Scattering of plane waves by rough surfaces in the sense of Born approximation

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Abstract

The topic of the present thesis is the scattering of electromagnetic plane waves by rough surfaces, i.e. by smooth and bounded perturbations of planar faces. Moreover, the contrast between the cover material and the substrate beneath the rough surface is supposed to be low. In this case, a modification of Stearns' far-field formula for the scattered field, based on Born approximation and Fourier techniques, is derived for a special class of surfaces. This class contains the graphs of functions, where the interface function is a radially modulated almost periodic function. For the Born formula to converge, a sufficient and almost necessary condition is given. The obtained far field contains plane waves, far-field terms like those for bounded scatterers, and, additionally, a new type of terms. Furthermore, it is proven that Stearns' conclusions concerning an approximate formula for the reduced efficiencies in the specular directions also hold for the presented class of interface functions. The derived formulas can be used for the fast numerical computations of far fields and for the statistics of random rough surfaces, which is shown for a simple example.

"The history of science teaches only too plainly the lesson
that no single method is absolutely to be relied upon,
that sources of error lurk where they are least expected,
and that they may escape the notice of the most experienced
and conscientious worker."

Sir John William Strutt, Lord Rayleigh
Transactions of the Sections' (1883)

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Contents

Chapter 1

Introduction

1.1 Background

The progress of modern technology vitally relies on computer chips or other electronic components with small and smaller details. The production of such components, on the other hand, usually involves lithographic processes employing light with wavelengths depending on the size of the desired structure details. Therefore, it is necessary to manufacture optical devices (e.g. optical gratings) designed for very short wavelengths. However, at some point, a perfect fabrication of such devices in accordance with the guidelines of design becomes either too difficult or is even not possible. Instead, the manufactured components of the optical devices deviate from ideal components by random aberrations. In the simplest case, a planar interface separating two different materials has typically a lot of tiny corrugations called roughness. In the present thesis, the term 'roughness' denotes a mostly smooth perturbation from a flat surface. Using such an interface to refract electromagnetic waves, the surface deviations, now almost in the size of the small wavelengths, become visible. Though the example of a planar interface is simple, a full understanding of the roughness phenomena is crucial for many applications. For example, the lithographic fabrication of computer chips in the extreme ultraviolet light (EUV) range, say of about 13 nm, requires the use of multi-layer systems (MLS) as Bragg mirrors, and each of the interfaces in this MLS has a specific roughness. To understand the impact of such an MLS on the reflection of light, the roughness effects on the reflection and transmission of light at each of the interfaces must be clarified. Naturally, the MLS is not the only source of roughness in an EUV-grating. These can also include roughness of the absorber structures above the MLS, e.g. line edge or line width roughness. Understanding the impact of this kind of roughness is especially important when considering the inverse problem in scattering metrology or the optimal design problem. These problems, however, will not be subject of this thesis. The aspects, how these roughness effects of grating structures influence the scattered field and may be included into the inverse problem, were, for example, studied in [26], [21] and [20].

One of the models to describe MLS' is used in the software of Windt [40] and is based on formulas derived by Stearns [36]. Note that similar models have been proposed for MLS' earlier by e.g. Bousquet et al. [7] and Elson et al. [16]. Stearns' formulas for a single interface scattering are obtained as follows: Suppose the rough interface is a fixed smooth interface, which is a bounded non-local perturbation of the ideal planar interface, and suppose a time-harmonic electromagnetic plane wave is incident from above. Manipulating Maxwell's equations according to Jackson [23, Sect. 10.2.A], the partial differential equations can be reduced to an inhomogeneous vector Helmholtz equation for the scattered electric displacement field. On the right-hand side, however, there appears a second order derivative of the total electric field, i.e., of the sum of the incoming field and the scattered field. On the other hand, if the scattered field is small in comparison with the incoming field, the first order Born approximation suggests to neglect the scattered electric field on the right-hand side. In other words, it remains to solve a vector Helmholtz equation with unknown displacement field and with known right-hand side. This is done by applying Fourier transform to both sides of the equation and by dividing with the coefficient of the Fourier transformed displacement field. The inverse Fourier transform now yields an explicit formula for the displacement field. This formula is an integral over the three-dimensional space. However, the integration in one of the three dimensions can be computed analytically by the residue theorem. Finally, taking limits and analysing the asymptotic behaviour, a corresponding far-field formula can be derived.

Of course, the Born approximation is not always justified (cf. [27] for a study on the validity for bounded scatterers, or [11] in the 2D case of an inhomogeneous layer on top of a perfectly conducting plate). However, for electromagnetic waves in the range of X-rays or EUV light, the optical contrast of the materials is often relatively small, i.e., the refractive index is often close to one. In this case, if the corrugations of the interface are not too large, and if the interface is smooth, the scattered field is expected to be small in comparison to the incoming wave field, assuming the incident direction is not to close to grazing direction. In this sense, the total field, as the sum of the scattered and incoming field, is almost identical to the incoming field alone, leading to the above described manipulation of the right-hand side of the Helmholtz equation. Moreover, Born approximation should be meaningful even if the scattered displacement field in the vector Helmholtz equation is replaced by the deviation of the scattered displacement field from the field resulting from an ideal planar interface. In this case a small term concentrated close to the interface and the deviation of the scattered electric field from that of the ideal interface is neglected.

Besides the formula of Stearns, there exist many alternative approximate formulas or rigorous numerical methods. These results are reported in the monographs by Beckmann et al. [4], Ogilvy [33], and Voronovich [38] as well as in the overview articles of DeSanto [14] and Elfouhaily et al. [15]. Among the approximate methods, the perturbation theory and the Kirchhoff theory are the most commonly used. Both theories are restricted to so called 'slightly rough' surfaces. This property is, for example, determined by the Rayleigh criterion (cf. [33, Sect. 1.2]), which is based on the phase shift and the resulting constructive or destructive interference when a wave is scattered at two arbitrary points of the interface. In the sense of 'slightly rough', it is usually assumed that the deviations from a planar surface are much smaller than the wavelength of the incident light.

In perturbation theory the total field, as a functional of the interface height function f, is represented as a Taylor series w.r.t. the interface height at the mean scattering surface, which is mostly commonly the zero plane. The introduced assumption of 'slightly rough' is necessary for the convergence of this Taylor representation. The series is then truncated after finitely many terms. By assuming that this truncated series also satisfies the boundary condition at the interface, a new and simplified boundary condition on the mean interface, here a plane, is obtained. Moreover, assuming that the scattered field can be represented as a series of functions that behave as $\mathcal{O}(f^n)$ for $n \to \infty$ and by plugging this into the new boundary condition, an approximate solution of the scattered field on the boundary is acquired by equating terms of the same order in f. An expression of the field away from the interface is obtained by using an integral representation of the field w.r.t. the mean interface. Usually this integral has to be evaluated numerically, which may involve computationally expensive calculations. However, when considering the stochastically averaged intensity, it may be reduced to the power spectrum density of the random process defining the rough interface. In special cases this term can be obtained analytically. The accuracy of the theory naturally depends on the accuracy and order of the truncated Taylor series. Effects like multiple scattering are included up to the order of the series expansion, while shadowing effects are neglected. More details on this theory and its accuracy can be found in Chapter 3 of the book by Ogilvy [33] and Chapter 4 of the book by Voronovich [38]. A general introduction into perturbation theory can be found in [30] by Nayfeh.

In Kirchhoff theory, also called tangent plane theory, as in the perturbation theory, an approximate expression of the total field on the interface is constructed and an integral formula is used to extend this result beyond the interface. The expression on the interface is acquired by approximating the interface at any point by an infinite tangent plane and using the analytically known scattering result at this plane as a local solution of the scattered field. Integrating appropriately over all these local solution gives an approximate solution of the wanted scattered field at the interface. In some special cases, e.g. scattering at a perfectly conducting surface, the integral representation of the field away from the interface can be further simplified to an analytical expression. In all other cases the integral has to be evaluated in other ways, for example by integrating numerically, which has the disadvantage of being computationally expensive. Obviously, the Kirchhoff approach considers the interface as a single scatterer and neglects multiple scattering and shadowing effects. Moreover, the local approximation of the surface by infinite planes restricts the approach to interfaces with sufficiently small curvature depending on the wavelength of the incoming field. More details on this theory can again be found in the books by Ogilvy [33], see Chapter 4, and by Voronovich [38], see Chapter 5, as well as the book by Beckmann and Spizzichino [4].

Note that for Stearns' approximated far-field formula, the assumption 'slightly rough' can be relaxed in the sense that the height perturbation of the interface can be of the size of the wavelength of the incident light, as long as the material constants are similar enough to ensure a small scattered field. The approach also differs from the perturbation and Kirchhoff theory, in that it solves the approximated Helmholtz equation analytically and thus also includes multiple scattering and shadowing effects, as long as they do not result in a strong scattered field such that Born approximation can no longer be applied. Another big advantage of the approach by Born approximation is the explicit far-field formula for the scattered field, where no additional integration is necessary. Note that for the previous two approximation methods, this is only the case in very specific situations, e.g. scattering at a perfectly conducting surface. Moreover, in theory it is also possible to consider continuous material transitions using Born approximation. In fact Stearns [36] also addresses this issue in his paper. However, this will not be a topic in the present thesis. The disadvantage of this approach, compared with perturbation and Kirchhoff theory, is its restriction to the low contrast case. On the other hand, since it is the goal of this thesis to examine scattering effects at rough interfaces for small wavelengths, e.g. EUV lithography, this can be assumed to be satisfied.

Among the rigorous approaches, boundary integral equation methods and finite elements methods are the most prominent. To arrive at the former, the field is represented by potentials or simplified potentials over the interface. Born approximation can also be used here to derive simple explicit formulas. On the other hand, to get rigorous formulas, the corresponding transmission problem for Maxwell's equation is to be solved, e.g. using boundary elements or finite elements, depending on the preferred method. Clearly, this can only be done numerically, i.e. up to a small error of the numerical method depending on the computing power. This, however, has the distinctive drawback that a numerical solution for the rigorous approach will take much longer computing times then the evaluation of the approximate formulas. Additionally, the numerical evaluation requires a bounded domain, which is usually obtained by truncation. These truncations introduce additional errors and have to be taken into account. One way is to use absorbing boundary layers to avoid reflection at the artificial boundaries or, in the case of periodic interfaces, to reduce the domain of calculation to one period of the interface. However, even in this case, if the period is very big compared to the incident wavelength the computing time will be considerable. Apart from this, the analysis of the numerical algorithms in the rigorous case is also difficult. Even for the simpler acoustic case in the three-dimensional space, there seems not to be any analytic theory for rough interfaces involving incident and reflected plane waves. The case of point sources is treated by Chandler-Wilde et al. [10, 9] using a variational approach. The uniqueness of a solution for plane wave incidence in 2D is considered in [12] and [29].

So far, the rough interface has been considered as a single smooth interface. In applications, however, the shape is not known explicitly. Realistically, the interface is an unknown realisation of some random process, which is for example described by distribution and correlation functions. Usually this is relaxed by considering special classes of random processes, e.g. stationary Gaussian processes, which are then characterised by only a few parameters like the size of the corrugations (standard deviation) and the smoothness (correlation length) of the interface. On the other hand, the incoming plane wave is in reality a ray with a diameter much larger than the wavelength and the dimension of the corrugations. The processing of the wave often acts like averaging over the local corrugations. Hence, the rough interface should be considered as a random process and the statistics of the resulting stochastic electric field is the entity of interest (cf. the above-mentioned monographs). The overview article [34] by Ogura and Takahashi gives an introduction into a stochastic functional approach to obtain the scattered stochastic field. In the present thesis, the stochastic view will not be considered analytically. Note, however, that a fast approximate formula for a single realisation of the stochastic process is a good starting point for a statistical analysis, for example using a Monte-Carlo approach. This is illustrated in a simple numerical example.

1.2 Contribution of the present work

The aim of this thesis is to check the validity of the Stearns' formula. No doubt, whenever the Born approximation is meaningful, the formulas yield accurate results when compared to physical measurements. From the mathematical point of view, however, the integrals in the formula do not exist for general bounded rough surfaces, even not for smooth ones. Therefore, in the present thesis, a mathematically rigorous modification of Stearns' formula is sought. For this, the following points are required.

- The vector Helmholtz equation for the scattered displacement field is replaced by that for the deviation to the displacement field of the ideal planar interface.
- A special variant of the limiting absorption principle is to be applied.
- The direct and inverse Fourier transforms are applied in the generalised sense, i.e. in the sense of Schwartz distributions.
- In order to justify the change in the order of integration, the unbounded domains of integration are to be truncated. After all manipulations are performed, the limit of the resulting formula for the truncated domains tending to the original unbounded domains is to be accessed.
- To get the inverse Fourier transform, a Fourier transform of bounded functions along the radial directions is to be evaluated. This requires a specific behaviour of the radial functions at infinity. For example, the class of interfaces can be restricted to special combinations of Fourier modes.

In fact, the rough interfaces in the present thesis are restricted to graphs of functions belonging to a special class. This class contains the algebra of almost periodic functions as well as almost periodic functions modulated by radial functions decaying at infinity. Note that almost periodic functions have been used already by Stover [37] and simpler biperiodic functions by Rice [35] to model rough surfaces. Moreover, combinations of Fourier modes play an important role for stochastic processes (cf. e.g. Yaglom [41, Equ. (2.61) in Sect. 8]).

In this way, the formula by Stearns [36], restricted to 'rough' interfaces, is given a strong mathematical foundation. The present thesis establishes two main novelties over Stearns' approach. Firstly, a special variation of the limiting absorption principle is employed. Secondly, the target field is replaced by that for the deviation to the displacement field of the ideal planar interface. Only these changes to Stearns' approach make it possible to obtain a mathematically rigorous formula for the scattered far field. Moreover, note that the presented approach is not restricted to the introduced class of interfaces. The presented techniques to derive far-field formulas may also be used for different classes of interfaces or potentially even in the case of continuous material transitions, provided that the Born approximation is justified and that some criteria are met, e.g. the interface class is a Banach space with known Fourier transforms of the contained functions. In the context of rough interfaces it may also be possible to apply the proposed approach to real random processes instead of 'known' interface realisations. A suggestion how this may be realised is given in Chapter 7.

The main result of the present thesis is a formula in the sense of Born approximation for the electromagnetic far field, which is adapted to the above-mentioned class of interfaces. Combining these formulas for reflection and transmission over several interfaces, the case of MLS' can be treated like in e.g. [36]. This, however, will also not be shown in the present thesis. Moreover, the approach of treating MLS' in [36] only considers the specular reflection modes, which is not enough, as is shown in the upcoming publication by Haase [18]. Here, the importance of including further refraction orders into the modelling of the MLS is illustrated. Even though the class of interfaces is already restricted, for the formula to be well defined, a further condition on the interface function is needed. Namely, if the evanescent Fourier modes for the fields with limited absorption tend to a plane-wave mode propagating parallel to the surface plane, then the coefficients of these Fourier modes diverge, and no limit of limiting absorption exists. In particular, for the special case of gratings, the formula of Born approximation converges if there is no Rayleigh mode, i.e., no reflected plane-wave mode propagating parallel to the plane of the grating. Since the differentiated formulas converge as well, it is clear that the Born approximation is a solution of the vector Helmholtz equation, in the sense that the transmission conditions are satisfied approximately. In summary, the following assumptions were made:

- **Low contrast**, e.g. short wavelengths
- Time-harmonic **plane wave incidence**
- **Non-grazing** incident
- **Almost periodic interface** with no or radial decay of polynomial order
- **No surface waves**

Under these assumption, the far-field formulas can be derived. The obtained far field consists of plane waves and far-field terms like those for bounded scatterers. Additionally, there appears a new type of terms, for which it is yet unclear whether they are physically meaningful. The derived formulas can be used for fast numerical computations of far fields as well as for the statistics of random rough surfaces.

This thesis is structured as follows. The notation and the inhomogeneous vector Helmholtz equation in the sense of Born approximation is introduced in Chapter 2. A general formula for its reflected near-field solution, based on the Fourier transform, is given at the beginning of Chapter 3. The validity of this formula is proven in the remainder of that chapter. To be precise, in the first two subsections of Section 3.2 the Helmholtz equation is solved by using generalised Fourier transforms. The resulting integrals are represented as Cauchy principle value limits of integrals truncated at infinity to change the order of integration of the truncated integrals. It can then be shown in the following two subsections that the integration in one of the three dimensions, as well as all the Cauchy principle value limits but one can be evaluated explicitly. To evaluate the remaining limit in Section 3.3, a class of special interface functions is defined in Subsection 3.3.1 and the limit is evaluated for such functions in the two subsequent subsections.

Similarly to Chapter 3, the main result of this thesis, namely the formula for the reflected (Thm. 4.1) and transmitted far-field (Thm. 5.1), are given at the beginning of their respective chapters 4 and 5. These results are proven in the following sections. In particular, the far-field formula for the reflected field is proven in detail. To prove the far-field asymptotics, the integral representation of the reflected field is split into two integrals corresponding to bounded integrands of evanescent and plane-wave modes, and weakly singular integrands with a small domain of integration (cf. Sect. 4.2.1). In the last two sections of Chapter 4 the obtained far-field formula is compared with Stearns' formula. To be more specific, Stearns' formula for the reduced efficiency in specular reflection direction is confirmed in Subsection 4.3. In Subsection 4.4 it is proven that Stearns' far-field formula in the sense of Born approximation is asymptotically the same to the one presented in this thesis for the specific example of a sinusoidal grating.

Since the proof for the near- and far-field formula of the transmitted field is very similar to the reflected case, Chapter 5 only gives an overview on how the proofs in Chapters 2–4 have to be modified to obtain the formulas proposed at the beginning of Chapter 5. Part of the far-field formula of Theorem 4.1, and thus Theorem 5.1, is proven in the Chapters A and B of the appendix. In the former, the field scattered at an ideal interface, which is a well-known result from Fresnel's formulas, is considered. In Chapter B the far field for interfaces with very specific parameters, for which the order of the singularity of the integral representation of the field increases, is derived.

Finally, in Chapter 6, the derived far-field formulas will be used to calculate the scattered field for random surface realisations. These 'realisations' of the scattered field are then used in a simple Monte-Carlo approach to get the averaged field that would usually be observed when measuring the scattered field in an experimental setup. The main part of this thesis is concluded by Chapter 7, which gives a short summary of the results as well as some ideas on how these may be extended in future work.

Throughout this thesis constants c with or without index are used for estimates and inequality chains. If not defined otherwise, these denote generic positive constants the values of which vary from instance to instance.

Chapter 2

Born approximation

In this chapter Maxwell's equations will be used to describe the total reflected field in form of a solution of an inhomogeneous vector Helmholtz equation. This equation will then be approximated in the sense of the first order Born approximation used by Stearns [36]. It will also be seen that a similar equation holds for the approximation of the desired reflected field minus the reflected field that results from illuminating an ideal interface, which is an interface defined by a plane. The approximate equation for this 'difference field' is then solved analytically using generalised Fourier transform, in the following chapter. Some minor preparations for these examinations will end Chapter 2.

2.1 Incident wave

Consider a time-harmonic incident plane wave $\mathcal{E}_0(\vec{x},t) = \vec{E}^0(\vec{x})\, e^{-i\omega t}$ illuminating the interface between two constant materials from above. The function $\vec{E}^0(\vec{x}) = \vec{e}^{\,0}\, e^{i\vec{k}\cdot\vec{x}}$ denotes the time independent part of $\mathcal{E}_0(\vec{x},t)$, where $\vec{k} := (k_x, k_y, k_z)^\top = k\vec{n}^0 \in \mathbb{R}^3$ is the wave vector, with $k := \|\vec{k}\| := \sqrt{\mu_0\epsilon_0}\omega > 0$ the real valued wave number, $k_z < 0$ and $\vec{n}^0$ a normalised vector that describes the direction of propagation of the incident field in the coordinate system shown in Figure 2.1. The values $\epsilon_0 > 0$ and $\mu_0 > 0$ denote the electric permittivity resp. magnetic permeability of the medium above the interface, while ϵ_0' and μ_0' denote the same below the interface. Note that ϵ_0, ϵ_0', μ_0 and μ_0' are not necessarily the free space values for the vacuum. The symbol $\vec{e}^{\,0}$ denotes the constant vector fixing polarisation and phase. Naturally, $\vec{e}^{\,0}$ is assumed to be perpendicular to $\vec{k}$.

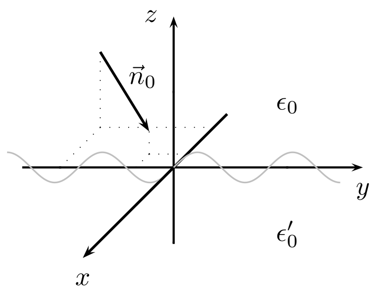


Figure 2.1: Coordinate system and propagation direction of incident field

2.2 Inhomogeneous vector Helmholtz equation

Note that, since the wave number $k = \sqrt{\epsilon_0\mu_0}\omega$ is assumed to be real valued, the material above the interface is non-absorbing. The physical background on the other hand, states that there are no materials that do not absorb at least a very small amount of the energy of an electromagnetic field travelling through. To incorporate this information into the solution of the subsequently established vector Helmholtz equation, the limiting absorption principle (first used in [22]) is applied. In this sense the examinations in this and the following sections of this chapter will be done for an adapted wave vector $\vec{k}_\tau$ of the incident field with a complex valued third component, i.e. $\vec{k}_\tau := (k_x, k_y, k_{z,\tau})^\top$ with $k_{z,\tau} := k_z + i\tau$, a negative $\tau \in \mathbb{R}$ close to zero and $k_z < 0$. Afterwards, for the solution of this slightly perturbed problem, the limit $\tau \nearrow 0$ is applied to obtain a solution of the unperturbed problem in the sense of the limiting absorption principle. For technical reasons only the third component of the wave vector instead of the whole vector is chosen complex. This is motivated by the fact that only waves that propagate away from the interface are of interest, while surface waves will be excluded in the context of this thesis. In this context, surface waves are to be understood as plane waves, whose propagation direction is parallel to the mean plane of the surface heights, e.g. the x-y-plane in Figure 2.1. Indeed, the subsequently derived formulas for the reflected field will not be valid in the case that such surface waves occur. For simplicity, define $\epsilon_\tau := \epsilon_0 - \tau^2/(\mu_0\omega^2) + i2\tau k_z/(\mu_0\omega^2)$, with which $k_\tau^2 := \vec{k}_\tau \cdot \vec{k}_\tau = \mu_0\epsilon_\tau\omega^2$ and $\operatorname{Im}\epsilon_\tau > 0$. In the course of this thesis a number of definitions will be introduced. To make the reading of this thesis more accessible, a list of the most important of these definitions is attached at the end.

The Maxwell equations that describe the field in the absence of sources are

$$\nabla \cdot \vec{\mathcal{B}} = 0, \qquad \nabla \times \vec{\mathcal{E}} = -\partial_t \vec{\mathcal{B}}, \tag{2.2.1}$$

$$\nabla \cdot \vec{\mathcal{D}} = 0, \qquad \nabla \times \vec{\mathcal{H}} = \partial_t \vec{\mathcal{D}}, \tag{2.2.2}$$

where $\vec{\mathcal{E}}$ is the electric field, $\vec{\mathcal{D}}$ the displacement field, $\vec{\mathcal{H}}$ the magnetic field and $\vec{\mathcal{B}}$ the magnetic induction. The system of equations (2.2.1) and (2.2.2) can be reduced to one equation, namely an inhomogeneous vector Helmholtz equation. Following [23, Sect. 10.2.A], consider $\nabla^2\vec{\mathcal{D}} - \mu_0\epsilon_\tau\partial_t^2\vec{\mathcal{D}}$, which using the equality $\nabla \times \nabla \times \vec{\mathcal{D}} = \nabla(\nabla \cdot \vec{\mathcal{D}}) - \nabla^2\vec{\mathcal{D}}$ and the first of the equations (2.2.2) equals $-\nabla \times \nabla \times \vec{\mathcal{D}} - \mu_0\epsilon_\tau\partial_t(\partial_t\vec{\mathcal{D}})$. Moreover, with the second equation and by adding a zero it transforms to $-\nabla \times \nabla \times (\vec{\mathcal{D}} - \epsilon_\tau\vec{\mathcal{E}}) + \epsilon_\tau\nabla \times (-\nabla \times \vec{\mathcal{E}} - \mu_0\partial_t\vec{\mathcal{H}})$. In the context of this thesis, the magnetic permeability $\mu_0 = \mu_0'$ will be assumed to be everywhere constant. Following (2.2.1), $-\nabla \times \vec{\mathcal{E}} = \partial_t\vec{\mathcal{B}}$, which leads to the wave equation

$$\nabla^2\vec{\mathcal{D}} - \mu_0\epsilon_\tau\partial_t^2\vec{\mathcal{D}} = -\nabla \times \nabla \times \left(\vec{\mathcal{D}} - \epsilon_\tau\vec{\mathcal{E}}\right) + \epsilon_\tau\partial_t\nabla \times \left(\vec{\mathcal{B}} - \mu_0\vec{\mathcal{H}}\right), \tag{2.2.3}$$

by changing the order of the spatial and time derivatives in the second summand on the right-hand side. As mentioned above, for this thesis, a harmonic time variation $e^{-i\omega t}$ with a frequency ω for the incident field is assumed, which results in time-harmonic total fields $\vec{\mathcal{D}}$, $\vec{\mathcal{B}}$, $\vec{\mathcal{E}}$ and $\vec{\mathcal{H}}$. Furthermore, these fields will be identified with the time-independent amplitude factors $\vec{D}$, $\vec{B}$, $\vec{E}$ and $\vec{H}$ of the fields, which multiplied with $e^{-i\omega t}$ will give the time dependent fields. With this, equation (2.2.3) reduces to

$$\left(\nabla^2 + k_\tau^2\right)\vec{D} = -\nabla \times \nabla \times \left(\vec{D} - \epsilon_\tau\vec{E}\right),$$

since $\vec{B} = \mu_0\vec{H}$ if μ_0 is everywhere constant. The solution function $\vec{D}$ of this equation is defined on the whole $\mathbb{R}^3$. On the other hand, a physical interpretation for the function can only be given above the interface, where it describes the total displacement field. Defining $\vec{E}^0(\vec{x}) := \vec{e}^{\,0}e^{i\vec{k}_\tau\cdot\vec{x}}$ as the incoming and $\vec{E}(\vec{x})$ as the total electric field, the reflected field is defined as $\vec{E}^r(\vec{x}) := \vec{E}(\vec{x}) - \vec{E}^0(\vec{x})$, where, once more, a physical interpretation exists only for the function above the interface. To continue, let the interface between the two media be described by the graph $\{(x', f(x')) : x' \in \mathbb{R}^2\}$ of a function $f \in L^\infty_{\mathcal{Q}}(\mathbb{R}^2)$, with

$$L^\infty_{\mathcal{Q}}(\mathbb{R}^2) := \left\{ f \in L^\infty(\mathbb{R}^2) \,\middle|\, \lim_{R\to\infty} \frac{1}{4R^2} \int_{[-R,R]^2} f(\eta')\,\mathrm{d}\eta' = 0 \right\}. \tag{2.2.4}$$

Note that for any function f, where $\lim_{R\to\infty} 1/(4R^2)\int_{[-R,R]^2} f(\eta')\,\mathrm{d}\eta' = c \neq 0$, the coordinate system can be shifted by c in the z-direction to get a function in $L^\infty_{\mathcal{Q}}(\mathbb{R}^2)$. Employing the definitions of the displacement fields of the incoming $\vec{D}^0(\vec{x}) := \epsilon_\tau\vec{E}^0(\vec{x})$ and the total electric field $\vec{D}(\vec{x}) := \varepsilon_\tau(\vec{x})\vec{E}(\vec{x})$, with

$$\varepsilon_{\mathcal{T}}(\vec{x}) := \begin{cases} \epsilon_{\mathcal{T}} & \text{if } z > f(x') \\ \epsilon_0' & \text{if } z < f(x') \end{cases}$$

for all $\vec{x} = (x', z)^\top \in \mathbb{R}^3$, the definition for the reflected part of the displacement field $\vec{D}^r(\vec{x}) := \vec{D}(\vec{x}) - \vec{D}^0(\vec{x})$ takes the form $\varepsilon_{\mathcal{T}}(\vec{x})\vec{E}(\vec{x}) - \epsilon_{\mathcal{T}}\vec{E}^0(\vec{x})$. Unlike ϵ_0, the electric permittivity ϵ_0' of the material below the interface is allowed to be complex valued. Note that $|\epsilon_{\mathcal{T}} - \epsilon_0'|$ is assumed to be small to satisfy the low contrast assumption, which is necessary for the validity of the subsequently used Born approximation.

It is well established, that the incoming field satisfies the homogeneous vector Helmholtz equation $(\nabla^2 + k_{\mathcal{T}}^2)\vec{D}^0 = 0$ above the interface. Applying this, the inhomogeneous Helmholtz equation for the reflected field is obtained as

$$\left(\nabla^2 + k_{\mathcal{T}}^2\right) \vec{D}^r = -\nabla \times \left[\nabla \times \left(\alpha(\vec{E}^0 + \vec{E}^r)\right)\right], \tag{2.2.5}$$

where $\alpha(\vec{x}) := \varepsilon_{\mathcal{T}}(\vec{x}) - \epsilon_{\mathcal{T}}$. Note that α is zero everywhere above the interface.

2.3 Born approximation

Neglecting the term $\vec{E}^r(\vec{x})$ in (2.2.5), a solution in the sense of the first order Born approximation is acquired.

$$\left(\nabla^2 + k_{\mathcal{T}}^2\right) \vec{D}^r = -\nabla \times \left[\nabla \times \left(\alpha\vec{E}^0\right)\right] \tag{2.3.1}$$

This approximation is motivated by the fact, that in special situations, e.g. for X-rays in the case of interfaces with low material contrast, small perturbation or/and small gradients, the scattered field is very small compared to the incident field, such that $\vec{E}^0 + \vec{E}^r \sim \vec{E}^0$.

Note that the existence of a mathematically rigorous treatment of the Born approximation of

$$\left(\nabla^2 + k^2\right) \vec{D} = -\nabla \times \left[\nabla \times \left(\alpha\vec{E}\right)\right]$$

is not yet clear. The mathematical formalism would have to look as following. First, a corresponding solution theory would have to be defined on two Banach spaces $\mathcal{B}_1$ and $\mathcal{B}_2$, where the operator $\nabla^2 + k^2$ maps from $\mathcal{B}_1$ to $\mathcal{B}_2$ and the inverse operator, i.e. the solution operator, maps from $\mathcal{B}_2$ to $\mathcal{B}_1$. Consequently, $\mathcal{B}_1$ contains the scattered wave solution $\vec{D}$ and includes a sufficient radiation condition that ensures the uniqueness of the solution. On the other hand, the space $\mathcal{B}_2$ has to contain $-\nabla \times [\nabla \times (\alpha\,\vec{E})]$ for all $\vec{E} \in \mathcal{B}_1$. Moreover, $\|\nabla \times [\nabla \times (\alpha\,\vec{E})]\|_{\mathcal{B}_2}$ has to go to zero as $\|\alpha\|_\infty \to 0$ and $\|\nabla \times [\nabla \times \vec{E}^r]\|_{\mathcal{B}_2}$ has to go to zero as $\|\vec{E}^r\|_{\mathcal{B}_1} \to 0$. In such a setting, it would be assumed that any general solution $\vec{D} = \epsilon_0\vec{E} \in \mathcal{B}_1$ consists of the sum of a particular solution $\vec{D}^r = \epsilon_0\vec{E}^r \in \mathcal{B}_1$ and a solution of the corresponding homogeneous equation, i.e. the incoming plane wave $\vec{E}^0$. Consequently, the particular solution $\vec{E}^r = \vec{E} - \vec{E}^0$ can be obtained as the solution of

$$\left(\nabla^2 + k^2\right) \vec{D}^r = -\nabla \times \left[\nabla \times \left(\alpha(\vec{E}^r + \vec{E}^0)\right)\right], \tag{2.3.2}$$

since $(\nabla^2 + k^2)\vec{E}^0 = 0$. The radiation condition in $\mathcal{B}_1$ ensures that $\vec{E}^r$ is a unique solution in this space. It now follows that $\|\vec{E}^r\|_{\mathcal{B}_1}$ tends to zero as the material contrast $\epsilon_0 - \epsilon_0'$ and thus $\|\alpha\|_\infty$ tends to zero, since then $\|\nabla \times [\nabla \times (\alpha\,\vec{E})]\|_{\mathcal{B}_2} \to 0$ and thus $\vec{E} \to \vec{E}^0$.

In this sense, the error of the Born approximation can be bounded by the error on the right-hand side of (2.3.2) or (2.2.5) if $\vec{E}^r$ is neglected, i.e. the error can be bounded by $\|\vec{E}^r\|_{\mathcal{B}_1}$. Furthermore, under the low contrast assumption, it is feasible to assume that the bulk of the reflected energy is reflected in specular direction $\vec{k}^r := (k_x, k_y, -k_z)^\top$, such that $\vec{E}^r$ can be represented as the sum of a plane wave $\vec{a}\,e^{i\vec{k}^r\cdot\vec{x}}$ in this direction and a small remainder $\vec{e}^r$. As a consequence,

$$\left\|\alpha\,\vec{E}^r\right\|_{\mathcal{B}_1} = \left\|\alpha\left(\vec{a}\,e^{i\vec{k}^r\cdot\vec{x}} + \vec{e}^r\right)\right\|_{\mathcal{B}_1} \leq \left\|\alpha\,\vec{a}\,e^{i\vec{k}^r\cdot\vec{x}}\right\|_{\mathcal{B}_1} + \left\|\alpha\,\vec{e}^r\right\|_{\mathcal{B}_1}. \tag{2.3.3}$$

This would directly correspond to the approach made by Stearns [36]. In this thesis, a slightly modified approach was chosen, introduced in the following.

In the special case of an ideal interface $f_Q \equiv 0$ and the corresponding $\alpha_Q(\vec{x})$, let $\vec{D}^{sc}_Q(\vec{x})$ be the solution of (2.2.5). On the other hand, the field reflected from an ideal interface can also be calculated directly using Fresnel's formulas (cf. Chapter A). With this in mind, set, for an arbitrary interface function $f \in L^\infty_Q(\mathbb{R}^2)$, $\alpha_d(\vec{x}) := \alpha(\vec{x}) - \alpha_Q(\vec{x})$ and $\vec{D}^d(\vec{x}) := \vec{D}^r(\vec{x}) - \vec{D}^r_Q(\vec{x})$ and use (2.2.5) for the difference field $\vec{D}^d$ to get

$$\begin{aligned}
\left(\nabla^2 + k_\tau^2\right) \vec{D}^d(\vec{x}) &= -\nabla\times\left[\nabla\times\left(\alpha(\vec{x})\left(\vec{E}^0(\vec{x}) + \vec{E}^r(\vec{x})\right)\right)\right] + \nabla\times\left[\nabla\times\left(\alpha_Q(\vec{x})\left(\vec{E}^0(\vec{x}) + \vec{E}^r_Q(\vec{x})\right)\right)\right]\\
&= -\nabla\times\left[\nabla\times\left(\alpha_d(\vec{x})\,\vec{E}^0(\vec{x})\right)\right] - \nabla\times\left[\nabla\times\left(\alpha(\vec{x})\,\vec{E}^r(\vec{x})\right)\right] + \nabla\times\left[\nabla\times\left(\alpha_Q(\vec{x})\,\vec{E}^r_Q(\vec{x})\right)\right]\\
&= -\nabla\times\left[\nabla\times\left(\alpha_d(\vec{x})\left(\vec{E}^0(\vec{x}) + \vec{E}^r(\vec{x})\right)\right)\right] - \nabla\times\left[\nabla\times\left(\alpha_Q(\vec{x})\,\vec{E}^r(\vec{x})\right)\right]\\
&\quad + \nabla\times\left[\nabla\times\left(\alpha_Q(\vec{x})\,\vec{E}^r_Q(\vec{x})\right)\right] \qquad (2.3.4)\\
&= -\nabla\times\left[\nabla\times\left(\alpha_d(\vec{x})\left(\vec{E}^0(\vec{x}) + \vec{E}^r(\vec{x})\right)\right)\right] - \nabla\times\left[\nabla\times\left(\alpha_Q(\vec{x})\left(\vec{E}^r(\vec{x}) - \vec{E}^r_Q(\vec{x})\right)\right)\right].
\end{aligned}$$

In the sense of Born approximation the terms $\vec{E}^r$ and $\vec{E}^r_Q := \vec{D}^r_Q/\epsilon_0$ are again neglected on the right-hand side, such that (2.3.4) reduces to

$$\left(\nabla^2 + k_\tau^2\right) \vec{D}^d(\vec{x}) = -\nabla\times\left[\nabla\times\left(\alpha_d(\vec{x})\vec{E}^0(\vec{x})\right)\right]. \qquad (2.3.5)$$

The advantage of considering this equation instead of (2.3.2) is that $\alpha_d(\vec{x})$ has a compact support w.r.t. z if $f \in L^\infty_Q(\mathbb{R}^2) \subset L^\infty(\mathbb{R}^2)$, since then $\alpha_d(\vec{x}) \equiv 0$ for $|z| > \|f\|_\infty$, while $\alpha(\vec{x})$ has an unbounded support in all three arguments. This is needed later, when the Fourier transform of α_d is evaluated. As before (cf. (2.3.3)), assuming an appropriate solution theory, the error of such an approximation can be bounded by the error introduced on the right-hand side to reach (2.3.5). In this case, the approximation error would be bounded by a constant times

$$\begin{aligned}
&\left\|\alpha_d\,\vec{E}^r + \alpha_Q(\vec{E}^r - \vec{E}^r_Q)\right\|_{\mathcal{B}_1}\\
&\quad\le \left\|\alpha_d\,\vec{E}^r\right\|_{\mathcal{B}_1} + \left\|\alpha_Q(\vec{E}^r - \vec{E}^r_Q)\right\|_{\mathcal{B}_1}\\
&\quad\le \left\|\alpha_d\,(\vec{a}\,e^{i\vec{k}^r\cdot\vec{x}} + \vec{e}^{\,r})\right\|_{\mathcal{B}_1} + \left\|\alpha_Q(\vec{a}\,e^{i\vec{k}^r\cdot\vec{x}} + \vec{e}^{\,r} - \vec{a}_Q\,e^{i\vec{k}^r\cdot\vec{x}})\right\|_{\mathcal{B}_1}\\
&\quad\le \left\|\alpha_d\,\vec{a}\,e^{i\vec{k}^r\cdot\vec{x}}\right\|_{\mathcal{B}_1} + \left\|\alpha_Q(\vec{a} - \vec{a}_Q)\right\|_{\mathcal{B}_1} + \left\|\alpha_d\,\vec{e}^{\,r}\right\|_{\mathcal{B}_1} + \left\|\alpha_Q\,\vec{e}^{\,r}\right\|_{\mathcal{B}_1}. \qquad (2.3.6)
\end{aligned}$$

Note that it can be expected that this bound is smaller than (2.3.3). Indeed, especially in the case of small perturbations of the interface, the field reflected in non-specular directions is much smaller than that in the specular direction $\vec{k}^r$ such that $\|\vec{e}^{\,r}\|$ and $\|\vec{a} - \vec{a}_Q\|$ are very small. Moreover, the bound $\|\alpha_d\,\vec{a}\,e^{i\vec{k}^r\cdot\vec{x}}\|_{\mathcal{B}_1}$ in (2.3.6) is smaller than $\|\alpha\,e^{i\vec{k}^r\cdot\vec{x}}\|_{\mathcal{B}_1}$ in (2.3.3), since α_d has a compact support in its third argument. For the remainder of this thesis, except in Chapter 5 where a very similar Born approximation is introduced for the transmitted field, the term 'Born approximation' is used to reference the approximation that leads from (2.3.4) to (2.3.5).

To solve equation (2.3.5) in the following sections by using Fourier transformation, it is necessary to specify the set of interface functions. In a first step this will now be done very roughly to ensure the validity of the Fourier transform. In Section 3.3.1 this set will then be reduced even further to a very specific space based on almost periodic functions (cf. [5]) to get explicit solution formulas.

Observe, that the set of interface functions f can be chosen in such a way that α_d identifies a functional of the dual space of the Schwartz space (cf. Definition C.1), i.e. $\int_{\mathbb{R}^3} \alpha_d(\vec{x})\varphi(\vec{x})\,\mathrm{d}\vec{x}$ is finite for all $\varphi \in \mathcal{S}(\mathbb{R}^3)$. In this sense α_d is an element of $\mathcal{S}'(\mathbb{R}^3)$, the dual space of $\mathcal{S}(\mathbb{R}^3)$. As mentioned above, this especially holds true for all $f \in L^\infty(\mathbb{R}^2)$, in which case the support of $\alpha_d(\vec{x})$ is bounded in the direction of z. In the following, such a function f will be assumed with $\|f\|_\infty = h/2$ and $h > 0$. With this the Fourier transform $\hat{\alpha}_d := \mathcal{F}(\alpha_d)$ of α_d, which is needed later on, is well defined in the generalised sense. To be precise, for smooth functions φ and ψ with compact support, the Fourier transform and its inverse are defined by

$$\mathcal{F}\varphi(\vec{s}) := \hat{\varphi}(\vec{s}) := \int\limits_{\mathbb{R}^3} \varphi(\vec{x})\, e^{-i\vec{x}\cdot\vec{s}}\, \mathrm{d}\vec{x}, \tag{2.3.7}$$

$$\mathcal{F}^{-1}\psi(\vec{x}) := \check{\psi}(\vec{x}) := \frac{1}{(2\pi)^3} \int\limits_{\mathbb{R}^3} \psi(\vec{s})\, e^{i\vec{s}\cdot\vec{x}}\, \mathrm{d}\vec{s} \tag{2.3.8}$$

and $\varphi(\vec{x}) = (\hat{\varphi})\check{}(\vec{x})$. Furthermore, if the duality $\langle f, g\rangle$ of the spaces C_0^∞ and $(C_0^\infty)^*$ is the extension of the scalar product $\int f\bar{g}$, then the generalised Fourier transform $\hat{\alpha}_d$ of the Schwartz distribution α_d is defined by

$$\langle \hat{\alpha}_d(\vec{s}), \varphi(\vec{s})\rangle := (2\pi)^3 \langle \alpha_d(\vec{\eta}), \check{\varphi}(\vec{\eta})\rangle \tag{2.3.9}$$

for all $\varphi \in \mathcal{S}(\mathbb{R}^3)$.

In the next section a similar formula will be used, where the argument of $\hat{\alpha}_d$ is shifted by $\vec{k}_\tau$. For $\vec{\eta} := (\eta_x, \eta_y, \eta_z)$, there holds

$$\begin{aligned}\left\langle \hat{\alpha}_d(\vec{s} - \vec{k}_\tau), \varphi(\vec{s})\right\rangle &= (2\pi)^3 \left\langle \alpha_d(\vec{\eta})\, e^{i\vec{k}_\tau\cdot\vec{\eta}}, \check{\varphi}(\vec{\eta})\right\rangle \\ &= (2\pi)^3 \left\langle \alpha_d(\vec{\eta})\, e^{i\vec{k}\cdot\vec{\eta}}\, e^{-\tau\eta_z}, \check{\varphi}(\vec{\eta})\right\rangle .\end{aligned}$$

Chapter 3

The reflected near field

3.1 The near-field formula

In this chapter it will be shown that

Theorem 3.1 (The reflected near field). *Assume an interface that is described by the graph of a function*

$$f \in \mathcal{A} := \Bigg\{ f : \mathbb{R}^2 \to \mathbb{R} \,\Big|\, f \in \mathrm{L}^\infty(\mathbb{R}^2),\ f(\eta') = \sum_{\ell=0}^{3} \left[\frac{1}{\sqrt{1+|\eta'|^2}^{\,\ell}} \sum_{j\in\mathbb{Z}} \lambda_{\ell,j}\, e^{i\omega'_{\ell,j}\cdot\eta'} \right] + g(\eta'),$$
$$\lambda_{\ell,j} \in \mathbb{C},\ \omega'_{\ell,j} \in \mathbb{R}^2,\ \sum_{\ell=0}^{3}\sum_{j\in\mathbb{Z}} |\lambda_{\ell,j}| + \big\|(1+|\eta'|^2)^2\, g(\eta')\big\|_\infty < \infty \Bigg\},$$

where $\lambda_{0,j_0} = 0$ *if* $\omega'_{0,j_0} = (0,0)^\top$, *and satisfies the condition*

$$k \notin \mathrm{cl} \left\{ \Big| k' + \sum_{j\in\mathbb{Z}} m_j \omega'_{0,j} \Big| :\ m_j \in \mathbb{N}_0 \text{ s.t.} \sum_{j\in\mathbb{Z}} m_j < \infty \right\}, \tag{3.1.1}$$

where $\mathbb{N}_0$ *is the set of non-negative integers and* $k' := (k_x, k_y)^\top$. *Moreover, such an interface is assumed to be illuminated by an incoming plane wave as in Subsection 2.1. Then the introduced Born approximation, as defined by (2.3.5), in the case of limiting absorption has, for the absorption going to zero, the following well-defined limit for the reflected electric field for* $z > 2h$:

$$\vec{E}^r(\vec{x}) = \vec{E}^r_d(\vec{x}) + \vec{E}_Q(\vec{x}) = E_Q - E_0 - E_1 - E_2 - E_3 - E_4, \tag{3.1.2}$$

where

$$E_Q := r(\vec{k}, \vec{e}^{\,0})\, \frac{e^{i\vec{k}^r\cdot\vec{x}}}{|k'|^2}, \tag{3.1.3}$$

$$E_0 := i\,\frac{\Delta}{2\epsilon_0} \sum_{n\in\mathbb{N}_0}\sum_{j\in\mathbb{Z}} \int_0^1 \tilde{\lambda}^n_{0,j}\, \frac{(-i\zeta)^n}{n!}\, \mathrm{d}\zeta\ \left[(\vec{\omega}_j \times \vec{e}^{\,0}) \times \vec{\omega}_j \right] \left(\omega^j_z\right)^{n-1} e^{i\vec{\omega}_j\cdot\vec{x}}, \tag{3.1.4}$$

$$E_1 := i\,\frac{\Delta}{4\pi\epsilon_0} \sum_{n\in\mathbb{N}_0}\sum_{j\in\mathbb{Z}} \int_0^1 \tilde{\lambda}^n_{1,j}\, \frac{(-i\zeta)^n}{n!}\, \mathrm{d}\zeta \int_{\mathbb{R}^2} \xi^{n-1}\, \frac{e^{-|s'-(k'+\tilde{\omega}'_{1,j})|}}{|s'-(k'+\tilde{\omega}'_{1,j})|} \left[(\vec{s}_\xi \times \vec{e}^{\,0}) \times \vec{s}_\xi \right] e^{i\vec{s}_\xi\cdot\vec{x}}\, \mathrm{d}s', \tag{3.1.5}$$

$$E_2 := i\,\frac{\Delta}{4\pi\epsilon_0} \sum_{n\in\mathbb{N}_0}\sum_{j\in\mathbb{Z}} \int_0^1 \tilde{\lambda}^n_{2,j}\, \frac{(-i\zeta)^n}{n!}\, \mathrm{d}\zeta \int_{\mathbb{R}^2} \xi^{n-1}\, K_0\big(|s'-(k'+\tilde{\omega}'_{2,j})|\big) \left[(\vec{s}_\xi \times \vec{e}^{\,0}) \times \vec{s}_\xi \right] e^{i\vec{s}_\xi\cdot\vec{x}}\, \mathrm{d}s', \tag{3.1.6}$$

$$E_3 := i\,\frac{\Delta}{4\pi\epsilon_0}\sum_{n\in\mathbb{N}_0}\sum_{j\in\mathbb{Z}}\int_0^1 \tilde{\lambda}_{3,j}^n\frac{(-i\zeta)^n}{n!}\,\mathrm{d}\zeta\int_{\mathbb{R}^2}\xi^{n-1}\,e^{-\left|s'-(k'+\tilde{\omega}'_{3,j})\right|}\left[(\vec{s}_\xi\times\vec{e}^{\,0})\times\vec{s}_\xi\right]e^{i\vec{s}_\xi\cdot\vec{x}}\,\mathrm{d}s', \tag{3.1.7}$$

$$E_4 := i\,\frac{\Delta}{8\pi^2\epsilon_0}\sum_{n\in\mathbb{N}_0}\int_0^1\frac{(-i\zeta)^n}{n!}\int_{\mathbb{R}^2}\xi^{n-1}\int_{\mathbb{R}^2}\tilde{g}_n(\eta',\zeta)\,e^{-i\eta'\cdot(s'-k')}\,\mathrm{d}\eta'\left[(\vec{s}_\xi\times\vec{e}^{\,0})\times\vec{s}_\xi\right]e^{i\vec{s}_\xi\cdot\vec{x}}\,\mathrm{d}s'\,\mathrm{d}\zeta, \tag{3.1.8}$$

$$\begin{aligned} r(\vec{k},\vec{e}^{\,0}) := \Bigg[&\frac{k_z+\sqrt{\tilde{k}^2-|k'|^2}}{k_z-\sqrt{\tilde{k}^2-|k'|^2}}\,(k_y e_x^0 - k_x e_y^0)\begin{pmatrix} k_y\\ -k_x\\ 0\end{pmatrix}\\ &+\frac{\tilde{k}^2k_z+k^2\sqrt{\tilde{k}^2-|k'|^2}}{\tilde{k}^2k_z-k^2\sqrt{\tilde{k}^2-|k'|^2}}\,\frac{k_z(k_xe_x^0+k_ye_y^0)-|k'|^2\,e_z^0}{k^2}\begin{pmatrix}-k_xk_z\\ -k_yk_z\\ -|k'|^2\end{pmatrix}\Bigg], \end{aligned}\tag{3.1.9}$$

$\xi := \sqrt{k^2-s'^2}$, $\vec{s}_w := (s_x,s_y,w)^\top$, $\tilde{k} := \sqrt{\mu_0\epsilon'_0}\omega$, $\vec{k}^r := (k_x,k_y,-k_z)^\top$, $\vec{\omega}_j := (k'+\tilde{\omega}'_{0,j},\omega_z^j)^\top$, $\omega_z^j := \sqrt{k^2-\left|k'+\tilde{\omega}'_{0,j}\right|^2}$ and $\vec{e}^{\,0}$ the incident polarisation vector $(e_x^0,e_y^0,e_z^0)^\top$. The terms $\tilde{\lambda}_{\ell,j}^n$, $\tilde{\omega}'_{\ell,j}$ and $\tilde{g}_n$ are defined as in the subsequent Lemma 3.9. Furthermore, there exists a $z_0>0$ such that the sums in E_ℓ, $\ell=0,\dots,4$, are absolutely and uniform convergent for any $z\geq z_0$.

Remark 3.2. *Examining the definintions (3.1.3) to (3.1.8) it is easily seen that $\vec{E}^r$ is a linear combination of plane waves and evanescent modes as well as integrals over plane waves and evanescent modes. By formally applying the differential operator $\nabla_{\vec{x}}\times\nabla_{\vec{x}}\times$ to E_Q and E_0 to E_4 it can be shown that they individually solve the homogeneous vector Helmholtz equation $\nabla\times\nabla\times E+k^2E=0$. Indeed, this follows since for any vector $\vec{s}$ with $\|\vec{s}\|=k$,*

$$\begin{aligned}\nabla_{\vec{x}}\times\nabla_{\vec{x}}\times\left[(\vec{s}\times\vec{e}^{\,0})\times\vec{s}\,e^{i\vec{s}\cdot\vec{x}}\right] &= -\vec{s}\times\left(\vec{s}\times\left[(\vec{s}\times\vec{e}^{\,0})\times\vec{s}\right]\right)e^{i\vec{s}\cdot\vec{x}}\\ &= \left(\vec{s}\cdot\left[(\vec{s}\times\vec{e}^{\,0})\times\vec{s}\right]\right)\vec{s}e^{i\vec{s}\cdot\vec{x}} - k^2\left[(\vec{s}\times\vec{e}^{\,0})\times\vec{s}\right]e^{i\vec{s}\cdot\vec{x}}\\ &= -k^2\left[(\vec{s}\times\vec{e}^{\,0})\times\vec{s}\right]e^{i\vec{s}\cdot\vec{x}}.\end{aligned}$$

Since ω, the third component of the propagation direction $\vec{\omega}_j$, and ξ, the third component of the propagation direction $\vec{s}_\xi$, are either non-negative real valued or complex valued with a vanishing real part and a positive imaginary part, only waves travelling upwards or parallel to the interface are added or integrated to obtain (3.1.2). Condition (3.1.1) ensures that only waves travelling away from the interface are included into the sum in (3.1.4).

Remark 3.3. *In the very simple case of scattering at an ideal interface, i.e. $f(\eta')=0$ or equivalently $g(\eta')=0$ and $\lambda_{\ell,j}=0$ for all $\ell=0,\dots,3$ and $j\in\mathbb{Z}$, all terms in (3.1.2) except for E_Q (cf. (3.1.3)) are zero. Thus $\vec{E}^r(\vec{x})=E_Q$. Indeed, this follows directly from the definitions (3.3.18) to (3.3.20) of $\tilde{\lambda}_{\ell,j}^n$ for all $\ell=0,\dots,3$ and $j\in\mathbb{Z}$ and $\tilde{g}_n$ in the subsequent Lemma 3.9. Consequently, for scattering at an ideal interface Formula (3.1.2) is the exact solution of the scattering problem.*

The proof of this theorem encompasses the entire Chapter 3. As a first step, the Helmholtz equation (2.3.5) for the difference field will be solved by applying the generalised Fourier transform, resulting in an integral representation of the reflected displacement field. These integrals will then be interpreted as Cauchy principal value integrals at infinity, which allows to interchange the order of integration in the following subsection. In the last two subsections of this section, one of the integrals is evaluated explicitly by applying contour integration and all but one of the limits of the Cauchy principal values are evaluated. Since the evaluation of the remaining limit requires the additional restrictions and considerations formulated in the theorem, it is examined separately in Section 3.3. In the last section of this chapter, the formula for the reflected electric field will be derived and the absolute and uniform convergence of the sums in E_ℓ for $\ell=0,\dots,4$ will be proven.

3.2 Solving the Helmholtz equation

3.2.1 Formula for the solution via Fourier transform

Applying the generalised Fourier transform (cf. (2.3.9)) to both sides of (2.3.5), the following equation is reached (cf. $\vec{E}^0(\vec{x}) = \vec{e}^{\,0}\, e^{i\vec{k}_\tau\cdot\vec{x}}$)

$$\left(-s^2 + k_\tau^2\right) \hat{D}^d(\vec{s}) = -\left[\left(\vec{s}\times\vec{e}^{\,0}\right)\times\vec{s}\right] \hat{\alpha}_d(\vec{s}-\vec{k}_\tau), \tag{3.2.1}$$

where $\hat{D}^d(\vec{s}) := \mathcal{F}(\vec{D}^d(\cdot))(\vec{s})$ is applied component-wise, $s^2 := \|\vec{s}\|^2$ and where the constants of the classical Fourier transform and its inverse (see (2.3.7) and (2.3.8)) are used. Equation (3.2.1) can then be resolved w.r.t. $\hat{D}^d(\vec{s})$ to get

$$\hat{D}^d(\vec{s}) = \left[\left(\vec{s}\times\vec{e}^{\,0}\right)\times\vec{s}\right] \frac{\hat{\alpha}_d(\vec{s}-\vec{k}_\tau)}{s^2 - k_\tau^2},$$

where $s^2 \neq k_\tau^2$ for all $\vec{s}\in\mathbb{R}^3$ and $\tau<0$. To get an expression for $\vec{D}^d(\vec{x})$, the inverse Fourier transform has to be applied. This is also to be done in the generalised way. Consequently,

$$\begin{aligned}
\left\langle \vec{D}^d(\vec{x}), \varphi(\vec{x})\right\rangle &= \left\langle \vec{D}^d(\vec{x}), (\hat{\varphi})\check{}\,(\vec{x})\right\rangle \\
&= \frac{1}{(2\pi)^3}\left\langle \hat{D}^d(\vec{s}), \hat{\varphi}(\vec{s})\right\rangle \\
&= \frac{1}{(2\pi)^3}\left\langle \hat{\alpha}_d(\vec{s}-\vec{k}_\tau)\,\frac{\left[\left(\vec{s}\times\vec{e}^{\,0}\right)\times\vec{s}\right]}{s^2-k_\tau^2}, \hat{\varphi}(\vec{s})\right\rangle \\
&= \frac{1}{(2\pi)^3}\left\langle \hat{\alpha}_d(\vec{s}-\vec{k}_\tau), \overline{\left[\frac{\left[\left(\vec{s}\times\vec{e}^{\,0}\right)\times\vec{s}\right]}{s^2-k_\tau^2}\right]\hat{\varphi}(\vec{s})}\right\rangle
\end{aligned}$$

for all $\varphi\in C_0^\infty(\mathbb{R}^3)$. Indeed, the last equation in the equality chain is valid since $s^2 - \vec{k}_\tau^2 \neq 0$ for all $\vec{s}\in\mathbb{R}^3$ and $\tau<0$, which shows that $[(\vec{s}\times\vec{e}^{\,0})\times\vec{s}]/(s^2-k_\tau^2)\,\hat{\varphi}(\vec{s})$ is a Schwartz function. Thus, by definition (cf. (2.3.9)),

$$\begin{aligned}
\left\langle \vec{D}^d(\vec{x}), \varphi(\vec{x})\right\rangle &= \left\langle \alpha_d(\vec{\eta})\, e^{i\vec{k}_\tau\cdot\vec{\eta}}, \mathcal{F}_{\vec{s}}^{-1}\left(\overline{\left[\frac{\left[\left(\vec{s}\times\vec{e}^{\,0}\right)\times\vec{s}\right]}{s^2-k_\tau^2}\right]\hat{\varphi}(\vec{s})}\right)(\vec{\eta})\right\rangle \\
&= \frac{1}{(2\pi)^3}\int\limits_{\mathbb{R}^3} \alpha_d(\vec{\eta})\, e^{i\vec{k}_\tau\cdot\vec{\eta}} \int\limits_{\mathbb{R}^3} \frac{\left[\left(\vec{s}\times\vec{e}^{\,0}\right)\times\vec{s}\right]}{s^2-k_\tau^2}\,\overline{\hat{\varphi}(\vec{s})}\, e^{-i\vec{\eta}\cdot\vec{s}}\,\mathrm{d}\vec{s}\,\mathrm{d}\vec{\eta} \\
&= \int\limits_{\mathbb{R}^3} \alpha_d(\vec{\eta})\, e^{i\vec{k}_\tau\cdot\vec{\eta}} \int\limits_{\mathbb{R}^3} \frac{\left[\left(\vec{s}\times\vec{e}^{\,0}\right)\times\vec{s}\right]}{s^2-k_\tau^2}\,(\overline{\varphi})\check{}\,(\vec{s})\, e^{-i\vec{\eta}\cdot\vec{s}}\,\mathrm{d}\vec{s}\,\mathrm{d}\vec{\eta},
\end{aligned} \tag{3.2.2}$$

where the integrals are well defined, since

$$\mathcal{F}_{\vec{s}}^{-1}\left(\frac{\left[\left(\vec{s}\times\vec{e}^{\,0}\right)\times\vec{s}\right]}{s^2-k_\tau^2}\,(\overline{\varphi})\check{}\,(\vec{s})\right)(\vec{\eta}) = \int\limits_{\mathbb{R}^3} \frac{\left[\left(\vec{s}\times\vec{e}^{\,0}\right)\times\vec{s}\right]}{s^2-k_\tau^2}\,(\overline{\varphi})\check{}\,(\vec{s})\, e^{-i\vec{\eta}\cdot\vec{s}}\,\mathrm{d}\vec{s},$$

the Fourier transform of a Schwartz function, is a Schwartz function (cf. Theorem C.2) and since $\alpha_d(\vec{\eta})\, e^{i\vec{k}_\tau\cdot\vec{\eta}}$ is uniformly bounded w.r.t. $\eta' := (\eta_x,\eta_y)^\top \in\mathbb{R}^2$ and $\eta_z\in\mathbb{R}$ and $\alpha_d(\vec{\eta})$ has a compact support w.r.t. η_z. Using these arguments, it is also easily seen that the outer integral in (3.2.2) exists absolutely.

3.2.2 Interchanging the order of integration

It is the goal of the next subsection to integrate analytically w.r.t. s_z, the third component of $\vec{s} := (s_x, s_y, s_z)^\top$ in (3.2.2) such that only the integrals w.r.t. s_x and s_y remain. To reach this goal the order of integration is interchanged. In order to enable such a change and the application of Lebesgue's dominated convergence theorem (cf. Theorem C.3), hereafter called Lebesgue's theorem, bounded domains of integration would be helpful. A switch to finite sections of the unbounded domain can be realised by the limit of a Cauchy principal value. Since the outer integral w.r.t. $\vec{\eta}$ in (3.2.2) exists absolutely for a complex valued k_τ^2, it is equal to its Cauchy principal value at infinity

$$\left\langle \vec{D}^d(\vec{x}), \varphi(\vec{x}) \right\rangle = \lim_{\tilde{r}\to\infty} \int\limits_{C_3(\tilde{r})} \alpha_d(\vec{\eta})\, e^{i\vec{k}_\tau\cdot\vec{\eta}} \int\limits_{\mathbb{R}^3} \frac{\left[\left(\vec{s}\times\vec{e}^{\,0}\right)\times\vec{s}\right]}{s^2-k_\tau^2}\, (\bar{\varphi})\check{}\,(\vec{s})\, e^{-i\vec{\eta}\cdot\vec{s}}\, \mathrm{d}\vec{s}\,\mathrm{d}\vec{\eta},$$

where $C_3(\tilde{r}) := B_2(\tilde{r})\times[-\tilde{r},\tilde{r}]$ and $B_2(\tilde{r}) := \left\{\eta' \in \mathbb{R}^2 : |\eta'| \le \tilde{r}\right\}$. On the other hand, for any fixed $\tilde{r}$, the integrals w.r.t. $\vec{\eta}$ and $\vec{s}$ are also absolutely integrable, since $(\bar{\varphi})\check{} \in \mathcal{S}(\mathbb{R}^3)$ decays faster than any polynomial as $\|\vec{s}\|$ tends to infinity. This allows Fubini's theorem (cf. Theorem C.4) to be applied. Thus

$$\left\langle \vec{D}^d(\vec{x}), \varphi(\vec{x}) \right\rangle = \lim_{\tilde{r}\to\infty} \int\limits_{\mathbb{R}^3}\int\limits_{C_3(\tilde{r})} \alpha_d(\vec{\eta})\, e^{-i\vec{\eta}\cdot(\vec{s}-\vec{k}_\tau)}\,\mathrm{d}\vec{\eta}\, \frac{\left[\left(\vec{s}\times\vec{e}^{\,0}\right)\times\vec{s}\right]}{s^2-k_\tau^2}\, (\bar{\varphi})\check{}\,(\vec{s})\,\mathrm{d}\vec{s}.$$

In the following subsections the term

$$\left\langle \vec{D}^d_{\tilde{r}}(\vec{x}), \varphi(\vec{x}) \right\rangle := \frac{1}{(2\pi)^3} \int\limits_{\mathbb{R}^3}\int\limits_{C_3(\tilde{r})} \alpha_d(\vec{\eta})\, e^{-i\vec{\eta}\cdot(\vec{s}-\vec{k}_\tau)}\,\mathrm{d}\vec{\eta}\, \frac{\left[\left(\vec{s}\times\vec{e}^{\,0}\right)\times\vec{s}\right]}{s^2-k_\tau^2} \int\limits_{\mathbb{R}^3} \bar{\varphi}(\vec{x})\, e^{i\vec{s}\cdot\vec{x}}\,\mathrm{d}\vec{x}\,\mathrm{d}\vec{s} \tag{3.2.3}$$

will be considered under the assumption that $\tilde{r} > h$ is arbitrarily fixed. The limit $\tilde{r}\to\infty$ will be examined later in Subsection 3.3.

Again, since the integral w.r.t. $\vec{s}$ in (3.2.3) is absolutely integrable and thus equal to its Cauchy principal value at infinity,

$$\left\langle \vec{D}^d_{\tilde{r}}(\vec{x}), \varphi(\vec{x}) \right\rangle := \frac{1}{(2\pi)^3} \lim_{r,R\to\infty} \int\limits_{B_2(r)}\int\limits_{-R}^{R}\int\limits_{C_3(\tilde{r})} \alpha_d(\vec{\eta})\, e^{-i\vec{\eta}\cdot(\vec{s}-\vec{k}_\tau)}\,\mathrm{d}\vec{\eta}\, \frac{\left[\left(\vec{s}\times\vec{e}^{\,0}\right)\times\vec{s}\right]}{s^2-k_\tau^2} \int\limits_{\mathbb{R}^3} \bar{\varphi}(\vec{x})\, e^{i\vec{s}\cdot\vec{x}}\,\mathrm{d}\vec{x}\,\mathrm{d}s_z\,\mathrm{d}s',$$

with $s' := (s_x, s_y)^\top$. Since φ has a compact support, the integrand of the integrals w.r.t. $\vec{x}$ and $\vec{s}$ is absolutely integrable for any fixed $r, R \in \mathbb{R}$. Hence, for the bounded domain of integration, Fubini's theorem can be applied and the order of integration can be interchanged to obtain

$$\left\langle \vec{D}^d_{\tilde{r}}(\vec{x}), \varphi(\vec{x}) \right\rangle$$
$$:= \frac{1}{(2\pi)^3} \lim_{r,R\to\infty} \int\limits_{\mathbb{R}^3} \bar{\varphi}(\vec{x}) \int\limits_{B_2(r)}\int\limits_{-R}^{R}\int\limits_{C_3(\tilde{r})} \alpha_d(\vec{\eta})\, e^{-i\vec{\eta}\cdot(\vec{s}-\vec{k}_\tau)}\,\mathrm{d}\vec{\eta}\, \frac{\left[\left(\vec{s}\times\vec{e}^{\,0}\right)\times\vec{s}\right]}{s_z^2-\xi_\tau^2}\, e^{i\vec{s}\cdot\vec{x}}\,\mathrm{d}s_z\,\mathrm{d}s'\,\mathrm{d}\vec{x}, \tag{3.2.4}$$

where $\xi_\tau := \sqrt{k_\tau^2 - s_x^2 - s_y^2}$. Here and in the remainder of this thesis the square root of a complex number w will be chosen in such a way that the argument of the complex number $\sqrt{w}$ is an element of the interval $[0,\pi)$. Thus, by definition, the imaginary part of ξ_τ is positive and the integrand of the integration w.r.t. s_z in (3.2.4) has no poles for any fixed $s' \in \mathbb{R}^2$.

3.2.3 Analytical integration

It is the goal of this subsection to resolve the limit w.r.t. R using contour integration and by applying Lebesgue's theorem to evaluate the limit before the integrals w.r.t. s' and $\vec{x}$. To apply Lebesgue's theorem, it will be shown that the integrand of the integral w.r.t. s' of (3.2.4) is uniformly bounded and pointwise convergent w.r.t. $R\to\infty$ and $R > |\vec{k}_\tau|$, for any fixed $r\in\mathbb{R}$. Note that, for the bound to be integrable w.r.t. s' and $\vec{x}$, it is sufficient that the integral w.r.t. s_z is absolutely integrable with uniform bound for any fixed $s' \in B_2(r)$ and $\vec{x}\in\mathbb{R}^3$, since $B_2(r)$ is bounded and φ has a compact

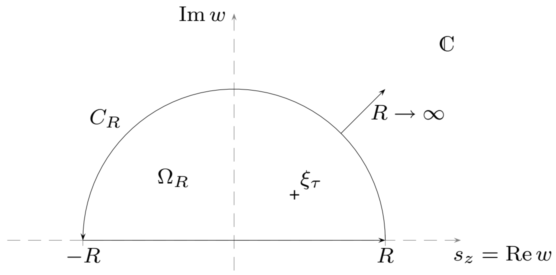


Figure 3.1: Contour integration path

support. From this point onwards, it will be assumed that the field is only evaluated outside the interface region, i.e. it is assumed that $|z| > h$, where z is the third component of $\vec{x}$.

For convenience, suppose $\tilde{r} > h$ and define $\Delta := \Delta_\tau := \epsilon_\tau - \epsilon_0'$ and

$$\begin{aligned}
\hat{\alpha}_{\tilde{r}}(\vec{s} - \vec{k}_\tau) &:= \int\limits_{C_3(\tilde{r})} \alpha_d(\vec{\eta})\, e^{-i\vec{\eta}\cdot(\vec{s}-\vec{k}_\tau)}\, \mathrm{d}\vec{\eta} \\
&= \int\limits_{C_3(\tilde{r})} \big[\alpha(\vec{\eta}) - \alpha_{\mathcal{Q}}(\vec{\eta})\big]\, e^{-i\vec{\eta}\cdot(\vec{s}-\vec{k}_\tau)}\, \mathrm{d}\vec{\eta} \\
&= -\Delta \int\limits_{B_2(\tilde{r})} \int\limits_0^{f(\eta')} e^{-i\eta_z(s_z - k_{z,\tau})}\, \mathrm{d}\eta_z\, e^{-i\eta'\cdot(s'-k')}\, \mathrm{d}\eta' \\
&= -\Delta \int\limits_{B_2(\tilde{r})} \left[-\frac{1}{i(s_z - k_{z,\tau})}\, e^{-i\eta_z(s_z - k_{z,\tau})}\right]_{\eta_z=0}^{f(\eta')} e^{-i\eta'\cdot(s'-k')}\, \mathrm{d}\eta' \\
&= i\Delta \int\limits_{B_2(\tilde{r})} \frac{1 - e^{-i(s_z-k_{z,\tau})\, f(\eta')}}{s_z - k_{z,\tau}}\, e^{-i\eta'\cdot(s'-k')}\, \mathrm{d}\eta',
\end{aligned} \tag{3.2.5}$$

such that

$$\hat{\alpha}_{\tilde{r}}(\vec{s} - \vec{k}_\tau) = -\Delta \int\limits_{B_2(\tilde{r})} \int\limits_0^1 e^{-i(s_z-k_{z,\tau})\,\zeta\, f(\eta')}\, \mathrm{d}\zeta\, f(\eta')\, e^{-i\eta'\cdot(s'-k')}\, \mathrm{d}\eta', \tag{3.2.6}$$

which is continuously differentiable and uniformly bounded w.r.t. $\vec{s}$. By analytic continuation of the function $\hat{\alpha}_{\tilde{r}}(\vec{s} - \vec{k}_\tau)\, [(\vec{s} \times \vec{e}^{\,0}) \times \vec{s}]/(s_z^2 - \xi_\tau^2)\, e^{is_z z}$ w.r.t. s_z onto $\mathbb{C}$ for all $z > h$, a meromorphic function (cf. Definition C.6) is obtained. Thus the residue theorem (cf. Theorem C.7) can be applied to the integration over the closed path $\partial\Omega_R := C_R \cup [-R, R]$, with $C_R := \{z \in \mathbb{C} : \mathrm{Im}\, z \geq 0, |z| = R\}$. The curve C_R is assumed to be oriented counter-clockwise. The integral w.r.t. s_z in (3.2.4) can then be written as (cf. Figure 3.1)

$$\begin{aligned}
\int\limits_{-R}^{R} \hat{\alpha}_{\tilde{r}}(\vec{s} - \vec{k}_\tau)\, \frac{\big[(\vec{s} \times \vec{e}^{\,0}) \times \vec{s}\big]}{s_z^2 - \xi_\tau^2}\, e^{is_z z}\, \mathrm{d}s_z = &- \int\limits_{C_R} \hat{\alpha}_{\tilde{r}}(\vec{s}_w - \vec{k}_\tau)\, \frac{\big[(\vec{s}_w \times \vec{e}^{\,0}) \times \vec{s}_w\big]}{w^2 - \xi_\tau^2}\, e^{iwz}\, \mathrm{d}w \\
&+ 2\pi i\, \hat{\alpha}_{\tilde{r}}(\vec{s}_{\xi_\tau} - \vec{k}_\tau)\, \frac{\big[(\vec{s}_{\xi_\tau} \times \vec{e}^{\,0}) \times \vec{s}_{\xi_\tau}\big]}{2\xi_\tau}\, e^{i\xi_\tau z},
\end{aligned} \tag{3.2.7}$$

where $\vec{s}_w = (s_x, s_y, w)^\top$ for $w \in \mathbb{C}$. The second summand on the right-hand side of (3.2.7) corresponds to $2\pi i$ times the winding number of the integration path around ξ_τ times the residue of the integrand at $w = \xi_\tau$. The point $w = \xi_\tau$ is enclosed by the path $\partial\Omega_R$, since $R > |\vec{k}_\tau| \geq |\xi_\tau|$ was assumed. Parametrising the curve C_R by $R\, e^{i\phi}$ for $\phi \in [0, \pi]$, the absolute value of the first summand in (3.2.7) can be estimated as

$$\begin{aligned}
&\left| \int\limits_{C_R} \hat{\alpha}_{\tilde{r}}(\vec{s}_w - \vec{k}_\tau) \, \frac{\left[\left(\vec{s}_w \times \vec{e}^{\,0} \right) \times \vec{s}_w \right]}{(w-\xi_\tau)(w+\xi_\tau)} \, e^{iwz} \, \mathrm{d}w \right| \\
&\qquad = \left| \int\limits_0^\pi \hat{\alpha}_{\tilde{r}}(\vec{s}_{Re^{i\phi}} - \vec{k}_\tau) \, \frac{\left[\left(\vec{s}_{Re^{i\phi}} \times \vec{e}^{\,0} \right) \times \vec{s}_{Re^{i\phi}} \right]}{(Re^{i\phi}-\xi_\tau)(Re^{i\phi}+\xi_\tau)} \, e^{izRe^{i\phi}} iRe^{i\phi} \, \mathrm{d}\phi \right| \\
&\qquad \le \int\limits_0^\pi \left| \hat{\alpha}_{\tilde{r}}(\vec{s}_{Re^{i\phi}} - \vec{k}_\tau) \, \frac{\left[\left(\vec{s}_{Re^{i\phi}} \times \vec{e}^{\,0} \right) \times \vec{s}_{Re^{i\phi}} \right]}{(Re^{i\phi}-\xi_\tau)(Re^{i\phi}+\xi_\tau)} \, iRe^{i\phi} \, e^{izRe^{i\phi}} \right| \mathrm{d}\phi \\
&\qquad \le \sup_{\phi\in[0,\pi]} \left| \frac{\left[\left(\vec{s}_{Re^{i\phi}} \times \vec{e}^{\,0} \right) \times \vec{s}_{Re^{i\phi}} \right]}{(Re^{i\phi}-\xi_\tau)(Re^{i\phi}+\xi_\tau)} \, \hat{\alpha}_{\tilde{r}}(\vec{s}_{Re^{i\phi}} - \vec{k}_\tau) \, R \, e^{i\frac{z}{2}Re^{i\phi}} \right| \int\limits_0^\pi \left| e^{i\frac{z}{2}Re^{i\phi}} \right| \mathrm{d}\phi \\
&\qquad = \sup_{\phi\in[0,\pi]} \left| \frac{\left[\left(\vec{s}_{Re^{i\phi}} \times \vec{e}^{\,0} \right) \times \vec{s}_{Re^{i\phi}} \right]}{(Re^{i\phi}-\xi_\tau)(Re^{i\phi}+\xi_\tau)} \, \hat{\alpha}_{\tilde{r}}(\vec{s}_{Re^{i\phi}} - \vec{k}_\tau) \, R \, e^{i\frac{z}{2}Re^{i\phi}} \right| \int\limits_0^\pi e^{-\frac{z}{2}R\sin\phi} \, \mathrm{d}\phi \\
&\qquad \le 2C(s') \int\limits_0^{\pi/2} e^{-\frac{z}{2}R\sin\phi} \, \mathrm{d}\phi \le \pi \, C(s').
\end{aligned} \tag{3.2.8}$$

It will be shown subsequently that the constant $C(s') := c_1 \, c_2(s')$ with

$$c_1 := \sup_{s'\in\mathbb{R}^2} \sup_{R\in[|\vec{k}_\tau|,\infty)} \sup_{\phi\in[0,\pi]} \left| \hat{\alpha}_{\tilde{r}}(\vec{s}_{Re^{i\phi}} - \vec{k}_\tau) \, R \, e^{i\frac{z}{2}Re^{i\phi}} \right|$$

and

$$c_2(s') := \sup_{R\in[|\vec{k}_\tau|,\infty)} \sup_{\phi\in[0,\pi]} \left| \frac{\left[\left(\vec{s}_{Re^{i\phi}} \times \vec{e}^{\,0} \right) \times \vec{s}_{Re^{i\phi}} \right]}{(Re^{i\phi}-\xi_\tau)(Re^{i\phi}+\xi_\tau)} \right|$$

is finite for any fixed $s' \in \mathbb{R}^2$.

It is easily seen that the supremum $c_2(s')$ is finite, since the numerator is a polynomial of order two of $Re^{i\phi}$, while the second order polynomial in the denominator has no zeros. It can also be shown that c_1 is finite. Together with (3.2.5) consider

$$\begin{aligned}
&\sup_{\phi\in[0,\pi]} \left| \hat{\alpha}_{\tilde{r}}(\vec{s}_{Re^{i\phi}} - \vec{k}_\tau) \, R \, e^{i\frac{z}{2}Re^{i\phi}} \right| \\
&\qquad = \sup_{\phi\in[0,\pi]} \left| \Delta \int\limits_{B_2(\tilde{r})} \frac{1 - e^{-i(Re^{i\phi}-k_{z,\tau})\, f(\eta')}}{Re^{i\phi}-k_{z,\tau}} \, e^{-i\eta'\cdot(s'-k')} \, \mathrm{d}\eta' \, R \, e^{i\frac{z}{2}Re^{i\phi}} \right| \\
&\qquad = \sup_{\phi\in[0,\pi]} \left| \frac{\Delta \, R}{Re^{i\phi}-k_{z,\tau}} \int\limits_{B_2(\tilde{r})} \left[e^{i\frac{z}{2}Re^{i\phi}} - e^{iRe^{i\phi}\left(\frac{z}{2}-f(\eta')\right)} \, e^{ik_{z,\tau} f(\eta')} \right] e^{-i\eta'\cdot(s'-k')} \, \mathrm{d}\eta' \right| \\
&\qquad \le \sup_{\phi\in[0,\pi]} \frac{|\Delta| \; R}{|R-|k_{z,\tau}||} \int\limits_{B_2(\tilde{r})} \left[e^{-\frac{z}{2}R\sin\phi} + e^{-R\sin\phi\left(\frac{z}{2}-f(\eta')\right)} \, e^{-\tau f(\eta')} \right] \mathrm{d}\eta' \\
&\qquad \le \frac{|\Delta| \; R}{|R-|k_{z,\tau}||} \int\limits_{B_2(\tilde{r})} \left[1 + e^{-\tau f(\eta')} \right] \mathrm{d}\eta',
\end{aligned}$$

where it was used that both z and $z/2 - f(\eta')$ are positive for all $z > h$ and $\eta' \in \mathbb{R}^2$ and where the last term is uniformly bounded w.r.t. R for any fixed $\tilde{r}$, since R was chosen larger than $|\vec{k}_\tau| \ge |k_{z,\tau}|$.

The second term of (3.2.7) is also uniformly bounded w.r.t. s' for any fixed $r \in \mathbb{R}$ and $z > h$, as will be shown in the following. First note that the supremum

$$c_3 := \sup_{s' \in \mathbb{R}^2} \left| \frac{\left[\left(\vec{s}_{\xi_\tau} \times \vec{e}^{\,0}\right) \times \vec{s}_{\xi_\tau}\right]}{\xi_\tau^2} \right| = \sup_{s' \in \mathbb{R}^2} \left| \frac{\left[\left(\vec{s}_{\xi_\tau} \times \vec{e}^{\,0}\right) \times \vec{s}_{\xi_\tau}\right]}{k_\tau^2 - s_x^2 - s_y^2} \right| \tag{3.2.9}$$

is finite since the denominator is a second order polynomial of s' without zeros, while the absolute value of the numerator is bounded from above by a polynomial with a total degree of two. Now consider (cf. (3.2.6))

$$\begin{aligned}
&\left| \hat{\alpha}_{\tilde{r}}(\vec{s}_{\xi_\tau} - \vec{k}_\tau) \, \frac{\left[\left(\vec{s}_{\xi_\tau} \times \vec{e}^{\,0}\right) \times \vec{s}_{\xi_\tau}\right]}{\xi_\tau} \, e^{i\xi_\tau z} \right| \\
&\quad = \left| \hat{\alpha}_{\tilde{r}}(\vec{s}_{\xi_\tau} - \vec{k}_\tau) \, \xi_\tau \, e^{i\xi_\tau z} \, \frac{\left[\left(\vec{s}_{\xi_\tau} \times \vec{e}^{\,0}\right) \times \vec{s}_{\xi_\tau}\right]}{\xi_\tau^2} \right| \\
&\quad \le c_3 \left| \hat{\alpha}_{\tilde{r}}(\vec{s}_{\xi_\tau} - \vec{k}_\tau) \, \xi_\tau \, e^{i\xi_\tau z} \right| \\
&\quad = c_3 \left| \Delta \int_{B_2(\tilde{r})} \int_0^1 e^{-i(\xi_\tau - k_{z,\tau}) \, \zeta \, f(\eta')} \, \mathrm{d}\zeta f(\eta') \, e^{-i\eta' \cdot (s' - k')} \, \mathrm{d}\eta' \, \xi_\tau \, e^{i\xi_\tau z} \right| \\
&\quad \le c_3 \left| \Delta \, \xi_\tau \right| \int_{B_2(\tilde{r})} \int_0^1 \left| e^{i\xi_\tau \left(z - \zeta \, f(\eta')\right)} \, e^{ik_{z,\tau} \, \zeta \, f(\eta')} \right| \, \mathrm{d}\zeta \, \mathrm{d}\eta' \\
&\quad = c_3 \left| \Delta \, \xi_\tau \right| \int_{B_2(\tilde{r})} \int_0^1 e^{-\left(z - \zeta \, f(\eta')\right) \sqrt{|k_\tau^2 - s'^2|} \sin\theta} \, e^{-\tau \, \zeta \, f(\eta')} \, \mathrm{d}\zeta \, \mathrm{d}\eta' \\
&\quad \le c_3 \left| \Delta \, \xi_\tau \right| \, e^{-\frac{h}{2} \sqrt{|k_\tau^2 - s'^2|} \sin\theta} \int_{B_2(\tilde{r})} \int_0^1 e^{-\tau \, \zeta \, f(\eta')} \, \mathrm{d}\zeta \, \mathrm{d}\eta',
\end{aligned} \tag{3.2.10}$$

where $\theta := \arg \sqrt{k_\tau^2 - s'^2} \in (0, \pi)$, $(z - \zeta \, f(\eta')) \ge h/2$ and $s'^2 := |s'|^2 = s_x^2 + s_y^2$. Note that $\lim_{|s'| \to \infty} \theta = \pi/2$. Therefore, $\lim_{|s'| \to \infty} |\xi_\tau| \, \exp(-\frac{h}{2} \sqrt{|k_\tau^2 - s'^2|} \sin\theta) = 0$, which shows that (3.2.10) is uniformly bounded w.r.t. $s' \in \mathbb{R}^2$ for any fixed $\tilde{r}$ and $z > h = 2\|f\|_\infty$. Hence the supremum

$$c_4(\tilde{r}) := \sup_{s' \in \mathbb{R}^2} \left| \hat{\alpha}_{\tilde{r}}(\vec{s}_{\xi_\tau} - \vec{k}_\tau) \, \frac{\left[\left(\vec{s}_{\xi_\tau} \times \vec{e}^{\,0}\right) \times \vec{s}_{\xi_\tau}\right]}{\xi_\tau} \, e^{i\xi_\tau z} \right| \tag{3.2.11}$$

is finite for any fixed $\tilde{r} > h$ and $\tau < 0$. Consequently, the integral w.r.t. s_z in (3.2.4) is absolutely bounded by $\pi \, C(s') + 2\pi \, c_4(\tilde{r})$ (cf. (3.2.8)), which is integrable on the bounded set $B_2(r)$.

With this, Lebesgue's theorem can be applied to evaluate the limit $R \to \infty$. Using estimate (3.2.8) it can be shown, that the limit of the integral over C_R tends to zero as R tends to infinity. In fact, by showing that the non-negative upper bound (3.2.8) of the absolute value of the integral over C_R tends to zero for any fixed $z > h > 0$, the same holds for the integral itself. To show this, the integral in the upper bound (3.2.8) is divided into the sum of the integrals over the interval $[0, \pi/4]$ and $[\pi/4, \pi/2]$, such that

$$\int_0^{\pi/2} e^{-\frac{z}{2} R \sin\phi} \, \mathrm{d}\phi = \int_0^{\pi/4} e^{-\frac{z}{2} R \sin\phi} \, \mathrm{d}\phi + \int_{\pi/4}^{\pi/2} e^{-\frac{z}{2} R \sin\phi} \, \mathrm{d}\phi.$$

The limit $R \to \infty$ of these integrals can then be estimated as

$$\lim_{R \to \infty} \int_{\pi/4}^{\pi/2} e^{-\frac{z}{2} R \sin\phi} \, \mathrm{d}\phi \le \lim_{R \to \infty} \frac{\pi}{4} e^{-\frac{z}{2} R \sin\frac{\pi}{4}} = \lim_{R \to \infty} \frac{\pi}{4} e^{-\frac{z}{2} R \frac{1}{\sqrt{2}}} = 0 \tag{3.2.12}$$

and, since $2\cos\phi > 1$ for $\phi \in \left[0, \frac{\pi}{4}\right]$,

$$\begin{aligned}
\lim_{R\to\infty} \int_0^{\pi/4} e^{-\frac{z}{2}R\sin\phi}\,\mathrm{d}\phi &< \lim_{R\to\infty} \int_0^{\pi/4} e^{-\frac{z}{2}R\sin\phi}\,2\cos\phi\,\mathrm{d}\phi \\
&= \lim_{R\to\infty} -\frac{4}{zR} \int_0^{\pi/4} e^{-\frac{z}{2}R\sin\phi} \left(-\frac{zR}{2}\cos\phi\right)\mathrm{d}\phi \\
&= \lim_{R\to\infty} -\frac{4}{z}\left(\frac{e^{-\frac{z}{2\sqrt{2}}R}-1}{R}\right) = 0. \qquad (3.2.13)
\end{aligned}$$

Therefore, (cf. (3.2.7))

$$\lim_{R\to\infty} \int_{-R}^{R} \hat{\alpha}_{\tilde{r}}(\vec{s}-\vec{k}_\tau)\,\frac{\left[\left(\vec{s}\times\vec{e}^{\,0}\right)\times\vec{s}\right]}{s_z^2-\xi_\tau^2}\,e^{is_z z}\,\mathrm{d}s_z = \pi i\,\hat{\alpha}_{\tilde{r}}(\vec{s}_{\xi_\tau}-\vec{k}_\tau)\,\frac{\left[\left(\vec{s}_{\xi_\tau}\times\vec{e}^{\,0}\right)\times\vec{s}_{\xi_\tau}\right]}{\xi_\tau}\,e^{i\xi_\tau z}$$

and it follows that (cf. (3.2.4))

$$\left\langle \vec{D}^d_{\tilde{r}}(\vec{x}),\varphi(\vec{x})\right\rangle = \frac{i}{8\pi^2}\lim_{r\to\infty}\int_{\mathbb{R}^3}\bar{\varphi}(\vec{x})\int_{B_2(r)}\hat{\alpha}_{\tilde{r}}(\vec{s}_{\xi_\tau}-\vec{k}_\tau)\,\frac{\left[\left(\vec{s}_{\xi_\tau}\times\vec{e}^{\,0}\right)\times\vec{s}_{\xi_\tau}\right]}{\xi_\tau}\,e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}}\,\mathrm{d}s'\,\mathrm{d}\vec{x}, \qquad (3.2.14)$$

if $\varphi(\vec{x}) \equiv 0$ for $z \le h$.

3.2.4 Resolution of one Cauchy principal value

The goal of this subsection is to evaluate the limit $r\to\infty$ in equation (3.2.14). To achieve this, it will be shown that the integrand of the integral w.r.t. s' in this equation is absolutely integrable for all fixed $x' \in \mathbb{R}^2$ and $z > h$. Afterwards it will be proven that this absolute integral is also uniformly bounded w.r.t. $r > 0$ for any fixed $x' \in \mathbb{R}^2$ and $z > h$. The absolute value of the product of $\varphi \in C_0^\infty(\mathbb{R}^3)$ and the integral w.r.t. s' in equation (3.2.14) is then dominated by a non-negative integrable function independent of r. Therefore Lebesgue's theorem can be applied.

First, the term $\xi_\tau = \sqrt{k_\tau^2 - s'^2}$, with $k_{z,\tau} = k_z + i\tau$ and $k_z < 0$ will be examined more closely. Assuming $s'^2 > 2\|\vec{k}_\tau\|^2$, it is easily seen that $\mathrm{Re}(k_\tau^2 - s'^2) = k^2-\tau^2-s'^2 < 0$ and $\mathrm{Im}(k_\tau^2-s'^2) = 2k_z\tau > 0$. Moreover, the argument $\arctan(2k_z\tau/(k^2-\tau^2-s'^2))+\pi$ of the complex number $k_\tau^2 - s'^2$ is an element of the interval $(\pi/2,\pi)$, for $\arctan\colon\mathbb{R}\to(-\pi/2,\pi/2)$. Hence the angle θ, defined as the argument of the complex number $\sqrt{k_\tau^2-s'^2}$, lies in $(\pi/4,\pi/2)$ leading to $\sin\theta > 1/\sqrt{2}$. With this in mind and the fact that $|z - f(\eta')| > h/2$ for all $|z| > h$, consider the following estimates together with (3.2.9), (3.2.10) and (3.2.11).

$$\begin{aligned}
&\left|\int_{B_2(r)} \hat{\alpha}_{\tilde{r}}(\vec{s}_{\xi_\tau}-\vec{k}_\tau)\,\frac{\left[\left(\vec{s}_{\xi_\tau}\times\vec{e}^{\,0}\right)\times\vec{s}_{\xi_\tau}\right]}{\xi_\tau}\,e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}}\,\mathrm{d}s'\right| \\
&\quad\le \int_{B_2(r)} \left|\hat{\alpha}_{\tilde{r}}(\vec{s}_{\xi_\tau}-\vec{k}_\tau)\,\frac{\left[\left(\vec{s}_{\xi_\tau}\times\vec{e}^{\,0}\right)\times\vec{s}_{\xi_\tau}\right]}{\xi_\tau}\,e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}}\right|\mathrm{d}s' \\
&\quad\le \int_{\mathbb{R}^2} \left|\hat{\alpha}_{\tilde{r}}(\vec{s}_{\xi_\tau}-\vec{k}_\tau)\,\frac{\left[\left(\vec{s}_{\xi_\tau}\times\vec{e}^{\,0}\right)\times\vec{s}_{\xi_\tau}\right]}{\xi_\tau}\,e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}}\right|\mathrm{d}s' \\
&\quad\le \int_{B_2(\sqrt{2}|\vec{k}_\tau|)} \left|\hat{\alpha}_{\tilde{r}}(\vec{s}_{\xi_\tau}-\vec{k}_\tau)\,\frac{\left[\left(\vec{s}_{\xi_\tau}\times\vec{e}^{\,0}\right)\times\vec{s}_{\xi_\tau}\right]}{\xi_\tau}\,e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}}\right|\mathrm{d}s' \\
&\qquad+ \int_{\mathbb{R}^2\setminus B_2(\sqrt{2}|\vec{k}_\tau|)} \left|\hat{\alpha}_{\tilde{r}}(\vec{s}_{\xi_\tau}-\vec{k}_\tau)\,\frac{\left[\left(\vec{s}_{\xi_\tau}\times\vec{e}^{\,0}\right)\times\vec{s}_{\xi_\tau}\right]}{\xi_\tau}\,e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}}\right|\mathrm{d}s'
\end{aligned}$$

$$
\begin{aligned}
&\leq 2\pi|\vec{k}_\tau|^2 c_4(\tilde{r}) + c_3 \int\limits_{\mathbb{R}^2\setminus B_2(\sqrt{2}|\vec{k}_\tau|)} \left|\hat{\alpha}_{\tilde{r}}(\vec{s}_{\xi_\tau} - \vec{k}_\tau)\, \xi_\tau \, e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}}\right| \mathrm{d}s' \\
&\leq 2\pi|\vec{k}_\tau|^2 c_4(\tilde{r}) \\
&\quad + c_3\,\Delta \int\limits_{\mathbb{R}^2\setminus B_2(\sqrt{2}|\vec{k}_\tau|)} \left|\frac{\xi_\tau}{\xi_\tau - k_{z,\tau}}\right| \int\limits_{B_2(\tilde{r})} \left[e^{-|z|\sqrt{|k_\tau^2 - s'^2|}\sin\theta} + e^{-|z-f(\eta')|\sqrt{|k_\tau^2-s'^2|}\sin\theta}\, e^{-\tau f(\eta')}\right] \mathrm{d}\eta'\,\mathrm{d}s' \\
&\leq 2\pi|\vec{k}_\tau|^2 c_4(\tilde{r}) + c_3\,\Delta \int\limits_{\mathbb{R}^2\setminus B_2(\sqrt{2}|\vec{k}_\tau|)} \left|\frac{\xi_\tau\,\pi\,\tilde{r}^2}{\xi_\tau - k_{z,\tau}}\right| \left[e^{-\frac{|z|}{\sqrt{2}}\sqrt{|k_\tau^2-s'^2|}} + e^{-\frac{h}{2\sqrt{2}}\sqrt{|k_\tau^2-s'^2|}}\, e^{\tau h}\right] \mathrm{d}s'. \quad (3.2.15)
\end{aligned}
$$

Similar to the estimate (3.2.10), the remaining quotient is uniformly bounded w.r.t. s'. This shows that the integral is finite for any fixed $x' \in \mathbb{R}^2$ and $z > h$ since the integrand decreases exponentially. Thus Lebesgue's theorem can be applied to evaluate the limit $r \to \infty$ and

$$
\left\langle \vec{D}^d_{\tilde{r}}(\vec{x}), \varphi(\vec{x}) \right\rangle = \frac{i}{8\pi^2} \int\limits_{\mathbb{R}^3} \bar{\varphi}(\vec{x}) \int\limits_{\mathbb{R}^2} \hat{\alpha}_{\tilde{r}}(\vec{s}_{\xi_\tau} - \vec{k}_\tau)\, \frac{\left[\left(\vec{s}_{\xi_\tau} \times \vec{e}^{\,0}\right) \times \vec{s}_{\xi_\tau}\right]}{\xi_\tau}\, e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}}\, \mathrm{d}s'\,\mathrm{d}\vec{x}, \tag{3.2.16}
$$

if $\varphi(\vec{x}) = 0$ for all $z \leq h$.

3.3 Resolution of remaining limits for a special interface space

To evaluate the last remaining limit $\tilde{r} \to \infty$ from the Cauchy principal values as well as the limit $\tau \nearrow 0$ of the limiting absorption principle, the set of interface function has to be reduced from $L^\infty_Q(\mathbb{R}^2)$ to a subset with specific properties. Defining the subset as in Theorem 3.1, it will be shown in the following subsection that the remaining limits exist for interfaces from this set. In the last part of this section the limits will then be evaluated to finally obtain formula (3.1.2) for the reflected field outside the interface region.

3.3.1 Almost periodic and decaying interface functions

Unfortunately, we were not able to treat general bounded and smooth interface functions f, so we have to restrict our analysis to a special class. Interface functions from this class must have an explicit Fourier transform. Furthermore, they should contain functions with a superposition of corrugations, e.g. almost periodic functions (cf. [5]), and functions of the same type, but with an integer order of decay at infinity. The idea is to model rough surfaces by superposition of corrugations while, at the same time, including interfaces with decaying properties.

Consider the following linear vector space of interface functions.

$$
\mathcal{A} := \left\{ f : \mathbb{R}^2 \to \mathbb{R} \;\middle|\; f \in \mathcal{A}^{\mathbb{C}} \right\}, \tag{3.3.1}
$$

$$
\begin{aligned}
\mathcal{A}^{\mathbb{C}} := \Bigg\{ f : \mathbb{R}^2 \to \mathbb{C} \;\Big|\; f \in \mathrm{L}^\infty(\mathbb{R}^2),\; f(\eta') = \sum_{\ell=0}^{3} \left[\frac{1}{\sqrt{1+|\eta'|^2}^{\,\ell}} \sum_{j\in\mathbb{Z}} \lambda_{\ell,j}\, e^{i\omega'_{\ell,j}\cdot\eta'} \right] + g(\eta') \\
\lambda_{\ell,j} \in \mathbb{C},\; \omega'_{\ell,j} \in \mathbb{R}^2,\; ||f||_{\mathcal{A}} < \infty \Bigg\}
\end{aligned}
$$

where

$$
||f||_{\mathcal{A}} := \sum_{\ell=0}^{3} \sum_{j\in\mathbb{Z}} |\lambda_{\ell,j}| + ||g||_{4,\infty} \tag{3.3.2}
$$

and $\left|\left|g(\eta')\right|\right|_{4,\infty} := \left|\left|(1+|\eta'|^2)^2\, g(\eta')\right|\right|_\infty$. Note, that the restrictions $\omega'_{\ell,j} = -\omega'_{\ell,-j}$ and $\lambda_{\ell,j} = \overline{\lambda_{\ell,-j}}$ for $\ell = 0,1,2,3$ and $j \in \mathbb{Z}$ ensure that the function f, given as a sum in the definition of $\mathcal{A}^{\mathbb{C}}$, is real

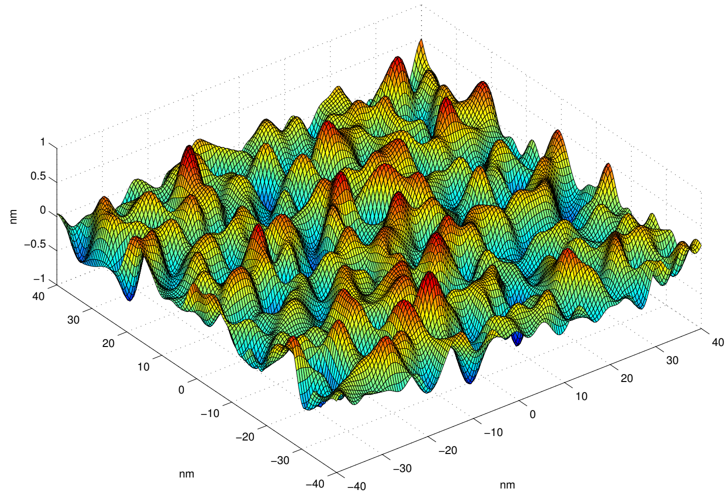


Figure 3.2: Example of an interface function from $\mathcal{A}$ using only the almost periodic portion and choosing a finite number of uniformly distributed random parameters $\omega'_{0,j}$ with corresponding $\lambda_{0,j}$ to get a given correlation function (cf. Chap. 6).

valued. Furthermore, it is assumed that the $\omega'_{\ell,j}$ of a function $f \in \mathcal{A}^{\mathbb{C}}$ are unique, meaning that from $\omega'_{\ell,j} = \omega'_{\ell,\iota}$ follows that $j = \iota$. Note that the function $\sum_{j\in\mathbb{Z}} \lambda_{\ell,j}\, e^{i\omega'_{\ell,j}\cdot\eta'}$ in the definition of $\mathcal{A}^{\mathbb{C}}$ fits the framework of almost periodic functions (cf. [5]). These type of functions have been used before by Stover [37] to characterise rough surfaces as superpositions of sinusoidal gratings. There holds

Remark 3.4. *It is easily seen that for any $f \in \mathcal{A}$ where $\lambda_{0,j_0} = 0$ if $\omega'_{0,j_0} = (0,0)^\top$, the function f is also an element of $L^\infty_{\mathbb{Q}}(\mathbb{R}^2)$ (cf. (2.2.4)), since it is not hard to show that in this case*

$$\lim_{R\to\infty} \int_{[-R,R]^2} \sum_{j\in\mathbb{Z}} \lambda_{0,j}\, e^{i\omega'_{0,j}\cdot\eta'}\, \mathrm{d}\eta' = 0,$$

as is shown in the proof of the subsequent lemma.

Lemma 3.5. *Any function $f \in \mathcal{A}$ is uniquely determined by the terms $\lambda_{\ell,j}$, $\omega'_{\ell,j}$ and g, i.e. two different sets of terms $(\lambda_{\ell,j}, \omega'_{\ell,j}, g)$ and $(\tilde{\lambda}_{\ell,j}, \tilde{\omega}'_{\ell,j}, \tilde{g}_2)$ will result in two different functions f and $\tilde{f}$.*

Proof. Assume a function $f \in \mathcal{A}$ can be represented by two different parameter sets

$$S_1 := \left((\lambda_{\ell,j})_{\left(\substack{\ell=0,\dots,3\\ j\in\mathbb{Z}}\right)}, (\omega'_{\ell,j})_{\left(\substack{\ell=0,\dots,3\\ j\in\mathbb{Z}}\right)}, g \right), \qquad S_2 := \left((\tilde{\lambda}_{\ell,j})_{\left(\substack{\ell=0,\dots,3\\ j\in\mathbb{Z}}\right)}, (\tilde{\omega}'_{\ell,j})_{\left(\substack{\ell=0,\dots,3\\ j\in\mathbb{Z}}\right)}, \tilde{g} \right).$$

Note that the mean value of a function $h : \mathbb{R}^2 \to \mathbb{C}$, defined as $\lim_{R\to\infty} 1/(4R^2) \int_{-R}^{R}\int_{-R}^{R} h(\eta')\,\mathrm{d}\eta'$, is zero for any function $h(\eta') = e^{i\omega'_{\ell,j}\cdot\eta'}$ with $\omega'_{\ell,j} \neq (0,0)^\top$, since such a function h is periodic with period $p' := \omega'_{\ell,j}$ such that $\int_{-m\,p_x/2}^{m\,p_x/2}\int_{-m\,p_y/2}^{m\,p_y/2} h(\eta')\,\mathrm{d}\eta' = 0$ for all $m \in \mathbb{Z}$. On the other hand, for an absolutely summable sequence $\lambda_{\ell,j}$ with $j \in \mathbb{Z}$, the mean value of $\sum_{j\in\mathbb{Z}} \lambda_{\ell,j}\, e^{i\omega'_{\ell,j}\cdot\eta'}$ is

$$\lim_{R\to\infty} \frac{1}{4R^2} \int_{-R}^{R}\int_{-R}^{R} \sum_{j\in\mathbb{Z}} \lambda_{\ell,j}\, e^{i\omega'_{\ell,j}\cdot\eta'}\,\mathrm{d}\eta' = \sum_{j\in\mathbb{Z}} \lim_{R\to\infty} \frac{\lambda_{\ell,j}}{4R^2} \int_{-R}^{R}\int_{-R}^{R} e^{i\omega'_{\ell,j}\cdot\eta'}\,\mathrm{d}\eta' = \lambda_{\ell,j_1},$$

where $j_1 \in \mathbb{Z}$ is the unique index with $\omega'_{\ell,j_1} = (0,0)^\top$. Moreover, for $\ell = 1,\dots,3$ it is easily seen that

$$\lim_{R\to\infty} \frac{1}{4R^2} \int_{-R}^{R}\int_{-R}^{R} \frac{1}{\sqrt{1+|\eta'|^2}^{\ell}} \sum_{j\in\mathbb{Z}} \lambda_{\ell,j}\, e^{i\omega'_{\ell,j}\cdot\eta'}\,\mathrm{d}\eta' = \sum_{j\in\mathbb{Z}} \lambda_{\ell,j} \lim_{R\to\infty} \frac{1}{4R^2} \int_{-R}^{R}\int_{-R}^{R} \frac{e^{i\omega'_{\ell,j}\cdot\eta'}}{\sqrt{1+|\eta'|^2}^{\ell}}\,\mathrm{d}\eta' = 0.$$

Since $g(\eta')$ tends to zero as $|\eta'| \to \infty$, it is also easily seen that $\lim_{R\to\infty} 1/(4R^2) \int_{-R}^{R}\int_{-R}^{R} g(\eta')\,\mathrm{d}\eta' = 0$. Naturally, the same properties hold for the parameter set S_2.

This is now used to show that the two different parameter sets of $f \in \mathcal{A}$, defined above, are identical. First, assume that a spatial frequency $\omega'_{0,\iota}$ with $\lambda_{0,\iota} \neq 0$ exists in S_1 that does not exists in S_2, i.e. $\omega'_{0,\iota} \neq \tilde{\omega}'_{0,j}$ for all $j \in \mathbb{Z}$. Defining

$$\mu(l,\omega'_{l,\iota}) := \lim_{R\to\infty} \frac{1}{4R^2} \int_{-R}^{R}\int_{-R}^{R} \left\{ \sum_{\ell=l}^{3} \frac{1}{\sqrt{1+|\eta'|^2}^{\ell}} \sum_{j\in\mathbb{Z}} \lambda_{\ell,j}\, e^{i\omega'_{\ell,j}\cdot\eta'} + g(\eta') \right\} \sqrt{1+|\eta'|^2}^{l}\, e^{-i\omega'_{0,\iota}\cdot\eta'}\,\mathrm{d}\eta',$$

and

$$\tilde{\mu}(l,\tilde{\omega}'_{l,\iota}) := \lim_{R\to\infty} \frac{1}{4R^2} \int_{-R}^{R}\int_{-R}^{R} \left\{ \sum_{\ell=l}^{3} \frac{1}{\sqrt{1+|\eta'|^2}^{\ell}} \sum_{j\in\mathbb{Z}} \tilde{\lambda}_{\ell,j}\, e^{i\tilde{\omega}'_{\ell,j}\cdot\eta'} + \tilde{g}(\eta') \right\} \sqrt{1+|\eta'|^2}^{l}\, e^{-i\tilde{\omega}'_{0,\iota}\cdot\eta'}\,\mathrm{d}\eta',$$

it follows that $\mu(0,\omega'_{0,\iota}) = \lambda_{0,\iota}$, while $\tilde{\mu}(0,\omega'_{0,\iota}) = 0$. This, however, is a contradiction, since both parameter sets represent the function f. Thus, it can be assumed w.l.o.g. that $\omega_{0,j} = \tilde{\omega}_{0,j}$ for all $j \in \mathbb{Z}$. Now it is easily shown that $\lambda_{0,\iota} = \tilde{\lambda}_{0,\iota}$ for any $\iota \in \mathbb{Z}$, since $\mu(0,\omega'_{0,\iota}) = \lambda_{0,\iota}$ and $\tilde{\mu}(0,\omega'_{0,\iota}) = \tilde{\mu}(0,\tilde{\omega}'_{0,\iota}) = \tilde{\lambda}_{0,\iota}$ have to be the same. Consequently $(\lambda_{0,j})_{j\in\mathbb{Z}} = (\tilde{\lambda}_{0,j})_{j\in\mathbb{Z}}$ and $\sum_{j\in\mathbb{Z}} \lambda_{0,j}\, e^{i\omega'_{0,j}\cdot\eta'} = \sum_{j\in\mathbb{Z}} \tilde{\lambda}_{0,j}\, e^{i\tilde{\omega}'_{0,j}\cdot\eta'}$. Naturally, this shows that $f(\eta') - \sum_{j\in\mathbb{Z}} \lambda_{0,j}\, e^{i\omega'_{0,j}\cdot\eta'} = f(\eta') - \sum_{j\in\mathbb{Z}} \tilde{\lambda}_{0,j}\, e^{i\tilde{\omega}'_{0,j}\cdot\eta'}$.

Similar to the parameters with $\ell = 0$, it can be shown that the parameters in S_1 and S_2 are identical for $l = 1$. As before, a spatial frequency $\omega'_{l,\iota}$ with $\lambda_{l,\iota} \neq 0$ in S_1 can be assumed such that $\omega'_{l,\iota} \neq \tilde{\omega}'_{l,j}$ for all $j \in \mathbb{Z}$. Again, the contradiction that $\mu(1,\omega'_{l,\iota}) = \lambda_{l,\iota}$ is not equal to $\tilde{\mu}(1,\omega'_{l,\iota}) = 0$ can be observed. Hence, it can be assumed w.l.o.g. that $\omega_{l,j} = \tilde{\omega}_{l,j}$ for all $j \in \mathbb{Z}$. Once more, it is now easily proven that $\lambda_{l,\iota} = \tilde{\lambda}_{l,\iota}$ for any $\iota \in \mathbb{Z}$, since $\mu(l,\omega'_{l,\iota}) = \lambda_{l,\iota}$ and $\tilde{\mu}(l,\omega'_{l,\iota}) = \tilde{\mu}(l,\tilde{\omega}'_{l,\iota}) = \tilde{\lambda}_{l,\iota}$ have to be identical. Thus, $\sum_{j\in\mathbb{Z}} \lambda_{l,j}\, e^{i\omega'_{l,j}\cdot\eta'} = \sum_{j\in\mathbb{Z}} \tilde{\lambda}_{l,j}\, e^{i\tilde{\omega}'_{l,j}\cdot\eta'}$. This can now be repeated for $l = 2, 3$, finally leading to

$$\sum_{\ell=l}^{3} \frac{1}{\sqrt{1+|\eta'|^2}^{\ell}} \sum_{j\in\mathbb{Z}} \lambda_{\ell,j}\, e^{i\omega'_{\ell,j}\cdot\eta'} = \sum_{\ell=l}^{3} \frac{1}{\sqrt{1+|\eta'|^2}^{\ell}} \sum_{j\in\mathbb{Z}} \tilde{\lambda}_{\ell,j}\, e^{i\tilde{\omega}'_{\ell,j}\cdot\eta'}$$

and

$$g(\eta') = f(\eta') - \sum_{\ell=l}^{3} \frac{1}{\sqrt{1+|\eta'|^2}^{\ell}} \sum_{j\in\mathbb{Z}} \lambda_{\ell,j}\, e^{i\omega'_{\ell,j}\cdot\eta'} = f(\eta') - \sum_{\ell=l}^{3} \frac{1}{\sqrt{1+|\eta'|^2}^{\ell}} \sum_{j\in\mathbb{Z}} \tilde{\lambda}_{\ell,j}\, e^{i\tilde{\omega}'_{\ell,j}\cdot\eta'} = \tilde{g}(\eta'),$$

which concludes the proof of the lemma. ■

It can also be shown that

Lemma 3.6. *The spaces $\mathcal{A}$ and $\mathcal{A}^{\mathbb{C}}$, together with the norm $\|\cdot\|_{\mathcal{A}}$ and pointwise multiplication, form Banach algebras.*

Proof. To show that $\mathcal{A}^{\mathbb{C}}$ is a Banach algebra, it has to be shown that $\mathcal{A}^{\mathbb{C}}$ with the norm $\|\cdot\|_{\mathcal{A}}$ is a complete, normed $\mathbb{C}$-vector space, which together with the pointwise multiplication forms an associative algebra, which is sub-multiplicative w.r.t. the vector space norm. It is not hard to shown that $(\mathcal{A}^{\mathbb{C}}, \|\cdot\|_{\mathcal{A}})$ with pointwise summation is a normed $\mathbb{C}$-vector space. Indeed, since for $f_n \in \mathcal{A}^{\mathbb{C}}$ for all $n \in \mathbb{N}_0$,

$$\begin{aligned}
(f_1+f_2)(\eta') &:= f_1(\eta') + f_2(\eta') \\
&= \sum_{\ell=0}^{3}\left[\frac{1}{\sqrt{1+|\eta'|^2}^{\ell}} \sum_{j\in\mathbb{Z}} \lambda^1_{\ell,j}\, e^{i\omega^1_{\ell,j}\cdot\eta'}\right] + g_1(\eta') + \sum_{\ell=0}^{3}\left[\frac{1}{\sqrt{1+|\eta'|^2}^{\ell}} \sum_{j\in\mathbb{Z}} \lambda^2_{\ell,j}\, e^{i\omega^2_{\ell,j}\cdot\eta'}\right] + g_2(\eta') \\
&= \sum_{\ell=0}^{3}\left[\frac{1}{\sqrt{1+|\eta'|^2}^{\ell}} \sum_{j\in\mathbb{Z}} (\tilde{\lambda}^1_{\ell,j} + \tilde{\lambda}^1_{\ell,j})\, e^{i\tilde{\omega}'_{\ell,j}\cdot\eta'}\right] + g_1(\eta') + g_2(\eta'),
\end{aligned}$$

where $\{\tilde\omega'_{\ell,j} | j \in \mathbb{Z}\} := \{\omega^1_{\ell,j} | \, j \in \mathbb{Z}\} \cup \{\omega^2_{\ell,j} | \, j \in \mathbb{Z}\}$ and

$$\tilde\lambda^n_{\ell,j} := \begin{cases} \lambda^n_{\ell,\iota} & \text{if } \tilde\omega'_{\ell,j} = \omega^n_{\ell,\iota} \\ 0 & \text{else} \end{cases}$$

for $n = 1, 2$, the summation is well defined in $\mathcal{A}^{\mathbb{C}}$. Furthermore, since the representation of any $f \in \mathcal{A}^{\mathbb{C}}$ is unique, $f \equiv 0$ is the unique zero element in $\mathcal{A}^{\mathbb{C}}$ with $\|f\|_{\mathcal{A}} = 0$. Using the fact that $\|\cdot\|_{\mathcal{A}}$ is a sum of the l^1 and L^∞-norm, it is then easily proven that $\|\cdot\|_{\mathcal{A}}$ is also a norm and that $(\mathcal{A}^{\mathbb{C}}, \|\cdot\|_{\mathcal{A}})$ is a normed $\mathbb{C}$-vector space. Moreover, since the spaces of absolutely summable series' l^1 and uniformly bounded functions L^∞ are complete spaces, this can also be shown for $\mathcal{A}^{\mathbb{C}}$. To be precise, assuming f_n is a Cauchy sequence in $\mathcal{A}^{\mathbb{C}}$, it follows that for any $\epsilon > 0$ there exists an $N > 0$, such that for all $n, m > N$

$$\|f_n - f_m\|_{\mathcal{A}} = \sum_{\ell=0}^{3} \sum_{j\in\mathbb{Z}} |\tilde\lambda^n_{\ell,j} - \tilde\lambda^m_{\ell,j}| + \left\|(1 + |\eta'|^2)^2 \, g_n(\eta') - (1 + |\eta'|^2)^2 \, g_m(\eta')\right\|_\infty < \epsilon,$$

where $\{\tilde\omega'_{\ell,j} | \, j \in \mathbb{Z}\} := \bigcup_{n\in\mathbb{N}_0} \{\omega^n_{\ell,j} | \, j \in \mathbb{Z}\}$ and $\tilde\lambda^n_{\ell,j}$ as above, but for all $n \in \mathbb{N}_0$, not just $n = 1, 2$. Since both l^1 and L^∞ are complete vector spaces, it follows that a $\tilde\lambda_{\ell,j} \in l^1(\mathbb{C})$ and a $G \in L^\infty(\mathbb{R}^2)$ exists, such that $\tilde\lambda^n_{\ell,j}$ tends to $\tilde\lambda_{\ell,j}$ in the l^1-norm and $(1 + |\eta'|^2)^2 \, g_n(\eta')$ tends to $G(\eta')$ in the L^∞-norm as n tends to infinity. With this, a potential limit of f_n can be defined as

$$f(\eta') := \sum_{\ell=0}^{3} \left[\frac{1}{\sqrt{1 + |\eta'|^2}^{\,\ell}} \sum_{j\in\mathbb{Z}} \tilde\lambda_{\ell,j} \, e^{i\tilde\omega'_{\ell,j}\cdot\eta'} \right] + \frac{G(\eta')}{(1 + |\eta'|^2)^2},$$

which is an element of $\mathcal{A}^{\mathbb{C}}$. Since the two parts of f converge in l^1 and L^∞, respectively, it holds that for any $\epsilon > 0$ there exists a constant $N > 0$ such that for all $n > N$, $\|(\tilde\lambda^n_{\ell,j})_{j\in\mathbb{Z}} - (\tilde\lambda_{\ell,j})_{j\in\mathbb{Z}}\|_{l^1} < \epsilon/5$ for all $\ell = 0, \ldots, 3$ and that $\|(1 + |\eta'|^2)^2 \, g_n(\eta') - G(\eta')\|_\infty < \epsilon/5$. Consequently $\|f_n - f\|_{\mathcal{A}} < \epsilon$ for all $n > N$, which shows that $f \in \mathcal{A}^{\mathbb{C}}$ is the limit of f_n w.r.t. $\|\cdot\|_{\mathcal{A}}$ and thus that $\mathcal{A}^{\mathbb{C}}$ is complete.

Next it will be shown that $(\mathcal{A}^{\mathbb{C}}, \|\cdot\|_{\mathcal{A}})$ with pointwise multiplication is an associative Algebra, where the product is sub-multiplicative w.r.t. $\|\cdot\|_{\mathcal{A}}$. By virtue of the pointwise definition of the product it is easily seen that it is indeed an associative Algebra, if the product of two elements from the space is an element of the space itself. For convenience, define $\Lambda^n_\ell := \Lambda^n_\ell(\eta') := \sum_{j\in\mathbb{Z}} \lambda^n_{\ell,j} \, e^{i\omega^n_{\ell,j}\cdot\eta'}$ for $n = 1, 2$, such that

$$\begin{aligned}
(f_1 \cdot f_2)(\eta') &:= f_1(\eta') \, f_2(\eta') \\
&= \left[\sum_{\ell=0}^{3} \frac{1}{\sqrt{1 + |\eta'|^2}^{\,\ell}} \sum_{j\in\mathbb{Z}} \lambda^1_{\ell,j} \, e^{i\omega^1_{\ell,j}\cdot\eta'} + g_1(\eta') \right] \left[\sum_{\ell=0}^{3} \frac{1}{\sqrt{1 + |\eta'|^2}^{\,\ell}} \sum_{j\in\mathbb{Z}} \lambda^2_{\ell,j} \, e^{i\omega^2_{\ell,j}\cdot\eta'} + g_2(\eta') \right] \\
&= \Lambda^1_0\Lambda^2_0 + \frac{\Lambda^1_0\Lambda^2_1 + \Lambda^1_1\Lambda^2_0}{\sqrt{1 + |\eta'|^2}} + \frac{\Lambda^1_0\Lambda^2_2 + \Lambda^1_1\Lambda^2_1 + \Lambda^1_2\Lambda^2_0}{1 + |\eta'|^2} + \frac{\Lambda^1_0\Lambda^2_3 + \Lambda^1_1\Lambda^2_2 + \Lambda^1_2\Lambda^2_1 + \Lambda^1_3\Lambda^2_0}{\sqrt{1 + |\eta'|^2}^{\,3}} \\
&\quad + \frac{\Lambda^1_1\Lambda^2_3 + \Lambda^1_2\Lambda^2_2 + \Lambda^1_3\Lambda^2_1}{(1 + |\eta'|^2)^2} + \frac{\Lambda^1_2\Lambda^2_3 + \Lambda^1_3\Lambda^2_2}{\sqrt{1 + |\eta'|^2}^{\,5}} + \frac{\Lambda^1_3\Lambda^2_3}{(1 + |\eta'|^2)^3} + g_1(\eta') \sum_{\ell=0}^{3} \frac{\Lambda^2_\ell}{\sqrt{1 + |\eta'|^2}^{\,\ell}} \\
&\quad + g_2(\eta') \sum_{\ell=0}^{3} \frac{\Lambda^1_\ell}{\sqrt{1 + |\eta'|^2}^{\,\ell}} + g_1(\eta') \, g_2(\eta') \\
&= \sum_{\kappa=0}^{6} \frac{1}{\sqrt{1 + |\eta'|^2}^{\,\kappa}} \sum_{\ell=\max\{0,\kappa-3\}}^{\min\{3,\kappa\}} \Lambda^1_\ell \Lambda^2_{\kappa-\ell} + g_1(\eta') \sum_{\ell=0}^{3} \frac{\Lambda^2_\ell}{\sqrt{1 + |\eta'|^2}^{\,\ell}} + g_2(\eta') \sum_{\ell=0}^{3} \frac{\Lambda^1_\ell}{\sqrt{1 + |\eta'|^2}^{\,\ell}} \\
&\quad + g_1(\eta') \, g_2(\eta'),
\end{aligned} \tag{3.3.3}$$

where

$$\Lambda_\ell^1 \Lambda_{\kappa-\ell}^2 = \left[\sum_{j\in\mathbb{Z}} \lambda_{\ell,j}^1 \, e^{i\omega_{\ell,j}^1\cdot\eta'}\right]\left[\sum_{\iota\in\mathbb{Z}} \lambda_{\kappa-\ell,\iota}^2 \, e^{i\omega_{\kappa-\ell,\iota}^2\cdot\eta'}\right] = \sum_{j\in\mathbb{Z}}\sum_{\iota\in\mathbb{Z}} \lambda_{\ell,j}^1 \, \lambda_{\kappa-\ell,\iota}^2 e^{i(\omega_{\ell,j}^1+\omega_{\kappa-\ell,\iota}^2)\cdot\eta'}.$$

The sum on the right-hand side can easily be transformed to get

$$\Lambda_\ell^1 \Lambda_{\kappa-\ell}^2 = \sum_{j\in\mathbb{Z}} \bar{\lambda}_{\kappa,j}^\ell \, e^{i\bar{\omega}_{\kappa,j}^\ell\cdot\eta'}. \tag{3.3.4}$$

Next, the order of the summations w.r.t. κ and ℓ on the right-hand side of (3.3.3) is interchanged. To do so, all the $\bar{\omega}_{\kappa,j}^\ell$ for a fixed κ and all ℓ are collected, i.e. $\{\bar{\omega}'_{\kappa,j} | \, j\in\mathbb{Z}\} := \bigcup_{\ell=\max\{0,\kappa-3\}}^{\min\{3,\kappa\}} \{\bar{\omega}_{\kappa,j}^\ell | \, j\in\mathbb{Z}\}$. Moreover, the $\bar{\lambda}_{\kappa,j}^\ell$, where the corresponding $\bar{\omega}_{\kappa,j}^\ell$ is equal to a given $\bar{\omega}'_{\kappa,\iota}$, are added, i.e.

$$\bar{\lambda}_{\kappa,\iota} := \sum_{\ell=\max\{0,\kappa-3\}}^{\min\{3,\kappa\}} \sum_{j\in\mathbb{Z}} \mathbb{1}_{\bar{\omega}'_{\kappa,\iota}}(\bar{\omega}_{\kappa,j}^\ell) \, \bar{\lambda}_{\kappa,j}^\ell, \tag{3.3.5}$$

such that new pairs $(\bar{\lambda}_{\kappa,\iota}, \bar{\omega}'_{\kappa,\iota})$ are obtained, where $\bar{\omega}'_{\kappa,\iota_1} \neq \bar{\omega}'_{\kappa,\iota_2}$ for $\iota_1 \neq \iota_2$. Here, the symbol $\mathbb{1}$ is used for the indicator function, i.e. for a set M the value $\mathbb{1}_M(\mathtt{m})$ is one if $\mathtt{m}\in M$ and zero otherwise. For a singleton $M = \{\mathtt{m}_0\}$, $\mathbb{1}_M(\mathtt{m})$ is shortly written as $\mathbb{1}_{\mathtt{m}_0}(\mathtt{m})$. Consequently,

$$\sum_{\ell=\max\{0,\kappa-3\}}^{\min\{3,\kappa\}} \Lambda_\ell^1 \Lambda_{\kappa-\ell}^2 = \sum_{\ell=\max\{0,\kappa-3\}}^{\min\{3,\kappa\}} \sum_{j\in\mathbb{Z}} \bar{\lambda}_{\kappa,j}^\ell \, e^{i\bar{\omega}_{\kappa,j}^\ell\cdot\eta'} = \sum_{\iota\in\mathbb{Z}} \bar{\lambda}_{\kappa,\iota} \, e^{i\bar{\omega}'_{\kappa,\iota}\cdot\eta'}$$

since the summation on the right-hand side of (3.3.4) exists absolutely, which shows that the summations w.r.t. ℓ and j can be rearranged freely. Replacing ι by j for consistency, this leads to

$$(f_1\cdot f_2)(\eta') = \sum_{\kappa=0}^{3} \frac{1}{\sqrt{1+|\eta'|^2}^\kappa} \sum_{j\in\mathbb{Z}} \bar{\lambda}_{\kappa,j} \, e^{i\bar{\omega}'_{\kappa,j}\cdot\eta'} + g(\eta'),$$

where

$$\begin{aligned} g(\eta') := {} & \frac{1}{(1+|\eta'|^2)^2} \sum_{\kappa=4}^{6} \frac{1}{\sqrt{1+|\eta'|^2}^{\kappa-4}} \sum_{j\in\mathbb{Z}} \bar{\lambda}_{\kappa,j} \, e^{i\bar{\omega}'_{\kappa,j}\cdot\eta'} + g_1(\eta') \sum_{\ell=0}^{3} \frac{\Lambda_\ell^2}{\sqrt{1+|\eta'|^2}^\ell} \\ & + g_2(\eta') \sum_{\ell=0}^{3} \frac{\Lambda_\ell^1}{\sqrt{1+|\eta'|^2}^\ell} + g_1(\eta') \, g_2(\eta'). \end{aligned}$$

It remains to show that $\|f_1\cdot f_2\|_{\mathcal{A}}$ is finite by showing that the norm is sub-multiplicative, or to be precise, that $\|f_1\cdot f_2\|_{\mathcal{A}} \leq \|f_1\|_{\mathcal{A}} \|f_2\|_{\mathcal{A}}$. For convenience, define $\Sigma_\ell^n := \sum_{j\in\mathbb{Z}} |\lambda_{\ell,j}^n|$ for $n = 1, 2$ and $\bar{\Sigma}_\kappa := \sum_{j\in\mathbb{Z}} |\bar{\lambda}_{\kappa,j}|$, such that

$$\|f_1\cdot f_2\|_{\mathcal{A}} = \sum_{\kappa=0}^{3} \bar{\Sigma}_\kappa + \|(1+|\eta'|^2)^2 \, g(\eta')\|_\infty, \tag{3.3.6}$$

where

$$\begin{aligned} \|(1+|\eta'|^2)^2 \, g(\eta')\|_\infty \leq {} & \left\| \sum_{\kappa=4}^{6} \frac{1}{\sqrt{1+|\eta'|^2}^{\kappa-4}} \sum_{j\in\mathbb{Z}} \bar{\lambda}_{\kappa,j} \, e^{i\bar{\omega}'_{\kappa,j}\cdot\eta'} \right\|_\infty + \left\| (1+|\eta'|^2)^2 \, g_1(\eta') \sum_{\ell=0}^{3} \frac{\Lambda_\ell^2}{\sqrt{1+|\eta'|^2}^\ell} \right\|_\infty \\ & + \left\| (1+|\eta'|^2)^2 \, g_2(\eta') \sum_{\ell=0}^{3} \frac{\Lambda_\ell^1}{\sqrt{1+|\eta'|^2}^\ell} \right\|_\infty + \left\| (1+|\eta'|^2)^2 \, g_1(\eta') \, g_2(\eta') \right\|_\infty \end{aligned}$$

$$\leq \sum_{\kappa=4}^{6} \bar{\Sigma}_\kappa + \|g_1\|_{4,\infty} \sum_{\ell=0}^{3} \Sigma_\ell^2 + \|g_2\|_{4,\infty} \sum_{\ell=0}^{3} \Sigma_\ell^1 + \|g_1\|_{4,\infty} \|g_2\|_{4,\infty}. \tag{3.3.7}$$

On the other hand, (cf. (3.3.4) and (3.3.5))

$$\begin{aligned}
\bar{\Sigma}_\kappa &\leq \sum_{j\in\mathbb{Z}} \sum_{\ell=\max\{0,\kappa-3\}}^{\min\{3,\kappa\}} \mathbb{1}_{\bar{\omega}'_{\kappa,j}}(\bar{\omega}^\ell_{\kappa,\iota}) \left|\bar{\lambda}^\ell_{\kappa,\iota}\right| = \sum_{\ell=\max\{0,\kappa-3\}}^{\min\{3,\kappa\}} \sum_{j\in\mathbb{Z}} \left|\bar{\lambda}^\ell_{\kappa,\iota}\right| \\
&= \sum_{\ell=\max\{0,\kappa-3\}}^{\min\{3,\kappa\}} \sum_{j\in\mathbb{Z}} \sum_{\iota\in\mathbb{Z}} \left|\lambda^1_{\ell,j}\right| \left|\lambda^2_{\kappa-\ell,\iota}\right| = \sum_{\ell=\max\{0,\kappa-3\}}^{\min\{3,\kappa\}} \Sigma^1_\ell \, \Sigma^2_{\kappa-\ell}.
\end{aligned}$$

It is not hard to check that

$$\sum_{\kappa=0}^{6} \bar{\Sigma}_\kappa \leq \sum_{\kappa=0}^{6} \sum_{\ell=\max\{0,\kappa-3\}}^{\min\{3,\kappa\}} \Sigma^1_\ell \, \Sigma^2_{\kappa-\ell} = \sum_{\ell=0}^{3} \sum_{\kappa=0}^{3} \Sigma^1_\ell \, \Sigma^2_\kappa = \left[\sum_{\ell=0}^{3} \Sigma^1_\ell\right] \left[\sum_{\kappa=0}^{3} \Sigma^2_\kappa\right].$$

Altogether, (cf. (3.3.6) and (3.3.7))

$$\|f_1 \cdot f_2\|_{\mathcal{A}} \leq \left[\sum_{\ell=0}^{3} \Sigma^1_\ell + \|g_1\|_{4,\infty}\right] \left[\sum_{\ell=0}^{3} \Sigma^2_\ell + \|g_2\|_{4,\infty}\right] = \|f_1\|_{\mathcal{A}} \, \|f_2\|_{\mathcal{A}}.$$

Thus $\|\cdot\|_{\mathcal{A}}$ is a sub-multiplicative norm w.r.t. the associative algebra and Banach space $\mathcal{A}^{\mathbb{C}}$, proving the statement of the lemma for $\mathcal{A}^{\mathbb{C}}$. The same arguments can also be used to show identical properties for $\mathcal{A}$, with the small difference that it is an $\mathbb{R}$-vector space. ■

Remark 3.7. *The coefficients $\lambda_{l,j}$ depend continuously on $f \in \mathcal{A}$. Moreover, the term g depends continuously on $f \in \mathcal{A}$ w.r.t. to the norm $\|\cdot\|_{4,\infty}$.*

3.3.2 Existence of the remaining Cauchy principal value and the limit of the limiting absorption principle

It is the goal of this subsection to show that the limits $\tau \nearrow 0$ and $\tilde{r} \to \infty$ of (3.2.16) exist under the assumption that f is an element of $\mathcal{A}$. To be precise, this subsection solely consists of the proof that

Theorem 3.8. *For any function $f(\eta')$ from $\mathcal{A}$ the limit*

$$\left\langle \vec{D}^d(\vec{x}), \varphi(\vec{x}) \right\rangle = \frac{i}{8\pi^2} \lim_{\tau\nearrow 0} \lim_{\tilde{r}\to\infty} \int_{\mathbb{R}^3} \bar{\varphi}(\vec{x}) \int_{\mathbb{R}^2} \hat{\alpha}_{\tilde{r}}(\vec{s}_{\xi_\tau} - \vec{k}_\tau) \frac{\left[\left(\vec{s}_{\xi_\tau} \times \vec{e}^{\,0}\right) \times \vec{s}_{\xi_\tau}\right]}{\xi_\tau} e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}} \, \mathrm{d}s' \, \mathrm{d}\vec{x} \tag{3.3.8}$$

exists.

Consider only the integral w.r.t. s' for an interface function $f \in \mathcal{A}$. Using the equations (3.2.5) and (3.2.6) for $\hat{\alpha}_{\tilde{r}}$, (3.3.8) transforms to

$$\left\langle \vec{D}^d(\vec{x}), \varphi(\vec{x}) \right\rangle = -\frac{\Delta}{8\pi^2} \lim_{\tau\nearrow 0} \lim_{\tilde{r}\to\infty} \int_{\mathbb{R}^3} \bar{\varphi}(\vec{x}) \, \Gamma_{\tau,\tilde{r}}(\vec{x}) \, \mathrm{d}\vec{x}, \tag{3.3.9}$$

where from now on $\Delta := \Delta_0 = \epsilon_0 - \epsilon'_0$ and

$$\begin{aligned}
\Gamma_{\tau,\tilde{r}}(\vec{x}) &:= \int_{\mathbb{R}^2} \int_{B_2(\tilde{r})} \frac{1 - e^{-i(\xi_\tau - k_{z,\tau}) f(\eta')}}{\xi_\tau - k_{z,\tau}} e^{-i\eta'\cdot\left(s'-k'\right)} \, \mathrm{d}\eta' \, \frac{\left[\left(\vec{s}_{\xi_\tau} \times \vec{e}^{\,0}\right) \times \vec{s}_{\xi_\tau}\right]}{\xi_\tau} e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}} \, \mathrm{d}s' \qquad (3.3.10) \\
&= i \int_{\mathbb{R}^2} \int_{B_2(\tilde{r})} \int_0^1 e^{-i(\xi_\tau - (k_z + i\tau))\zeta f(\eta')} \, \mathrm{d}\zeta \, f(\eta') \, e^{-i\eta'\cdot\left(s'-k'\right)} \, \mathrm{d}\eta' \, \frac{\left[\left(\vec{s}_{\xi_\tau} \times \vec{e}^{\,0}\right) \times \vec{s}_{\xi_\tau}\right]}{\xi_\tau} e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}} \, \mathrm{d}s'
\end{aligned}$$

Here it can easily be shown that Fubini's theorem can be applied for any fixed $\tilde{r}$ and $\tau < 0$, since $e^{i\xi_\tau\left(z-\zeta f(\eta')\right)}$ decays exponentially as $|s'|$ tends to infinity and since the integrand is uniformly bounded w.r.t. $\eta' \in B_2(\tilde{r})$. Hence, the order of integration can be interchanged. Additionally replacing the exponential function in $e^{-i(\xi_\tau - i\tau)\zeta f(\eta')}$ by its power series,

$$\begin{aligned}
\Gamma_{\tau,\tilde{r}}(\vec{x}) &= i\int_0^1 \int_{\mathbb{R}^2} \left\{ \int_{B_2(\tilde{r})} e^{-i(\xi_\tau - i\tau)\zeta f(\eta')}\, e^{ik_z\zeta f(\eta')}\, f(\eta')\, e^{-i\eta'\cdot\left(s'-k'\right)}\,\mathrm{d}\eta'\, \frac{\left[\left(\vec{s}_{\xi_\tau}\times\vec{e}^{\,0}\right)\times\vec{s}_{\xi_\tau}\right]}{\xi_\tau}\, e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}} \right\} \mathrm{d}s'\,\mathrm{d}\zeta \\
&= i\int_0^1 \int_{\mathbb{R}^2} \left\{ \int_{B_2(\tilde{r})} \sum_{n\in\mathbb{N}_0} (-i\zeta)^n\; f(\eta')^{n+1}\frac{\left(\xi_\tau - i\tau\right)^n}{n!}\, e^{ik_z\zeta f(\eta')}\, e^{-i\eta'\cdot\left(s'-k'\right)}\,\mathrm{d}\eta' \right. \\
&\qquad\qquad \left. \frac{\left[\left(\vec{s}_{\xi_\tau}\times\vec{e}^{\,0}\right)\times\vec{s}_{\xi_\tau}\right]}{\xi_\tau}\, e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}} \right\} \mathrm{d}s'\,\mathrm{d}\zeta \\
&= i\,\mathrm{I}_1 + i\,\mathrm{I}_2,
\end{aligned} \tag{3.3.11}$$

where

$$\begin{aligned}
\mathrm{I}_1 := \int_0^1 \int_{\mathbb{R}^2} &\left\{ \int_{B_2(\tilde{r})} \sum_{n=0}^{8} (-i\zeta)^n\; f(\eta')^{n+1}\frac{\left(\xi_\tau - i\tau\right)^n}{n!}\, e^{ik_z\zeta f(\eta')}\, e^{-i\eta'\cdot\left(s'-k'\right)}\,\mathrm{d}\eta' \right. \\
&\qquad \left. \frac{\left[\left(\vec{s}_{\xi_\tau}\times\vec{e}^{\,0}\right)\times\vec{s}_{\xi_\tau}\right]}{\xi_\tau}\, e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}} \right\} \mathrm{d}s'\,\mathrm{d}\zeta,
\end{aligned} \tag{3.3.12}$$

$$\begin{aligned}
\mathrm{I}_2 := \int_0^1 \int_{\mathbb{R}^2} &\left\{ \int_{B_2(\tilde{r})} \sum_{n=9}^{\infty} (-i\zeta)^n\; f(\eta')^{n+1}\frac{\left(\xi_\tau - i\tau\right)^n}{n!}\, e^{ik_z\zeta f(\eta')}\, e^{-i\eta'\cdot\left(s'-k'\right)}\,\mathrm{d}\eta' \right. \\
&\qquad \left. \frac{\left[\left(\vec{s}_{\xi_\tau}\times\vec{e}^{\,0}\right)\times\vec{s}_{\xi_\tau}\right]}{\xi_\tau}\, e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}} \right\} \mathrm{d}s'\,\mathrm{d}\zeta.
\end{aligned} \tag{3.3.13}$$

First, examine integral (3.3.12) by pulling the finite sum outside the integrals and replace $e^{ik_z\zeta f(\eta')}$ by the power series of the exponential function, giving

$$\begin{aligned}
\mathrm{I}_1 &= \sum_{n=0}^{8} \int_0^1 \frac{(-i\zeta)^n}{n!} \int_{\mathbb{R}^2} \left\{ \frac{\left(\xi_\tau - i\tau\right)^n}{\xi_\tau} \int_{B_2(\tilde{r})} f(\eta')^{n+1}\, e^{ik_z\zeta f(\eta')}\, e^{-i\eta'\cdot\left(s'-k'\right)}\,\mathrm{d}\eta' \right. \\
&\qquad\qquad \left. \left[\left(\vec{s}_{\xi_\tau}\times\vec{e}^{\,0}\right)\times\vec{s}_{\xi_\tau}\right]\, e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}} \right\} \mathrm{d}s'\,\mathrm{d}\zeta \\
&= \sum_{n=0}^{8} \int_0^1 \frac{(-i\zeta)^n}{n!} \int_{\mathbb{R}^2} \left\{ \frac{\left(\xi_\tau - i\tau\right)^n}{\xi_\tau} \int_{B_2(\tilde{r})} f(\eta')^{n+1} \sum_{m\in\mathbb{N}_0} \frac{\left(ik_z\zeta\, f(\eta')\right)^m}{m!}\, e^{-i\eta'\cdot\left(s'-k'\right)}\,\mathrm{d}\eta' \right. \\
&\qquad\qquad \left. \left[\left(\vec{s}_{\xi_\tau}\times\vec{e}^{\,0}\right)\times\vec{s}_{\xi_\tau}\right]\, e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}} \right\} \mathrm{d}s'\,\mathrm{d}\zeta
\end{aligned} \tag{3.3.14}$$

Since f is an element of the Banach algebra $\mathcal{A} \subset \mathcal{A}^{\mathbb{C}}$, the term

$$f_n(\eta') := f_{n,k_z,\zeta}(\eta'), \qquad f_{n,k_z,\zeta} := f^{n+1}\, e^{ik_z\zeta f} = \sum_{m\in\mathbb{N}_0} \frac{(ik_z\zeta)^m}{m!}\, f^{m+n+1} \tag{3.3.15}$$

is also an element of $\mathcal{A}^{\mathbb{C}}$, such that (cf. subsequent Lemma 3.9)

$$f_n(\eta') = \sum_{\ell=0}^{3} \left[\frac{1}{\sqrt{1+|\eta'|^2}^{\,\ell}} \sum_{j\in\mathbb{Z}} \tilde{\lambda}^n_{\ell,j}\, e^{i\tilde{\omega}'_{\ell,j}\cdot\eta'} \right] + \tilde{g}_n(\eta',\zeta).$$

Note that this reformulation could already be plugged into $\Gamma_{\tau,\tilde{r}}(\vec{x})$ (cf. (3.3.11)) to get (cf. (3.3.9))

$$\begin{aligned}&\left\langle \vec{D}^d(\vec{x}), \varphi(\vec{x})\right\rangle \\ &= -i\frac{\Delta}{8\pi^2} \lim_{\tau\nearrow 0} \lim_{\tilde{r}\to\infty} \int_{\mathbb{R}^3} \int_0^1 \int_{\mathbb{R}^2} \Bigg\{ \bar{\varphi}(\vec{x}) \frac{\left[\left(\vec{s}_{\xi_\tau} \times \vec{e}^{\,0}\right) \times \vec{s}_{\xi_\tau}\right]}{\xi_\tau} e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}} \\ &\quad \int_{B_2(\tilde{r})} \sum_{n\in\mathbb{N}_0} \frac{[-i\zeta\,(\xi_\tau - i\tau)]^n}{n!} \left[\sum_{\ell=0}^{3}\sum_{j\in\mathbb{Z}} \frac{\tilde{\lambda}^n_{\ell,j}(\zeta)\, e^{i\tilde{\omega}'_{\ell,j}\cdot\eta'}}{\sqrt{1+|\eta'|^2}^{\,\ell}} + \tilde{g}_n(\eta',\zeta)\right] e^{-i\eta'\cdot(s'-k')}\,\mathrm{d}\eta' \Bigg\}\,\mathrm{d}s'\,\mathrm{d}\zeta\,\mathrm{d}\vec{x}.\end{aligned}$$

It is the overall goal of this and the next subsection to show in which sense the sums w.r.t. n, j and ℓ can be pulled outside the integrals, while the limits w.r.t. $\tilde{r}$ and τ are evaluated before the integrals. Applying this formally would lead to

$$\begin{aligned}&\left\langle \vec{D}^d(\vec{x}), \varphi(\vec{x})\right\rangle \\ &= -i\frac{\Delta}{8\pi^2} \sum_{\ell=0}^{3} \sum_{n\in\mathbb{N}_0} \sum_{j\in\mathbb{Z}} \Bigg\{ \int_0^1 \tilde{\lambda}^n_{\ell,j}(\zeta) \frac{[-i\zeta]^n}{n!}\,\mathrm{d}\zeta \\ &\quad \int_{\mathbb{R}^3} \bar{\varphi}(\vec{x}) \int_{\mathbb{R}^2}\int_{\mathbb{R}^2} \frac{1}{\sqrt{1+|\eta'|^2}^{\,\ell}} e^{-i\eta'\cdot\left(s'-(k'+\tilde{\omega}'_{\ell,j})\right)}\,\mathrm{d}\eta' \,\left[\left(\vec{s}_{\xi_0} \times \vec{e}^{\,0}\right) \times \vec{s}_{\xi_0}\right] \xi_0^{n-1}\, e^{i\vec{s}_{\xi_0}\cdot\vec{x}}\,\mathrm{d}s'\,\mathrm{d}\vec{x} \Bigg\} \\ &\quad - i\frac{\Delta}{8\pi^2} \sum_{n\in\mathbb{N}_0} \Bigg\{ \int_{\mathbb{R}^3} \bar{\varphi}(\vec{x}) \int_0^1 \frac{[-i\zeta]^n}{n!} \\ &\qquad \int_{\mathbb{R}^2}\int_{\mathbb{R}^2} \tilde{g}_n(\eta',\zeta)\, e^{-i\eta'\cdot(s'-k')}\,\mathrm{d}\eta' \,\left[\left(\vec{s}_{\xi_0} \times \vec{e}^{\,0}\right) \times \vec{s}_{\xi_0}\right] \xi_0^{n-1}\, e^{i\vec{s}_{\xi_0}\cdot\vec{x}}\,\mathrm{d}s'\,\mathrm{d}\zeta\,\mathrm{d}\vec{x} \Bigg\},\end{aligned}$$

where the first integral w.r.t. η' can be evaluated explicitly using known solutions of generalised Fourier transforms. To do all of this rigorously, it will be shown in the current subsection that the limits w.r.t. $\tilde{r}$ and τ exist, by separating the sum w.r.t. n into a finite sum and the rest (cf. (3.3.11)). For the finite sum it is then shown in which sense the transformations of switching the order of the limits, the sums and the integrals can be applied. In the following Subsection 3.3.3 it will then be proven that this also holds for the entire infinite sum w.r.t. n by letting the number of terms in the finite sum tend to infinity and showing that the integral over the rest, i.e. I_2, tends to zero.

It is used that

Lemma 3.9. *For any function f in $\mathcal{A}$, the function f_n (cf. (3.3.15)) is equal to*

$$f_n(\eta') = \sum_{\ell=0}^{3} \left[\frac{1}{\sqrt{1+|\eta'|^2}^{\,\ell}} \sum_{j\in\mathbb{Z}} \tilde{\lambda}^n_{\ell,j}\, e^{i\tilde{\omega}'_{\ell,j}\cdot\eta'}\right] + \tilde{g}_n(\eta',\zeta), \tag{3.3.16}$$

where $\tilde{\omega}'_{\ell,j}$, $\ell = 0,1,2,3$ are defined by

$$\left\{\tilde{\omega}'_{0,j} : j\in\mathbb{Z}\right\} = \left\{ \sum_{\kappa\in\mathbb{Z}} m_\kappa \omega'_{0,\kappa} \,:\, m_\kappa \in \mathbb{N}_0,\, \sum_{\kappa\in\mathbb{Z}} m_\kappa < \infty \right\}, \tag{3.3.17}$$

$$\left\{\tilde{\omega}'_{\ell,j} : j\in\mathbb{Z}\right\} = \left\{ \sum_{l=0}^{\ell}\sum_{\kappa\in\mathbb{Z}} m^l_\kappa \omega'_{l,\kappa} \,:\, m^l_\kappa \in \mathbb{N}_0,\, \sum_{\kappa\in\mathbb{Z}} m^0_\kappa < \infty,\, \sum_{l=1}^{\ell} l \sum_{\kappa\in\mathbb{Z}} m^l_\kappa = \ell \right\}$$

and where

$$\tilde{\lambda}^n_{0,j} := \tilde{\lambda}^n_{0,j}(\zeta) := \sum_{\substack{m_\kappa\in\mathbb{N}_0:\\ \tilde{m}:=\sum_{\kappa\in\mathbb{Z}} m_\kappa \geq n+1,\, \tilde{m}<\infty \\ \sum_{\kappa\in\mathbb{Z}} m_\kappa\omega'_{0,\kappa} = \tilde{\omega}'_{0,j}}} (ik_z\zeta)^{\tilde{m}-n-1} \frac{\tilde{m}!}{(\tilde{m}-n-1)!} \left[\prod_{\kappa\in\mathbb{Z}} \frac{[\lambda_{0,\kappa}]^{m_\kappa}}{m_\kappa!}\right], \tag{3.3.18}$$

$$\tilde{\lambda}^n_{\ell,j} := \tilde{\lambda}^n_{\ell,j}(\zeta) := \sum_{\substack{m^l_\kappa \in \mathbb{N}_0: \\ \tilde{m} := \sum_{l=0}^{\ell} \sum_{\kappa\in\mathbb{Z}} m^l_\kappa \geq n+1,\, \tilde{m}<\infty \\ \sum_{l=1}^{\ell} l \sum_{\kappa\in\mathbb{Z}} m^l_\kappa = \ell,\, \sum_{l=0}^{\ell}\sum_{\kappa\in\mathbb{Z}} m^l_\kappa \omega'_{l,\kappa} = \tilde{\omega}'_{\ell,j}}} (ik_z\zeta)^{\tilde{m}-n-1} \frac{\tilde{m}!}{(\tilde{m}-n-1)!} \left[\prod_{l=0}^{\ell}\prod_{\kappa\in\mathbb{Z}} \frac{[\lambda_{l,\kappa}]^{m^l_\kappa}}{m^l_\kappa!}\right], \tag{3.3.19}$$

$$\tilde{g}_n(\eta',\zeta) := \sum_{m\in\mathbb{N}_0} \frac{(m+n+1)!}{m!} (ik_z\zeta)^m \sum_{\vec{n}_5 \in \mathrm{I}_{m+n+1} \setminus \left(\bigcup_{\ell=0}^{3} \mathrm{I}^\ell_{m+n+1}\right)} \left[\frac{g(\eta')^{n_4}}{n_4! \sqrt{1+|\eta'|^2}^{\left(\sum_{l=1}^{3} l n_l\right)}} \prod_{l=0}^{3} \sum_{m_\infty \in \mathrm{J}_{n_l}} \left\{\left[\prod_{j\in\mathbb{Z}} \frac{[\lambda_{l,j}]^{m_j}}{m_j!}\right] e^{i\eta'\cdot \sum_{j\in\mathbb{Z}} m_j \omega'_{l,j}}\right\}\right], \tag{3.3.20}$$

$$\mathrm{I}_a := \left\{\vec{n}_5 := (n_0,\dots,n_4) \in \mathbb{N}_0^5 \,\middle|\, \sum_{l=0}^{4} n_l = a\right\},$$

$$\mathrm{I}^\ell_a := \left\{\vec{n}_5 := (n_0,\dots,n_4) \in \mathbb{N}_0^5 \,\middle|\, \sum_{l=0}^{4} n_l = a,\ \sum_{l=1}^{4} l n_l = \ell\right\}, \quad \ell = 0,1,2,3$$

$$\mathrm{J}_a := \left\{m_\infty := (m_j)_{j\in\mathbb{Z}} \,\middle|\, m_j \in \mathbb{N}_0,\ \sum_{j\in\mathbb{Z}} m_j = a\right\}. \tag{3.3.21}$$

Proof. The existence of representation (3.3.16) is a simple consequence of the algebra structure of $\mathcal{A}$. It remains to derive the formulas for the coefficients and $\tilde{g}_n$.

Using the multinomial theorem (cf. Theorem C.8) twice it can be shown that, if $m_\infty := (m_j)_{j\in\mathbb{Z}}$ is a sequence of non-negative integers, $\vec{n}_5 := (n_0,\dots,n_4) \in \mathbb{N}_0^5$ and $m,n \geq 0$,

$$\begin{aligned}
f(\eta')^{m+n+1} &= \sum_{\vec{n}_5\in\mathrm{I}_{m+n+1}} \left[\frac{g(\eta')^{n_4}\,(m+n+1)!}{n_4!} \prod_{l=0}^{3}\left\{\frac{1}{n_l!\sqrt{1+|\eta'|^2}^{\,l n_l}} \left(\sum_{j\in\mathbb{Z}} \lambda_{l,j}\, e^{i\omega'_{l,j}\cdot\eta'}\right)^{n_l}\right\}\right] \\
&= \sum_{\vec{n}_5\in\mathrm{I}_{m+n+1}} \left[\frac{g(\eta')^{n_4}\,(m+n+1)!}{n_4!} \prod_{l=0}^{3}\left\{\frac{1}{n_l!\sqrt{1+|\eta'|^2}^{\,l n_l}} \sum_{m_\infty\in\mathrm{J}_{n_l}} \left(n_l! \left[\prod_{j\in\mathbb{Z}} \frac{[\lambda_{l,j}]^{m_j}}{m_j!}\right] e^{i\eta'\cdot\sum_{j\in\mathbb{Z}} m_j\omega'_{l,j}}\right)\right\}\right] \\
&= \sum_{\vec{n}_5\in\mathrm{I}_{m+n+1}} \left[\frac{g(\eta')^{n_4}\,(m+n+1)!}{n_4!\sqrt{1+|\eta'|^2}^{\left(\sum_{l=1}^{3} l n_l\right)}} \prod_{l=0}^{3} \sum_{m_\infty\in\mathrm{J}_{n_l}} \left\{\left[\prod_{j\in\mathbb{Z}} \frac{[\lambda_{l,j}]^{m_j}}{m_j!}\right] e^{i\eta'\cdot\sum_{j\in\mathbb{Z}} m_j\omega'_{l,j}}\right\}\right].
\end{aligned}$$

The sum over the 5-tuples $\vec{n}_5$ can then be separated into terms which contain the lower powers of $1/\sqrt{1+|\eta'|^2}$ without powers of $g(\eta')$ and a part with finite $\|\cdot\|_{4,\infty}$-norm. E.g., only the five-tuple $(m+n+1,0,0,0,0)$ will result in terms without the term $1/\sqrt{1+|\eta'|^2}$, positive powers of the same or $g(\eta')$, while only the five-tuple $(m+n,1,0,0,0)$ will result in terms with $1/\sqrt{1+|\eta'|^2}$ and without

$g(\eta')$. Note that n_4 in $\mathrm{I}^{\ell}_{m+n+1}$ is always zero for any $\ell = 1, 2, 3$. This then leads to

$$
\begin{aligned}
f(\eta')^{m+n+1} = (m+n+1)! \sum_{m_\infty \in \mathrm{J}_{m+n+1}} & \left\{ \left[\prod_{j\in\mathbb{Z}} \frac{[\lambda_{0,j}]^{m_j}}{m_j!} \right] e^{i\eta' \cdot \sum\limits_{j\in\mathbb{Z}} m_j \omega'_{0,j}} \right\} \\
+ \sum_{\ell=1}^{3} & \left[\frac{(m+n+1)!}{\sqrt{1+|\eta'|^2}^{\ell}} \sum_{\vec{n}_5 \in \mathrm{I}^{\ell}_{m+n+1}} \prod_{l=0}^{\ell} \sum_{m_\infty \in \mathrm{J}_{n_l}} \left\{ \left[\prod_{j\in\mathbb{Z}} \frac{[\lambda_{l,j}]^{m_j}}{m_j!} \right] e^{i\eta' \cdot \sum\limits_{j\in\mathbb{Z}} m_j \omega'_{l,j}} \right\} \right] \\
+ \sum_{\vec{n}_5 \in \mathrm{I}_{m+n+1} \setminus \left(\bigcup\limits_{\ell=0}^{3} \mathrm{I}^{\ell}_{m+n+1} \right)} & \left[\frac{(m+n+1)!\, g(\eta')^{n_4}}{n_4! \sqrt{1+|\eta'|^2}^{\left(\sum\limits_{l=1}^{3} l n_l\right)}} \right. \\
& \left. \prod_{l=0}^{3} \sum_{m_\infty \in \mathrm{J}_{n_l}} \left\{ \left[\prod_{j\in\mathbb{Z}} \frac{[\lambda_{l,j}]^{m_j}}{m_j!} \right] e^{i\eta' \cdot \sum\limits_{j\in\mathbb{Z}} m_j \omega'_{l,j}} \right\} \right]. \qquad (3.3.22)
\end{aligned}
$$

With this, define (cf. (3.3.15))

$$
\begin{aligned}
\bar{\lambda}^n_{0,m+n+1}(m_\infty) &:= (ik_z\zeta)^m \frac{(m+n+1)!}{m!} \left[\prod_{j\in\mathbb{Z}} \frac{[\lambda_{0,j}]^{m_j}}{m_j!} \right], \\
\bar{\omega}'_0(m_\infty) &:= \sum_{j\in\mathbb{Z}} m_j \omega'_{0,j},
\end{aligned}
$$

for all $m_\infty \in \mathrm{J}_{m+n+1}$, all $m \in \mathbb{N}_0$ and any fixed $n \in \mathbb{N}_0$. This can be extended by defining

$$
\tilde{\lambda}^n_0(\tilde{m}, m_\infty) := \begin{cases} \bar{\lambda}^n_{0,\tilde{m}}(m_\infty) & \text{if } \tilde{m} \geq n+1 \\ 0 & \text{else} \end{cases} \qquad (3.3.23)
$$

for all $\tilde{m} \in \mathbb{N}_0$. Assigning an index $j \in \mathbb{Z}$ to every pair $(\tilde{m}, m_\infty)$ leads to the desired expression

$$
\begin{aligned}
\sum_{m\in\mathbb{N}_0} (ik_z\zeta)^m \frac{(m+n+1)!}{m!} & \sum_{m_\infty \in \mathrm{J}_{m+n+1}} \left\{ \left[\prod_{j\in\mathbb{Z}} \frac{[\lambda_{0,j}]^{m_j}}{m_j!} \right] e^{i\eta' \cdot \sum\limits_{j\in\mathbb{Z}} m_j \omega'_{0,j}} \right\} \\
&= \sum_{\tilde{m}\in\mathbb{N}_0} \sum_{m_\infty \in \mathrm{J}_{\tilde{m}}} \tilde{\lambda}^n_0(\tilde{m}, m_\infty)\, e^{i\eta' \cdot \bar{\omega}'_0(m_\infty)} \\
&= \sum_{j\in\mathbb{Z}} \tilde{\lambda}^n_{0,j}\, e^{i\eta' \cdot \tilde{\omega}'_{0,j}},
\end{aligned}
$$

where $\tilde{\lambda}^n_{0,j}$ and $\tilde{\omega}'_{0,j}$ are defined by $\{\tilde{\omega}'_{0,j} : j \in \mathbb{Z}\} = \{\bar{\omega}'_0(m_\infty) : m_\infty \in \mathrm{J}_{\tilde{m}}, \tilde{m} \in \mathbb{N}_0\}$ and

$$
\tilde{\lambda}^n_{0,j} := \sum_{\tilde{m}, m_\infty : \bar{\omega}'_0(m_\infty) = \tilde{\omega}'_{0,j}} \tilde{\lambda}^n_0(\tilde{m}, m_\infty). \qquad (3.3.24)
$$

Thus (3.3.18) follows.

Similarly the second term of (3.3.22) can be transformed. First note that the product

$$
\prod_{l=0}^{\ell} \sum_{m^l_\infty \in \mathrm{J}_{n_l}} \left\{ \left[\prod_{j\in\mathbb{Z}} \frac{[\lambda_{l,j}]^{m^l_j}}{m^l_j!} \right] e^{i\eta' \cdot \sum\limits_{j\in\mathbb{Z}} m^l_j \omega'_{l,j}} \right\}
$$

can be rewritten as the sum

$$\sum_{\vec{m}_\ell:=(m^0_\infty,\ldots,m^\ell_\infty)\in \times_{l=0}^{\ell} \mathrm{J}_{n_l}} \left[\prod_{l=0}^{\ell}\prod_{j\in\mathbb{Z}} \frac{[\lambda_{l,j}]^{m^l_j}}{m^l_j!}\right] e^{i\eta'\cdot\sum\limits_{l=0}^{\ell}\sum\limits_{j\in\mathbb{Z}} m^l_j\omega'_{l,j}}.$$

With this, once more define

$$\bar{\lambda}^n_{\ell,m+n+1}(\vec{m}_\ell) := (ik_z\zeta)^m\,\frac{(m+n+1)!}{m!}\left[\prod_{l=0}^{\ell}\prod_{j\in\mathbb{Z}}\frac{[\lambda_{l,j}]^{m^l_j}}{m^l_j!}\right]$$

$$\bar{\omega}'_\ell(\vec{m}_\ell) := \sum_{l=0}^{\ell}\sum_{j\in\mathbb{Z}} m^l_j\omega'_{l,j}$$

for all $\vec{m}_\ell \in \times_{l=0}^{\ell}\mathrm{J}_{n_l}$, all $\vec{n}_5 \in \mathrm{I}^\ell_{m+n+1}$, all $m \in \mathbb{N}_0$ and any fixed $n \in \mathbb{N}_0$. Furthermore, this is again extended by defining

$$\tilde{\lambda}^n_\ell(\tilde{m},\vec{m}_\ell) := \begin{cases}\bar{\lambda}^n_{\ell,m+n+1}(\vec{m}_\ell) & \text{if } \tilde{m}\geq n+1\\ 0 & \text{else}\end{cases}$$

for all $\tilde{m} \in \mathbb{N}_0$, which leads to the reformulation

$$\begin{aligned}
&\sum_{m\in\mathbb{N}_0}(ik_z\zeta)^m\,\frac{(m+n+1)!}{m!}\sum_{\vec{n}_5\in\mathrm{I}^\ell_{m+n+1}}\prod_{l=0}^{\ell}\sum_{m_\infty\in\mathrm{J}_{n_l}}\left\{\prod_{j\in\mathbb{Z}}\left(\frac{[\lambda_{l,j}]^{m_j}}{m_j!}\right) e^{i\eta'\cdot\sum\limits_{j\in\mathbb{Z}} m_j\omega'_{l,j}}\right\}\\
&\quad=\sum_{m\in\mathbb{N}_0}\sum_{\vec{n}_5\in\mathrm{I}^\ell_{m+n+1}}\sum_{\vec{m}_\ell\in\times_{l=0}^{\ell}\mathrm{J}_{n_l}}\bar{\lambda}^n_{\ell,m+n+1}(\vec{m}_\ell)\,e^{i\eta'\cdot\bar{\omega}'_\ell(\vec{m}_\ell)}\\
&\quad=\sum_{\tilde{m}\in\mathbb{N}_0}\sum_{\vec{n}_5\in\mathrm{I}^\ell_{\tilde{m}}}\sum_{\vec{m}_\ell\in\times_{l=0}^{\ell}\mathrm{J}_{n_l}}\tilde{\lambda}^n_\ell(\tilde{m},\vec{m}_\ell)\,e^{i\eta'\cdot\bar{\omega}'_\ell(\vec{m}_\ell)}\\
&\quad=\sum_{j\in\mathbb{Z}}\tilde{\lambda}^n_{\ell,j}\,e^{i\eta'\cdot\tilde{\omega}'_{\ell,j}},
\end{aligned}$$

where every j corresponds with one triple $(\tilde{m},\vec{n}_5,\vec{m}_\ell)$ and where $\tilde{\lambda}^n_{\ell,j}$ and $\tilde{\omega}'_{\ell,j}$ are defined for any fixed $\ell = 1,2,3$ by $\{\tilde{\omega}'_{\ell,j} : j\in\mathbb{Z}\} = \{\bar{\omega}'_\ell(\vec{m}_\ell) : \vec{m}_\ell \in \times_{l=0}^{\ell}\mathrm{J}_{n_l}, \vec{n}_5\in\mathrm{I}^\ell_{\tilde{m}}, \tilde{m}\in\mathbb{N}_0\}$ and

$$\tilde{\lambda}^n_{\ell,j} = \sum_{\tilde{m},\vec{m}_\ell\in\times_{l=0}^{\ell}\mathrm{J}_{n_l},\vec{n}_5\in\mathrm{I}^\ell_{\tilde{m}}:\,\tilde{\omega}'_{\ell,j}=\bar{\omega}'_\ell(\vec{m}_\ell)}\tilde{\lambda}^n_\ell(\tilde{m},\vec{m}_\ell).$$

At last define $\tilde{g}_n$ as the last line in (3.3.22). ■

Remark 3.10. *Note that f_n also depends on the constant k_z and the variables $\zeta\in[0,1]$ and $n\in\{0,\ldots,8\}$. Consequently, $\tilde{\lambda}^n_{\ell,j}$ is dependent on k_z, ζ and n, while $\tilde{\omega}'_{\ell,j}$ is a constant for any fixed $\ell = 0,\ldots,3$ and $j\in\mathbb{Z}$. Similarly the function $\tilde{g}_n$ depends on k_z and ζ.*

Using the lemma, the limit $\tilde{r}\to\infty$ of I_1 (cf. (3.3.14)) can be evaluated as the sum of the three terms

$$\lim_{\tilde{r}\to\infty}\mathrm{I}_1 = \mathrm{I}_{1.1}+\mathrm{I}_{1.2}+\mathrm{I}_{1.3}, \tag{3.3.25}$$

where

$$\begin{aligned}\mathrm{I}_{1.1} := \lim_{\tilde{r}\to\infty}\sum_{n=0}^{8}\sum_{j\in\mathbb{Z}}\Bigg\{\int_0^1\tilde{\lambda}^n_{0,j}\,\frac{(-i\zeta)^n}{n!}\,\mathrm{d}\zeta\int_{\mathbb{R}^2}\Bigg\{\frac{(\xi_\tau-i\tau)^n}{\xi_\tau}\int_{B_2(\tilde{r})} e^{i\tilde{\omega}'_{0,j}\cdot\eta'}\,e^{-i\eta'\cdot(s'-k')}\,\mathrm{d}\eta'&\\
\left[(\vec{s}_{\xi_\tau}\times\vec{e}^{\,0})\times\vec{s}_{\xi_\tau}\right]\,e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}}\Bigg\}\,\mathrm{d}s'\Bigg\},&\end{aligned} \tag{3.3.26}$$

$$\mathrm{I}_{1.2} := \lim_{\tilde{r}\to\infty} \sum_{\ell=1}^{3} \sum_{n=0}^{8} \sum_{j\in\mathbb{Z}} \Bigg\{ \int_0^1 \tilde{\lambda}_{\ell,j}^n \frac{(-i\zeta)^n}{n!} \,\mathrm{d}\zeta \int_{\mathbb{R}^2} \Bigg\{ \frac{(\xi_\tau - i\tau)^n}{\xi_\tau} \int_{B_2(\tilde{r})} \frac{1}{\sqrt{1+|\eta'|^2}^{\,\ell}} \, e^{i\tilde{\omega}'_{\ell,j}\cdot\eta'} \, e^{-i\eta'\cdot(s'-k')} \,\mathrm{d}\eta' \\ \left[\left(\vec{s}_{\xi_\tau} \times \vec{e}^{\,0}\right) \times \vec{s}_{\xi_\tau}\right] e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}} \Bigg\} \,\mathrm{d}s' \Bigg\} \tag{3.3.27}$$

and

$$\mathrm{I}_{1.3} := \lim_{\tilde{r}\to\infty} \sum_{n=0}^{8} \int_0^1 \frac{(-i\zeta)^n}{n!} \int_{\mathbb{R}^2} \Bigg\{ \frac{(\xi_\tau - i\tau)^n}{\xi_\tau} \int_{B_2(\tilde{r})} \tilde{g}_n(\eta',\zeta) \, e^{-i\eta'\cdot(s'-k')} \,\mathrm{d}\eta' \\ \left[\left(\vec{s}_{\xi_\tau} \times \vec{e}^{\,0}\right) \times \vec{s}_{\xi_\tau}\right] e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}} \Bigg\} \,\mathrm{d}s' \,\mathrm{d}\zeta. \tag{3.3.28}$$

The limit (3.3.28) can easily be evaluated by applying Lebesgue's theorem, since for any $n \in \{0, \ldots, 8\}$ the function $\tilde{g}_n$ is independent of s', continuously dependent on ζ (cf. (3.3.20)) and absolutely integrable w.r.t. $\eta' \in \mathbb{R}^2$, such that there holds $|\int_{B_2(\tilde{r})} \tilde{g}_n(\eta',\zeta)\, e^{-i\eta'\cdot(s'-k')}\,\mathrm{d}\eta'| \le \max_{\zeta\in[0,1]} \int_{\mathbb{R}^2} |\tilde{g}_n(\eta',\zeta)|\,\mathrm{d}\eta' \le c_n < \infty$. Moreover, the term $(\xi_\tau - i\tau)^n/\xi_\tau\, [(\vec{s}_{\xi_\tau} \times \vec{e}^{\,0}) \times \vec{s}_{\xi_\tau}]\, e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}}$ is uniformly bounded and absolutely integrable w.r.t. $s' \in \mathbb{R}^2$ for any fixed $\tau < 0$, since $e^{i\xi_\tau z}$ decays exponentially.

To evaluate the limits (3.3.26) and (3.3.27) consider the Fourier transform

$$\int_{\mathbb{R}^2} \frac{1}{\sqrt{1+|\eta'|^2}^{\,\ell}} \, e^{-i\eta'\cdot\left(s'-(k'+\tilde{\omega}'_{\ell,j})\right)} \,\mathrm{d}\eta'$$

for $\ell \in \{0,1,2,3\}$, which can be evaluated as a Hankel transform of order zero defined as (cf. [1, Eqn. 9.1.18, p. 104] for the relation between Hankel and Fourier transform)

$$\int_0^\infty f(|\eta'|)\, J_0(|s'||\eta'|)\, |\eta'| \,\mathrm{d}|\eta'| = \frac{1}{2\pi} \int_{\mathbb{R}^2} f(|\eta'|)\, e^{-is'\cdot\eta'} \,\mathrm{d}\eta',$$

where J_0 is the zero order Bessel function of the first kind. Keeping in mind that the inverse Hankel transform coincides with the Hankel transform itself, the well-known Fourier transform for the Dirac delta and [31, Eqns. 2.19 and 2.20, p. 8 and Eqn. 2.110, p. 22] lead to

$$\int_{\mathbb{R}^2} e^{-i\eta'\cdot\left(s'-(k'+\tilde{\omega}'_{0,j})\right)} \,\mathrm{d}\eta' = 4\pi^2\, \delta\left(s' - (k' + \tilde{\omega}'_{0,j})\right), \tag{3.3.29}$$

$$\int_{\mathbb{R}^2} \frac{1}{\sqrt{1+|\eta'|^2}} \, e^{-i\eta'\cdot\left(s'-(k'+\tilde{\omega}'_{1,j})\right)} \,\mathrm{d}\eta' = 2\pi \frac{e^{-\left|s'-(k'+\tilde{\omega}'_{1,j})\right|}}{\left|s' - (k' + \tilde{\omega}'_{1,j})\right|}, \tag{3.3.30}$$

$$\int_{\mathbb{R}^2} \frac{1}{1+|\eta'|^2} \, e^{-i\eta'\cdot\left(s'-(k'+\tilde{\omega}'_{2,j})\right)} \,\mathrm{d}\eta' = 2\pi\, K_0\left(\left|s' - (k' + \tilde{\omega}'_{2,j})\right|\right) \tag{3.3.31}$$

and

$$\int_{\mathbb{R}^2} \frac{1}{\sqrt{1+|\eta'|^2}^{\,3}} \, e^{-i\eta'\cdot\left(s'-(k'+\tilde{\omega}'_{3,j})\right)} \,\mathrm{d}\eta' = 2\pi\, e^{-\left|s'-(k'+\tilde{\omega}'_{3,j})\right|}, \tag{3.3.32}$$

where $K_0(z)$ is the modified Bessel function of the second kind, which has a logarithmic singularity at $z = 0$. Note that the right-hand side of (3.3.30) is a weakly singular function, while that of (3.3.32) is uniformly bounded.

It can be shown that the limit of integral (3.3.26) and (3.3.27) is well defined in the sense of a limit in $\mathcal{S}'(\mathbb{R}^2)$, since

$$\varphi_n(s') := \frac{(\xi_\tau - i\tau)^n}{\xi_\tau} \left[\left(\vec{s}_{\xi_\tau} \times \vec{e}^{\,0} \right) \times \vec{s}_{\xi_\tau} \right] e^{i\vec{s}_{\xi_\tau} \cdot \vec{x}}$$

is a Schwartz function for $\tau < 0$ and $|z| > h$. For convenience, define

$$F_{\tilde{r},\ell,j}(\eta') := \mathbb{1}_{B_2(\tilde{r})}(\eta') \frac{1}{\sqrt{1+|\eta'|^2}^{\,\ell}} e^{i\eta' \cdot (\tilde{\omega}'_{\ell,j} + k')}.$$

With this, the limit of the integral w.r.t. s' in (3.3.26) and (3.3.27) is evaluated as

$$\begin{aligned}
\lim_{\tilde{r}\to\infty} \int_{\mathbb{R}^2} \int_{B_2(\tilde{r})} \frac{1}{\sqrt{1+|\eta'|^2}^{\,\ell}} e^{i\eta' \cdot (\tilde{\omega}'_{\ell,j} + k')} \, e^{-is' \cdot \eta'} \, \mathrm{d}\eta' \, \varphi_n(s') \, \mathrm{d}s' &= \lim_{\tilde{r}\to\infty} \int_{\mathbb{R}^2} \mathcal{F}F_{\tilde{r},\ell,j}(s') \, \varphi_n(s') \, \mathrm{d}s' \\
&= \lim_{\tilde{r}\to\infty} \int_{\mathbb{R}^2} F_{\tilde{r},\ell,j}(\eta') \, \mathcal{F}\varphi_n(\eta') \, \mathrm{d}\eta' \\
&= \int_{\mathbb{R}^2} F_{\infty,\ell,j}(\eta') \, \mathcal{F}\varphi_n(\eta') \, \mathrm{d}\eta' \qquad (3.3.33) \\
&= \int_{\mathbb{R}^2} \frac{1}{\sqrt{1+|\eta'|^2}^{\,\ell}} e^{i\eta' (\tilde{\omega}'_{\ell,j} + k')} \mathcal{F}\varphi_n(\eta') \, \mathrm{d}\eta',
\end{aligned}$$

which is finite for any $|z| > h$ and $\tau < 0$, since $\mathcal{F}\varphi_n \in \mathcal{S}(\mathbb{R}^2)$. Note that the limit is uniform w.r.t. j and ζ. Indeed, switching to absolute values in the formulas for $\mathrm{I}_{1.1}$ and $\mathrm{I}_{1.2}$ (cf. (3.3.26) and (3.3.27)) will lead to a product of a sum over j independent of $\tilde{r}$, times an integral independent of j, which is the third line of formula (3.3.33) switched to absolute values. To be exact,

$$\begin{aligned}
\lim_{\tilde{r}\to\infty} \left| \sum_{j\in\mathbb{Z}} \int_0^1 \tilde{\lambda}^n_{\ell,j} \frac{(-i\zeta)^n}{n!} \, \mathrm{d}\zeta \int_{\mathbb{R}^2} F_{\tilde{r},\ell,j}(\eta') \, \mathcal{F}\varphi_n(\eta') \, \mathrm{d}\eta' \right| &\le \lim_{\tilde{r}\to\infty} \sum_{j\in\mathbb{Z}} \int_0^1 |\tilde{\lambda}^n_{\ell,j}| \frac{\zeta^n}{n!} \, \mathrm{d}\zeta \int_{\mathbb{R}^2} |F_{\tilde{r},\ell,j}(\eta') \, \mathcal{F}\varphi_n(\eta')| \, \mathrm{d}\eta' \\
&= \lim_{\tilde{r}\to\infty} \sum_{j\in\mathbb{Z}} \int_0^1 \left|\tilde{\lambda}^n_{\ell,j}\right| \frac{\zeta^n}{n!} \, \mathrm{d}\zeta \int_{B_2(\tilde{r})} \frac{|\mathcal{F}\varphi_n(\eta')|}{\sqrt{1+|\eta'|^2}^{\,\ell}} \, \mathrm{d}\eta' \\
&\le \lim_{\tilde{r}\to\infty} \sum_{j\in\mathbb{Z}} \int_0^1 \left|\tilde{\lambda}^n_{\ell,j}\right| \frac{\zeta^n}{n!} \, \mathrm{d}\zeta \int_{\mathbb{R}^2} \frac{|\mathcal{F}\varphi_n(\eta')|}{\sqrt{1+|\eta'|^2}^{\,\ell}} \, \mathrm{d}\eta' \\
&= \sum_{j\in\mathbb{Z}} \int_0^1 \left|\tilde{\lambda}^n_{\ell,j}\right| \frac{\zeta^n}{n!} \, \mathrm{d}\zeta \int_{\mathbb{R}^2} \frac{|\mathcal{F}\varphi_n(\eta')|}{\sqrt{1+|\eta'|^2}^{\,\ell}} \, \mathrm{d}\eta' \\
&\le c_{\ell,n},
\end{aligned}$$

where $c_{\ell,n}$ is finite for all $\ell = 0, \ldots, 3$ and $n = 0, \ldots, 8$. This follows since $(\tilde{\lambda}^n_{\ell,j})_{j\in\mathbb{Z}}$ is an absolutely summable sequence w.r.t. j, while $\mathcal{F}\varphi_n$ is a Schwartz function and thus absolutely integrable.

Altogether, for the integral w.r.t. s' and η' in $\mathrm{I}_{1.2}$, i.e. for $\ell \in \{1, 2, 3\}$, this results in (cf. (3.3.33))

$$\lim_{\tilde{r}\to\infty} \int_{\mathbb{R}^2} \int_{B_2(\tilde{r})} \frac{1}{\sqrt{1+|\eta'|^2}^{\,\ell}} e^{i\eta' \cdot (\tilde{\omega}'_{\ell,j} + k')} \, e^{-is' \cdot \eta'} \, \mathrm{d}\eta' \, \varphi_n(s') \, \mathrm{d}s' = \int_{\mathbb{R}^2} \mathcal{F}F_{\infty,\ell,j}(s') \, \varphi_n(s') \, \mathrm{d}s'. \qquad (3.3.34)$$

Inserting this into (3.3.27) leads to

$$\begin{aligned}
\mathrm{I}_{1.2} &= \sum_{\ell=1}^{3}\sum_{n=0}^{8}\sum_{j\in\mathbb{Z}}\left\{\int_0^1 \tilde{\lambda}_{\ell,j}^n \frac{(-i\zeta)^n}{n!}\,\mathrm{d}\zeta \int_{\mathbb{R}^2} \mathcal{F}F_{\infty,\ell,j}(s')\,\varphi_n(s')\,\mathrm{d}s'\right\} \qquad (3.3.35)\\
&= \sum_{\ell=1}^{3}\sum_{n=0}^{8}\sum_{j\in\mathbb{Z}}\left\{\int_0^1 \tilde{\lambda}_{\ell,j}^n \frac{(-i\zeta)^n}{n!}\,\mathrm{d}\zeta \int_{\mathbb{R}^2} \mathcal{F}F_{\infty,\ell,j}(s')\,\frac{(\xi_\tau - i\tau)^n}{\xi_\tau}\,\left[\left(\vec{s}_{\xi_\tau}\times\vec{e}^{\,0}\right)\times\vec{s}_{\xi_\tau}\right]\,e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}}\,\mathrm{d}s'\right\}.
\end{aligned}$$

These integrals exist since the integrands are at most weakly singular, since the $\mathcal{F}F_{\infty,\ell,j}$ (cf. (3.3.30)–(3.3.32)) are bounded at infinity (cf. [1, Eqn. 9.7.2, p. 122]) and since $e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}}$ is exponentially decreasing and thus ensures the existence of the integral w.r.t. s'.

It remains to examine the limit $\tau \nearrow 0$ of (3.3.35). Note that the integral w.r.t. s' exists even if the singularity points of (3.3.30) or (3.3.31), that appear only for $\tau = 0$, coincide with the singularity point of $1/\xi_\tau = 1/\sqrt{k_\tau^2 - s'^2}$ for $\tau = 0$.

Lemma 3.11. *For any $k \in \mathbb{R}_+$ and $k' \in \mathbb{R}^2$, as well as a sufficiently large positive constant c, the absolute value*

$$\left|\int_{B_2(2k)} \frac{1}{\sqrt{k^2 - |s'|^2}}\,\frac{1}{|k'-s'|}\,\mathrm{d}s'\right| \le c \int_{B_2(2k)} \frac{1}{\sqrt{|k^2 - |s'|^2|}}\,\frac{|\log|k'-s'||}{|k'-s'|}\,\mathrm{d}s'$$

is finite.

Proof. Obviously this holds true if $|k'| \neq k$, since then the two quotients in the integrand are not coinciding weak singularities. For $|k'| = k$ assume w.l.o.g. that $k' = (0,k)^\top$. Otherwise, for polar coordinates (r,ϕ) the angle ϕ can be substituted by $\tilde{\phi} + \phi_k - \pi/2$, where $k' = k(\cos\phi_k, \sin\phi_k)^\top$. For $|k'| = k$ the neighbourhood of the point where the two singularities coincide is of particular interest, since the two singularities are again only weakly singular or even bounded, and thus integrable, outside of this neighbourhood. Hence, only a small neighbourhood of $s' = k'$, determined by the small constants $\epsilon_x, \epsilon_y > 0$, will be considered. In particular, the constant ϵ_y is assumed smaller than ϵ_x and $k_y = k$. For an appropriately chosen neighbourhood the integral on the right-hand side can be written as

$$\int_{-\epsilon_x}^{\epsilon_x}\int_{\sqrt{k^2-\epsilon_y^2-s_x^2}}^{\sqrt{k^2+\epsilon_y^2-s_x^2}} \frac{1}{\sqrt{|k^2-|s'|^2|}}\,\frac{|\log|k'-s'||}{|k'-s'|}\,\mathrm{d}s'.$$

Note that for this domain of integration, the term $1/\sqrt{|k^2-|s'|^2|}$ is weakly singular on a segment of a circle with radius k. Now a smooth coordinate transformation is introduced such that this term is modified to a weak singularity on one coordinate axis of the new system and the weak singularity at $s' = k'$ is moved to the origin. To be precise, s_x is substituted by t_x and s_y by $(t_y+1)\sqrt{k^2-t_x^2}$ leading to

$$\int_{-\epsilon_x}^{\epsilon_x}\int_{\sqrt{1-\frac{\epsilon_y^2}{k^2-t_x^2}}-1}^{\sqrt{1+\frac{\epsilon_y^2}{k^2-t_x^2}}-1} \frac{1}{\sqrt{2+t_y}}\,\frac{1}{\sqrt{|t_y|}}\,\frac{\left|\log\left|(0,k)^\top - (t_x,(t_y+1)\sqrt{k^2-t_x^2})^\top\right|\right|}{\left|(0,k)^\top - (t_x,(t_y+1)\sqrt{k^2-t_x^2})^\top\right|}\,\mathrm{d}t_y\,\mathrm{d}t_x.$$

It is not hard to show that for $\epsilon_y \to 0$,

$$\int\limits_{-\epsilon_x}^{\epsilon_x} \int\limits_{\sqrt{1-\frac{\epsilon_y^2}{k^2-t_x^2}}-1}^{\sqrt{1+\frac{\epsilon_y^2}{k^2-t_x^2}}-1} \frac{1}{\sqrt{2+t_y}} \frac{1}{\sqrt{|t_y|}} \frac{\left|\log\left|(0,k)^\top - (t_x,(t_y+1)\sqrt{k^2-t_x^2})^\top\right|\right|}{\left|(0,k)^\top - (t_x,(t_y+1)\sqrt{k^2-t_x^2})^\top\right|} \,\mathrm{d}t_y\,\mathrm{d}t_x$$

$$\leq c \int\limits_{-\epsilon_y}^{\epsilon_y} \int\limits_{-\epsilon_x}^{\epsilon_x} \frac{1}{\sqrt{|t_y|}} \frac{|\log|t'||}{|t'|} \,\mathrm{d}t_x\,\mathrm{d}t_y.$$

Here,

$$\begin{aligned}
\int\limits_{-\epsilon_y}^{\epsilon_y} \int\limits_{-\epsilon_x}^{\epsilon_x} \frac{1}{\sqrt{|t_y|}} \frac{|\log|t'||}{|t'|} \,\mathrm{d}t_x\,\mathrm{d}t_y &= \int\limits_{-\epsilon_y}^{\epsilon_y} \frac{1}{\sqrt{|t_y|}} \int\limits_{-\epsilon_x}^{\epsilon_x} \frac{\frac{1}{2}|\log(t_x^2+t_y^2)|}{\sqrt{t_x^2+t_y^2}} \,\mathrm{d}t_x\,\mathrm{d}t_y \\
&= 4\int\limits_{0}^{\epsilon_y} \frac{1}{\sqrt{t_y}} \int\limits_{0}^{\epsilon_x} \frac{\frac{1}{2}|\log(t_x^2+t_y^2)|}{\sqrt{t_x^2+t_y^2}} \,\mathrm{d}t_x\,\mathrm{d}t_y \\
&= 2\int\limits_{0}^{\epsilon_y} \frac{1}{\sqrt{t_y}} \int\limits_{0}^{\epsilon_x/t_y} \frac{|\log(t_y^2(1+t_x^2))|}{\sqrt{1+t_x^2}} \,\mathrm{d}t_x\,\mathrm{d}t_y \qquad (3.3.36) \\
&= 4\int\limits_{0}^{\epsilon_y} \frac{|\log t_y|}{\sqrt{t_y}} \int\limits_{0}^{\epsilon_x/t_y} \frac{1}{\sqrt{1+t_x^2}} \,\mathrm{d}t_x\,\mathrm{d}t_y + 2\int\limits_{0}^{\epsilon_y} \frac{1}{\sqrt{t_y}} \int\limits_{0}^{\epsilon_x/t_y} \frac{\log(1+t_x^2)}{\sqrt{1+t_x^2}} \,\mathrm{d}t_x\,\mathrm{d}t_y,
\end{aligned}$$

where

$$\begin{aligned}
\int\limits_{0}^{\epsilon_y} \frac{|\log t_y|}{\sqrt{t_y}} \int\limits_{0}^{\epsilon_x/t_y} \frac{1}{\sqrt{1+t_x^2}} \,\mathrm{d}t_x\,\mathrm{d}t_y &= \int\limits_{0}^{\epsilon_y} \frac{|\log t_y|}{\sqrt{t_y}} \operatorname{arsinh}\left(\frac{\epsilon_x}{t_y}\right) \mathrm{d}t_y \\
&= \int\limits_{0}^{\epsilon_y} \frac{|\log t_y|}{\sqrt{t_y}} \log\left(\frac{\epsilon_x}{t_y} + \sqrt{1+\frac{\epsilon_x^2}{t_y^2}}\right) \mathrm{d}t_y \\
&= \int\limits_{0}^{\epsilon_y} \frac{|\log t_y| \log\left(\epsilon_x + \sqrt{t_y^2+\epsilon_x^2}\right)}{\sqrt{t_y}} \,\mathrm{d}t_y - \int\limits_{0}^{\epsilon_y} \frac{(\log t_y)^2}{\sqrt{t_y}} \,\mathrm{d}t_y \qquad (3.3.37)
\end{aligned}$$

is finite. Note that $\epsilon_x/t_y \geq 1$ for $0 \leq t_y \leq \epsilon_y < \epsilon_x$. Thus, since $\log(1+t_x^2) \leq \log 2$ and $1/\sqrt{1+t_x^2} \leq 1$ for $0 \leq t_x \leq 1$ and since $\log(1+t_x^2) \leq c\,(1+t_x^2)^{1/6}$ and $1+t_x^2 \geq t_x^2$ for $1 \leq t_x \leq \epsilon_x/t_y$, the second, obviously positive, integral on the right-hand side of (3.3.36) can be bounded from above by

$$\begin{aligned}
\int\limits_{0}^{\epsilon_y} \frac{1}{\sqrt{t_y}} \int\limits_{0}^{\epsilon_x/t_y} \frac{\log(1+t_x^2)}{\sqrt{1+t_x^2}} \,\mathrm{d}t_x\,\mathrm{d}t_y &\leq \int\limits_{0}^{\epsilon_y} \frac{1}{\sqrt{t_y}} \int\limits_{0}^{1} \frac{\log(1+t_x^2)}{\sqrt{1+t_x^2}} \,\mathrm{d}t_x\,\mathrm{d}t_y + \int\limits_{0}^{\epsilon_y} \frac{1}{\sqrt{t_y}} \int\limits_{1}^{\epsilon_x/|t_y|} \frac{\log(1+t_x^2)}{\sqrt{1+t_x^2}} \,\mathrm{d}t_x\,\mathrm{d}t_y \\
&\leq \int\limits_{0}^{\epsilon_y} \frac{\log 2}{\sqrt{t_y}} \,\mathrm{d}t_y + c\int\limits_{0}^{\epsilon_y} \frac{1}{\sqrt{t_y}} \int\limits_{1}^{\epsilon_x/|t_y|} \frac{1}{(1+t_x^2)^{\frac{1}{3}}} \,\mathrm{d}t_x\,\mathrm{d}t_y \\
&\leq \int\limits_{0}^{\epsilon_y} \frac{\log 2}{\sqrt{t_y}} \,\mathrm{d}t_y + c\int\limits_{0}^{\epsilon_y} \frac{1}{\sqrt{t_y}} \int\limits_{1}^{\epsilon_x/|t_y|} \frac{1}{[t_x]^{\frac{2}{3}}} \,\mathrm{d}t_x\,\mathrm{d}t_y \\
&\leq \int\limits_{0}^{\epsilon_y} \frac{\log 2}{\sqrt{t_y}} \,\mathrm{d}t_y + 3c\int\limits_{0}^{\epsilon_y} \frac{1}{\sqrt{t_y}} \left[\frac{\epsilon_x^{\frac{1}{3}}}{[t_y]^{\frac{1}{3}}} - 1\right] \mathrm{d}t_y. \qquad (3.3.38)
\end{aligned}$$

It is easily seen that this bound is finite, since only weak singularities occur. Thus the lemma is proven. ∎

This can be used to apply Lebesgue's theorem to evaluate the limit $\tau \nearrow 0$ of the integrand w.r.t. s' in (3.3.35) and thus (3.3.27), such that

$$\lim_{\tau\nearrow 0} \mathrm{I}_{1.2} = \sum_{\ell=1}^{3}\sum_{n=0}^{8}\sum_{j\in\mathbb{Z}} \left\{ \int_0^1 \tilde{\lambda}^n_{\ell,j} \frac{(-i\zeta)^n}{n!}\,\mathrm{d}\zeta \int_{\mathbb{R}^2} \mathcal{F}F_{\infty,\ell,j}(s')\,\xi^{n-1}\left[\left(\vec{s}_\xi \times \vec{e}^{\,0}\right)\times \vec{s}_\xi\right] e^{i\vec{s}_\xi\cdot\vec{x}}\,\mathrm{d}s' \right\}. \tag{3.3.39}$$

On the other hand, for the integral w.r.t s' and η' in $\mathrm{I}_{1.1}$ the limit (cf. (3.3.29) and (3.3.34))

$$\lim_{\tilde{r}\to\infty} \int_{\mathbb{R}^2}\int_{B_2(\tilde{r})} e^{i\eta'\cdot(\tilde{\omega}'_{0,j}+k')}\,e^{-is'\cdot\eta'}\,\mathrm{d}\eta'\,\varphi_n(s')\,\mathrm{d}s' = 4\pi^2\varphi_n(\tilde{\omega}'_{0,j}+k')$$

is obtained. In this sense, the limit in (3.3.26) evaluates as

$$\mathrm{I}_{1.1} = 4\pi^2 \sum_{n=0}^{8}\sum_{j\in\mathbb{Z}} \int_0^1 \tilde{\lambda}^n_{0,j}\,(-i\zeta)^n\,\mathrm{d}\zeta\,\frac{\left(\omega^j_{z,\tau}-\tau\right)^n}{n!\;\omega^j_{z,\tau}}\left[\left(\vec{\omega}^j_\tau \times \vec{e}^{\,0}\right)\times\vec{\omega}^j_\tau\right] e^{i\vec{\omega}^j_\tau\cdot\vec{x}}, \tag{3.3.40}$$

with $\vec{\omega}^j_\tau := \left(k' + \tilde{\omega}'_{0,j}, \omega^j_{z,\tau}\right)^\top$ and $\omega^j_{z,\tau} := \sqrt{k_\tau^2 - \left|k' + \tilde{\omega}'_{0,j}\right|^2}$. Note again that the $\tilde{\lambda}^n_{0,j}$ are absolutely summable w.r.t. j, which is a consequence of the Banach algebra properties of $\mathcal{A}^{\mathrm{C}}$.

It remains to consider the limit $\tau \nearrow 0$ of the two terms $\mathrm{I}_{1.1}$ and $\mathrm{I}_{1.3}$ (cf. (3.3.40) and (3.3.28)). For $\mathrm{I}_{1.1}$, this limit is easily evaluated, since the sum w.r.t. j exists absolutely and the integral w.r.t. ζ is uniformly bounded w.r.t. τ. However, it has to be assumed that $\omega^j_{z,0} \neq 0$, i.e. that (cf. (3.3.17) for the connection between $\omega'_{0,j}$ and $\tilde{\omega}'_{0,j}$)

$$k \notin \mathrm{cl}\left\{ \left|k' + \sum_{j\in\mathbb{Z}} m_j\omega'_{0,j}\right| \,:\, m_j \in \mathbb{N}_0 \text{ s.t.} \sum_{j\in\mathbb{Z}} m_j < \infty \right\} \tag{3.3.41}$$

to obtain a finite value $\lim_{\tau\nearrow 0}\left(\omega^j_{z,\tau}-\tau\right)^n/\omega^j_{z,\tau}$ for $n=0$. Under this assumption,

$$\lim_{\tau\nearrow 0}\mathrm{I}_{1.1} = 4\pi^2 \sum_{n=0}^{8}\sum_{j\in\mathbb{Z}} \int_0^1 \tilde{\lambda}^n_{0,j}\,(-i\zeta)^n\,\mathrm{d}\zeta\,\frac{\left[\omega^j_{z,0}\right]^{n-1}}{n!}\left[\left(\vec{\omega}^j_0 \times \vec{e}^{\,0}\right)\times\vec{\omega}^j_0\right] e^{i\vec{\omega}^j_0\cdot\vec{x}}. \tag{3.3.42}$$

Remark 3.12 (Remarks on the restriction of wave numbers)**.**

i) *Condition (3.3.41) is not always necessary. If* $k = \left|k' + \sum_{j\in\mathbb{Z}} m_j\omega'_{0,j}\right|$ *for a special sequence* m_j *and if this is an isolated point of the set in the formula (3.3.41), and if, by chance, the coefficient*

$$\sum_{n\in\mathbb{N}_0}\int_0^1 \tilde{\lambda}^n_{0,j}\,(-i\zeta)^n\,\mathrm{d}\zeta\,[\omega^j_{z,0}]^n/n!$$

of the corresponding $1/\omega^j_{z,\tau}$ *(see the subsequent (3.1.4) and Theorem 3.1) vanishes, then the limit* $\tau \nearrow 0$ *may be possible even though (3.3.41) is violated.*

ii) *In the case of a decaying interface, i.e.* $\lambda_{0,j} = 0$ *and* $\omega'_{0,j} = (0,0)^\top$ *for all* $j \in \mathbb{Z}$, *condition (3.3.41) is always satisfied, since* $k_z < 0$ *such that* $k \neq |k'|$. *Moreover, it follows that* $\tilde{\lambda}^n_{0,j} = 0$ *for all* $j \in \mathbb{Z}$, *such that* $E_0 = 0$ *(cf. (3.1.4)).*

iii) *For a simple bi-periodic interface* $f(\eta') := \cos(\omega'\cdot\eta')$ *with a fixed* $\omega' \in \mathbb{R}^2$ *the spatial frequencies* $\omega'_{0,j}$ *are only non-zero for one pair* $(j,-j) \in \mathbb{Z}^2$, *e.g.* $\omega'_{0,1} = \omega'$ *and* $\omega'_{0,-1} = -\omega'$. *With this it is easily seen that condition (3.3.41) reduces to* $|k' + m\,\omega'|^2 \neq k^2$ *for all* $m \in \mathbb{Z}$. *By solving the quadratic equation w.r.t.* m *it can also be rewritten as* $\left[k'\cdot\omega'_0 \pm \sqrt{(k'\cdot\omega'_0)^2 + k_z^2}\right]/|\omega'| \notin \mathbb{Z}$ *with* $\omega'_0 := \omega'/|\omega'|$. *These are the so-called reflected (transmitted) Rayleigh modes of a grating.*

iv) *In the case where* $\mathcal{R} := \{\omega'_{0,j} \mid j \in \mathbb{Z}\} = \mathbb{Q}^2 \cap [-1,1]^2$, *the set of all pairs of rational numbers in* $[-1,1]^2$, *it is easily seen that for any value* $\omega'_r \in \mathbb{Q}^2$ *a finite subset* $\mathcal{M}$ *of* $\mathcal{R}$ *exists such that* $\omega'_r = \sum_{\mathcal{M}} \omega'_{0,j}$. *Naturally, it follows that all* $k \in [0,\infty)$ *are excluded by condition (3.3.41) and that the formulas derived in this thesis can not be applied.*

v) *A simple non-periodic interface function with only countably many wave number exclusions is* $f(\eta') = \cos(\eta_x) + \cos(\pi\,\eta_x) = 1/2\,e^{-i\pi\eta_x} + 1/2\,e^{-i\eta_x} + 1/2\,e^{i\eta_x} + 1/2\,e^{i\pi\eta_x}$ *(doubly periodic function). Here it can easily be confirmed that for normal incidence, i.e.* $k' = (0,0)^\top$, *condition (3.3.41) reduces to* $k \neq |m_1 + m_2\,\pi|$ *for all* $m_1, m_2 \in \mathbb{Z}$.

vi) *For any set* $\mathcal{R} := \{\omega'_{0,j} \mid j \in \mathbb{Z}\}$ *that has a subset* $\mathcal{D}$ *which is dense in some domain* $\Omega \subset \mathbb{R}^2$ *with* $(0,0)^\top \in \Omega$, *all non-negative real valued wave numbers are excluded by condition (3.3.41). Indeed, if* $\omega_m := \min_{\omega' \in \mathcal{D}} |\omega'|$, *a sufficiently large* $m \in \mathbb{N}$ *can be found such that* $m\,\omega_m > \sqrt{2}$. *As a consequence,* $m\,\mathcal{R}$ *has a subset that is dense in* $[-1,1]^2$, *which leads to a case very similar to the example in Remark 3.12* (iv).

vii) *A sufficient condition for the existence of wave numbers that satisfy condition (3.3.41) is to have only finitely many non-zero spatial frequencies* $\omega_{0,j}$. *This is the most relevant case for numerical simulations.*

Analogously to (3.3.40), the limit $\tau \nearrow 0$ of $\mathrm{I}_{1.3}$ (cf. (3.3.28)) is easily calculated using Lebesgue's theorem, since the absolute value of the integral $\int_{B_2(\tilde{r})} \tilde{g}_n(\eta',\zeta)\, e^{-i\eta'\cdot(s'-k')}\,\mathrm{d}\eta'$ is uniformly bounded w.r.t. s' by $\|\tilde{g}_n\|_{L^1(\mathbb{R}^2)} < \|\tilde{g}_n\|_{4,\infty}\, \|1/(1+|\eta'|^2)^2\|_{L^1(\mathbb{R}^2)} < \infty$ while the term $(\xi_\tau - i\tau)^n/\xi_\tau\, [(\vec{s}_{\xi_\tau} \times \vec{e}^{\,0}) \times \vec{s}_{\xi_\tau}]\, e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}}$ is pointwise convergent and uniformly bounded w.r.t. τ by a function that is integrable w.r.t. s'. It follows that the limits $\tilde{r} \to \infty$ and $\tau \nearrow 0$ of (3.3.14) can be evaluated.

Now consider the remaining integral I_2 (cf. (3.3.13))

$$
\begin{aligned}
\mathrm{I}_2 = \int_0^1 \int_{\mathbb{R}^2} \Bigg\{ \int_{B_2(\tilde{r})} & \sum_{n=9}^{\infty} (-i\zeta)^n\, f(\eta')^{n+1} \frac{(\xi_\tau - i\tau)^n}{n!}\, e^{ik_z\zeta f(\eta')}\, e^{-i\eta'\cdot(s'-k')}\,\mathrm{d}\eta' \\
& \frac{\left[(\vec{s}_{\xi_\tau} \times \vec{e}^{\,0}) \times \vec{s}_{\xi_\tau}\right]}{\xi_\tau}\, e^{is'\cdot x'}\, e^{iz\xi_\tau} \Bigg\}\,\mathrm{d}s'\,\mathrm{d}\zeta \\
= \int_0^1 \int_{\mathbb{R}^2} \Bigg\{ \int_{B_2(\tilde{r})} & \sum_{n=9}^{\infty} (-i\zeta)^n\, f(\eta')^{n+1} \frac{(\xi_\tau - i\tau)^n}{n!}\, e^{ik_z\zeta f(\eta')}\, \frac{1+|\eta'|_*^4}{1+|\eta'|_*^4}\, e^{-i\eta'\cdot(s'-k')}\,\mathrm{d}\eta' \\
& \frac{\left[(\vec{s}_{\xi_\tau} \times \vec{e}^{\,0}) \times \vec{s}_{\xi_\tau}\right]}{\xi_\tau}\, e^{is'\cdot x'}\, e^{iz\xi_\tau} \Bigg\}\,\mathrm{d}s'\,\mathrm{d}\zeta \\
= \int_0^1 \int_{\mathbb{R}^2} \Bigg\{ \int_{B_2(\tilde{r})} & \sum_{n=9}^{\infty} (-i\zeta)^n\, f(\eta')^{n+1} \frac{(\xi_\tau - i\tau)^n}{n!}\, e^{ik_z\zeta f(\eta')}\, \frac{\left(1+\nabla_{s'}^4\right)\, e^{-i\eta'\cdot(s'-k')}}{1+|\eta'|_*^4}\,\mathrm{d}\eta' \\
& \frac{\left[(\vec{s}_{\xi_\tau} \times \vec{e}^{\,0}) \times \vec{s}_{\xi_\tau}\right]}{\xi_\tau}\, e^{is'\cdot x'}\, e^{iz\xi_\tau} \Bigg\}\,\mathrm{d}s'\,\mathrm{d}\zeta,
\end{aligned}
\tag{3.3.43}
$$

where $\nabla_{s'}^4 := \partial_{s_x}^4 + \partial_{s_y}^4$ and $|\eta'|_*^4 := \eta_x^4 + \eta_y^4$. To further transform this expression, consider the following lemma.

Lemma 3.13. *For two complex valued functions* $f, g \in C^4(\mathbb{R}^2)$ *the following equation holds true.*

$$
f(s')\,\partial_{s_x}^4 g(s') = \sum_{m=0}^{4} (-1)^m \binom{4}{m}\, \partial_{s_x}^{4-m} \left[\partial_{s_x}^m f(s')\, g(s')\right]
$$

Proof. The Leibniz rule (cf. Theorem C.9) implies

$$
\begin{aligned}
\partial_{s_x}\left[\partial^3_{s_x} f(s')\, g(s')\right] &= \partial^4_{s_x} f(s')\, g(s') + \partial^3_{s_x} f(s')\, \partial_{s_x} g(s')\\
\partial^2_{s_x}\left[\partial^2_{s_x} f(s')\, g(s')\right] &= \partial^4_{s_x} f(s')\, g(s') + 2\partial^3_{s_x} f(s')\, \partial_{s_x} g(s') + \partial^2_{s_x} f(s')\, \partial^2_{s_x} g(s')\\
\partial^3_{s_x}\left[\partial_{s_x} f(s')\, g(s')\right] &= \partial^4_{s_x} f(s')\, g(s') + 3\partial^3_{s_x} f(s')\, \partial_{s_x} g(s') + 3\partial^2_{s_x} f(s')\, \partial^2_{s_x} g(s') + \partial_{s_x} f(s')\, \partial^3_{s_x} g(s').
\end{aligned}
$$

These are now used to replace all the terms from

$$
\partial^4_{s_x}\left[f(s')\, g(s')\right] = \partial^4_{s_x} f(s')\, g(s') + 4\partial^3_{s_x} f(s')\partial_{s_x} g(s') + 6\partial^2_{s_x} f(s')\partial^2_{s_x} g(s') + 4\partial_{s_x} f(s')\partial^3_{s_x} g(s') + f(s')\partial^4_{s_x} g(s')
$$

that contain derivatives of g. Or, to be more precise, all the terms of the form $\partial^{(4-\ell)}_{s_x} f(s')\, \partial^{\ell}_{s_x} g(s')$, where $1 \le \ell \le 3$, are removed. ∎

Naturally, Lemma 3.13 also holds for derivatives w.r.t. s_y, such that

$$
\begin{aligned}
f(s')\left(1+\nabla^4_{s'}\right) g(s') &= f(s')\, g(s') + f(s')\, \partial^4_{s_x} g(s') + f(s')\, \partial^4_{s_y} g(s')\\
&= f(s')\, g(s') + \sum_{m=0}^{4} (-1)^m \binom{4}{m} \partial^{4-m}_{s_x}\left[\partial^m_{s_x} f(s')\, g(s')\right]\\
&\quad + \sum_{m=0}^{4} (-1)^m \binom{4}{m} \partial^{4-m}_{s_y}\left[\partial^m_{s_y} f(s')\, g(s')\right]
\end{aligned}
$$

Applying this to the integrand w.r.t. η' in (3.3.43), the equation transforms to

$$
\begin{aligned}
\mathrm{I}_2 = &\sum_{j=0}^{2}\sum_{m=0}^{M_j} (-1)^m \binom{4}{m} \int_0^1 \int_{\mathbb{R}^2} \Bigg\{\\
&\partial^{(4-m)\alpha'_j}_{s'}\left[\int_{B_2(\tilde{r})} \partial^{m\alpha'_j}_{s'}\left[\sum_{n=9}^{\infty} (-i\zeta)^n\ f(\eta')^{n+1} \frac{(\xi_\tau - i\tau)^n}{n!}\, e^{i\frac{z}{2}\xi_\tau}\right] \frac{e^{ik_z\zeta\, f(\eta')}}{1+|\eta'|^4_*}\, e^{-i\eta'\cdot(s'-k')}\, \mathrm{d}\eta'\right]\\
&\frac{\left[\left(\vec{s}_{\xi_\tau}\times\vec{e}^{\,0}\right)\times\vec{s}_{\xi_\tau}\right]}{\xi_\tau}\, e^{is'\cdot x'}\, e^{i\frac{z}{2}\xi_\tau}\Bigg\}\, \mathrm{d}s'\, \mathrm{d}\zeta,
\end{aligned}
\tag{3.3.44}
$$

where α'_j is a multi-index defined as

$$
\alpha'_j := \begin{cases} (0,0) & \text{if } j=0\\ (1,0) & \text{if } j=1\\ (0,1) & \text{if } j=2 \end{cases}
$$

and

$$
M_j := \begin{cases} 0 & \text{if } j=0\\ 4 & \text{otherwise} \end{cases}.
$$

Applying integration by parts $(4-m)$ times to the integral w.r.t. s' leads to

$$
\begin{aligned}
\mathrm{I}_2 = &\sum_{j=0}^{2}\sum_{m=0}^{M_j} \binom{4}{m} \int_0^1 \int_{\mathbb{R}^2} \Bigg\{\\
&\int_{B_2(\tilde{r})} \partial^{m\alpha'_j}_{s'}\left[\sum_{n=9}^{\infty} (-i\zeta)^n\ f(\eta')^{n+1} \frac{(\xi_\tau - i\tau)^n}{n!}\, e^{i\frac{z}{2}\xi_\tau}\right] \frac{e^{ik_z\zeta\, f(\eta')}}{1+|\eta'|^4_*}\, e^{-i\eta'\cdot(s'-k')}\, \mathrm{d}\eta'\\
&\partial^{(4-m)\alpha'_j}_{s'}\left[\frac{\left[\left(\vec{s}_{\xi_\tau}\times\vec{e}^{\,0}\right)\times\vec{s}_{\xi_\tau}\right]}{\xi_\tau}\, e^{is'\cdot x'}\, e^{i\frac{z}{2}\xi_\tau}\right]\Bigg\}\, \mathrm{d}s'\, \mathrm{d}\zeta,
\end{aligned}
\tag{3.3.45}
$$

where the absolute value of

$$\sum_{n=9}^{\infty} (-i\zeta)^n \, f(\eta')^{n+1} \frac{(\xi_\tau - i\tau)^n}{n!} \, e^{i\frac{z}{2}\xi_\tau}$$
$$= f(\eta')\, e^{-i(\xi_\tau - i\tau)\left(\zeta f(\eta') - \frac{z}{2}\right)} \, e^{-\tau\frac{z}{2}} - \sum_{n=0}^{8} (-i\zeta)^n \, f(\eta')^{n+1} \frac{(\xi_\tau - i\tau)^n}{n!} \, e^{i\frac{z}{2}\xi_\tau} \tag{3.3.46}$$

is uniformly bounded w.r.t. η' and τ and decreases exponentially as $|s'|$ tends to infinity. Indeed, $f(\eta')$ is bounded, $|\tau| \le 1$ and the right-hand side of the last equation is an exponentially decaying function w.r.t. s', since $z > 0$ and $(\zeta\, f(\eta') - z/2) < 0$. Moreover, $e^{iz/2\,\xi_\tau}$ and all its derivatives decay exponentially for $|s'|$ to infinity, which shows that the boundary terms that would usually occur after integrating by parts are zero. Note, that the derivatives do not introduce singularities for $\tau < 0$. Thus, the limit $\tilde r \to \infty$ can now be evaluated, since the integrand w.r.t. η' is dominated by the term $1/(1 + |\eta'|_*^4)$ for $|\eta'| \to \infty$.

Furthermore, for the terms in the sum with the index $j = 0$, the same arguments can be used to evaluate the limit $\tau \nearrow 0$, since the term $1/\xi_\tau$ is only weakly singular for $\tau = 0$. To evaluate the limit $\tau \nearrow 0$ for any fixed $j = 1, 2$ it remains to be shown that

$$\left| \partial_{s'}^{m\alpha_j'} \left[\sum_{n=9}^{\infty} (-i\zeta)^n \, f(\eta')^{n+1} \frac{(\xi_\tau - i\tau)^n}{n!} \, e^{i\frac{z}{2}\xi_\tau} \right] \partial_{s'}^{(4-m)\alpha_j'} \left[\frac{\left[\left(\vec s_{\xi_\tau} \times \vec e^{\,0} \right) \times \vec s_{\xi_\tau} \right]}{\xi_\tau} \, e^{is'\cdot x'} \, e^{i\frac{z}{2}\xi_\tau} \right] \right| \tag{3.3.47}$$

is uniformly bounded w.r.t. η' and $-1 < \tau \le 0$ by a function integrable w.r.t. s'. If this condition is satisfied, Lebesgue's theorem can be applied. The existence of the integral w.r.t. η' is then ensured by the term $1/(1+|\eta'|_*^4)$. Before an estimate of (3.3.47) can be found, the derivatives have to be examined. This is done in two steps. After splitting the domain of integration w.r.t. s' in (3.3.45) into $B_2(2k)$ and $\mathbb{R}^2 \setminus B_2(2k)$, the behaviour of (3.3.47) at the singularity $s'^2 = k^2$ and at infinity are examined separately. To be precise,

$$\begin{aligned}
\lim_{\tilde r \to \infty} \mathrm{I}_2 = & \sum_{j=0}^{2} \sum_{m=0}^{M_j} \binom{4}{m} \int_0^1 \Bigg\{ \\
& \int_{B_2(2k)} \Bigg\{ \int_{\mathbb{R}^2} \partial_{s'}^{m\alpha_j'} \left[\sum_{n=9}^{\infty} (-i\zeta)^n \, f(\eta')^{n+1} \frac{(\xi_\tau - i\tau)^n}{n!} \, e^{i\frac{z}{2}\xi_\tau} \right] \frac{e^{ik_z\zeta\, f(\eta')}}{1 + |\eta'|_*^4} \, e^{-i\eta'\cdot(s'-k')} \, \mathrm{d}\eta' \\
& \qquad \partial_{s'}^{(4-m)\alpha_j'} \left[\frac{\left[\left(\vec s_{\xi_\tau} \times \vec e^{\,0} \right) \times \vec s_{\xi_\tau} \right]}{\xi_\tau} \, e^{is'\cdot x'} \, e^{i\frac{z}{2}\xi_\tau} \right] \Bigg\} \, \mathrm{d}s' \\
& + \int_{\mathbb{R}^2 \setminus B_2(2k)} \Bigg\{ \int_{\mathbb{R}^2} \partial_{s'}^{m\alpha_j'} \left[\sum_{n=9}^{\infty} (-i\zeta)^n \, f(\eta')^{n+1} \frac{(\xi_\tau - i\tau)^n}{n!} \, e^{i\frac{z}{2}\xi_\tau} \right] \frac{e^{ik_z\zeta\, f(\eta')}}{1 + |\eta'|_*^4} \, e^{-i\eta'\cdot(s'-k')} \, \mathrm{d}\eta' \\
& \qquad \partial_{s'}^{(4-m)\alpha_j'} \left[\frac{\left[\left(\vec s_{\xi_\tau} \times \vec e^{\,0} \right) \times \vec s_{\xi_\tau} \right]}{\xi_\tau} \, e^{is'\cdot x'} \, e^{i\frac{z}{2}\xi_\tau} \right] \Bigg\} \, \mathrm{d}s' \Bigg\} \, \mathrm{d}\zeta.
\end{aligned} \tag{3.3.48}$$

To study the behaviour around the singularity, the subsequent lemma is used to show that the differentiation and the summation in (3.3.47) can be interchanged.

Lemma 3.14. *For all s' in the compact set $B_2(2k)$, the sums*

$$\sum_{n=9}^{\infty} (-i\zeta)^n \, f(\eta')^{n+1} \frac{(\xi_\tau - i\tau)^n}{n!} \, e^{i\frac{z}{2}\xi_\tau}$$

and

$$\sum_{n=9}^{\infty} \frac{(-i\zeta)^n}{n!} \, f(\eta')^{n+1} \partial_{s'}^{m\alpha_j'} \left[(\xi_\tau - i\tau)^n \, e^{i\frac{z}{2}\xi_\tau} \right] \tag{3.3.49}$$

are uniformly bounded w.r.t. $s' \in B_2(2k)$ and $\tau \in [-1, 0]$ for any fixed $\eta' \in \mathbb{R}^2$.

Proof. This is obviously true for the first term since no singularities occur and $e^{-\frac{z}{2}\xi_\tau}$ decays exponentially for any fixed $\tau \in [0,1]$ as $|s'| \to \infty$. To show this for the second term, examine the derivative by using the Leibniz rule. But first, for convenience, define

$$F_{1,n}(\xi) := \left(\xi - i\tau\right)^n \tag{3.3.50}$$

and

$$F_2(\xi) := e^{i\frac{z}{2}\xi}. \tag{3.3.51}$$

With this

$$\begin{aligned}\partial_{s'}^{m\alpha'_j}\left[(\xi_\tau - i\tau)^n\, e^{i\frac{z}{2}\xi_\tau}\right] &= \partial_{s'}^{m\alpha'_j}\left[F_{1,n}(\xi_\tau)\; F_2(\xi_\tau)\right] \\ &= \sum_{l=0}^{m} \frac{m!}{l!\,(m-l)!}\partial_{s'}^{l\alpha'_j}\left[F_{1,n}(\xi_\tau)\right]\,\partial_{s'}^{(m-l)\alpha'_j}\left[F_2(\xi_\tau)\right].\end{aligned} \tag{3.3.52}$$

To further study these derivatives, Faà di Bruno's formula (cf. Theorem C.10), which is a generalisation of the chain rule for higher order derivatives, is used. Defining

$$T_l := \left\{(\ell_1,\ldots,\ell_l) \in \mathbb{N}_0^l : \sum_{o=1}^{l} o\,\ell_o = l\right\}, \tag{3.3.53}$$

$$s_l : \mathbb{N}_0^l \to \mathbb{N}_0, \quad (\ell_1,\ldots,\ell_l) \mapsto \sum_{o=1}^{l} \ell_o \tag{3.3.54}$$

and

$$p_l : \mathbb{N}_0^l \to \mathbb{N}_0, \quad (\ell_1,\ldots,\ell_l) \mapsto \prod_{o=1}^{l} \ell_o!$$

leads to

$$\partial_{s'}^{l\alpha'_j}\left[F_{1,n}(\xi_\tau)\right] = \sum_{\vec{\ell}_1 := (\ell_1^1,\ldots,\ell_l^1)\in T_l} \frac{l!}{p_l(\vec{\ell}_1)}\left[\partial_{\xi_\tau}^{s_l(\vec{\ell}_1)} F_{1,n}(\xi_\tau)\right] \prod_{\substack{o=1\\ \ell_o^1 \geq 1}}^{l} \left[\frac{\partial_{s'}^{o\alpha'_j}\xi_\tau}{o!}\right]^{\ell_o^1}$$

and

$$\partial_{s'}^{(m-l)\alpha'_j}\left[F_2(\xi_\tau)\right] = \sum_{\vec{\ell}_2 := (\ell_1^2,\ldots,\ell_{m-l}^2)\in T_{m-l}} \frac{(m-l)!}{p_{m-l}(\vec{\ell}_2)}\left[\partial_{\xi_\tau}^{s_{m-l}(\vec{\ell}_2)} F_2(\xi_\tau)\right] \prod_{\substack{o=1\\ \ell_o^2 \geq 1}}^{m-l} \left[\frac{\partial_{s'}^{o\alpha'_j}\xi_\tau}{o!}\right]^{\ell_o^2}.$$

Thus (cf. (3.3.52))

$$\begin{aligned}\partial_{s'}^{m\alpha'_j}\left[(\xi_\tau - i\tau)^n\, e^{i\frac{z}{2}\xi_\tau}\right] = \sum_{l=0}^{m} m! \sum_{(\vec{\ell}_1,\vec{\ell}_2)\in T_l\times T_{m-l}} &\left\{\frac{1}{p_l(\vec{\ell}_1)\,p_{m-l}(\vec{\ell}_2)}\left[\partial_{\xi_\tau}^{s_l(\vec{\ell}_1)} F_{1,n}(\xi_\tau)\; \partial_{\xi_\tau}^{s_{m-l}(\vec{\ell}_2)} F_2(\xi_\tau)\right]\right. \\ &\left.\prod_{\substack{o=1\\ \ell_o^1 \geq 1}}^{l} \left[\frac{\partial_{s'}^{o\alpha'_j}\xi_\tau}{o!}\right]^{\ell_o^1} \prod_{\substack{o=1\\ \ell_o^2 \geq 1}}^{m-l} \left[\frac{\partial_{s'}^{o\alpha'_j}\xi_\tau}{o!}\right]^{\ell_o^2}\right\},\end{aligned}$$

where (cf. (3.3.50) and (3.3.51))

$$\partial_{\xi_\tau}^{s_l(\vec{\ell}_1)} F_{1,n}(\xi_\tau) = \frac{n!}{(n - s_l(\vec{\ell}_1))!}\left(\xi_\tau - i\tau\right)^{n - s_l(\vec{\ell}_1)}$$

and

$$\partial_{\xi_\tau}^{s_{m-l}(\vec{\ell}_2)} F_2\left(\xi_\tau\right) = \left(i\frac{z}{2}\right)^{s_{m-l}(\vec{\ell}_2)} e^{i\frac{z}{2}\,\xi_\tau}.$$

This leads to

$$\begin{aligned}
&\partial_{s'}^{m\alpha'_j}\left[\left(\xi_\tau - i\tau\right)^n\, e^{i\frac{z}{2}\xi_\tau}\right] \\
&\quad = \sum_{l=0}^{m} m! \sum_{(\vec{\ell}_1,\vec{\ell}_2)\in T_l\times T_{m-l}} \left\{ \frac{1}{p_l(\vec{\ell}_1)\, p_{m-l}(\vec{\ell}_2)}\, \frac{n!}{(n-s_l(\vec{\ell}_1))!} \left(\xi_\tau - i\tau\right)^{n-s_l(\vec{\ell}_1)} \left(i\frac{z}{2}\right)^{s_{m-l}(\vec{\ell}_2)} e^{i\frac{z}{2}\,\xi_\tau} \right. \\
&\qquad\qquad \left. \prod_{\substack{o=1\\ \tilde{\ell}_o\geq 1}}^{\max\{l,m-l\}} \left[\frac{\partial_{s'}^{o\alpha'_j}\xi_\tau}{o!}\right]^{\tilde{\ell}_o} \right\},
\end{aligned} \tag{3.3.55}$$

where

$$\tilde{\ell}_o := \begin{cases} \ell_o^1 + \ell_o^2 & \text{if } o \leq \min\{l, m-l\} \\ \ell_o^1 & \text{if } m-l < o \leq l \\ \ell_o^2 & \text{if } l < o \leq m-l \end{cases}.$$

Now Faà di Bruno's formula is applied once more to evaluate the derivative

$$\begin{aligned}
\partial_{s'}^{o\alpha'_j}\xi_\tau &= \partial_{s'}^{o\alpha'_j}\left[\sqrt{k_\tau^2 - s'^2}\right] \\
&= \sum_{\vec{\ell}_3\in T_o} \frac{o!}{p_o(\vec{\ell}_3)} \left[\prod_{\iota=0}^{s_o(\vec{\ell}_3)-1}\left(\frac{1-2\iota}{2}\right)\right] \sqrt{k_\tau^2 - s'^2}^{\,1-2s_o(\vec{\ell}_3)} \prod_{\substack{\iota=1\\ \ell_\iota^3\geq 1}}^{o} \left[\frac{\partial_{s'}^{\iota\alpha'_j}\left[k_\tau^2 - s'^2\right]}{\iota!}\right]^{\ell_\iota^3}.
\end{aligned}$$

Thus, since

$$\left[\frac{\partial_{s'}^{\iota\alpha'_j}\left[k_\tau^2 - s'^2\right]}{\iota!}\right]^{\ell_\iota^3} = 0$$

if $\ell_\iota^3 \geq 1$ for $\iota > 2$, which shows that only those $\vec{\ell}_3$ contribute where $\ell_1^3 + 2\,\ell_2^3 = o$, and by defining $\kappa := \ell_2^3$

$$\begin{aligned}
&\partial_{s'}^{o\alpha'_j}\xi_\tau \\
&\quad = \sum_{\kappa=0}^{o/2} \frac{o!}{\kappa!\,(o-2\kappa)!} \left[\prod_{\iota=0}^{o-\kappa-1}\left(\frac{1-2\iota}{2}\right)\right] \sqrt{k_\tau^2 - s'^2}^{\,1-2(o-\kappa)} \left[\frac{\partial_{s'}^{\alpha'_j}\left[k_\tau^2 - s'^2\right]}{1!}\right]^{o-2\kappa} \left[\frac{\partial_{s'}^{2\alpha'_j}\left[k_\tau^2 - s'^2\right]}{2!}\right]^{\kappa} \\
&\quad = \sum_{\kappa=0}^{o/2} \frac{o!\,(-1)^{o-\kappa}\,2^{o-2\kappa}}{\kappa!\,(o-2\kappa)!} \left[\prod_{\iota=0}^{o-\kappa-1}\left(\frac{1-2\iota}{2}\right)\right] \sqrt{k_\tau^2 - s'^2}^{\,1-2(o-\kappa)} \left[s'\right]^{(o-2\kappa)\alpha'_j}.
\end{aligned}$$

It follows that (cf. (3.3.55))

$$\begin{aligned}
&\partial_{s'}^{m\alpha'_j}\left[\left(\xi_\tau - i\tau\right)^n\, e^{i\frac{z}{2}\xi_\tau}\right] \\
&\quad = \sum_{l=0}^{m} m! \sum_{(\vec{\ell}_1,\vec{\ell}_2)\in T_l\times T_{m-l}} \left\{ \frac{1}{p_l(\vec{\ell}_1)\, p_{m-l}(\vec{\ell}_2)}\, \frac{n!}{(n-s_l(\vec{\ell}_1))!} \left(\xi_\tau - i\tau\right)^{n-s_l(\vec{\ell}_1)} \left(i\frac{z}{2}\right)^{s_{m-l}(\vec{\ell}_2)} e^{i\frac{z}{2}\,\xi_\tau} \right. \\
&\qquad\qquad \left. \prod_{\substack{o=1\\ \tilde{\ell}_o\geq 1}}^{\max\{l,m-l\}} \left[\xi_\tau^{(1-2o)} \sum_{\kappa=0}^{o/2} C_{o,\kappa}\, \xi_\tau^{2\kappa} \left[s'\right]^{(o-2\kappa)\alpha'_j}\right]^{\tilde{\ell}_o} \right\},
\end{aligned}$$

where $C_{o,\kappa} := (-1)^{o-\kappa}\, 2^{o-2\kappa}/(\kappa!\,(o-2\kappa)!)\prod_{\iota=0}^{o-\kappa-1}\{(1-2\iota)/2\}$ and (cf. (3.3.53))

$$\begin{aligned}\prod_{\substack{o=1\\ \tilde{\ell}_o\geq 1}}^{\max\{l,m-l\}}\left[\xi_\tau^{(1-2o)}\right]^{\tilde{\ell}_o} &= \xi_\tau^{\left(\sum_{o=1}^{l}\ell_o^1(1-2o)+\sum_{o=1}^{m-l}\ell_o^2(1-2o)\right)}\\ &= \xi_\tau^{\left(s_l(\vec{\ell}_1)+s_{m-l}(\vec{\ell}_2)-2l-2(m-l)\right)}\\ &= \frac{1}{\xi_\tau^{\left(2m-s_l(\vec{\ell}_1)-s_{m-l}(\vec{\ell}_2)\right)}}.\end{aligned}$$

Hence

$$\begin{aligned}\partial_{s'}^{m\alpha_j'}\left[(\xi_\tau-i\tau)^n\, e^{i\frac{z}{2}\xi_\tau}\right] = \sum_{l=0}^{m} m! \sum_{(\vec{\ell}_1,\vec{\ell}_2)\in T_l\times T_{m-l}} &\left\{\frac{1}{p_l(\vec{\ell}_1)\,p_{m-l}(\vec{\ell}_2)}\,\frac{n!}{\left(n-s_l(\vec{\ell}_1)\right)!}\,\frac{\left(\xi_\tau-i\tau\right)^{n-s_l(\vec{\ell}_1)}}{\xi_\tau^{\left(2m-s_l(\vec{\ell}_1)-s_{m-l}(\vec{\ell}_2)\right)}}\right.\\ &\left.\left(i\frac{z}{2}\right)^{s_{m-l}(\vec{\ell}_2)}\prod_{\substack{o=1\\ \tilde{\ell}_o\geq 1}}^{\max\{l,m-l\}}\left[\sum_{\kappa=0}^{o/2} C_{o,\kappa}\,\xi_\tau^{2\kappa}\,[s']^{(o-2\kappa)\alpha_j'}\right]^{\tilde{\ell}_o}\right\} e^{i\frac{z}{2}\xi_\tau}. \quad (3.3.56)\end{aligned}$$

Note that

$$\frac{\left(\xi_\tau-i\tau\right)^{n-s_l(\vec{\ell}_1)}}{\xi_\tau^{\left(2m-s_l(\vec{\ell}_1)-s_{m-l}(\vec{\ell}_2)\right)}}$$

is uniformly bounded w.r.t. $s'\in B_2(2k)$ for any $\tau<0$ and $n\geq 9$, since the denominator only has zeros in the complex plane. On the other hand, for the limit $\tau\nearrow 0$,

$$\lim_{\tau\searrow 0}\frac{\left(\xi_\tau-i\tau\right)^{n-s_l(\vec{\ell}_1)}}{\xi_\tau^{\left(2m-s_l(\vec{\ell}_1)-s_{m-l}(\vec{\ell}_2)\right)}} = \frac{\xi^{n-s_l(\vec{\ell}_1)}}{\xi^{\left(2m-s_l(\vec{\ell}_1)-s_{m-l}(\vec{\ell}_2)\right)}} = \frac{\xi^n}{\xi^{2m-s_{m-l}(\vec{\ell}_2)}}, \qquad (3.3.57)$$

which is uniformly bounded w.r.t. $s'\in B_2(2k)$ for any $n\geq 9$, since $m\leq 4$ and $s_{m-l}(\vec{\ell}_2)\geq 0$. Summing up over n in (3.3.49), the $n!$ cancels and the factor $1/(n-s_l(\vec{\ell}_1))!$ ensures the convergence. ■

Consequently, the left derivative in (3.3.47) can be evaluated by differentiating every summand separately. In view of (3.3.57), consider

$$\frac{\left(\xi_\tau-i\tau\right)^{n-s_l(\vec{\ell}_1)}}{\xi_\tau^{\left(2m-s_l(\vec{\ell}_1)-s_{m-l}(\vec{\ell}_2)\right)}} = \frac{\left(\xi_\tau-i\tau\right)^{-s_l(\vec{\ell}_1)}}{\xi_\tau^{-s_l(\vec{\ell}_1)}}\,\frac{\left(\xi_\tau-i\tau\right)^{n}}{\xi_\tau^{\left(2m-s_{m-l}(\vec{\ell}_2)\right)}}$$

and formula (3.3.56) can be transformed further. Now collect all factors of $(\xi_\tau-i\tau)^n/\xi_\tau^{(2m-s_{m-l}(\vec{\ell}_2))}$ with fixed $s_{m-l}(\vec{\ell}_2)$ into one function to get

$$\partial_{s'}^{m\alpha_j'}\left[(\xi_\tau-i\tau)^n\, e^{i\frac{z}{2}\xi_\tau}\right] = n!\, e^{i\frac{z}{2}\,\xi_\tau}\sum_{l=0}^{m}\sum_{\vec{\ell}_1\in T_l}\sum_{\tilde{l}=0}^{\tilde{l}_b}\frac{1}{\left(n-s_l(\vec{\ell}_1)\right)!}\,q^m_{j,\tilde{l},\vec{\ell}_1}(s',z)\,\frac{(\xi_\tau-i\tau)^n}{\xi_\tau^{(2m-s_{m-l}(\vec{\ell}_2))}},$$

where

$$q^m_{j,\tilde{l},\vec{\ell}_1}(s',z) := q^m_{j,l,\tilde{l},\vec{\ell}_1}(s',z,\tau)$$

$$:= \sum_{\substack{\vec{\ell}_2 \in T_{m-l} \\ s_{m-l}(\vec{\ell}_2)=\tilde{l}}} \Bigg\{ \frac{m!}{p_l(\vec{\ell}_1)\, p_{m-l}(\vec{\ell}_2)} \frac{\big(\xi_\tau - i\tau\big)^{-s_l(\vec{\ell}_1)}}{\xi_\tau^{-s_l(\vec{\ell}_1)}} \Big(i\frac{z}{2}\Big)^{s_{m-l}(\vec{\ell}_2)}$$
$$\prod_{\substack{o=1 \\ \tilde{\ell}_o \geq 1}}^{\max\{l,m-l\}} \left[\sum_{\kappa=0}^{o/2} C_{o,\kappa}\, \xi_\tau^{\frac{o}{2}-\kappa} \, [s']^{(o-2\kappa)\alpha_j'} \right]^{\tilde{\ell}_o} \Bigg\}$$

and (cf. (3.3.53) and (3.3.54))

$$\tilde{l}_b := \tilde{l}_b(m) := \max_{l=0,\dots,m} \; \max_{\vec{\ell}_2 \in T_{m-l}} s_{m-l}(\vec{\ell}_2) \leq m \leq 4.$$

For convenience, define $\mathrm{S}_m := \{(l, \vec{\ell}_1, \tilde{l}) : l = 0, \dots, m,\ \vec{\ell}_1 \in T_l,\ \tilde{l} = 0, \dots, \tilde{l}_b\}$. This leads to (cf. (3.3.47))

$$\sum_{n=9}^{\infty} \frac{(-i\zeta)^n}{n!} f(\eta')^{n+1} \partial_{s'}^{m\alpha_j'} \left[(\xi_\tau - i\tau)^n \, e^{i\frac{z}{2}\xi_\tau} \right]$$
$$= \sum_{n=9}^{\infty} \frac{(-i\zeta)^n}{n!} f(\eta')^{n+1} \sum_{(l,\vec{\ell}_1,\tilde{l}) \in \mathrm{S}_m} \frac{n!}{\big(n - s_l(\vec{\ell}_1)\big)!} q^m_{j,\tilde{l},\vec{\ell}_1}(s', z) \frac{\big(\xi_\tau - i\tau\big)^n}{\xi_\tau^{\left(2m-\tilde{l}\right)}} e^{i\frac{z}{2}\xi_\tau}$$
$$= \sum_{n=9}^{\infty} (-i\zeta)^n \, f(\eta')^{n+1} \sum_{(l,\vec{\ell}_1,\tilde{l}) \in \mathrm{S}_m} \frac{q^m_{j,\tilde{l},\vec{\ell}_1}(s', z)}{\big(n - s_l(\vec{\ell}_1)\big)!} \frac{\big(\xi_\tau - i\tau\big)^n}{\xi_\tau^{\left(2m-\tilde{l}\right)}} e^{i\frac{z}{2}\xi_\tau}. \tag{3.3.58}$$

Similarly, the derivative on the right of (3.3.47) can be evaluated as

$$\partial_{s'}^{(4-m)\alpha_j'} \left[\frac{\left[\left(\vec{s}_{\xi_\tau} \times \vec{e}^{\,0}\right) \times \vec{s}_{\xi_\tau}\right]}{\xi_\tau} e^{is'\cdot x'} \, e^{i\frac{z}{2}\xi_\tau} \right] = \frac{\vec{q}_j(s', \xi_\tau)}{\xi_\tau^{(9-2m)}} e^{is'\cdot x'} \, e^{i\frac{z}{2}\xi_\tau}, \tag{3.3.59}$$

where $\vec{q}_j(s', \xi_\tau) := \vec{q}_j(s', \xi_\tau, z)$ is a vector valued polynomial of positive finite order that collects the remaining terms resulting from the differentiation. Thus (cf. (3.3.47))

$$\partial_{s'}^{m\alpha_j'} \left[\sum_{n=9}^{\infty} (-i\zeta)^n \, f(\eta')^{n+1} \frac{(\xi_\tau - i\tau)^n}{n!} e^{i\frac{z}{2}\xi_\tau} \right] \partial_{s'}^{(4-m)\alpha_j'} \left[\frac{\left[\left(\vec{s}_{\xi_\tau} \times \vec{e}^{\,0}\right) \times \vec{s}_{\xi_\tau}\right]}{\xi_\tau} e^{is'\cdot x'} \, e^{i\frac{z}{2}\xi_\tau} \right]$$
$$= \sum_{n=9}^{\infty} (-i\zeta)^n \, f(\eta')^{n+1} \sum_{(l,\vec{\ell}_1,\tilde{l}) \in \mathrm{S}_m} \frac{q^m_{j,\tilde{l},\vec{\ell}_1}(s', z)}{\big(n - s_l(\vec{\ell}_1)\big)!} \frac{(\xi_\tau - i\tau)^n}{\xi_\tau^{9-\tilde{l}}} \vec{q}_j(s', \xi_\tau) \, e^{is'\cdot x'} \, e^{iz\xi_\tau} \tag{3.3.60}$$

for $s' \in B_2(2k)$. However, this is bounded uniformly w.r.t. τ and η' by a function that is integrable w.r.t. s', since $\lim_{\tau \nearrow 0} (\xi_\tau - i\tau)^n / \xi_\tau^{9-\tilde{l}} = \xi^{n-9+\tilde{l}}$, where $n - 9 + \tilde{l} \geq 0$ for $n \geq 9$. Hence, Lebesgue's theorem can be applied for this part of integral (3.3.48), i.e. for the integration w.r.t. s' over $B_2(2k)$ (cf. second and third line on the right-hand side of (3.3.48)), to evaluate the limits w.r.t. $\tilde{r}$ and τ before the integrals.

For all $s' \in \mathbb{R}^2 \setminus B_2(2k)$ (cf. fourth and fifth line on the right-hand side of (3.3.48)) the derivatives in (3.3.47) can be evaluated by considering the right-hand side of (3.3.58) for these s'. Since the sums in this term exist absolutely,

$$\sum_{n=9}^{\infty} (-i\zeta)^n \, f(\eta')^{n+1} \sum_{(l,\vec{\ell}_1,\tilde{l}) \in \mathrm{S}_m} \frac{q^m_{j,\tilde{l},\vec{\ell}_1}(s', z)}{\big(n - s_l(\vec{\ell}_1)\big)!} \frac{\big(\xi_\tau - i\tau\big)^n}{\xi_\tau^{\left(2m-\tilde{l}\right)}} e^{i\frac{z}{2}\xi_\tau}$$
$$= \sum_{(l,\vec{\ell}_1,\tilde{l}) \in \mathrm{S}_m} \Bigg\{ q^m_{j,\tilde{l},\vec{\ell}_1}(s', z) \frac{\big(\xi_\tau - i\tau\big)^{s_l(\vec{\ell}_1)}}{\xi_\tau^{\left(2m-\tilde{l}\right)}} f(\eta')^{s_l(\vec{\ell}_1)+1} \, (-i\zeta)^{s_l(\vec{\ell}_1)}$$
$$\sum_{n=9}^{\infty} (-i\zeta)^{n-s_l(\vec{\ell}_1)} \, f(\eta')^{n-s_l(\vec{\ell}_1)} \frac{\big(\xi_\tau - i\tau\big)^{n-s_l(\vec{\ell}_1)}}{\big(n - s_l(\vec{\ell}_1)\big)!} \Bigg\} e^{i\frac{z}{2}\xi_\tau}$$

$$= \sum_{(l,\vec{\ell}_1,\tilde{l})\in \mathrm{S}_m} \Bigg\{ q^m_{j,\tilde{l},\vec{\ell}_1}(s',z) \frac{\left(\xi_\tau - i\tau\right)^{s_l(\vec{\ell}_1)}}{\xi_\tau^{\left(2m-\tilde{l}\right)}} f(\eta')^{s_l(\vec{\ell}_1)+1} (-i\zeta)^{s_l(\vec{\ell}_1)}$$
$$\sum_{n=9-s_l(\vec{\ell}_1)}^{\infty} (-i\zeta)^n f(\eta')^n \frac{\left(\xi_\tau - i\tau\right)^n}{n!} \Bigg\} e^{i\frac{z}{2}\xi_\tau} \tag{3.3.61}$$
$$= \sum_{(l,\vec{\ell}_1,\tilde{l})\in \mathrm{S}_m} \Bigg\{ q^m_{j,\tilde{l},\vec{\ell}_1}(s',z) \frac{\left(\xi_\tau - i\tau\right)^{s_l(\vec{\ell}_1)}}{\xi_\tau^{\left(2m-\tilde{l}\right)}} f(\eta')^{s_l(\vec{\ell}_1)+1} (-i\zeta)^{s_l(\vec{\ell}_1)}$$
$$\left(e^{-i(\xi_\tau - i\tau)\zeta f(\eta')} - \sum_{n=0}^{8-s_l(\vec{\ell}_1)} (-i\zeta)^n f(\eta')^n \frac{\left(\xi_\tau - i\tau\right)^n}{n!} \right) \Bigg\} e^{i\frac{z}{2}\xi_\tau}$$

which is uniformly bounded w.r.t. τ and η' by a function that is integrable w.r.t. s', since $|\xi_\tau| \geq c > 0$ for $|s'| > 2k$. The same holds again true for (3.3.59). Note, that the integrand in (3.3.48) is uniformly bounded w.r.t. η' as well. Hence, Lebesgue's theorem can also be applied to the integrals on the fourth and fifth line on the right-hand side of (3.3.48) to evaluate the limits before the integrals.

3.3.3 Evaluation of the remaining Cauchy principal value and the limit of the limiting absorption principle

Thus it has been shown that the limits $\tau \nearrow 0$ and $\tilde{r} \to \infty$ of $\Gamma_{\tau,\tilde{r}}(\vec{x})$ (cf. (3.3.11)) exist, by showing that they exist for I_1 (cf. (3.3.12)) and I_2 (cf. (3.3.13)). Note, that the splitting of the sum over n in (3.3.11) can be done for 8 replaced by any fixed $N \geq 8$. The existence of the limits of (3.3.12) and (3.3.13) will still hold. This will now be used to prove

Lemma 3.15. *Defining* $\lim\limits_{\substack{\tau\nearrow 0\\ \tilde{r}\to\infty}} := \lim\limits_{\tau\nearrow 0} \lim\limits_{\tilde{r}\to\infty}$ *and*

$$w_n(\zeta,\eta',s',\tilde{r},\tau) := (-i\zeta)^n\ f(\eta')^{n+1} \mathbb{1}_{B_2(\tilde{r})}(\eta') \frac{\left(\xi_\tau - i\tau\right)^n}{n!} e^{ik_z\zeta f(\eta')} e^{-i\eta'\cdot(s'-k')} \frac{\left[\left(\vec{s}_{\xi_\tau}\times\vec{e}^{\,0}\right)\times\vec{s}_{\xi_\tau}\right]}{\xi_\tau} e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}}.$$

the limits w.r.t. τ and $\tilde{r}$ can be evaluated before taking the sum w.r.t. n on the right hand side of (3.3.11), such that

$$\lim_{\substack{\tau\nearrow 0\\ \tilde{r}\to\infty}} (\mathrm{I}_1 + \mathrm{I}_2) = \lim_{\substack{\tau\nearrow 0\\ \tilde{r}\to\infty}} \int_0^1 \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} \sum_{n\in\mathbb{N}_0} w_n(\zeta,\eta',s',\tilde{r},\tau)\,\mathrm{d}\eta'\,\mathrm{d}s'\,\mathrm{d}\zeta$$
$$= \sum_{n\in\mathbb{N}_0} \lim_{\substack{\tau\nearrow 0\\ \tilde{r}\to\infty}} \int_0^1 \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} w_n(\zeta,\eta',s',\tilde{r},\tau)\,\mathrm{d}\eta'\,\mathrm{d}s'\,\mathrm{d}\zeta. \tag{3.3.62}$$

Proof. Note, that the existence of the left-hand side of (3.3.62) has been shown in the previous subsection. Consider,

$$\sum_{n\in\mathbb{N}_0} \lim_{\substack{\tau\nearrow 0\\ \tilde{r}\to\infty}} \int_0^1 \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} w_n(\zeta,\eta',s',\tilde{r},\tau)\,\mathrm{d}\eta'\,\mathrm{d}s'\,\mathrm{d}\zeta$$
$$= \lim_{\substack{N\to\infty\\ N\geq 8}} \sum_{n=0}^{N} \lim_{\substack{\tau\nearrow 0\\ \tilde{r}\to\infty}} \int_0^1 \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} w_n(\zeta,\eta',s',\tilde{r},\tau)\,\mathrm{d}\eta'\,\mathrm{d}s'\,\mathrm{d}\zeta$$
$$= \lim_{\substack{N\to\infty\\ N\geq 8}} \lim_{\substack{\tau\nearrow 0\\ \tilde{r}\to\infty}} \int_0^1 \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} \sum_{n=0}^{N} w_n(\zeta,\eta',s',\tilde{r},\tau)\,\mathrm{d}\eta'\,\mathrm{d}s'\,\mathrm{d}\zeta$$

$$= \lim_{\substack{N\to\infty\\N\geq 8}} \lim_{\substack{\tau\nearrow 0\\ \tilde r\to\infty}} \int_0^1 \int_{\mathbb{R}^2}\int_{\mathbb{R}^2} \left[\sum_{n\in\mathbb{N}_0} w_n(\zeta,\eta',s',\tilde r,\tau) - \sum_{n=N+1}^{\infty} w_n(\zeta,\eta',s',\tilde r,\tau)\right] \mathrm{d}\eta'\,\mathrm{d}s'\,\mathrm{d}\zeta$$
$$= \lim_{\substack{\tau\nearrow 0\\ \tilde r\to\infty}} \int_0^1 \int_{\mathbb{R}^2}\int_{\mathbb{R}^2} \sum_{n\in\mathbb{N}_0} w_n(\zeta,\eta',s',\tilde r,\tau)\,\mathrm{d}\eta'\,\mathrm{d}s'\,\mathrm{d}\zeta$$
$$- \lim_{\substack{N\to\infty\\N\geq 8}} \lim_{\substack{\tau\nearrow 0\\ \tilde r\to\infty}} \int_0^1 \int_{\mathbb{R}^2}\int_{\mathbb{R}^2} \sum_{n=N+1}^{\infty} w_n(\zeta,\eta',s',\tilde r,\tau)\,\mathrm{d}\eta'\,\mathrm{d}s'\,\mathrm{d}\zeta,$$

where it was used that $\sum_{n\in\mathbb{N}_0} w_n(\zeta,\eta',s',\tilde r,\tau)$ is absolutely integrable w.r.t. ζ, η' and s' for any fixed $\tilde r > 0$. The existence of the first term on the right-hand side has already been shown. It remains to evaluate the limit

$$\lim_{\substack{N\to\infty\\N\geq 8}} \lim_{\substack{\tau\nearrow 0\\ \tilde r\to\infty}} \int_0^1 \int_{\mathbb{R}^2}\int_{\mathbb{R}^2} \sum_{n=N+1}^{\infty} w_n(\zeta,\eta',s',\tilde r,\tau)\,\mathrm{d}\eta'\,\mathrm{d}s'\,\mathrm{d}\zeta = \lim_{\substack{N\to\infty\\N\geq 8}} \lim_{\substack{\tau\nearrow 0\\ \tilde r\to\infty}} \mathrm{I}_2$$

for 8 replaced by N in I_2 (cf. (3.3.13)), by applying Lebesgue's theorem. To do so, the same transformations that led to (3.3.45) are applied here. Furthermore, the integral w.r.t. s' is again split into the sums of integrals over the two domains $B_2(2k)$ and $\mathbb{R}^2 \setminus B_2(2k)$. As before, this allows to evaluate the limits $\tilde r \to \infty$ and $\tau \nearrow 0$ by evaluating the limits of the integrand before evaluating the integrals. Thus

$$\lim_{\substack{N\to\infty\\N\geq 8}} \lim_{\substack{\tau\nearrow 0\\ \tilde r\to\infty}} \int_0^1 \int_{\mathbb{R}^2}\int_{\mathbb{R}^2} \sum_{n=N+1}^{\infty} w_n(\zeta,\eta',s',\tilde r,\tau)\,\mathrm{d}\eta'\,\mathrm{d}s'\,\mathrm{d}\zeta$$
$$= \lim_{\substack{N\to\infty\\N\geq 8}} \int_0^1 \int_{\mathbb{R}^2}\int_{\mathbb{R}^2} \sum_{n=N+1}^{\infty} w_n(\zeta,\eta',s',\infty,0)\,\mathrm{d}\eta'\,\mathrm{d}s'\,\mathrm{d}\zeta. \tag{3.3.63}$$

In view of (3.3.45), for $\tau = 0$ the limit (3.3.63) transforms to

$$\lim_{\substack{N\to\infty\\N\geq 8}} \lim_{\substack{\tau\nearrow 0\\ \tilde r\to\infty}} \int_0^1 \int_{\mathbb{R}^2}\int_{\mathbb{R}^2} \sum_{n=N+1}^{\infty} w_n(\zeta,\eta',s',\tilde r,\tau)\,\mathrm{d}\eta'\,\mathrm{d}s'\,\mathrm{d}\zeta = \lim_{\substack{N\to\infty\\N\geq 8}} \int_0^1 \int_{B_2(2k)}\int_{\mathbb{R}^2} \sum_{n=N+1}^{\infty} \tilde w_1(n,\zeta,\eta',s')\,\mathrm{d}\eta'\,\mathrm{d}s'\,\mathrm{d}\zeta$$
$$+ \lim_{\substack{N\to\infty\\N\geq 8}} \int_0^1 \int_{\mathbb{R}^2\setminus B_2(2k)}\int_{\mathbb{R}^2} \tilde w_2(N,\zeta,\eta',s')\,\mathrm{d}\eta'\,\mathrm{d}s'\,\mathrm{d}\zeta,$$

where (cf. (3.3.45) and (3.3.60))

$$\tilde w_1(n,\zeta,\eta',s') := \sum_{j=0}^{2}\sum_{m=0}^{M_j} \sum_{(l,\vec\ell_1,\tilde l)\in \mathrm{S}_m} \Bigg\{ \binom{4}{m} (-i\zeta)^n\, f(\eta')^{n+1} \frac{q^m_{j,\tilde l,\vec\ell_1}(s',z)}{\big(n - s_l(\vec\ell_1)\big)!}\,\frac{\xi^n}{\xi^{9-\tilde l}}$$
$$\vec q_j(s',\xi)\, e^{is'\cdot x'}\, e^{iz\xi}\, e^{ik_z\zeta\, f(\eta')}\, \frac{1}{1+|\eta'|_*^4}\, e^{-i\eta'\cdot(s'-k')} \Bigg\}$$

and (cf. (3.3.45), (3.3.58), (3.3.59) and the third line of (3.3.61))

$$\tilde{w}_2(N,\zeta,\eta',s') := \sum_{j=0}^{2}\sum_{m=0}^{M_j}\Bigg\{ \sum_{(l,\vec{\ell}_1,\tilde{l})\in \mathrm{S}_m} \Bigg[q^m_{j,\tilde{l},\vec{\ell}_1}(s',z)\,\frac{\xi^{s_l(\vec{\ell}_1)}}{\xi^{9-\tilde{l}}}\,(-i\zeta)^{s_l(\vec{\ell}_1)}\, f(\eta')^{s_l(\vec{\ell}_1)+1} \sum_{n=N+1-s_l(\vec{\ell}_1)}^{\infty} \frac{\big(-i\zeta f(\eta')\big)^n}{n!}\,\xi^n\Bigg] \binom{4}{m}\vec{q}_j(s',\xi)\, e^{i\vec{s}_\xi\cdot\vec{x}}\, e^{ik_z\zeta f(\eta')}\,\frac{1}{1+|\eta'|_*^4}\, e^{-i\eta'\cdot(s'-k')}\Bigg\}.$$

It remains to apply Lebesgue's theorem to evaluate the limit $N\to\infty$. First consider

$$\left|\sum_{n=N+1}^{\infty}\tilde{w}_1(n,\zeta,\eta',s')\right| \le \sum_{n=N+1}^{\infty}|\tilde{w}_1(n,\zeta,\eta',s')| \le \sum_{n=9}^{\infty}|\tilde{w}_1(n,\zeta,\eta',s')|\,.$$

However, estimating (3.3.60), it has already be shown that this function is integrable w.r.t. η', s' and ζ. Hence, Lebesgue's theorem can be applied. At last, consider the term

$$\begin{aligned}
|\tilde{w}_2(N,\zeta,\eta',s')| &\le \sum_{j=0}^{2}\sum_{m=0}^{M_j}\Bigg\{\sum_{(l,\vec{\ell}_1,\tilde{l})\in \mathrm{S}_m}\Bigg[\left|\frac{q^m_{j,\tilde{l},\vec{\ell}_1}(s',z)}{\xi^{9-\tilde{l}}}\, f(\eta')^{s_l(\vec{\ell}_1)+1}\right| \zeta^{s_l(\vec{\ell}_1)} \sum_{n=N+1-s_l(\vec{\ell}_1)}^{\infty}\frac{|-i\zeta f(\eta')\xi|^n}{n!}\Bigg] \\
&\qquad \left|\binom{4}{m}\vec{q}_j(s',\xi)\, e^{i\vec{s}_\xi\cdot\vec{x}}\, e^{ik_z\zeta f(\eta')}\,\frac{1}{1+|\eta'|_*^4}\, e^{-i\eta'\cdot(s'-k')}\right|\Bigg\} \\
&\le \sum_{j=0}^{2}\sum_{m=0}^{M_j}\Bigg\{\sum_{(l,\vec{\ell}_1,\tilde{l})\in \mathrm{S}_m}\Bigg[\left|\frac{q^m_{j,\tilde{l},\vec{\ell}_1}(s',z)}{\xi^{9-\tilde{l}}}\, f(\eta')^{s_l(\vec{\ell}_1)+1}\right| \zeta^{s_l(\vec{\ell}_1)} \sum_{n=0}^{\infty}\frac{|-i\zeta f(\eta')\xi|^n}{n!}\Bigg] \\
&\qquad \left|\binom{4}{m}\vec{q}_j(s',\xi)\, e^{i\vec{s}_\xi\cdot\vec{x}}\, e^{ik_z\zeta f(\eta')}\,\frac{1}{1+|\eta'|_*^4}\, e^{-i\eta'\cdot(s'-k')}\right|\Bigg\} \\
&= \sum_{j=0}^{2}\sum_{m=0}^{M_j}\Bigg\{\sum_{(l,\vec{\ell}_1,\tilde{l})\in \mathrm{S}_m}\Bigg[\left|\frac{q^m_{j,\tilde{l},\vec{\ell}_1}(s',z)}{\xi^{9-\tilde{l}}}\, f(\eta')^{s_l(\vec{\ell}_1)+1}\right| \zeta^{s_l(\vec{\ell}_1)}\, e^{|-i\zeta f(\eta')\xi|}\,\left|e^{iz\xi}\right|\Bigg] \\
&\qquad \left|\binom{4}{m}\vec{q}_j(s',\xi)\, e^{is'\cdot x'}\, e^{ik_z\zeta f(\eta')}\,\frac{1}{1+|\eta'|_*^4}\, e^{-i\eta'\cdot(s'-k')}\right|\Bigg\} \\
&= \sum_{j=0}^{2}\sum_{m=0}^{M_j}\Bigg\{\sum_{(l,\vec{\ell}_1,\tilde{l})\in \mathrm{S}_m}\Bigg[\left|\frac{q^m_{j,\tilde{l},\vec{\ell}_1}(s',z)}{\xi^{9-\tilde{l}}}\, f(\eta')^{s_l(\vec{\ell}_1)+1}\right| \zeta^{s_l(\vec{\ell}_1)}\, e^{-\left(z-\zeta f(\eta')\right)\sqrt{s'^2-k^2}}\Bigg] \\
&\qquad \left|\binom{4}{m}\vec{q}_j(s',\xi)\, e^{is'\cdot x'}\, e^{ik_z\zeta f(\eta')}\,\frac{1}{1+|\eta'|_*^4}\, e^{-i\eta'\cdot(s'-k')}\right|\Bigg\},
\end{aligned}$$

which is integrable w.r.t. $s'\in\mathbb{R}^2\setminus B_2(2k)$, η' and ζ for $z>h$. Thus Lebesgue's theorem can be applied to show that

$$\begin{aligned}
\lim_{\substack{N\to\infty\\ N\ge 8}} \int_0^1\int_{\mathbb{R}^2}\int_{\mathbb{R}^2} \sum_{n=N+1}^{\infty} w_n(\zeta,\eta',s',\infty,0)\,\mathrm{d}\eta'\,\mathrm{d}s'\,\mathrm{d}\zeta
&= \int_0^1\int_{\mathbb{R}^2}\int_{\mathbb{R}^2} \lim_{\substack{N\to\infty\\ N\ge 8}}\sum_{n=N+1}^{\infty} w_n(\zeta,\eta',s',\infty,0)\,\mathrm{d}\eta'\,\mathrm{d}s'\,\mathrm{d}\zeta \\
&= 0,
\end{aligned}$$

since

$$\lim_{\substack{N\to\infty \\ N\geq 8}} \sum_{n=N+1}^{\infty} w_n(\zeta,\eta',s',\infty,0)$$

converges pointwise to zero. Consequently, equation (3.3.62) holds true. ■

Thus it was shown that both limits in (3.3.8) can be evaluated by applying Lebesgue's theorem, integration by parts and the generalised Fourier transform, which then formally leads to

$$\left\langle \vec{D}^d(\vec{x}), \varphi(\vec{x}) \right\rangle = \frac{i}{8\pi^2} \int\limits_{\mathbb{R}^3} \bar{\varphi}(\vec{x}) \int\limits_{\mathbb{R}^2} \hat{\alpha}(\vec{s}_\xi - \vec{k})\, \frac{\left[\left(\vec{s}_\xi \times \vec{e}^{\,0}\right) \times \vec{s}_\xi\right]}{\xi}\, e^{i\vec{s}_\xi\cdot\vec{x}}\,\mathrm{d}s'\,\mathrm{d}\vec{x},$$

where (cf. (3.2.5))

$$\hat{\alpha}(\vec{s}_\xi - \vec{k}) := i\Delta \int\limits_{\mathbb{R}^2} \frac{1-e^{-i(\xi-k_z)f(\eta')}}{\xi - k_z}\, e^{-i\eta'\cdot(s'-k')}\,\mathrm{d}\eta'$$

and where the above manipulations are needed to define the integral (see the subsequent formula (3.3.65)). Since the integral w.r.t. s' is a locally bounded integrable function w.r.t. $\vec{x}$ with $z > h$, the distribution $\vec{D}^d(\vec{x})$ can be identified with the locally integrable function

$$\vec{D}^d(\vec{x}) = \frac{i}{8\pi^2} \int\limits_{\mathbb{R}^2} \hat{\alpha}(\vec{s}_\xi - \vec{k})\, \frac{\left[\left(\vec{s}_\xi \times \vec{e}^{\,0}\right) \times \vec{s}_\xi\right]}{\xi}\, e^{i\vec{s}_\xi\cdot\vec{x}}\,\mathrm{d}s'. \tag{3.3.64}$$

More precisely, the last integral is well defined in the sense (cf. (3.3.8)–(3.3.11), (3.3.25), (3.3.28), (3.3.30)–(3.3.32), (3.3.42), (3.3.39) and (3.3.62))

$$\begin{aligned}
\vec{D}^d(\vec{x}) = &-i\,\frac{\Delta}{2} \sum_{n\in\mathbb{N}_0} \sum_{j\in\mathbb{Z}} \int_0^1 \tilde{\lambda}^n_{0,j}\, \frac{(-i\zeta)^n}{n!}\,\mathrm{d}\zeta\, \left[\left(\vec{\omega}_j \times \vec{e}^{\,0}\right)\times\vec{\omega}_j\right] \left(\omega^j_z\right)^{n-1} e^{i\vec{\omega}_j\cdot\vec{x}} \\
&- i\,\frac{\Delta}{4\pi} \sum_{n\in\mathbb{N}_0} \sum_{j\in\mathbb{Z}} \int_0^1 \tilde{\lambda}^n_{1,j}\, \frac{(-i\zeta)^n}{n!}\,\mathrm{d}\zeta \int\limits_{\mathbb{R}^2} \Bigg\{ \xi^{n-1}\, \frac{e^{-\left|s'-(k'+\tilde{\omega}'_{1,j})\right|}}{\left|s'-(k'+\tilde{\omega}'_{1,j})\right|} \\
&\qquad\qquad \left[\left(\vec{s}_\xi \times \vec{e}^{\,0}\right)\times\vec{s}_\xi\right] e^{i\vec{s}_\xi\cdot\vec{x}} \Bigg\}\,\mathrm{d}s' \\
&- i\,\frac{\Delta}{4\pi} \sum_{n\in\mathbb{N}_0} \sum_{j\in\mathbb{Z}} \int_0^1 \tilde{\lambda}^n_{2,j}\, \frac{(-i\zeta)^n}{n!}\,\mathrm{d}\zeta \int\limits_{\mathbb{R}^2} \Bigg\{ \xi^{n-1}\, K_0\left(\left|s'-(k'+\tilde{\omega}'_{2,j})\right|\right) \\
&\qquad\qquad \left[\left(\vec{s}_\xi \times \vec{e}^{\,0}\right)\times\vec{s}_\xi\right] e^{i\vec{s}_\xi\cdot\vec{x}} \Bigg\}\,\mathrm{d}s' \\
&- i\,\frac{\Delta}{4\pi} \sum_{n\in\mathbb{N}_0} \sum_{j\in\mathbb{Z}} \int_0^1 \tilde{\lambda}^n_{3,j}\, \frac{(-i\zeta)^n}{n!}\,\mathrm{d}\zeta \int\limits_{\mathbb{R}^2} \Bigg\{ \xi^{n-1}\, e^{-\left|s'-(k'+\tilde{\omega}'_{3,j})\right|} \\
&\qquad\qquad \left[\left(\vec{s}_\xi \times \vec{e}^{\,0}\right)\times\vec{s}_\xi\right] e^{i\vec{s}_\xi\cdot\vec{x}} \Bigg\}\,\mathrm{d}s' \\
&- i\,\frac{\Delta}{8\pi^2} \sum_{n\in\mathbb{N}_0} \int_0^1 \frac{(-i\zeta)^n}{n!} \int\limits_{\mathbb{R}^2} \Bigg\{ \xi^{n-1} \int\limits_{\mathbb{R}^2} \tilde{g}_n(\eta',\zeta)\, e^{-i\eta'\cdot\left(s'-k'\right)}\,\mathrm{d}\eta' \\
&\qquad\qquad \left[\left(\vec{s}_\xi \times \vec{e}^{\,0}\right)\times\vec{s}_\xi\right] e^{i\vec{s}_\xi\cdot\vec{x}} \Bigg\}\,\mathrm{d}s'\,\mathrm{d}\zeta,
\end{aligned} \tag{3.3.65}$$

with $\vec{\omega}_j = (k' + \tilde{\omega}'_{0,j}, \omega^j_z)^\top$, $\omega^j_z = \sqrt{k^2 - |k'+\tilde{\omega}'_{0,j}|^2}$ and $\tilde{\lambda}^n_{\ell,j}$, $\tilde{\omega}'_{\ell,j}$ and $\tilde{g}_n$ as in Lemma 3.9.

3.4 Reflected electric field

Following the definitions and notation introduced in Section 2.2 the reflected displacement field $\vec{D}_d^r(\vec{x})$, which equals $\vec{D}^d(\vec{x})$ for $z > h$, can be reduced to its underlying electric fields.

$$\vec{D}_d^r(\vec{x}) = \vec{D}^{sc}(\vec{x}) - \vec{D}_{\mathcal{Q}}^{sc}(\vec{x}) = \epsilon_0 \vec{E}^{sc}(\vec{x}) - \epsilon_0 \vec{E}_{\mathcal{Q}}^{sc}(\vec{x}) = \epsilon_0 \vec{E}_d^r(\vec{x}),$$

where $\vec{E}_d^r(\vec{x}) := \vec{E}^{sc}(\vec{x}) - \vec{E}_{\mathcal{Q}}^{sc}(\vec{x})$ for $z > h$. Define

$$\begin{aligned} \vec{D}^r(\vec{x}) &:= \vec{D}^{sc}(\vec{x}) = \vec{D}(\vec{x}) - \vec{D}^0(\vec{x}) & \qquad \vec{E}^r(\vec{x}) &:= \vec{E}^{sc}(\vec{x}) = \vec{E}(\vec{x}) - \vec{E}^0(\vec{x}) \\ \vec{D}_{\mathcal{Q}}^r(\vec{x}) &:= \vec{D}_{\mathcal{Q}}^{sc}(\vec{x}) = \vec{D}_{\mathcal{Q}}(\vec{x}) - \vec{D}^0(\vec{x}) & \qquad \vec{E}_{\mathcal{Q}}^r(\vec{x}) &:= \vec{E}_{\mathcal{Q}}^{sc}(\vec{x}) = \vec{E}_{\mathcal{Q}}(\vec{x}) - \vec{E}^0(\vec{x}) \end{aligned}$$

where $\vec{D}^r(\vec{x}) = \epsilon_0 \vec{E}^r(\vec{x})$, $\vec{D}_{\mathcal{Q}}^r(\vec{x}) = \epsilon_0 \vec{E}_{\mathcal{Q}}^r(\vec{x})$. Hence, when applying this to equation (3.3.65), the reflected electric difference field is represented by $\vec{E}_d^r(\vec{x}) = 1/\epsilon_0 \ \vec{D}^d(\vec{x}) = -\sum_{\ell=0}^4 E_\ell$ (cf. (3.1.4)–(3.1.8)) for all $\vec{x} \in \mathbb{R}^2 \times (h, \infty)$. With this, formula (3.1.2) from Theorem 3.1, $\vec{E}^r(\vec{x}) = \vec{E}_d^r(\vec{x}) + \vec{E}_{\mathcal{Q}}(\vec{x}) = E_{\mathcal{Q}} - \sum_{\ell=0}^4 E_\ell$ for all $\vec{x} \in \mathbb{R}^2 \times (h, \infty)$, where $E_{\mathcal{Q}} = \vec{E}_{\mathcal{Q}}(\vec{x})$, is reached. The explicit formula of $E_{\mathcal{Q}}$ (cf. (3.1.3)), describing the electric field reflected from an ideal interface, is shown in Section A.3 in the appendix (cf. Eqn. (A.3.2)). Apart from this, it only remains to proof the absolute convergence of the infinite sums in E_0 to E_4.

The definition of the algebra norm in (3.3.2) implies that, for any $\zeta \in [0,1]$,

$$\sum_{j\in\mathbb{Z}} \left|\tilde{\lambda}_{\ell,j}^n\right| \le \left\| f^{n+1}\, e^{ik_z \zeta f} \right\|_{\mathcal{A}} \le c\, \|f\|_{\mathcal{A}}^{n+1}, \tag{3.4.1}$$

with a constant $c > 0$ independent of n. Furthermore, for any $\ell = 0, \dots, 3$, the function $\tilde{\lambda}_{\ell,j}^n(\zeta) := \tilde{\lambda}_{\ell,j}^n$ (cf. (3.3.18) and (3.3.19)) is continuous w.r.t. ζ by the algebra property of $\mathcal{A}^{\mathbb{C}}$. The absolute convergence of the sums will be shown separately for E_0, E_ℓ for $\ell = 1,2,3$ and E_4, starting with E_0.

Split E_0 according to (cf. (3.1.4))

$$\begin{aligned} E_0 &= E_0^a + E_0^b, \\ E_0^a &:= i\,\frac{\Delta}{2\epsilon_0} \sum_{n\in\mathbb{N}_0} \sum_{\substack{j\in\mathbb{Z} \\ \left|k' + \tilde{\omega}_{0,j}'\right| < k}} \int_0^1 \tilde{\lambda}_{0,j}^n \frac{(-i\zeta)^n}{n!}\, \mathrm{d}\zeta \ \left[\left(\vec{\omega}_j \times \vec{e}^{\,0}\right) \times \vec{\omega}_j\right] \left(\omega_z^j\right)^{n-1} e^{i\vec{\omega}_j\cdot\vec{x}}, \\ E_0^b &:= E_0 - E_0^a. \end{aligned}$$

Note that condition (3.3.41) implies that a constant $\epsilon > 0$ exists such that

$$\sup_{j\in\mathbb{Z}} \left|k^2 - \left|k' + \tilde{\omega}_{0,j}'\right|\right| \ge \epsilon$$

and thus $|\omega_z^j| > \epsilon$. Moreover, since $\tilde{\omega}_{0,j}'$ is independent of n, the same holds for ϵ.

First consider E_0^a, i.e. where $\omega_z^j \in \mathbb{R}$. Thus

$$|E_0^a| \le c \sum_{n\in\mathbb{N}_0} \sum_{\substack{j\in\mathbb{Z} \\ \left|k' + \tilde{\omega}_{0,j}'\right| < k}} \frac{1}{n!} \int_0^1 \left|\tilde{\lambda}_{0,j}^n(\zeta)\right| \mathrm{d}\zeta\, \frac{k^{n+2}}{\epsilon} \le c \sum_{n\in\mathbb{N}_0} \sum_{\substack{j\in\mathbb{Z} \\ \left|k' + \tilde{\omega}_{0,j}'\right| < k}} \frac{1}{n!} \int_0^1 \left|\tilde{\lambda}_{0,j}^n(\zeta_0)\right| \mathrm{d}\zeta\, \frac{k^{n+2}}{\epsilon},$$

where $\zeta_0 := \operatorname{argmax}_{\zeta\in[0,1]} |\tilde{\lambda}_{0,j}^n(\zeta)|$. However, (3.4.1) implies

$$|E_0^a| \le \frac{c}{\epsilon} \sum_{n\in\mathbb{N}_0} \frac{1}{n!} \sum_{j\in\mathbb{Z}} \left|\tilde{\lambda}_{0,j}^n(\zeta_0)\right| k^{n+2} \le \frac{ck^2}{\epsilon} \|f\|_{\mathcal{A}} \sum_{n\in\mathbb{N}_0} \frac{k^n\ \|f\|_{\mathcal{A}}^n}{n!} = \frac{ck^2}{\epsilon} \|f\|_{\mathcal{A}} e^{k\|f\|_{\mathcal{A}}} < \infty.$$

For E_0^b define a z_0 with $z_0 > \|f\|_{\mathcal{A}}$, and assume $z > z_0$. It follows that

$$\begin{aligned}\left|E_0^b\right| &\le c \sum_{n\in\mathbb{N}_0} \frac{1}{n!} \sum_{\substack{j\in\mathbb{Z}\\ \left|k'+\tilde{\omega}'_{0,j}\right|\ge k}} \int_0^1 \left|\tilde{\lambda}_{0,j}^n\right| \mathrm{d}\zeta\, k^2 \frac{|\omega_z^j|^n}{|\omega_z^j|} e^{-\left|\omega_z^j\right| z_0} \\ &\le \frac{c}{\epsilon} \sum_{n\in\mathbb{N}_0} \frac{1}{n!} \sum_{\substack{j\in\mathbb{Z}\\ \left|k'+\tilde{\omega}'_{0,j}\right|\ge k}} \int_0^1 \left|\tilde{\lambda}_{0,j}^n\right| \mathrm{d}\zeta\, k^2 \left|\omega_z^j\right|^n e^{-\left|\omega_z^j\right| z_0}.\end{aligned}$$

To find the supremum of $\left|\omega_z^j\right|^n e^{-\left|\omega_z^j\right| z_0}$ w.r.t. $\left|\omega_z^j\right|$, consider the continuous function $h(t) := t^n\, e^{-t\, z_0}$, which is non-negative for $t \ge 0$. Moreover, the function is zero at $t = 0$ and for $t \to \infty$. Thus, since the derivative

$$h'(t) = n\, t^{n-1}\, e^{-t\, z_0} - z_0\, t^n\, e^{-t\, z_0} = (n - z_0\, t)\, t^{n-1}\, e^{-t\, z_0}$$

has only one zero, apart from $t = 0$, at $t = n/z_0$, this is the argument of the global maximum of h for $t \in [0, \infty)$. Consequently, $\sup_{t\ge 0} h(t) = (n/z_0)^n e^{-n} = (n/e)^n z_0^{-n}$ and with Stirling's formula (cf. [3, p. 75])

$$\sup_{t\ge 0} \left[t^n\, e^{-t\, z_0}\right] \overset{n\to\infty}{\sim} \frac{n!}{\sqrt{2\pi\, n}}\, z_0^{-n}. \tag{3.4.2}$$

Using (3.4.1) once more, it follows that

$$\left|E_0^b\right| \le \frac{c}{\epsilon} \sum_{n\in\mathbb{N}_0} \frac{k^2}{\sqrt{2\pi\, n}} \sum_{\substack{j\in\mathbb{Z}\\ \left|k'+\tilde{\omega}'_{0,j}\right|\ge k}} \int_0^1 \left|\tilde{\lambda}_{0,j}^n\right| \mathrm{d}\zeta\, z_0^{-n} \le \frac{c}{\epsilon} \sum_{n\in\mathbb{N}_0} \frac{k^2\, \|f\|_{\mathcal{A}}}{\sqrt{2\pi\, n}} \left(\frac{\|f\|_{\mathcal{A}}}{z_0}\right)^n < \infty$$

for $z_0 > \|f\|_{\mathcal{A}}$. Hence, E_0^b and therewith E_0 is absolutely and uniformly convergent for any $z \ge z_0$.

Similarly, this can be shown for E_ℓ, with $\ell = 1, 2, 3$ (cf. (3.1.5) to (3.1.7)). This time the domain of integration of the integral w.r.t. s' is split into the two parts $B_2(\sqrt{2}k)$ and $\mathbb{R}^2 \setminus B_2(\sqrt{2}k)$. For the first part, there holds $|\xi| \le k$ and

$$\begin{aligned}&\sum_{n\in\mathbb{N}_0} \sum_{j\in\mathbb{Z}} \left| \int_0^1 \tilde{\lambda}_{\ell,j}^n \frac{(-i\zeta)^n}{n!} \mathrm{d}\zeta \int\limits_{B_2(\sqrt{2}k)} \left\{ \xi^{n-1}\, r_{\ell,j}(s')\, \left[\left(\vec{s}_\xi \times \vec{e}^{\,0}\right) \times \vec{s}_\xi\right]\, e^{i\vec{s}_\xi\cdot\vec{x}} \right\} \mathrm{d}s' \right| \\ &\qquad \le c \sum_{n\in\mathbb{N}_0} \frac{1}{n!} \sum_{j\in\mathbb{Z}} \int_0^1 \left|\tilde{\lambda}_{\ell,j}^n\right| \mathrm{d}\zeta\, k^{n+2} \int\limits_{B_2(\sqrt{2}k)} \frac{|r_{\ell,j}(s')|}{|\xi|} \mathrm{d}s',\end{aligned} \tag{3.4.3}$$

where $\|\vec{s}_\xi\| = k$ for $s' \in B_2(\sqrt{2}k)$ and where

$$r_{1,j}(s') := \frac{e^{-\left|s'-(k'+\tilde{\omega}'_{1,j})\right|}}{\left|s' - (k' + \tilde{\omega}'_{1,j})\right|}, \qquad r_{2,j}(s') := K_0\left(\left|s' - (k' + \tilde{\omega}'_{2,j})\right|\right), \qquad r_{3,j}(s') := e^{-\left|s'-(k'+\tilde{\omega}'_{3,j})\right|}.$$

Since $K_0\left(\left|s' - (k' + \tilde{\omega}'_{2,j})\right|\right)$ has a logarithmic singularity at $s' = k' + \tilde{\omega}'_{2,j}$ and is otherwise continuous, it is easily shown that $|r_{\ell,j}(s')| \le c/|s' - (k' + \tilde{\omega}'_{\ell,j})|$ for $\ell = 1, 2, 3$, where c is independent of j. Thus, since $c/|s' - (k' + \tilde{\omega}'_{\ell,j})|$ is a weakly singular function w.r.t. s', where j only determines the position of the singularity, Lemma 3.11 shows that there exists another $c > 0$ independent of j such that $\int_{B_2(\sqrt{2}k)} |r_{\ell,j}(s')|/|\xi|\, \mathrm{d}s' \le c < \infty$. Using this and (3.4.1), it follows that (cf. (3.4.3))

$$\begin{aligned}&\sum_{n\in\mathbb{N}_0} \sum_{j\in\mathbb{Z}} \left| \int_0^1 \tilde{\lambda}_{1,j}^n \frac{(-i\zeta)^n}{n!} \mathrm{d}\zeta \int\limits_{B_2(\sqrt{2}k)} \left\{ \xi^{n-1}\, r_{\ell,j}(s')\, \left[\left(\vec{s}_\xi \times \vec{e}^{\,0}\right) \times \vec{s}_\xi\right]\, e^{i\vec{s}_\xi\cdot\vec{x}} \right\} \mathrm{d}s' \right| \\ &\qquad \le ck^2\, \|f\|_{\mathcal{A}} \sum_{n\in\mathbb{N}_0} \frac{k^n\, \|f\|_{\mathcal{A}}^n}{n!} = ck\, \|f\|_{\mathcal{A}} e^{k\, \|f\|_{\mathcal{A}}} < \infty.\end{aligned}$$

On the other hand, for the integral in E_ℓ over the complementary domain $\mathbb{R}^2 \setminus B_2(\sqrt{2}k)$, the same z_0 as before is used to show that for $|\xi| \geq k$ with $s' \in \mathbb{R}^2 \setminus B_2(\sqrt{2}k)$, (cf. (3.4.2) with $t = |\xi|$)

$$\begin{aligned}
&\sum_{n\in\mathbb{N}_0}\sum_{j\in\mathbb{Z}}\left|\int_0^1 \tilde{\lambda}_{1,j}^n \frac{(-i\zeta)^n}{n!}\,\mathrm{d}\zeta \int\limits_{\mathbb{R}^2\setminus B_2(\sqrt{2}k)} \left\{\xi^{n-1}\, r_{\ell,j}(s')\,\left[\left(\vec{s}_\xi \times \vec{e}^{\,0}\right)\times \vec{s}_\xi\right]\, e^{i\vec{s}_\xi\cdot\vec{x}}\right\}\mathrm{d}s'\right| \\
&\qquad \leq c \sum_{n\in\mathbb{N}_0}\frac{1}{n!}\sum_{j\in\mathbb{Z}}\int_0^1\left|\tilde{\lambda}_{1,j}^n\right|\,\mathrm{d}\zeta\, k^2 \int\limits_{\mathbb{R}^2\setminus B_2(\sqrt{2}k)} \frac{|\xi|^n}{|\xi|}\, e^{-|\xi|\,z_0}\, |r_{\ell,j}(s')|\,\mathrm{d}s' \\
&\qquad \leq c \sum_{n\in\mathbb{N}_0}\frac{1}{n!}\sum_{j\in\mathbb{Z}}\int_0^1\left|\tilde{\lambda}_{1,j}^n\right|\,\mathrm{d}\zeta\, k \int\limits_{\mathbb{R}^2\setminus B_2(\sqrt{2}k)} |\xi|^n\, e^{-|\xi|\,z_0}\, |r_{\ell,j}(s')|\,\mathrm{d}s' \\
&\qquad \leq c \sum_{n\in\mathbb{N}_0}\frac{1}{\sqrt{n}\,z_0^n}\sum_{j\in\mathbb{Z}}\int_0^1\left|\tilde{\lambda}_{1,j}^n\right|\,\mathrm{d}\zeta \int\limits_{\mathbb{R}^2\setminus B_2(\sqrt{2}k)} |r_{\ell,j}(s')|\,\mathrm{d}s'.
\end{aligned}$$

In addition to the weak singularity it is now also used that $r_{\ell,j}(s')$ decays exponentially as $|s'|$ tends to infinity (cf. [1, Eqn. 9.7.2, p. 122]). Again, a constant c independent of j can be found such that $\int_{\mathbb{R}^2\setminus B_2(k)} |r_{\ell,j}(s')|\,\mathrm{d}s' < c$. Thus (3.4.1) shows that

$$\begin{aligned}
&\sum_{n\in\mathbb{N}_0}\sum_{j\in\mathbb{Z}}\left|\int_0^1 \tilde{\lambda}_{1,j}^n \frac{(-i\zeta)^n}{n!}\,\mathrm{d}\zeta \int\limits_{\mathbb{R}^2\setminus B_2(\sqrt{2}k)} \left\{\xi^{n-1}\, r_{\ell,j}(s')\,\left[\left(\vec{s}_\xi \times \vec{e}^{\,0}\right)\times \vec{s}_\xi\right]\, e^{i\vec{s}_\xi\cdot\vec{x}}\right\}\mathrm{d}s'\right| \\
&\qquad \leq c \sum_{n\in\mathbb{N}_0}\frac{k\,\|f\|_{\mathcal{A}}}{\sqrt{2\pi\,n}}\left(\frac{\|f\|_{\mathcal{A}}}{z_0}\right)^n < \infty
\end{aligned}$$

for $z_0 > \|f\|_{\mathcal{A}}$. It follows that E_ℓ is absolutely and uniformly convergent for any $\ell = 1, 2, 3$ and $z > \|f\|_{\mathcal{A}}$.

Now only E_4 (cf. (3.1.8)) remains. Note that the function $\tilde{g}_n(\eta', \zeta)$ (cf. (3.3.20)) also depends continuously on ζ. Similar to (3.4.1) it can also be shown that (cf. (3.3.2))

$$\int_{\mathbb{R}^2} |\tilde{g}_n(\eta',\zeta)|\,\mathrm{d}\eta' = \int_{\mathbb{R}^2}\frac{\left(1+|\eta'|^2\right)^2}{\left(1+|\eta'|^2\right)^2}\,|\tilde{g}_n(\eta',\zeta)|\,\mathrm{d}\eta' \leq \|\tilde{g}_n(\eta',\zeta)\|_{4,\infty}\int_{\mathbb{R}^2}\frac{1}{\left(1+|\eta'|^2\right)^2} \tag{3.4.4}$$

$$\leq c\,\|\tilde{g}_n(\eta',\zeta)\|_{4,\infty} \leq c\,\left\|f^{n+1}\,e^{ik_z\zeta f}\right\|_{\mathcal{A}} \leq c\,\|f\|_{\mathcal{A}}^{n+1} \tag{3.4.5}$$

for any fixed $\zeta \in [0, 1]$. As for E_1 to E_3 the domain of integration of the integral w.r.t. s' in E_4 is split into the two parts $B_2(\sqrt{2}k)$ and $\mathbb{R}^2 \setminus B_2(\sqrt{2}k)$. The first part can be estimated as

$$\begin{aligned}
&\sum_{n\in\mathbb{N}_0}\left|\int_0^1 \frac{(-i\zeta)^n}{n!}\int\limits_{B_2(\sqrt{2}k)}\left\{\xi^{n-1}\int_{\mathbb{R}^2}\tilde{g}_n(\eta',\zeta)\,e^{-i\eta'\cdot(s'-k')}\,\mathrm{d}\eta'\,\left[\left(\vec{s}_\xi\times\vec{e}^{\,0}\right)\times\vec{s}_\xi\right]\,e^{i\vec{s}_\xi\cdot\vec{x}}\right\}\mathrm{d}s'\,\mathrm{d}\zeta\right| \\
&\qquad \leq \sum_{n\in\mathbb{N}_0}\frac{1}{n!}\int_0^1\int_{\mathbb{R}^2}|\tilde{g}_n(\eta',\zeta)|\,\mathrm{d}\eta'\,\mathrm{d}\zeta\,k^{n+2}\int\limits_{B_2(\sqrt{2}k)}\frac{1}{|\xi|}\,\mathrm{d}s',
\end{aligned}$$

where the integral w.r.t. s' is finite. Since $\tilde{g}_n(\eta', \zeta)$ is a continuous function w.r.t. ζ, the integral $\int_{\mathbb{R}^2} |\tilde{g}_n(\eta', \zeta)|\,\mathrm{d}\eta'$ is also a continuous function w.r.t. ζ. Hence, the first mean value theorem for integration can be used to show that there exists a $\zeta_0 \in [0, 1]$ such that (cf. (3.4.5))

$$\int_0^1\int_{\mathbb{R}^2}|\tilde{g}_n(\eta',\zeta)|\,\mathrm{d}\eta'\,\mathrm{d}\zeta = \int_{\mathbb{R}^2}|\tilde{g}_n(\eta',\zeta_0)|\,\mathrm{d}\eta' \leq c\,\|f\|_{\mathcal{A}}^{n+1}.$$

Hence

$$\sum_{n\in\mathbb{N}_0}\left|\int_0^1 \frac{(-i\zeta)^n}{n!}\int_{B_2(k)}\left\{\xi^{n-1}\int_{\mathbb{R}^2}\tilde{g}_n(\eta',\zeta)\,e^{-i\eta'\cdot(s'-k')}\,\mathrm{d}\eta'\ \left[\left(\vec{s}_\xi\times\vec{e}^{\,0}\right)\times\vec{s}_\xi\right]\,e^{i\vec{s}_\xi\cdot\vec{x}}\right\}\mathrm{d}s'\,\mathrm{d}\zeta\right|$$
$$\leq ck^2\,\|f\|_{\mathcal{A}}\sum_{n\in\mathbb{N}_0}\frac{k^n\,\|f\|_{\mathcal{A}}^n}{n!}=ck^2\,\|f\|_{\mathcal{A}}e^{k\,\|f\|_{\mathcal{A}}}<\infty.$$

For the second part of the integral, z_0 is this time chosen such that $z_0>2\,\|f\|_{\mathcal{A}}$. Assume $z\geq z_0$ and note that $|\xi|\geq k$ for $s'\in\mathbb{R}^2\setminus B_2(\sqrt{2}k)$. Thus (cf. (3.4.2))

$$\sum_{n\in\mathbb{N}_0}\left|\int_0^1 \frac{(-i\zeta)^n}{n!}\int_{\mathbb{R}^2\setminus B_2(\sqrt{2}k)}\left\{\xi^{n-1}\int_{\mathbb{R}^2}\tilde{g}_n(\eta',\zeta)\,e^{-i\eta'\cdot(s'-k')}\,\mathrm{d}\eta'\ \left[\left(\vec{s}_\xi\times\vec{e}^{\,0}\right)\times\vec{s}_\xi\right]\,e^{i\vec{s}_\xi\cdot\vec{x}}\right\}\mathrm{d}s'\,\mathrm{d}\zeta\right|$$
$$\leq c\sum_{n\in\mathbb{N}_0}\frac{k^2}{n!}\int_0^1\int_{\mathbb{R}^2}|\tilde{g}_n(\eta',\zeta)|\,\mathrm{d}\eta'\,\mathrm{d}\zeta\int_{\mathbb{R}^2\setminus B_2(\sqrt{2}k)}\frac{|\xi|^n}{|\xi|}\,e^{-|\xi|\,z_0}\,\mathrm{d}s'$$
$$\leq c\sum_{n\in\mathbb{N}_0}\frac{k}{n!}\int_0^1\int_{\mathbb{R}^2}|\tilde{g}_n(\eta',\zeta)|\,\mathrm{d}\eta'\,\mathrm{d}\zeta\int_{\mathbb{R}^2\setminus B_2(\sqrt{2}k)}|\xi|^n\,e^{-|\xi|\,\frac{z_0}{2}}\,e^{-|\xi|\,\frac{z_0}{2}}\,\mathrm{d}s'$$
$$\leq c\sum_{n\in\mathbb{N}_0}\frac{1}{\sqrt{n}\,\left(\frac{z_0}{2}\right)^n}\int_0^1\int_{\mathbb{R}^2}|\tilde{g}_n(\eta',\zeta)|\,\mathrm{d}\eta'\,\mathrm{d}\zeta\int_{\mathbb{R}^2\setminus B_2(\sqrt{2}k)}e^{-|\xi|\,\frac{z_0}{2}}\,\mathrm{d}s'.$$

Using the first mean value theorem for integration w.r.t. ζ and (3.4.5) for a final time then leads to

$$\sum_{n\in\mathbb{N}_0}\left|\int_0^1 \frac{(-i\zeta)^n}{n!}\int_{\mathbb{R}^2\setminus B_2(k)}\left\{\xi^{n-1}\int_{\mathbb{R}^2}\tilde{g}_n(\eta',\zeta)\,e^{-i\eta'\cdot(s'-k')}\,\mathrm{d}\eta'\ \left[\left(\vec{s}_\xi\times\vec{e}^{\,0}\right)\times\vec{s}_\xi\right]\,e^{i\vec{s}_\xi\cdot\vec{x}}\right\}\mathrm{d}s'\,\mathrm{d}\zeta\right|$$
$$\leq c\sum_{n\in\mathbb{N}_0}\frac{k\,\|f\|_{\mathcal{A}}}{\sqrt{2\pi\,n}}\left(\frac{2\,\|f\|_{\mathcal{A}}}{z_0}\right)^n<\infty$$

for $z_0>2\,\|f\|_{\mathcal{A}}$. Consequently, E_4 is also absolutely and uniformly convergent for any $z\geq z_0$. This concludes the proof of Theorem 3.1.

Chapter 4

The reflected far field

4.1 The far-field formula

The primary goal of this chapter is to determine the far-field pattern for the solution of the reflected electric field in the case of interface functions from $\mathcal{A} \cap L^\infty_Q$. In the context of this thesis, the reflected far field is understood as the reflected field many wavelengths above the highest points of the 'rough' surface. This far-field pattern can be described by the asymptotic behaviour of (3.1.2) for $\|\vec{x}\| \to \infty$ with $\vec{x} = \|\vec{x}\|\,\vec{m}$ and a fixed direction $\vec{m} = (m_x, m_y, m_z)^\top$ s.t. $m_z > 0$. For this thesis, only the terms of the asymptotic expansion that decay at most with the order $1/\|\vec{x}\|$ are considered for the far-field pattern. All other terms will be neglected. There holds,

Theorem 4.1 (The reflected far field). *Assume the interface is the graph of a function $f \in \mathcal{A} \cap L^\infty_Q$ as described in Remark 3.4 that satisfies condition (3.3.41). Moreover, suppose this interface is illuminated by an incoming plane wave as described in Subsection 2.1. Then the far-field asymptotics of the reflected polarised electric field for $z > \max\{2\|f\|_{\mathcal{A}}, 2\|f\|_\infty\}$, $\vec{x} =: R\vec{m}$ and $R := \|\vec{x}\|$ in the sense of the Born approximation is*

$$
\begin{aligned}
\vec{E}^r(R\vec{m}) = {} & r(\vec{k}, \vec{e}^{\,0})\, \frac{e^{ikR\vec{n}_0^r \cdot \vec{m}}}{|k'|^2} \\
& - i\,\frac{\Delta}{2\epsilon_0} \sum_{n\in\mathbb{N}_0} \sum_{\substack{j\in\mathbb{Z} \\ |k'+\tilde{\omega}'_{0,j}|<k}} \int_0^1 \tilde{\lambda}^n_{0,j}(\zeta) \frac{(-i\zeta)^n}{n!}\,\mathrm{d}\zeta \;\left[\left(\vec{\omega}_j \times \vec{e}^{\,0}\right) \times \vec{\omega}_j\right] \left(\omega^j_z\right)^{n-1} e^{iR\vec{\omega}_j\cdot\vec{m}} \\
& - \frac{\Delta\, k^3}{2\epsilon_0}\, \mathcal{H}(\vec{m}) \left[\left(\vec{m} \times \vec{e}^{\,0}\right) \times \vec{m}\right] \frac{e^{ikR}}{kR} \\
& - i\,\frac{\Delta}{2\epsilon_0} \sum_{\substack{j\in\mathbb{Z} \\ |k'+\tilde{\omega}'_{1,j}|=k}} \int_0^1 \tilde{\lambda}^0_{1,j}(\zeta)\,\mathrm{d}\zeta \left[\left((k'+\tilde{\omega}'_{1,j}, 0)^\top \times \vec{e}^{\,0}\right) \times (k'+\tilde{\omega}'_{1,j}, 0)^\top\right] \frac{e^{iR(k'+\tilde{\omega}'_{1,j})\cdot m'}}{kRm_z} \\
& - \frac{\Delta\, k^2}{4\pi\epsilon_0}\, \mathcal{H}_1(\vec{m}) \left[\left(\vec{m} \times \vec{e}^{\,0}\right) \times \vec{m}\right] \left(\frac{1}{kR} + \sqrt{i\pi}\,\frac{e^{ikR}}{\sqrt{kR}}\right) \\
& - \frac{\Delta\, k^3}{4\epsilon_0}\, \mathcal{H}_2(\vec{m}) \left[\left(\vec{m} \times \vec{e}^{\,0}\right) \times \vec{m}\right] \frac{\log R}{kR}\, e^{ikR} + o\left(\frac{1}{R}\right),
\end{aligned}
\tag{4.1.1}
$$

where $\vec{n}_0^r := (n^0_x, n^0_y, -n^0_z)^\top$ (cf. def. of $\vec{n}^{\,0}$ in Sect. 2.1), $\vec{\omega}_j = (k' + \tilde{\omega}'_{0,j}, \omega^j_z)^\top$, $\omega^j_z = \sqrt{k^2 - |k' + \tilde{\omega}'_{0,j}|^2}$, $r(\vec{k}, \vec{e}^{\,0})$ is defined by Equation (3.1.9) in Theorem 3.1,

$$
\mathcal{H}(\vec{m}) := \sum_{n\in\mathbb{N}_0} \sum_{j\in\mathbb{Z}} \sum_{\ell=1}^{4} \int_0^1 \tilde{\lambda}^n_{\ell,j}(\zeta)\, \frac{(-ikm_z\,\zeta)^n}{n!}\, \tilde{h}_{\ell,j,n}(\vec{m}, \zeta)\,\mathrm{d}\zeta,
$$

$$\mathcal{H}_1(\vec{m}) := \sqrt{2}\,\tilde{F}(\pi \setminus \alpha) \sum_{n\in\mathbb{N}_0} \sum_{\substack{j\in\mathbb{Z}\\ \tilde{\omega}'_{1,j}=km'-k'}} \int_0^1 \tilde{\lambda}^n_{1,j}(\zeta)\,\frac{(-ikm_z\,\zeta)^n}{n!}\,\mathrm{d}\zeta,$$

$$\mathcal{H}_2(\vec{m}) := \sum_{n\in\mathbb{N}_0} \sum_{\substack{j\in\mathbb{Z}\\ \tilde{\omega}'_{2,j}=km'-k'}} \int_0^1 \tilde{\lambda}^n_{2,j}(\zeta)\,\frac{(-ikm_z\,\zeta)^n}{n!}\,\mathrm{d}\zeta,$$

$\tilde{\lambda}^n_{\ell,j}$, $\tilde{\omega}_{\ell,j}$ and $\tilde{g}_n$ defined as in Lemma 3.9, $\tilde{F}$ denotes the elliptic integral of the first kind (cf. [1, Eqn. 17.2.6, p. 234]) and

$$\tilde{h}_{\ell,j,n}(\vec{m},\zeta) := \begin{cases} \frac{e^{-\left|km'-(k'+\tilde{\omega}'_{1,j})\right|}}{\left|km'-(k'+\tilde{\omega}'_{1,j})\right|} & \text{if } \ell=1 \text{ and } m' \neq \frac{k'+\tilde{\omega}'_{1,j}}{k} \\ -1 & \text{if } \ell=1 \text{ and } m' = \frac{k'+\tilde{\omega}'_{1,j}}{k} \\ K_0\left(\left|km'-(k'+\tilde{\omega}'_{2,j})\right|\right) & \text{if } \ell=2 \text{ and } m' \neq \frac{k'+\tilde{\omega}'_{2,j}}{k} \\ -\frac{1}{2}\left[\tilde{\gamma}+\log\left(\frac{k}{8}\,(1+m_z)^2\right)-i\frac{\pi}{2}\right] & \text{if } \ell=2 \text{ and } m' = \frac{k'+\tilde{\omega}'_{2,j}}{k} \\ e^{-\left|km'-(k'+\tilde{\omega}'_{3,j})\right|} & \text{if } \ell=3 \\ \frac{1}{2\pi}\int_{\mathbb{R}^2} \tilde{g}_n(\eta',\zeta)\,e^{-i\eta'\cdot(km'-k')}\,\mathrm{d}\eta' & \text{if } \ell=4 \end{cases}. \tag{4.1.2}$$

Remark 4.2 (Appearance of far-field terms)**.**

i) *The sum of plane waves in the second line of (4.1.1) is the far field corresponding to the near-field term E_0 (cf. (3.1.4)) in Equation (3.1.2). Similarly, the index $\ell = 1,\ldots,4$ of $\tilde{h}_{\ell,j,n}$ corresponds to the near-field terms E_1 to E_4 (cf. (3.1.5) to (3.1.8)) in (3.1.2). Moreover, the fourth line of (4.1.1) as well as the following line containing the function $\mathcal{H}_1$ are additional far-field terms corresponding to E_1, while the line containing $\mathcal{H}_2$ is an additional far-field term for E_2.*

ii) *In the case of a purely almost periodic interface function, i.e. $g(\eta') \equiv 0$ and $\lambda_{\ell,j} = 0$ for all $\ell = 1,2,3$ and $j \in \mathbb{Z}$, only the plane wave terms in the first two lines of Equation (4.1.1) remain. This can be seen by considering the definitions (3.3.19) and (3.3.20) of $\tilde{g}_n$ and $\tilde{\lambda}^n_{\ell,j}$ for all $\ell = 1,\ldots,3$ and $j \in \mathbb{Z}$ in Lemma 3.9 or, more easily, by examining equation (3.3.22) in the proof of this lemma.*

   The same terms of (4.1.1) will also remain, if the interface is further simplified to be periodic or bi-periodic. This case is examined in the numerical example of Chapter 6. This chapter also discusses how the calculation of the amplitude factors $\tilde{\lambda}^n_{0,j}$ may be simplified in these cases. Moreover, the sum w.r.t. j in the second line of (4.1.1) will reduce to only finitely many plane wave terms.

iii) *In the case of an interface function with the lowest decay order towards infinity, e.g. $f(\eta') := \cos(\omega'\cdot\eta')/\sqrt{1+|\eta'|^2}$ or equivalently $g(\eta') \equiv 0$, $\lambda_{1,-1} = \lambda_{1,1} = 1/2$, $-\omega'_{1,-1} = \omega'_{1,1} = \omega'$ and all other $\lambda_{\ell,j}$ are equal to zero, all terms of Equation (4.1.1), except for the plane waves in the second line, will be non-zero.*

   Increasing the decay further by using an interface function with compact support, all terms except the first line of (4.1.1) and the summand with $\ell = 4$ in $\mathcal{H}$ will be zero. This shows that a locally bounded perturbation of a planar interface results in a reflected far field, described as the superposition of one plane wave, resulting from the scattering at an ideal plane, and the usual radially decaying wave resulting from scattering at a bounded obstacle.

iv) *Apart from the usual plane wave and radial decay terms, i.e. terms with $e^{iR\vec{\omega}_j\cdot\vec{m}}$ or e^{ikR}/R, Equation (4.1.1) also contains some terms with more unusual decay orders. However, these come only into play in very specific instances. For example, consider the function $\tilde{h}_{1,j,n}(\vec{m},\zeta)$ (cf. first two lines of (4.1.2)) contained in the definition of $\mathcal{H}(\vec{m})$, which is the amplitude function of the radial decay term e^{ikR}/R. The function $\tilde{h}_{1,j,n}$ has to be defined piecewise to avoid the possible singularity at $km' = k' + \tilde{\omega}'_{1,j}$. When proving Theorem 4.1, this means that in this situation the* *far-field asymptotics have to be derived separately. Consequently, in this case, and only in this case, the new decay order terms $1/R$ and $e^{ikR}/\sqrt{R}$ come into play. Or in other words, the function $\mathcal{H}_1$ is zero in all other cases. Examining the singularity point $km' = k' + \tilde{\omega}'_{1,j}$, where $\tilde{\omega}'_{1,j}$ is defined by Lemma 3.9, it is apparent that this situation only occurs for very specific combinations of wave vectors $\vec{k}$ with $k = \|\vec{k}\|$ and spatial frequencies $\omega'_{\ell,j}$ of the interface. Even then, the singularity, which is to be avoided, only manifests in one reflection direction $\vec{m} = (m', \sqrt{1-|m'|^2})^\top$ with $m' = (k' + \tilde{\omega}'_{1,j})/k$. Similarly, $\mathcal{H}_2$ corresponds to the possible singularity in $\tilde{h}_{2,j,n}$.*

Similar to Chapter 3 and Theorem 3.1, this chapter is mainly dedicated to proving Theorem 4.1. Additionally, the last two sections contain remarks comparing the here presented far-field solution with the results by Stearns [36].

In the following two sections the main terms of asymptotic behaviour of (3.1.2) will be derived. For the plane waves in E_Q and (3.1.4) the asymptotic expansion is already the plane wave formula itself. For the remaining terms (3.1.5)–(3.1.8), the basic approach is to transform the integral w.r.t. s' to polar or spherical coordinates, as needed. The resulting integrals are then integrated by parts w.r.t. the radius or the polar angle such that the resulting terms either contribute to the far-field pattern or can be shown, mostly by using the Riemann-Lebesgue lemma (cf. Thm. C.11), to decay faster than $1/\|\vec{x}\|$. Special care is taken for weakly singular integrands (cf. (3.1.5) and (3.1.6)). This is done by introducing a cut-off function with a support in a small neighbourhood around the singularity and thus splitting the integrand into singular and non-singular parts. The resulting integrals are treated separately in Subsections 4.2.2, 4.2.3 and 4.2.4. The idea for determining the asymptotic behaviour of the weakly singular integrals is to further split the integrands step by step. Finally, there remain non-singular integrands and one singular integrand, which can be evaluated explicitly. In Subsection 4.2.4.4 all is put together to obtain the far-field asymptotics formulated in Theorem 4.1. In the last two sections 4.3 and 4.4 these results will be compared with those by Stearns (cf. [36]) for two special cases, i.e. the formula for the reduced energy reflected in specular direction and the scattering at a sinusoidal grating.

4.2 Several parts of the field in correspondence to a partition of the domain of integration

4.2.1 Splitting of the field

To obtain an approximation of the far field, the terms on the right-hand side of (3.1.2) will be treated separately, starting with the second, i.e. (3.1.4). Examining the exponent of

$$e^{i\vec{\omega}_j\cdot\vec{x}} = e^{i(k'+\tilde{\omega}'_{0,j})\cdot x'}\, e^{iz\sqrt{k^2-|k'+\tilde{\omega}'_{0,j}|^2}},$$

it can be deduced that the electric field E_0 is a superposition of plane waves and evanescent modes, which correspond to $|k'+\tilde{\omega}'_{0,j}| < k$ and $|k'+\tilde{\omega}'_{0,j}| > k$, respectively. This is a result of $\sqrt{k^2 - |k' + \tilde{\omega}'_{0,j}|^2}$ being either real or purely imaginary with a non-negative imaginary part. To evaluate the far field, the far-field direction is fixed by a unit vector $\vec{m}$ with $m_z > 0$ and the far-field behaviour at the points $\vec{x} =: R\vec{m}$, where R tends to infinity, is considered. In (3.1.4) all summands, for which $|k' + \tilde{\omega}'_{0,j}|^2 > k^2$, decay exponentially as R tends to infinity and are thus negligible evanescent modes of the electric field. Only the remaining terms, as well as E_Q (cf. (3.1.3)), contribute as plane wave modes to the far-field.

Next, the remaining terms (3.1.5) to (3.1.8) are examined. For convenience in the following examinations, define the new normalised variable $\vec{n}^r := \vec{s}_\xi/(s_x^2 + s_y^2 + \xi^2)^{1/2} = \vec{s}_\xi/k = (n_x, n_y, n_z^r)^\top$ with $n_z^r := \sqrt{1 - n'^2}$. It follows that $\mathrm{d}s' = k^2\,\mathrm{d}n'$ and

$$E_\ell = \sum_{n\in\mathbb{N}_0}\sum_{j\in\mathbb{Z}}\int_0^1 \tilde{\lambda}^n_{\ell,j}\,\frac{(-ik\zeta)^n}{n!}\int_{\mathbb{R}^2}\frac{h_{\ell,j}(n')}{n_z^r}\,e^{ik\vec{n}^r\cdot\vec{x}}\,\mathrm{d}n'\,\mathrm{d}\zeta \tag{4.2.1}$$

for $\ell = 1,\dots,4$, where $\tilde{\lambda}^n_{4,j} = 1$ for $j = 0$ and $n \in \mathbb{N}_0$ and $\tilde{\lambda}^n_{4,j} = 0$ for $j \in \mathbb{Z}\setminus\{0\}$ and $n \in \mathbb{N}_0$,

$$h_{1,j}(n') := h_{1,j,n}(n') := i\,\frac{\Delta\, k^3}{4\pi\epsilon_0}\,[n_z^r]^n\,\frac{e^{-\left|kn'-(k'+\tilde{\omega}'_{1,j})\right|}}{\left|kn' - (k'+\tilde{\omega}'_{1,j})\right|}\;\left[\left(\vec{n}^r\times\vec{e}^{\,0}\right)\times\vec{n}^r\right], \tag{4.2.2}$$

$$h_{2,j}(n') := h_{2,j,n}(n') := i\,\frac{\Delta\, k^3}{4\pi\epsilon_0}\,[n_z^r]^n K_0\left(\left|kn' - (k' + \tilde{\omega}'_{2,j})\right|\right)\ \left[\left(\vec{n}^r \times \vec{e}^{\,0}\right) \times \vec{n}^r\right], \tag{4.2.3}$$

$$h_{3,j}(n') := h_{3,j,n}(n') := i\,\frac{\Delta\, k^3}{4\pi\epsilon_0}\,[n_z^r]^n\, e^{-\left|kn' - (k' + \tilde{\omega}'_{1,j})\right|}\ \left[\left(\vec{n}^r \times \vec{e}^{\,0}\right) \times \vec{n}^r\right] \tag{4.2.4}$$

and

$$h_{4,0}(n') := h_{4,0,n}(n') := i\,\frac{\Delta\, k^3}{8\pi^2\epsilon_0}\,[n_z^r]^n \int\limits_{\mathbb{R}^2} \tilde{g}_n(\eta', \zeta)\, e^{-i\eta'\cdot(kn'-k')}\,\mathrm{d}\eta'\ \left[\left(\vec{n}^r \times \vec{e}^{\,0}\right) \times \vec{n}^r\right]. \tag{4.2.5}$$

Examining the exponent of $e^{ik\vec{n}^r\cdot\vec{x}} = e^{ikn'\cdot x'}\, e^{ikz\sqrt{1-n'^2}}$ it can be deduced that this part of the electric field is also a superposition of plane waves and evanescent modes, which correspond to $n'^2 \leq 1$ and $n'^2 > 1$, respectively. Moreover, the functions $h_{1,j}(n')$ and $h_{2,j}(n')$ possess weak singularities at $kn' = k' + \tilde{\omega}'_{1,j}$ and $kn' = k' + \tilde{\omega}'_{2,j}$, respectively. Note that these singularities coincide with the weak singularity $1/n_z^r = 1/\sqrt{1-n'^2}$, if $|k' + \tilde{\omega}'_{1,j}| = k$ or $|k' + \tilde{\omega}'_{2,j}| = k$. In these cases, the integrals are still absolutely integrable (cf. Lemma 3.11) but introduce additional challenges when deriving the far-field asymptotics. These challenges can be overcome by examining the integrals in these cases very carefully and adapting the methods, used in the following for the cases of non-intersecting singularities, appropriately. Since the examinations of the asymptotic behaviour for $|k' + \tilde{\omega}'_{\ell,j}| = k$, for $\ell = 1, \ldots, 4$, are quite extensive but otherwise very similar to those shown in the following, they are presented in the appendix in Section B.

To study the integrals in the case that $|k' + \tilde{\omega}'_{\ell,j}| \neq k$ for $\ell = 1, \ldots, 4$, the domain of integration w.r.t. n' will be separated according to the areas of integration corresponding to plane waves ($|n'| \leq 1$) and evanescent modes ($|n'| \geq 1$) and a small neighbourhood around the singularity point $k' = \tilde{\omega}'_{\ell,j}$, $\ell = 1, \ldots, 4$ (cf. Figure 4.1). Consequently, (cf. (4.2.1))

$$\int\limits_{\mathbb{R}^2} \frac{h_{\ell,j}(n')}{n_z^r}\, e^{ik\vec{n}^r\cdot\vec{x}}\,\mathrm{d}n' = W^1_{\ell,j} + W^2_{\ell,j} + W^3_{\ell,j}, \tag{4.2.6}$$

where

$$W^1_{\ell,j} := \int\limits_{B_2(1)} \left(1 - \chi_\epsilon(kn' - k' - \tilde{\omega}'_{\ell,j})\right) \frac{h_{\ell,j}(n')}{n_z^r}\, e^{ik\vec{n}^r\cdot\vec{x}}\,\mathrm{d}n', \tag{4.2.7}$$

$$W^2_{\ell,j} := \int\limits_{\mathbb{R}^2\setminus B_2(1)} \left(1 - \chi_\epsilon(kn' - k' - \tilde{\omega}'_{\ell,j})\right) \frac{h_{\ell,j}(n')}{n_z^r}\, e^{ik\vec{n}^r\cdot\vec{x}}\,\mathrm{d}n',$$

and

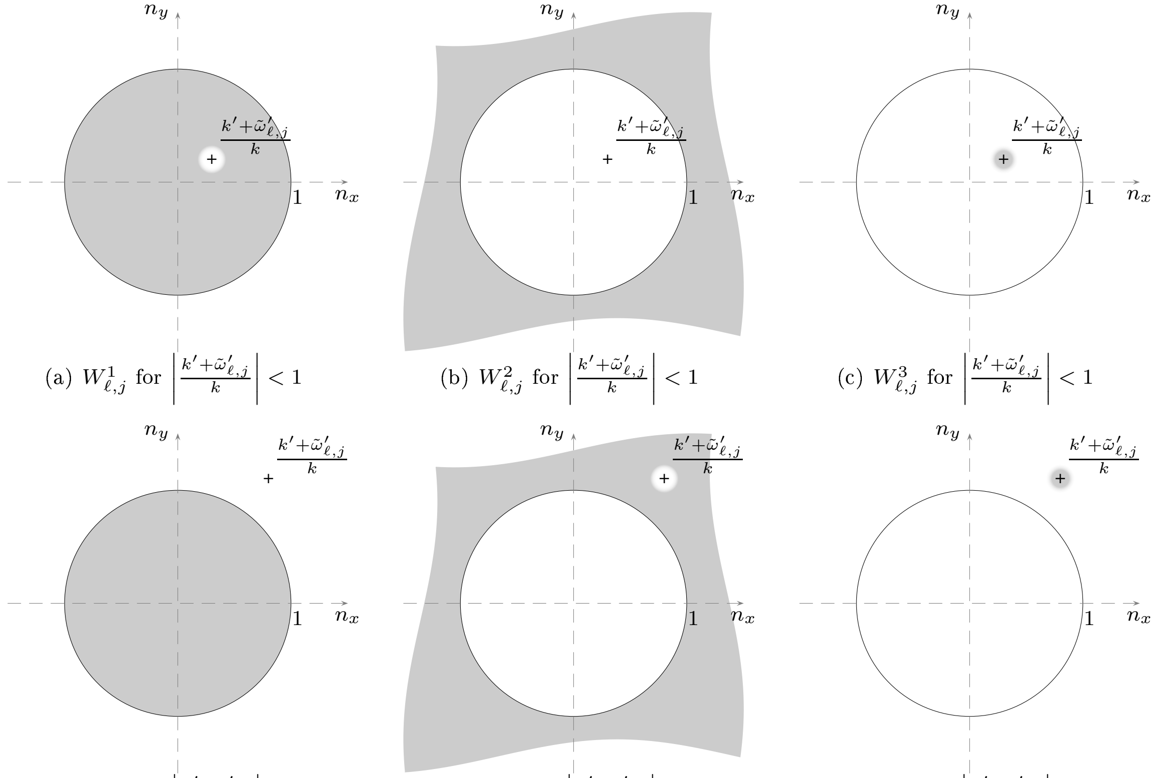
$$W^3_{\ell,j} := \int\limits_{\mathbb{R}^2} \chi_\epsilon(kn' - k' - \tilde{\omega}'_{\ell,j})\, \frac{h_{\ell,j}(n')}{n_z^r}\, e^{ik\vec{n}^r\cdot\vec{x}}\,\mathrm{d}n'. \tag{4.2.8}$$

Here $\chi_\epsilon \in C_0^\infty(\mathbb{R}^2)$, $\mathrm{supp}\chi_\epsilon \subset B_2(\epsilon)$, $\chi_\epsilon(n') = 1$ for $n' \in B_2(\epsilon/2)$ and a small constant $\epsilon > 0$ with $\epsilon < |k - |k' + \tilde{\omega}'_{\ell,j}||$ for $\ell = 1, \ldots, 4$. This choice of ϵ ensures that either $\mathrm{supp}\chi_\epsilon(k\,\cdot\, - k' - \tilde{\omega}'_{\ell,j}) \subset B_2(1)$ or $\mathrm{supp}\chi_\epsilon(k\,\cdot\, - k' - \tilde{\omega}'_{\ell,j}) \subset \mathbb{R}^2 \setminus B_2(1)$. The asymptotics for $R \to \infty$ of these three integrals will be examined separately in the following three subsections.

4.2.2 Smooth integrands of evanescent modes

First consider $W^2_{\ell,j}$ by introducing polar coordinates $n' = \rho n'_0$, with $n'_0 := (\cos\phi, \sin\phi)^\top$. Integration by parts w.r.t. ρ leads to

$$\begin{aligned}
W^2_{\ell,j} &= \int\limits_0^{2\pi}\int\limits_1^{\infty} \left(1 - \chi_\epsilon(k\rho n'_0 - k' - \tilde{\omega}'_{\ell,j})\right) h_{\ell,j}(\rho n'_0)\, e^{ik\rho R n'_0\cdot m'}\, \frac{\rho}{\sqrt{1-\rho^2}}\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho\,\mathrm{d}\phi \\
&= -\frac{1}{ikRm_z}\int\limits_0^{2\pi}\int\limits_1^{\infty} \left(1 - \chi_\epsilon(k\rho n'_0 - k' - \tilde{\omega}'_{\ell,j})\right) h_{\ell,j}(\rho n'_0)\, e^{ik\rho R n'_0\cdot m'}\, \partial_\rho\left[e^{-kRm_z\sqrt{\rho^2-1}}\right]\,\mathrm{d}\rho\,\mathrm{d}\phi
\end{aligned}$$



(a) $W^1_{\ell,j}$ for $\left|\frac{k'+\tilde{\omega}'_{\ell,j}}{k}\right| < 1$ (b) $W^2_{\ell,j}$ for $\left|\frac{k'+\tilde{\omega}'_{\ell,j}}{k}\right| < 1$ (c) $W^3_{\ell,j}$ for $\left|\frac{k'+\tilde{\omega}'_{\ell,j}}{k}\right| < 1$

(d) $W^1_{\ell,j}$ for $\left|\frac{k'+\tilde{\omega}'_{\ell,j}}{k}\right| > 1$ (e) $W^2_{\ell,j}$ for $\left|\frac{k'+\tilde{\omega}'_{\ell,j}}{k}\right| > 1$ (f) $W^3_{\ell,j}$ for $\left|\frac{k'+\tilde{\omega}'_{\ell,j}}{k}\right| > 1$

Figure 4.1: Domains of integration of $W^1_{\ell,j}$, $W^2_{\ell,j}$ and $W^3_{\ell,j}$

$$
\begin{aligned}
&= -\frac{1}{ikRm_z} \int_0^{2\pi} \left[\Big(1 - \chi_\epsilon(k\rho n_0' - k' - \tilde{\omega}'_{\ell,j})\Big)\, h_{\ell,j}(\rho n_0')\, e^{ik\rho R n_0'\cdot m'}\, e^{-kRm_z\sqrt{\rho^2-1}} \right]_{\rho=1}^{\infty} \mathrm{d}\phi \\
&\quad + \frac{1}{ikRm_z} \int_0^{2\pi}\int_1^{\infty} \partial_\rho \left[\Big(1 - \chi_\epsilon(k\rho n_0' - k' - \tilde{\omega}'_{\ell,j})\Big)\, h_{\ell,j}(\rho n_0')\, e^{ik\rho R n_0'\cdot m'} \right] e^{-kRm_z\sqrt{\rho^2-1}}\, \mathrm{d}\rho\, \mathrm{d}\phi \\
&= \frac{1}{ikRm_z}\, W^{2.1}_{\ell,j} + \frac{1}{ikRm_z}\, W^{2.2}_{\ell,j},
\end{aligned}
\tag{4.2.9}
$$

where

$$
W^{2.1}_{\ell,j} := \int_0^{2\pi} \Big(1 - \chi_\epsilon(k n_0' - k' - \tilde{\omega}'_{\ell,j})\Big)\, h_{\ell,j}(n_0')\, e^{ikRn_0'\cdot m'}\, \mathrm{d}\phi \tag{4.2.10}
$$

and

$$
W^{2.2}_{\ell,j} := \int_0^{2\pi}\int_1^{\infty} \partial_\rho \left[\Big(1 - \chi_\epsilon(k\rho n_0' - k' - \tilde{\omega}'_{\ell,j})\Big)\, h_{\ell,j}(\rho n_0')\, e^{ik\rho R n_0'\cdot m'} \right] e^{-kRm_z\sqrt{\rho^2-1}}\, \mathrm{d}\rho\, \mathrm{d}\phi. \tag{4.2.11}
$$

First, consider $W^{2.1}_{\ell,j}$ for $m' \neq (0,0)^\top$ and $\frac{m'}{|m'|} = (\cos\phi', \sin\phi')^\top$. Substitute $u = u(\phi) := kn_0' \cdot m' = k\,|m'|\cos(\phi - \phi')$. Naturally this has to be done separately for the two sets $\phi - \phi' \in [0, \pi)$ and

$\phi - \phi' \in [\pi, 2\pi)$ leading to

$$W_{\ell,j}^{2.1} = \int_{\phi'}^{2\pi+\phi'} \left(1 - \chi_\epsilon(kn_0' - k' - \tilde{\omega}_{\ell,j}')\right) h_{\ell,j}(n_0')\, e^{ikRn_0'\cdot m'}\, \mathrm{d}\phi$$

$$= - \int_{k|m'|}^{-k|m'|} \left(1 - \chi_\epsilon(kn_{0,1}'(u) - k' - \tilde{\omega}_{\ell,j}')\right) h_{\ell,j}\left(n_{0,1}'(u)\right) \frac{1}{\sqrt{k^2 \left|m'\right|^2 - u^2}}\, e^{iRu}\, \mathrm{d}u$$

$$- \int_{-k|m'|}^{k|m'|} \left(1 - \chi_\epsilon(kn_{0,2}'(u) - k' - \tilde{\omega}_{\ell,j}')\right) h_{\ell,j}\left(n_{0,2}'(u)\right) \frac{1}{\sqrt{k^2 \left|m'\right|^2 - u^2}}\, e^{iRu}\, \mathrm{d}u,$$

where

$$n_{0,\iota}'(u) := \begin{pmatrix} \cos\left[(-1)^{\iota+1}\arccos\left(\frac{u}{k|m'|}\right) + \phi' + (\iota-1)2\pi\right] \\ \sin\left[(-1)^{\iota+1}\arccos\left(\frac{u}{k|m'|}\right) + \phi' + (\iota-1)2\pi\right] \end{pmatrix}$$

for $\iota = 1, 2$. Note that the integrand of both integrals is absolutely integrable w.r.t. u on the compact set $[-k\left|m'\right|, k\left|m'\right|]$. Thus, according to the Riemann-Lebesgue lemma, the integral converges to zero as R tends to infinity. Furthermore, this shows for $m' \neq (0,0)^\top$ that the first term on the right-hand side of (4.2.9) tends to zero faster than $1/R$ as R tends to infinity. In the case of $m' = (0,0)^\top$ the term

$$\frac{1}{ikR} \int_0^{2\pi} \left(1 - \chi_\epsilon(kn_0' - k' - \tilde{\omega}_{\ell,j}')\right) h_{\ell,j}(n_0')\, \mathrm{d}\phi \tag{4.2.12}$$

remains. Later on, when examining $W_{\ell,j}^1$, it will be seen that this term also occurs for the integral over $B_2(1)$ but with opposite sign, which shows that the sum of the two (cf. (4.2.6)) is equal to zero.

For $W_{\ell,j}^{2.2}$ (cf. (4.2.11)) examine the derivative

$$\begin{aligned}
&\partial_\rho \left[\left(1 - \chi_\epsilon(k\rho n_0' - k' - \tilde{\omega}_{\ell,j}')\right) h_{\ell,j}(\rho n_0')\, e^{ik\rho R n_0'\cdot m'}\right] \\
&\quad = -kn_0' \cdot \nabla\chi_\epsilon(k\rho n_0' - k' - \tilde{\omega}_{\ell,j}')\, h_{\ell,j}(\rho n_0')\, e^{ik\rho R n_0'\cdot m'} \\
&\qquad + \left(1 - \chi_\epsilon(k\rho n_0' - k' - \tilde{\omega}_{\ell,j}')\right) n_0' \cdot \nabla h_{\ell,j}(\rho n_0')\, e^{ik\rho R n_0'\cdot m'} \\
&\qquad + ikRn_0' \cdot m' \left(1 - \chi_\epsilon(k\rho n_0' - k' - \tilde{\omega}_{\ell,j}')\right) h_{\ell,j}(\rho n_0')\, e^{ik\rho R n_0'\cdot m'}.
\end{aligned} \tag{4.2.13}$$

Since, for some arbitrary $\nu; \in \mathbb{R}^2$,

$$\left|\nabla\left[n_z^r(n')\right]\right| = \left|\nabla\left[\sqrt{1-n'^2}\right]\right| = \left|-\frac{n'}{\sqrt{1-n'^2}}\right| = \frac{\rho}{\sqrt{\rho^2-1}},$$

$$\left|\nabla\left[\frac{1}{|n'-\nu'|}\right]\right| = \left|-\frac{n'-\nu'}{|n'-\nu'|^3}\right| \leq \frac{c}{|n'-\nu'|^2}$$

and

$$\left|\nabla\left[e^{-k|n'-\nu'|}\right]\right| = \left|-k\,\frac{n'-\nu'}{|n'-\nu'|}\, e^{-k|n'-\nu'|}\right| \leq c, \tag{4.2.14}$$

it follows for $\ell = 1$ (cf. (4.2.2)) that

$$\left|n_0' \cdot \nabla h_{\ell,j}(\rho n_0')\right| e^{-\frac{k}{2}Rm_z\sqrt{\rho^2-1}} \leq \frac{c}{\left|k\rho n_0' - k' + \tilde{\omega}_{\ell,j}'\right|} \left(\frac{1}{\left|k\rho n_0' - k' + \tilde{\omega}_{\ell,j}'\right|} + \frac{\rho}{\sqrt{\rho^2-1}} + 1\right),$$

for $\rho \in [1,\infty)$. The same estimate also holds for $\ell = 2,3,4$, since $h_{\ell,j}(\rho n_0')$ has a weaker singularity at the same position in these cases. This shows that

$$\left|\left(1-\chi_\epsilon(k\rho n_0' - k' - \tilde\omega_{\ell,j}')\right) n_0'\cdot\nabla h_{\ell,j}(\rho n_0')\right| e^{-\frac{k}{2}Rm_z\sqrt{\rho^2-1}} \le c\left(1+\frac{\rho}{\sqrt{\rho^2-1}}\right).$$

It follows that (cf. (4.2.13))

$$\left|\partial_\rho\left[\left(1-\chi_\epsilon(k\rho n_0' - k' - \tilde\omega_{\ell,j}')\right) h_{\ell,j}(\rho n_0')\, e^{ik\rho R n_0'\cdot m'}\right]\right| e^{-\frac{k}{2}Rm_z\sqrt{\rho^2-1}} \le c\left(1+\frac{\rho}{\sqrt{\rho^2-1}}+R\right)$$

for $\rho \in [1,\infty)$, since $\nabla\chi_\epsilon(k\rho n_0' - k' - \tilde\omega_{\ell,j}') \equiv 0$ in a small neighbourhood of $k\rho n_0' = k' + \tilde\omega_{\ell,j}'$. Substituting $u := R\sqrt{\rho^2-1}$ in this estimate, (cf. (4.2.11))

$$\begin{aligned}
\left|W_{\ell,j}^{2,2}\right| &\le 2\pi\, c\int_1^\infty \left(1+\frac{\rho}{\sqrt{\rho^2-1}}+R\right) e^{-\frac{k}{2}Rm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho\\
&= 2\pi\,\frac{c}{R}\int_0^\infty \left(\frac{1}{R}\frac{u}{\sqrt{\frac{u^2}{R^2}+1}} + 1 + \frac{u}{\sqrt{\frac{u^2}{R^2}+1}}\right) e^{-\frac{k}{2}m_z\,u}\,\mathrm{d}u\\
&\le \frac{c}{R}\int_0^\infty \left(\frac{1}{R}+1\right) e^{-\frac{k}{4}m_z\,u}\,\mathrm{d}u\\
&= \mathcal{O}\left(\frac{1}{R}\right),
\end{aligned}$$

since $u^2/R^2 \ge 0$ and $u\,e^{-k/4m_z\,u} \le c$ for all $u \in [0,\infty)$ and $R > 0$. Consequently the second term on the right-hand side of (4.2.9) has an asymptotic behaviour of $o(1/R)$ and

$$W_{\ell,j}^2 = \mathbb{1}_0(|m'|)\,\frac{1}{ikR}\int_0^{2\pi}\left(1-\chi_\epsilon(kn_0' - k' - \tilde\omega_{\ell,j}')\right) h_{\ell,j}(n_0')\,\mathrm{d}\phi + o\left(\frac{1}{R}\right). \tag{4.2.15}$$

4.2.3 Smooth integrands of plane waves

Recall that (cf. (4.2.7))

$$W_{\ell,j}^1 := \int_{B_2(1)} \left(1-\chi_\epsilon(kn' - k' - \tilde\omega_{\ell,j}')\right) \frac{h_{\ell,j}(n')}{n_z^r}\, e^{ikR\vec n^r\cdot\vec m}\,\mathrm{d}n'. \tag{4.2.16}$$

To examine this integral, observe that $n' = (n_x, n_y)^\top \mapsto \vec n^r = (n_x, n_y, \sqrt{1-n_x^2-n_y^2})^\top$ is a bijective mapping of the points of the unit disk onto the upper hemisphere of the unit ball. For convenience, the vector $\vec n^r$ will be transformed to spherical coordinates (θ,ϕ), where the direction of the polar axes is chosen as $\vec m$. As a result $\vec n^r\cdot\vec m$ equals $\cos\theta$. If

$$\vec m = (\sin\alpha\cos\beta, \sin\alpha\sin\beta, \cos\alpha)^\top, \tag{4.2.17}$$

with the z-axis as polar axis, then $\vec n^r$ can be represented as

$$\begin{aligned}
\vec n^r(\theta,\phi) &:= A\cdot(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)^\top\\
&= \begin{pmatrix} \sin\alpha\cos\beta\cos\theta + (\cos\alpha\cos\beta\cos\phi - \sin\beta\sin\phi)\sin\theta \\ \sin\alpha\sin\beta\cos\theta + (\cos\alpha\sin\beta\cos\phi + \cos\beta\sin\phi)\sin\theta \\ \cos\alpha\,\cos\theta - \sin\alpha\cos\phi\sin\theta \end{pmatrix},
\end{aligned} \tag{4.2.18}$$

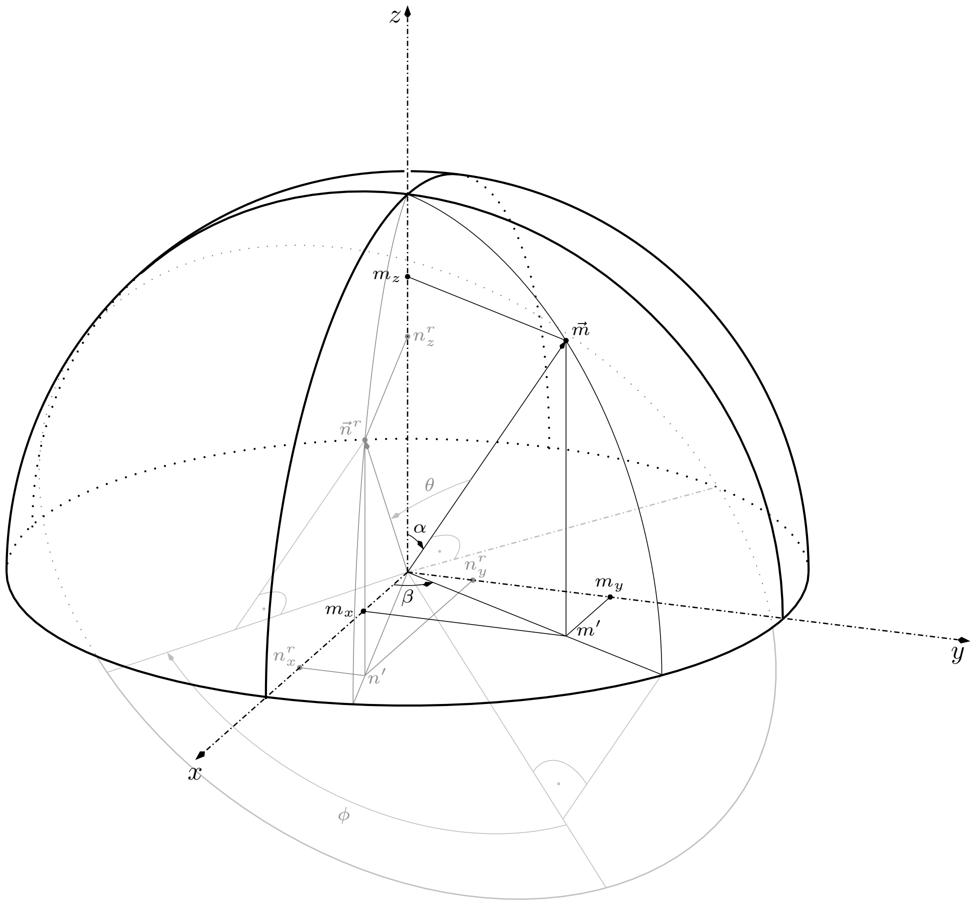


Figure 4.2: Spherical coordinates w.r.t. $\vec{m}$

with

$$A = \begin{pmatrix} \cos\alpha\cos\beta & -\sin\beta & \sin\alpha\cos\beta \\ \cos\alpha\sin\beta & \cos\beta & \sin\alpha\sin\beta \\ -\sin\alpha & 0 & \cos\alpha \end{pmatrix} = \begin{pmatrix} \cos\beta & -\sin\beta & 0 \\ \sin\beta & \cos\beta & 0 \\ 0 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} \cos\alpha & 0 & \sin\alpha \\ 0 & 1 & 0 \\ -\sin\alpha & 0 & \cos\alpha \end{pmatrix},$$

as visualised in Figure 4.2. Now n_x and n_y can be substituted in integral (4.2.16). For this, the determinant of the Jacobian matrix $\partial(n_x, n_y)/\partial(\theta, \phi)$ needs to be calculated, which leads to

$$\det\left(\frac{\partial(n_x, n_y)}{\partial(\theta, \phi)}\right) = \sin\theta(-\sin\alpha\sin\theta\cos\phi + \cos\alpha\cos\theta) = n_z^r(\theta, \phi)\sin\theta. \tag{4.2.19}$$

Since the calculation of the determinant is a lengthy process but otherwise contains no difficulties, it will not be shown in more detail. As a result, the differential $\mathrm{d}n'$ is replaced by $n_z^r(\theta, \phi)\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi$. Thus

$$W_{\ell,j}^1 = \int_0^{2\pi}\int_0^{\theta(\phi)} \Big(1 - \chi_\epsilon(kn'(\theta, \phi) - k' - \tilde{\omega}_{\ell,j}')\Big)\, h_{\ell,j}\Big(n'(\theta, \phi)\Big)\, \sin\theta\, e^{ikR\cos\theta}\,\mathrm{d}\theta\,\mathrm{d}\phi \tag{4.2.20}$$

where $\theta(\phi) \leq \pi$ is the angle at which $\vec{n}^r(\theta(\phi), \phi)$ lies in the $x-y$ plane, i.e. $n_z^r(\theta(\phi), \phi) = 0$, and $n'(\theta, \phi)$ is defined as $(n_x^r(\theta, \phi), n_y^r(\theta, \phi))^\top$. Further substituting $\cos\theta$ by ψ, where $\theta \in [0, \theta(\phi)] \subset [0, \pi]$, and applying integration by parts to the integral w.r.t. ψ leads to the expression

$$
\begin{aligned}
W^1_{\ell,j} &= \int_0^{2\pi}\int_{\cos\theta(\phi)}^{1} \Big(1-\chi_\epsilon(kn'(\psi,\phi)-k'-\tilde{\omega}'_{\ell,j})\Big)\, h_{\ell,j}\Big(n'(\psi,\phi)\Big)\, e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi \\
&= \frac{1}{ikR}\int_0^{2\pi} \Big(1-\chi_\epsilon(km'-k'-\tilde{\omega}'_{\ell,j})\Big)\, h_{\ell,j}(m')\, e^{ikR}\,\mathrm{d}\phi \\
&\quad - \frac{1}{ikR}\int_0^{2\pi} \Big(1-\chi_\epsilon(kn'_0(\phi)-k'-\tilde{\omega}'_{\ell,j})\Big)\, h_{\ell,j}\Big(n'_0(\phi)\Big)\, e^{ikR\cos\theta(\phi)}\,\mathrm{d}\phi \\
&\quad - \frac{1}{ikR}\int_0^{2\pi}\int_{\cos\theta(\phi)}^{1} \partial_\psi\left[\Big(1-\chi_\epsilon(kn'(\psi,\phi)-k'-\tilde{\omega}'_{\ell,j})\Big)\, h_{\ell,j}\Big(n'(\psi,\phi)\Big)\right] e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi \\
&= 2\pi\Big(1-\chi_\epsilon(km'-k'-\tilde{\omega}'_{\ell,j})\Big)\, h_{\ell,j}(m')\,\frac{e^{ikR}}{ikR} \\
&\quad - \frac{1}{ikR}\int_0^{2\pi} \Big(1-\chi_\epsilon(kn'_0(\phi)-k'-\tilde{\omega}'_{\ell,j})\Big)\, h_{\ell,j}\Big(n'_0(\phi)\Big)\, e^{ikR\cos\theta(\phi)}\,\mathrm{d}\phi \\
&\quad - \frac{1}{ikR}\int_0^{2\pi}\int_{\cos\theta(\phi)}^{1} \partial_\psi\left[\Big(1-\chi_\epsilon(kn'(\psi,\phi)-k'-\tilde{\omega}'_{\ell,j})\Big)\, h_{\ell,j}\Big(n'(\psi,\phi)\Big)\right] e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi
\end{aligned}
\tag{4.2.21}
$$

where $n'(1,\phi) = m'$,

$$
n'(\psi,\phi) := \begin{pmatrix} \sin\alpha\cos\beta\,\psi + (\cos\alpha\cos\beta\cos\phi - \sin\beta\sin\phi)\sqrt{1-\psi^2} \\ \sin\alpha\sin\beta\,\psi + (\cos\alpha\sin\beta\cos\phi + \cos\beta\sin\phi)\sqrt{1-\psi^2} \end{pmatrix}, \tag{4.2.22}
$$

$$
n^r_z(\psi,\phi) := \cos\alpha\,\psi - \sin\alpha\cos\phi\sqrt{1-\psi^2} \tag{4.2.23}
$$

and $n'_0(\phi) := n'\big(\cos\theta(\phi),\phi\big)$. Similarly to (4.2.10) and (4.2.11), define

$$
W^{1.1}_{\ell,j} := \int_0^{2\pi} \Big(1-\chi_\epsilon(kn'_0(\phi)-k'-\tilde{\omega}'_{\ell,j})\Big)\, h_{\ell,j}\Big(n'_0(\phi)\Big)\, e^{ikR\cos\theta(\phi)}\,\mathrm{d}\phi
$$

and

$$
W^{1.2}_{\ell,j} := \int_0^{2\pi}\int_{\cos\theta(\phi)}^{1} \partial_\psi\left[\Big(1-\chi_\epsilon(kn'(\psi,\phi)-k'-\tilde{\omega}'_{\ell,j})\Big)\, h_{\ell,j}\Big(n'(\psi,\phi)\Big)\right] e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi, \tag{4.2.24}
$$

such that (cf. (4.2.21))

$$
W^1_{\ell,j} = 2\pi\Big(1-\chi_\epsilon(kn'_0(\phi)-k'-\tilde{\omega}'_{\ell,j})\Big)\, h_{\ell,j}(m')\,\frac{e^{ikR}}{ikR} - \frac{1}{ikR}W^{1.1}_{\ell,j} - \frac{1}{ikR}W^{1.2}_{\ell,j}. \tag{4.2.25}
$$

To examine $W^{1.1}_{\ell,j}$ a closer look at $\cos\theta(\phi)$ is necessary. Since $\theta(\phi)$ is defined as the solution of

$$
n^r_z(\theta(\phi),\phi) = \cos\alpha\cos\theta(\phi) - \sin\alpha\sin\theta(\phi)\cos\phi = 0, \tag{4.2.26}
$$

the value $\cos\theta(\phi)$ is found as

$$
\cos\theta(\phi) = \begin{cases} \cos\left(\mathrm{Atan}\left(\frac{\cot\alpha}{\cos\phi}\right)\right) & \text{if } \phi\notin\left\{\frac{\pi}{2},\frac{3}{2}\pi\right\} \text{ and } \alpha\neq 0 \\ 0 & \text{if } \phi\in\left\{\frac{\pi}{2},\frac{3}{2}\pi\right\} \text{ or } \alpha = 0 \end{cases}, \tag{4.2.27}
$$

with

$$\begin{aligned}\mathrm{Atan} : \mathbb{R} \setminus \{0\} &\to [0,\pi] \setminus \{\frac{\pi}{2}\}\\ x \mapsto \mathrm{Atan}(x) &:= \begin{cases}\arctan(x) & \text{if } x > 0\\ \pi + \arctan(x) & \text{if } x < 0\end{cases}.\end{aligned}$$

On the other hand, replacing $\sin\theta(\phi)$ in (4.2.26) by $\sqrt{1-\cos^2\theta(\phi)}$ and dividing by $\cos\alpha$, the equation

$$\cos\theta(\phi) = \tan\alpha\cos\phi\,\sqrt{1-\cos^2\theta(\phi)}$$

is obtained. Squaring and rearranging this leads to

$$\left(1+\tan^2\alpha\cos^2\phi\right)\,\cos^2\theta(\phi) = \tan^2\alpha\cos^2\phi$$

and

$$\cos\theta(\phi) = \frac{\tan\alpha\cos\phi}{\sqrt{1+\tan^2\alpha\cos^2\phi}}, \tag{4.2.28}$$

which is an alternative representation of $\cos\theta(\phi)$, equivalent to (4.2.27). From this, it is easily deduced that $\cos\theta(\phi)$ is monotone for $\phi\in[0,\pi)$ and for $\phi\in[\pi,2\pi)$. Thus, unless $\alpha=0$ or equivalently $m'=(0,0)^\top$, the substitution $t:=\cos\theta(\phi)$ for these two intervals is possible. For now it is assumed that $\alpha\in(0,\pi/2)$. It is easily calculated that the inverse function $\phi(t)=\arccos(\cot\alpha\,t/\sqrt{1-t^2})$ such that $\mathrm{d}\phi = -\cos\alpha/[(1-t^2)\sqrt{\sin^2\alpha-t^2}]\,\mathrm{d}t$ with $\cos\theta(\phi)\in(-\sin\alpha,\sin\alpha]$ for $\phi\in[0,\pi)$. Thus

$$\begin{aligned}W^{1.1}_{\ell,j} = &\int\limits_{-\sin\alpha}^{\sin\alpha}\Big(1-\chi_\epsilon(kn'_{0,1}(t)-k'-\tilde{\omega}'_{\ell,j})\Big)\,h_{\ell,j}\Big(n'_{0,1}(t)\Big)\,\frac{\cos\alpha}{1-t^2}\,\frac{1}{\sqrt{\sin^2\alpha-t^2}}\,e^{ikR\,t}\,\mathrm{d}t\\ &-\int\limits_{-\sin\alpha}^{\sin\alpha}\Big(1-\chi_\epsilon(kn'_{0,2}(t)-k'-\tilde{\omega}'_{\ell,j})\Big)\,h_{\ell,j}\Big(n'_{0,2}(t)\Big)\,\frac{\cos\alpha}{1-t^2}\,\frac{1}{\sqrt{\sin^2\alpha-t^2}}\,e^{ikR\,t}\,\mathrm{d}t,\end{aligned}$$

where

$$n'_{0,l}(t) := n'_0\Big(\cos\theta\big(\phi(t)+(l-1)\,\pi\big),\phi(t)+(l-1)\,\pi\Big)$$

for $l=1,2$. Since $\alpha\in(0,\pi/2)$, or equivalently $|m'|\neq 0$, and thus $0<\sin\alpha<1$, the integrands of these integrals are only weakly singular at $t=\pm\sin\alpha$ and thus absolutely integrable. Hence, the asymptotic behaviour

$$\frac{1}{R}\,W^{1.1}_{\ell,j} = o\left(\frac{1}{R}\right)$$

for the second term on the right-hand side of (4.2.21) follows from the Riemann-Lebesgue lemma. In the case that $\alpha=0$ and thus $\cos\theta(\phi)\equiv 0$ the term

$$-\frac{1}{ikR}\int\limits_0^{2\pi}\Big(1-\chi_\epsilon(kn'_0(\phi)-k'-\tilde{\omega}'_{\ell,j})\Big)\,h_{\ell,j}\Big(n'_0(\phi)\Big)\,\mathrm{d}\phi, \tag{4.2.29}$$

with (cf. (4.2.22))

$$n'_0(\phi) = \begin{pmatrix}\cos\beta\cos\phi-\sin\beta\sin\phi\\ \sin\beta\cos\phi+\cos\beta\sin\phi\end{pmatrix} = \begin{pmatrix}\cos(\beta+\phi)\\ \sin(\beta+\phi)\end{pmatrix}$$

remains. Note that with this and $\alpha=0$, (4.2.29) is the negative of (4.2.12). Thus the two terms cancel when $W^1_{\ell,j}$ is added to $W^2_{\ell,j}$ (cf. (4.2.6)).

Next $W^{1,2}_{\ell,j}$ (cf. (4.2.24)) is examined. Note that the function $h_{\ell,j}(n')$ can also be written as a function $\tilde{h}_{\ell,j}(n', n^r_z)$, with $n^r_z := \sqrt{1-n'^2}$ (cf. (4.2.2)–(4.2.5)). For convenience this will be used until the end of this subsection. For $W^{1,2}_{\ell,j}$ examine the derivative

$$\begin{aligned}
&\partial_\psi \left[\Big(1-\chi_\epsilon(kn'(\psi,\phi)-k'-\tilde{\omega}'_{\ell,j})\Big)\, h_{\ell,j}\Big(n'(\psi,\phi)\Big)\right] \\
&\quad = \partial_\psi \left[\Big(1-\chi_\epsilon(kn'(\psi,\phi)-k'-\tilde{\omega}'_{\ell,j})\Big)\, \tilde{h}_{\ell,j}\Big(n'(\psi,\phi), n^r_z(\psi,\phi)\Big)\right] \\
&\quad = -k\,\partial_\psi n'(\psi,\phi)\cdot\nabla\chi_\epsilon(kn'(\psi,\phi)-k'-\tilde{\omega}'_{\ell,j})\,\tilde{h}_{\ell,j}\Big(n'(\psi,\phi), n^r_z(\psi,\phi)\Big) \\
&\qquad + \Big(1-\chi_\epsilon(kn'(\psi,\phi)-k'-\tilde{\omega}'_{\ell,j})\Big)\,\partial_\psi n'(\psi,\phi)\cdot\nabla_{n'}\tilde{h}_{\ell,j}\Big(n'(\psi,\phi), n^r_z(\psi,\phi)\Big) \\
&\qquad + \Big(1-\chi_\epsilon(kn'(\psi,\phi)-k'-\tilde{\omega}'_{\ell,j})\Big)\,\partial_\psi n^r_z(\psi,\phi)\,\partial_{n^r_z}\tilde{h}_{\ell,j}\Big(n'(\psi,\phi), n^r_z(\psi,\phi)\Big),
\end{aligned}$$

where (cf. (4.2.22))

$$\partial_\psi n'(\psi,\phi) = \begin{pmatrix} \sin\alpha\cos\beta + (\cos\alpha\cos\beta\cos\phi - \sin\beta\sin\phi)\,\frac{-\psi}{\sqrt{1-\psi^2}} \\ \sin\alpha\sin\beta + (\cos\alpha\sin\beta\cos\phi + \cos\beta\sin\phi)\,\frac{-\psi}{\sqrt{1-\psi^2}} \end{pmatrix} \tag{4.2.30}$$

and (cf. (4.2.23))

$$\partial_\psi n^r_z(\psi,\phi) = \cos\alpha + \sin\alpha\cos\phi\,\frac{\psi}{\sqrt{1-\psi^2}}. \tag{4.2.31}$$

Observe that $\tilde{h}_{\ell,j}(n', n^r_z)$ and its partial derivatives w.r.t. n' and n^r_z are uniformly bounded w.r.t. n' and n^r_z, except at the singularity $kn' = k' + \tilde{\omega}'_{\ell,j}$. Since the singularity is cut off by $1-\chi_\epsilon$ and $\nabla\chi_\epsilon$, it follows that for $|n'| \le 1$

$$\left|\partial_\psi \left[\Big(1-\chi_\epsilon(kn'(\psi,\phi)-k'-\tilde{\omega}'_{\ell,j})\Big)\, h_{\ell,j}\Big(n'(\psi,\phi)\Big)\right]\right| \le c\left(1+\frac{|\psi|}{\sqrt{1-\psi^2}}\right)$$

which is integrable on the compact domain of integration $\{(\phi,\psi)\,|\,0\le\phi\le 2\pi,\ \cos\theta(\phi)\le\psi\le 1\}$. Thus the absolute value of the integral w.r.t. ψ in (4.2.24) is uniformly bounded w.r.t. R by a function that is integrable w.r.t. ϕ. Furthermore, it follows from the Riemann-Lebesgue lemma that the integral w.r.t. ψ converges pointwise to zero as R tends to infinity. Consequently, Lebesgue's theorem shows that $W^{1,2}_{\ell,j}$ tends to zero as R tends to infinity. Hence, (cf. (4.2.25))

$$\begin{aligned}
W^1_{\ell,j} &= 2\pi\Big(1-\chi_\epsilon(km'-k'-\tilde{\omega}'_{\ell,j})\Big)\, h_{\ell,j}(m')\,\frac{e^{ikR}}{ikR} \\
&\quad - \mathbb{1}_0(|m'|)\frac{1}{ikR}\int_0^{2\pi}\Big(1-\chi_\epsilon(kn'_0(\phi)-k'-\tilde{\omega}'_{\ell,j})\Big)\, h_{\ell,j}\Big(n'_0(\phi)\Big)\,\mathrm{d}\phi + o\left(\frac{1}{R}\right).
\end{aligned}$$

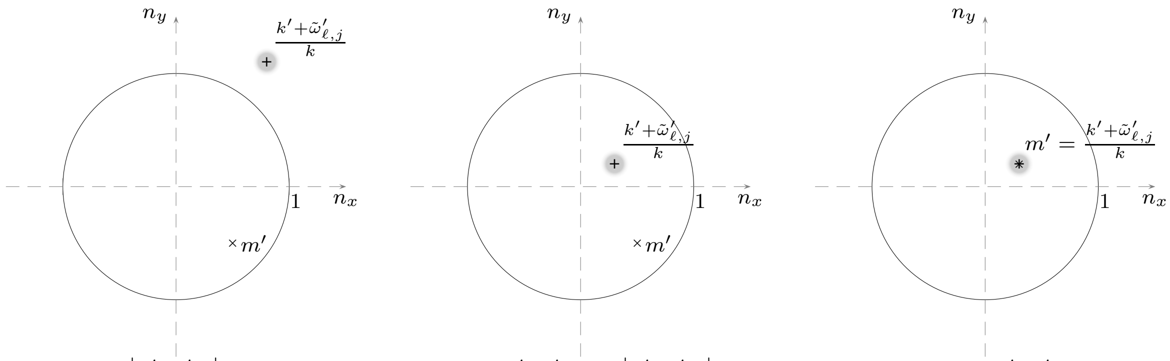
Now consider a fixed direction m'. Since ϵ can be chosen arbitrarily small, $\chi_\epsilon(km'-k'-\tilde{\omega}'_{\ell,j})$ is either zero if $km' \neq k' + \tilde{\omega}'_{\ell,j}$ or one if $km' = k' + \tilde{\omega}'_{\ell,j}$ such that

$$\begin{aligned}
W^1_{\ell,j} &= 2\pi\left(1-\mathbb{1}_{k'+\tilde{\omega}'_{\ell,j}}(km')\right) h_{\ell,j}(m')\,\frac{e^{ikR}}{ikR} \\
&\quad - \mathbb{1}_0(|m'|)\frac{1}{ikR}\int_0^{2\pi}\Big(1-\chi_\epsilon(kn'_0(\phi)-k'-\tilde{\omega}'_{\ell,j})\Big)\, h_{\ell,j}\Big(n'_0(\phi)\Big)\,\mathrm{d}\phi + o\left(\frac{1}{R}\right).
\end{aligned} \tag{4.2.32}$$

4.2.4 Singular integrands

Recall that (cf. (4.2.8))

$$W^3_{\ell,j} := \int_{\mathbb{R}^2} \chi_\epsilon(kn'-k'-\tilde{\omega}'_{\ell,j})\,\frac{h_{\ell,j}(n')}{n^r_z}\,e^{ikR\vec{n}^r\cdot\vec{m}}\,\mathrm{d}n'.$$



(a) $\left|\frac{k'+\tilde{\omega}'_{\ell,j}}{k}\right| > 1$ (b) $m' \neq \frac{k'-\tilde{\omega}'_{\ell,j}}{k}$ for $\left|\frac{k'+\tilde{\omega}'_{\ell,j}}{k}\right| < 1$ (c) $m' = \frac{k'+\tilde{\omega}'_{\ell,j}}{k}$

Figure 4.3: Three cases for integration of $W^3_{\ell,j}$

To examine this integral, three cases will be considered separately. To be precise, the support of the cut-off function can either lie outside of the unit disk (cf. Fig. 4.3(a)) or inside of it. If it is inside the unit disk the two cases of $km' \neq k' + \tilde{\omega}'_{\ell,j}$ (cf. Fig. 4.3(b)) and $km' = k' + \tilde{\omega}'_{\ell,j}$ (cf. Fig. 4.3(c)) are studied. These distinctions are necessary since different substitutions are applied to these different situations, to determine the asymptotic behaviour of the integral $W^3_{\ell,j}$.

4.2.4.1 Singularity on unit disc

First assume $km' \neq k' + \tilde{\omega}'_{\ell,j}$, $|k' + \tilde{\omega}'_{\ell,j}|/k < 1$ and a small ϵ such that $m' \notin \operatorname{supp}\chi_\epsilon(k(\,\cdot\,,\,\cdot\,)^\top - k' - \tilde{\omega}'_{\ell,j})$ (cf. Fig. 4.3(b)). Now, applying the same substitution as in Section 4.2.3, (cf. (4.2.30), (4.2.31) and the first line of (4.2.21))

$$W^3_{\ell,j} = \int_0^{2\pi} \int_{\cos\theta(\phi)}^1 \chi_\epsilon\big(kn'(\psi,\phi) - k' - \tilde{\omega}'_{\ell,j}\big)\, h_{\ell,j}\big(n'(\psi,\phi)\big)\, e^{ikR\psi}\, \mathrm{d}\psi\, \mathrm{d}\phi.$$

In the case of $\ell > 1$ the same approach as for $W^1_{\ell,j}$ can be applied, since here $h_{\ell,j}$ has at most a logarithmic singularity at the point $kn' = k' + \tilde{\omega}'_{\ell,j}$, which is still absolutely integrable after differentiating w.r.t. ψ. To be more precise, for $\ell = 2, 3$ it follows that even the derivative w.r.t. ψ of $h_{\ell,j}$ (cf. (4.2.3), (4.2.4) and for the derivative of K_0 in $h_{2,j}$ [1, Eqns. 9.6.27, 9.6.11 and 9.6.10, pp. 120 and 119]), occurring when applying integration by parts w.r.t. ψ (cf. (4.2.21)), is still integrable w.r.t. $\psi \in [\cos\theta(\phi), 1]$ and $\phi \in [0, 2\pi)$. For $\ell = 4$ the derivative w.r.t. ψ of $h_{4,0}$ is also integrable w.r.t. $\psi \in [\cos\theta(\phi), 1]$ and $\phi \in [0, 2\pi)$, since (cf. (4.2.5))

$$\nabla_{n'} \int_{\mathbb{R}^2} \tilde{g}_n(\eta', \zeta)\, e^{-i\eta'\cdot(kn'-k')}\, \mathrm{d}\eta' = -ik \int_{\mathbb{R}^2} \eta'\, \tilde{g}_n(\eta', \zeta)\, e^{-i\eta'\cdot(kn'-k')}\, \mathrm{d}\eta'$$

is uniformly bounded w.r.t. $n'(\psi,\phi) \in B_2(1)$ and $\partial_\psi n'(\psi,\phi)$ is weakly singular. Indeed the function $\tilde{g}_n(\eta', \zeta)$, as an element of the Banach algebra $\mathcal{A}^{\mathbb{C}}$ w.r.t. η', was defined in such a way that it can be shown that $\|\, |\eta'|\, \tilde{g}_n(\eta', \zeta)\|_{L^1(\mathbb{R}^2)}$ is finite for any fixed $\zeta \in [0, 1]$. Hence,

$$W^3_{\ell,j} = o\left(\frac{1}{R}\right), \qquad \ell = 2, 3, 4. \tag{4.2.33}$$

It remains to examine the case $\ell = 1$. Define

$$f_j(\psi,\phi) := h_{1,j}\big(n'(\psi,\phi)\big)\, |n'(\psi,\phi) - \nu'|\,, \tag{4.2.34}$$

where $\nu' := (k' + \tilde{\omega}'_{\ell,j})/k$. Integral $W^3_{1,j}$ transforms to

$$W^3_{1,j} = \int_0^{2\pi} \int_{\cos\theta(\phi)}^1 \chi_\epsilon\big(kn'(\psi,\phi) - k\nu'\big)\, \frac{f_j(\psi,\phi)}{|n'(\psi,\phi) - \nu'|}\, e^{ikR\psi}\, \mathrm{d}\psi\, \mathrm{d}\phi.$$

At this point, the cut-off function is specified further by defining it as the tensor product of two cut-off functions $\tilde{\chi}^1_\epsilon = \tilde{\chi}^2_\epsilon \in C_0^\infty(\mathbb{R})$, with the same or a smaller ϵ as before. Thus, by defining $(\psi_0, \phi_0)^\top$ such that $n'(\psi_0, \phi_0) = \nu'$ and $\epsilon < \psi_0 - \cos\theta(\phi)$ for all $\phi \in \operatorname{supp}\tilde{\chi}^1_\epsilon(\,\cdot\, - \phi_0)$,

$$W^3_{1,j} = \int\limits_0^{2\pi} \tilde{\chi}^1_\epsilon(\phi - \phi_0) \int\limits_{\psi_0-\epsilon}^{1} \tilde{\chi}^2_\epsilon(\psi - \psi_0)\, \frac{f_j(\psi, \phi)}{|n'(\psi, \phi) - \nu'|}\, e^{ikR\psi}\, \mathrm{d}\psi\, \mathrm{d}\phi.$$

The upper bound of one of the integral w.r.t. ψ could also have been replace by $\psi_0 + \epsilon$. For simplicity the one is left unchanged. The integral is now split into

$$W^3_{1,j} = W^{3.1}_j + g_j(\psi_0, \phi_0)\, W^{3.2}_j, \tag{4.2.35}$$

where

$$W^{3.1}_j := \int\limits_0^{2\pi} \tilde{\chi}^1_\epsilon(\phi - \phi_0) \int\limits_{\psi_0-\epsilon}^{1} \frac{\tilde{\chi}^2_\epsilon(\psi - \psi_0)\, [g_j(\psi, \phi) - g_j(\psi_0, \phi_0)]}{\sqrt{\tilde{a}\,(\psi - \psi_0)^2 + \tilde{b}\,(\phi - \phi_0)^2 + \tilde{c}\,(\psi - \psi_0)\,(\phi - \phi_0)}}\, e^{ikR\psi}\, \mathrm{d}\psi\, \mathrm{d}\phi \tag{4.2.36}$$

$$W^{3.2}_j := \int\limits_0^{2\pi} \tilde{\chi}^1_\epsilon(\phi - \phi_0) \int\limits_{\psi_0-\epsilon}^{1} \frac{\tilde{\chi}^2_\epsilon(\psi - \psi_0)}{\sqrt{\tilde{a}\,(\psi - \psi_0)^2 + \tilde{b}\,(\phi - \phi_0)^2 + \tilde{c}\,(\psi - \psi_0)\,(\phi - \phi_0)}}\, e^{ikR\psi}\, \mathrm{d}\psi\, \mathrm{d}\phi \tag{4.2.37}$$

$$g_j(\psi, \phi) := f_j(\psi, \phi)\, \frac{\sqrt{\tilde{a}\,(\psi - \psi_0)^2 + \tilde{b}\,(\phi - \phi_0)^2 + \tilde{c}\,(\psi - \psi_0)\,(\phi - \phi_0)}}{|n'(\psi, \phi) - \nu'|} \tag{4.2.38}$$

and

$$\tilde{a} := \left| \partial_\psi \Big[n'(\psi, \phi) \Big]_{\substack{\psi=\psi_0 \\ \phi=\phi_0}} \right|^2 = \left| \begin{pmatrix} \sin\alpha\cos\beta - (\cos\alpha\cos\beta\cos\phi_0 - \sin\beta\sin\phi_0)\, \frac{\psi_0}{\sqrt{1-\psi_0^2}} \\ \sin\alpha\sin\beta - (\cos\alpha\sin\beta\cos\phi_0 + \cos\beta\sin\phi_0)\, \frac{\psi_0}{\sqrt{1-\psi_0^2}} \end{pmatrix} \right|^2, \tag{4.2.39}$$

$$\tilde{b} := \left| \partial_\phi \Big[n'(\psi, \phi) \Big]_{\substack{\psi=\psi_0 \\ \phi=\phi_0}} \right|^2 = \left| \begin{pmatrix} (-\cos\alpha\cos\beta\sin\phi_0 - \sin\beta\cos\phi_0)\, \sqrt{1-\psi_0^2} \\ (-\cos\alpha\sin\beta\sin\phi_0 + \cos\beta\cos\phi_0)\, \sqrt{1-\psi_0^2} \end{pmatrix} \right|^2, \tag{4.2.40}$$

$$\tilde{c} := 2\Big\{ \partial_\psi \big[n'(\psi, \phi)\big] \cdot \partial_\phi \big[n'(\psi, \phi)\big] \Big\}_{\substack{\psi=\psi_0 \\ \phi=\phi_0}}.$$

Note that $\tilde{a}$, $\tilde{b}$ and $\tilde{c}$ are finite since $-1 < -\sin\alpha \le \cos\theta(\phi_0) \le \psi_0 < 1$ for $\alpha \in [0, \pi/2)$. There also holds

Lemma 4.3. *The function g_j, as defined in (4.2.38), is a continuous function for all $(\psi, \phi)^\top \neq (\psi_0, \phi_0)^\top$. Furthermore, g_j can be extended continuously by defining*

$$g_j(\psi_0, \phi_0) := \lim_{\substack{\psi \to \psi_0 \\ \phi \to \phi_0}} g_j(\psi, \phi).$$

Proof. It is easily seen that g_j is a continuous for all $(\psi, \phi)^\top \neq (\psi_0, \phi_0)^\top$, since this holds for f_j and since $|n'(\psi, \phi) - \nu'|$ is only zero at $(\psi_0, \phi_0)^\top$. Obviously, the limit $\lim_{(\psi,\phi)\to(\psi_0,\phi_0)} f_j(\psi, \phi) = f_j(\psi_0, \phi_0)$ is also finite, since f_j is defined by removing the singularity of $h_{1,j}$. Consider the limit $(\psi, \phi) \to (\psi_0, \phi_0)$ of the remaining factor in g_j by transforming the point $(\psi - \psi_0, \phi - \phi_0)^\top$ to the polar coordinates $r\,(\cos\gamma, \sin\gamma)$ and considering the limit $r \to 0$. It will be shown that all the radial limits exist and are independent of the angle γ. With

$$\tilde{a}\,(\psi - \psi_0)^2 + \tilde{b}\,(\phi - \phi_0)^2 + \tilde{c}\,(\psi - \psi_0)\,(\phi - \phi_0) + \sum_{\substack{(l_1,l_2)\in\mathbb{N}_0^2 \\ l_1+l_2\ge 3}} b_{l_1,l_2}\,(\psi - \psi_0)^{l_1}(\phi - \phi_0)^{l_2}$$

being the Taylor expansion of $|n'(\psi,\phi)-\nu'|^2$ at $(\psi,\phi)=(\psi_0,\phi_0)$, it can be concluded that

$$\begin{aligned}
&\lim_{(\psi,\phi)\to(\psi_0,\phi_0)} \frac{\sqrt{\tilde a\,(\psi-\psi_0)^2+\tilde b\,(\phi-\phi_0)^2+\tilde c\,(\psi-\psi_0)\,(\phi-\phi_0)}}{|n'(\psi,\phi)-\nu'|} \\
&= \lim_{(\psi,\phi)\to(\psi_0,\phi_0)} \frac{\sqrt{\tilde a\,(\psi-\psi_0)^2+\tilde b\,(\phi-\phi_0)^2+\tilde c\,(\psi-\psi_0)\,(\phi-\phi_0)}}{\sqrt{\tilde a\,(\psi-\psi_0)^2+\tilde b\,(\phi-\phi_0)^2+\tilde c\,(\psi-\psi_0)\,(\phi-\phi_0)+\sum\limits_{\substack{(l_1,l_2)\in\mathbb{N}_0^2\\ l_1+l_2\geq 3}} b_{l_1,l_2}\,(\psi-\psi_0)^{l_1}(\phi-\phi_0)^{l_2}}} \\
&= \lim_{r\to 0} \frac{r\sqrt{\tilde a\cos^2\gamma+\tilde b\sin^2\gamma+\tilde c\cos\gamma\sin\gamma}}{\sqrt{\tilde a r^2\cos^2\gamma+\tilde b r^2\sin^2\gamma+\tilde c r^2\cos\gamma\sin\gamma+r^3\sum\limits_{\substack{(l_1,l_2)\in\mathbb{N}_0^2\\ l_1+l_2\geq 3}} b_{l_1,l_2}\,r^{(l_1+l_2-3)}\cos^{l_1}\gamma\,\sin^{l_2}\gamma}} \\
&= \lim_{r\to 0} \frac{\sqrt{\tilde a\cos^2\gamma+\tilde b\sin^2\gamma+\tilde c\cos\gamma\sin\gamma}}{\sqrt{\tilde a\cos^2\gamma+\tilde b\sin^2\gamma+\tilde c\cos\gamma\sin\gamma+r\sum\limits_{\substack{(l_1,l_2)\in\mathbb{N}_0^2\\ l_1+l_2\geq 3}} b_{l_1,l_2}\,r^{(l_1+l_2-3)}\cos^{l_1}\gamma\,\sin^{l_2}\gamma}} \\
&= 1, \qquad (4.2.41)
\end{aligned}$$

where

$$\begin{aligned}
\tilde a\cos^2\gamma+&\tilde b\sin^2\gamma+\tilde c\cos\gamma\sin\gamma \\
&= (\partial_\psi n'(\psi_0,\phi_0)\cos\gamma+\partial_\phi n'(\psi_0,\phi_0)\sin\gamma)\cdot(\partial_\psi n'(\psi_0,\phi_0)\cos\gamma+\partial_\phi n'(\psi_0,\phi_0)\sin\gamma) \\
&= |\partial_\psi n'(\psi_0,\phi_0)\cos\gamma+\partial_\phi n'(\psi_0,\phi_0)\sin\gamma|^2\neq 0.
\end{aligned}$$

Indeed, this inequality follows only if the two vectors $\partial_\psi n'$ (cf. (4.2.39)) and $\partial_\phi n'$ (cf. (4.2.40)) are not parallel, i.e., if

$$\tilde d := \det\left(\frac{\partial n'(\psi,\phi)}{\partial(\psi,\phi)}\right)_{\substack{\psi=\psi_0\\ \phi=\phi_0}} \neq 0 \qquad (4.2.42)$$

for $\psi_0>\cos\theta(\phi_0)$. On the other hand, in view of (4.2.19) and with $\psi=\cos\theta$, this is easily proven since

$$\tilde d = \frac{1}{\partial_\theta[\cos\theta]}\,\det\left(\frac{\partial(n_x,n_y)}{\partial(\theta,\phi)}\right) = -n_z^r(\psi_0,\phi_0)$$

and since $n_z^r(\psi,\phi)$ is by construction only zero for $\psi=\cos\theta(\phi)$. Thus for $\psi_0\neq\cos\theta(\phi_0)$, which is equivalent to $|\nu'|\neq 1$ (cf. Sect. B of the appendix), it follows that $\tilde d\neq 0$. Note that this also shows that $\tilde a\neq 0$ and $\tilde b\neq 0$, since if either of them were zero the partial derivative of n' w.r.t. ψ or ϕ (cf. (4.2.39) or (4.2.40)) would be zero and thus $\tilde d$ (cf. (4.2.42)). ■

Using an approach similar to the one used for $W^1_{1,j}$ (cf. Sect. 4.2.3), it will now be shown that $W_j^{3.1}$ (cf. (4.2.36)) has an asymptotic behaviour of $o(1/R)$ as R tends to infinity. Applying integration by parts w.r.t. ψ to $W_j^{3.1}$ (cf. (4.2.36)), keeping in mind that $\tilde\chi^2_\epsilon(1-\psi_0)=\tilde\chi^2_\epsilon(-\epsilon)=0$,

$$\begin{aligned}
W_j^{3.1} = \frac{1}{ikR}\int_0^{2\pi}\tilde\chi^1_\epsilon(\phi-\phi_0)&\left[\frac{\tilde\chi^2_\epsilon(\psi-\psi_0)\,[g_j(\psi,\phi)-g_j(\psi_0,\phi_0)]}{\sqrt{\tilde a\,(\psi-\psi_0)^2+\tilde b\,(\phi-\phi_0)^2+\tilde c\,(\psi-\psi_0)\,(\phi-\phi_0)}}\,e^{ikR\psi}\right]_{\psi=\psi_0-\epsilon}^{1} \mathrm{d}\phi \\
-\frac{1}{ikR}\int_0^{2\pi}\tilde\chi^1_\epsilon(\phi-\phi_0)\int_{\psi_0-\epsilon}^{1}\partial_\psi&\left[\frac{\tilde\chi^2_\epsilon(\psi-\psi_0)\,[g_j(\psi,\phi)-g_j(\psi_0,\phi_0)]}{\sqrt{\tilde a\,(\psi-\psi_0)^2+\tilde b\,(\phi-\phi_0)^2+\tilde c\,(\psi-\psi_0)\,(\phi-\phi_0)}}\right]e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi
\end{aligned}$$

$$
\begin{aligned}
&= -\frac{1}{ikR} \int_0^{2\pi} \tilde{\chi}_\epsilon^1(\phi-\phi_0) \int_{\psi_0-\epsilon}^{1} \frac{\left[\tilde{\chi}_\epsilon^2\right]'(\psi-\psi_0)\left[g_j(\psi,\phi)-g_j(\psi_0,\phi_0)\right]}{\sqrt{\tilde{a}\,(\psi-\psi_0)^2+\tilde{b}\,(\phi-\phi_0)^2+\tilde{c}\,(\psi-\psi_0)\,(\phi-\phi_0)}}\, e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi \\
&\quad - \frac{1}{ikR} \int_0^{2\pi} \tilde{\chi}_\epsilon^1(\phi-\phi_0) \int_{\psi_0-\epsilon}^{1} \frac{\tilde{\chi}_\epsilon^2(\psi-\psi_0)\,\partial_\psi g_j(\psi,\phi)}{\sqrt{\tilde{a}\,(\psi-\psi_0)^2+\tilde{b}\,(\phi-\phi_0)^2+\tilde{c}\,(\psi-\psi_0)\,(\phi-\phi_0)}}\, e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi \\
&\quad + \frac{1}{ikR} \int_0^{2\pi} \Bigg\{ \tilde{\chi}_\epsilon^1(\phi-\phi_0) \\
&\qquad \int_{\psi_0-\epsilon}^{1} \frac{\tilde{\chi}_\epsilon^2(\psi-\psi_0)\,\left[\tilde{a}\,(\psi-\psi_0)+\frac{\tilde{c}}{2}\,(\phi-\phi_0)\right]\,\left[g_j(\psi,\phi)-g_j(\psi_0,\phi_0)\right]}{\sqrt{\tilde{a}\,(\psi-\psi_0)^2+\tilde{b}\,(\phi-\phi_0)^2+\tilde{c}\,(\psi-\psi_0)\,(\phi-\phi_0)}^{\,3}}\, e^{ikR\psi}\,\mathrm{d}\psi \Bigg\}\,\mathrm{d}\phi.
\end{aligned}
\tag{4.2.43}
$$

Here

$$
\begin{aligned}
\partial_\psi g_j(\psi,\phi) &= \partial_\psi \left[\frac{f_j(\psi,\phi)\sqrt{\tilde{a}\,(\psi-\psi_0)^2+\tilde{b}\,(\phi-\phi_0)^2+\tilde{c}\,(\psi-\psi_0)\,(\phi-\phi_0)}}{\sqrt{\tilde{a}\,(\psi-\psi_0)^2+\tilde{b}\,(\phi-\phi_0)^2+\tilde{c}\,(\psi-\psi_0)\,(\phi-\phi_0)+\sum\limits_{\substack{(l_1,l_2)\in\mathbb{N}_0^2\\ l_1+l_2\geq 3}} b_{l_1,l_2}\,(\psi-\psi_0)^{l_1}(\phi-\phi_0)^{l_2}}} \right] \\
&= \partial_\psi \left[\frac{f_j(\psi,\phi)}{\sqrt{1+\sum\limits_{\substack{(l_1,l_2)\in\mathbb{N}_0^2\\ l_1+l_2\geq 3}} b_{l_1,l_2}\,\frac{(\psi-\psi_0)^{l_1}(\phi-\phi_0)^{l_2}}{\tilde{a}\,(\psi-\psi_0)^2+\tilde{b}\,(\phi-\phi_0)^2+\tilde{c}\,(\psi-\psi_0)\,(\phi-\phi_0)}}} \right] \\
&= \frac{\partial_\psi f_j(\psi,\phi)}{\sqrt{1+\sum\limits_{\substack{(l_1,l_2)\in\mathbb{N}_0^2\\ l_1+l_2\geq 3}} b_{l_1,l_2}\,\frac{(\psi-\psi_0)^{l_1}(\phi-\phi_0)^{l_2}}{\tilde{a}\,(\psi-\psi_0)^2+\tilde{b}\,(\phi-\phi_0)^2+\tilde{c}\,(\psi-\psi_0)\,(\phi-\phi_0)}}} \\
&\quad - \frac{1}{2}\Bigg\{ \sum_{\substack{(l_1,l_2)\in\mathbb{N}_0^2\\ l_1+l_2\geq 3}} b_{l_1,l_2} \Bigg[\frac{l_1\,(\psi-\psi_0)^{l_1-1}(\phi-\phi_0)^{l_2}}{\tilde{a}\,(\psi-\psi_0)^2+\tilde{b}\,(\phi-\phi_0)^2+\tilde{c}\,(\psi-\psi_0)\,(\phi-\phi_0)} \\
&\qquad\qquad - \frac{(\psi-\psi_0)^{l_1}(\phi-\phi_0)^{l_2}\left[2\tilde{a}(\psi-\psi_0)+\tilde{c}(\phi-\phi_0)\right]}{\left[\tilde{a}\,(\psi-\psi_0)^2+\tilde{b}\,(\phi-\phi_0)^2+\tilde{c}\,(\psi-\psi_0)\,(\phi-\phi_0)\right]^2} \Bigg] \Bigg\} \\
&\qquad \frac{f_j(\psi,\phi)}{\sqrt{1+\sum\limits_{\substack{(l_1,l_2)\in\mathbb{N}_0^2\\ l_1+l_2\geq 3}} b_{l_1,l_2}\,\frac{(\psi-\psi_0)^{l_1}(\phi-\phi_0)^{l_2}}{\tilde{a}\,(\psi-\psi_0)^2+\tilde{b}\,(\phi-\phi_0)^2+\tilde{c}\,(\psi-\psi_0)\,(\phi-\phi_0)}}^{\,3}}
\end{aligned}
\tag{4.2.44}
$$

is uniformly bounded in a neighbourhood of $(\psi,\phi)=(\psi_0,\phi_0)$. Indeed, all quotients are bounded, while this can be seen for $\partial_\psi f_j(\psi,\phi)$ by considering (4.2.34), (4.2.2), (4.2.14), (4.2.30) and (4.2.31) for $\psi_0<1$. Furthermore, similar to (4.2.41), it will be shown subsequently that

$$
\frac{g_j(\psi,\phi)-g_j(\psi_0,\phi_0)}{\sqrt{\tilde{a}\,(\psi-\psi_0)^2+\tilde{b}\,(\phi-\phi_0)^2+\tilde{c}\,(\psi-\psi_0)\,(\phi-\phi_0)}}
\tag{4.2.45}
$$

is uniformly bounded in a neighbourhood of $(\psi,\phi)=(\psi_0,\phi_0)$. In fact, once more, the existence of radial limits is shown (cf. the evaluation of the limit in (4.2.41)). Consider the limit by applying L'Hôpital's rule w.r.t. r

$$\lim_{r\to 0} \frac{g_j(r\cos\gamma+\psi_0, r\sin\gamma+\phi_0) - g_j(\psi_0,\phi_0)}{r\sqrt{\tilde{a}\,\cos^2\gamma+\tilde{b}\,\sin^2\gamma+\tilde{c}\,\cos\gamma\sin\gamma}}$$
$$= \lim_{r\to 0} \frac{\frac{f_j\left(r\cos\gamma+\psi_0, r\sin\gamma+\phi_0\right)\sqrt{\tilde{a}\cos^2\gamma+\tilde{b}\sin^2\gamma+\tilde{c}\cos\gamma\sin\gamma}}{\sqrt{\tilde{a}\cos^2\gamma+\tilde{b}\sin^2\gamma+\tilde{c}\cos\gamma\sin\gamma+r\,S(r,\gamma)}} - f_j(\psi_0,\phi_0)}{r\sqrt{\tilde{a}\cos^2\gamma+\tilde{b}\sin^2\gamma+\tilde{c}\cos\gamma\sin\gamma}}$$
$$= \lim_{r\to 0}\left\{ \frac{\frac{(\cos\gamma,\sin\gamma)^\top\cdot\nabla f_j\left(r\cos\gamma+\psi_0, r\sin\gamma+\phi_0\right)\sqrt{\tilde{a}\cos^2\gamma+\tilde{b}\sin^2\gamma+\tilde{c}\cos\gamma\sin\gamma}}{\sqrt{\tilde{a}\cos^2\gamma+\tilde{b}\sin^2\gamma+\tilde{c}\cos\gamma\sin\gamma+r\,S(r,\gamma)}}}{\sqrt{\tilde{a}\cos^2\gamma+\tilde{b}\sin^2\gamma+\tilde{c}\cos\gamma\sin\gamma}} \right.$$
$$\left. - \frac{\frac{f_j\left(r\cos\gamma+\psi_0, r\sin\gamma+\phi_0\right)}{2}\,\frac{\partial_r[r\,S(r,\gamma)]\sqrt{\tilde{a}\cos^2\gamma+\tilde{b}\sin^2\gamma+\tilde{c}\cos\gamma\sin\gamma}}{\sqrt{\tilde{a}\cos^2\gamma+\tilde{b}\sin^2\gamma+\tilde{c}\cos\gamma\sin\gamma+r\,S(r,\gamma)}^3}}{\sqrt{\tilde{a}\cos^2\gamma+\tilde{b}\sin^2\gamma+\tilde{c}\cos\gamma\sin\gamma}}\right\}$$

where

$$S(r,\gamma) := \sum_{\substack{(l_1,l_2)\in\mathbb{N}_0^2\\ l_1+l_2\geq 3}} b_{l_1,l_2}\, r^{(l_1+l_2-3)}\cos^{l_1}\gamma\,\sin^{l_2}\gamma,$$
$$\partial_r\left[r\,S(r,\gamma)\right] = \sum_{\substack{(l_1,l_2)\in\mathbb{N}_0^2\\ l_1+l_2\geq 3}} b_{l_1,l_2}\,(l_1+l_2-2)\, r^{(l_1+l_2-3)}\cos^{l_1}\gamma\,\sin^{l_2}\gamma.$$

Moreover, the equations (4.2.34), (4.2.2), (4.2.14), (4.2.30) and (4.2.31) show that

$$|\nabla f_j(\psi,\phi)| \leq c\left(1+\frac{1}{\sqrt{1-\psi^2}}\right) = c\left(1+\frac{1}{\sqrt{1-(r\cos\gamma+\psi_0)^2}}\right) < \infty \tag{4.2.46}$$

for sufficiently small r, since $m' \neq \nu'$ and thus $|\psi_0| < 1$. Therefore,

$$\lim_{r\to 0} \frac{g_j(r\cos\gamma+\psi_0, r\sin\gamma+\phi_0) - g_j(\psi_0,\phi_0)}{r\sqrt{\tilde{a}\,\cos^2\gamma+\tilde{b}\,\sin^2\gamma+\tilde{c}\,\cos\gamma\sin\gamma}} \tag{4.2.47}$$
$$= \frac{(\cos\gamma,\sin\gamma)^\top\cdot\nabla f_j(\psi_0,\phi_0)}{\sqrt{\tilde{a}\cos^2\gamma+\tilde{b}\sin^2\gamma+\tilde{c}\cos\gamma\sin\gamma}} - \frac{f_j(\psi_0,\phi_0)}{2}\,\frac{\sum_{\substack{(l_1,l_2)\in\mathbb{N}_0^2\\ l_1+l_2=3}} b_{l_1,l_2}\,(l1+l2-2)\,\cos^{l_1}\gamma\,\sin^{l_2}\gamma}{\sqrt{\tilde{a}\cos^2\gamma+\tilde{b}\sin^2\gamma+\tilde{c}\cos\gamma\sin\gamma}^3}$$

is finite, since $\tilde{a}\cos^2\gamma+\tilde{b}\sin^2\gamma+\tilde{c}\cos\gamma\sin\gamma \neq 0$ has been shown above in context of the limit (4.2.41). With this, it also easily shown that the right-hand side of (4.2.47) is a continuous function w.r.t. γ and thus uniformly bounded. Consequently, the following lemma shows that (4.2.45) is uniformly bounded in a neighbourhood of $(\psi,\phi) = (\psi_0,\phi_0)$.

Lemma 4.4. *Assuming a compact set $D \subset \mathbb{R}^2$ and a function $F : D \to \mathbb{R}$ that is continuous for all $(\psi,\phi) \in D\setminus\{(\psi_0,\phi_0)\}$. Moreover, defining $(r\cos\gamma, r\sin\gamma) := (\psi-\psi_0, \phi-\phi_0)$ for $r \geq 0$ and $\gamma \in [0,2\pi]$, it is assumed that the function*

$$l(\gamma) := \lim_{r\to 0} F(r\cos\gamma+\psi_0, r\sin\gamma+\phi_0)$$

is uniformly bounded for all $\gamma \in [0,2\pi]$. For such a function, there holds

$$|F(\psi,\phi)| \leq c < \infty$$

for all $(\psi,\phi) \in D$.

Proof. Since F is continuous outside a neighbourhood $B_\delta(\psi_0,\phi_0) := \{(\psi,\phi) : \|(\psi,\phi)-(\psi_0,\phi_0)\| < \delta\| \subseteq D$ with $\delta > 0$ of $(\psi,\phi) = (\psi_0,\phi_0)$ and since D is a compact set, it follows that F is uniformly bounded outside this neighbourhood, i.e. $r \geq \delta$. Moreover, since F is continuous for $(\psi,\phi) \neq (\psi_0,\phi_0)$, and since $\cos\gamma$ and $\sin\gamma$ are continuous functions, the function $(r,\gamma) \mapsto F(r\cos\gamma+\psi_0, r\sin\gamma+\phi_0)$ is continuous for all $r \geq \delta$ and $\gamma \in [0,2\pi]$. Hence, the supremum over all $r \geq \delta$ and $\gamma \in [0,2\pi]$ is finite and attained either in the interior of $D \setminus B_\delta(\psi_0,\phi_0)$ or on its boundary. Thus, since the continuous continuation $l(\gamma)$ of $F(r\cos\gamma+\psi_0, r\sin\gamma+\phi_0)$ to $r=0$ is uniformly bounded w.r.t. $\gamma \in [0,2\pi]$, there either exists a $\delta_0 > 0$ such that the supremum no longer changes for δ smaller than δ_0 or the supremum over all $r \geq 0$ and $\gamma \in [0,2\pi]$ is attained at $r = 0$. In the latter case, however, the supremum is also finite, since $l(\gamma) = \lim_{r\to 0} F(r\cos\gamma+\psi_0, r\sin\gamma+\phi_0)$ is uniformly bounded w.r.t. $\gamma \in [0,2\pi]$, thus proving the lemma. ∎

Hence, using (4.2.44), (4.2.46) and (4.2.47), it is easily seen that all the integrands on the right-hand side of (4.2.43) are at most weakly singular and thus absolutely integrable w.r.t. ψ. Consequently, the integrals w.r.t. ψ are uniformly bounded w.r.t. R by a function that is integrable w.r.t. ϕ. Lebesgue's theorem and the Riemann-Lebesgue lemma then show that

$$W_j^{3.1} = o\left(\frac{1}{R}\right). \tag{4.2.48}$$

To examine $W_j^{3.2}$ (cf. (4.2.37)), substitute ψ and ϕ, after interchanging the order of integration, by introducing the new variables

$$\upsilon - \upsilon_0 := \tilde{d}\sqrt{\tilde{b}}\,(\psi-\psi_0)$$

and

$$\sigma - \sigma_0 := \sqrt{\tilde{b}}\frac{\tilde{c}}{2}\,(\psi-\psi_0) + \sqrt{\tilde{b}}^3\,(\phi-\phi_0).$$

Here $\tilde{d} = \sqrt{\tilde{a}\,\tilde{b} - \tilde{c}^2/4}$, $\upsilon_0 := \tilde{d}\sqrt{\tilde{b}}\,\psi_0$ and $\sigma_0 := \sqrt{\tilde{b}}\,(\tilde{c}/2\,\psi_0 + \tilde{b}\,\phi_0)$. Thus $\mathrm{d}\phi\,\mathrm{d}\psi = 1/(\tilde{d}\,\tilde{b}^2)\,\mathrm{d}\sigma\,\mathrm{d}\upsilon$ and

$$\begin{aligned}
&\sqrt{\tilde{a}\,(\psi-\psi_0)^2 + \tilde{b}\,(\phi-\phi_0)^2 + \tilde{c}\,(\psi-\psi_0)(\phi-\phi_0)} \\
&\quad = \Bigg\{\tilde{a}\,\frac{(\upsilon-\upsilon_0)^2}{\tilde{d}^2\tilde{b}} + \frac{1}{\tilde{b}^2}\left[(\sigma-\sigma_0)^2 + \frac{\tilde{c}^2}{4\tilde{d}^2}\,(\upsilon-\upsilon_0)^2 - \frac{\tilde{c}}{\tilde{d}}\,(\upsilon-\upsilon_0)(\sigma-\sigma_0)\right] \\
&\qquad + \frac{\tilde{c}}{\tilde{d}\tilde{b}^2}\,(\upsilon-\upsilon_0)(\sigma-\sigma_0) - \frac{\tilde{c}^2}{2\tilde{d}^2\tilde{b}^2}\,(\upsilon-\upsilon_0)^2\Bigg\}^{\frac{1}{2}} \\
&\quad = \frac{1}{\tilde{b}}\sqrt{\frac{\tilde{a}\,\tilde{b} - \frac{\tilde{c}^2}{4}}{\tilde{d}^2}\,(\upsilon-\upsilon_0)^2 + (\sigma-\sigma_0)^2} \\
&\quad = \frac{\sqrt{(\upsilon-\upsilon_0)^2 + (\sigma-\sigma_0)^2}}{\tilde{b}}.
\end{aligned}$$

It follows that (cf. (4.2.37))

$$\begin{aligned}
W_j^{3.2} &= \int_{\psi_0-\epsilon}^{1}\int_0^{2\pi} \tilde{\chi}_\epsilon^1(\phi-\phi_0)\frac{\tilde{\chi}_\epsilon^2(\psi-\psi_0)}{\sqrt{\tilde{a}\,(\psi-\psi_0)^2 + \tilde{b}\,(\phi-\phi_0)^2 + \tilde{c}\,(\psi-\psi_0)\,(\phi-\phi_0)}}\,\mathrm{d}\phi\, e^{ikR\psi}\,\mathrm{d}\psi \\
&= \frac{1}{\tilde{d}\tilde{b}}\int_{\tilde{d}\sqrt{\tilde{b}}\,(\psi_0-\epsilon)}^{\tilde{d}\sqrt{\tilde{b}}} \tilde{\chi}_\epsilon^2\left(\frac{\upsilon-\upsilon_0}{\tilde{d}\sqrt{\tilde{b}}}\right)\int_{\frac{\tilde{c}}{2\tilde{d}}\upsilon}^{\frac{\tilde{c}}{2\tilde{d}}\upsilon+2\pi\sqrt{\tilde{b}}^3}\frac{\tilde{\chi}_\epsilon^1\left(\frac{\sigma-\sigma_0-\frac{\tilde{c}}{2\tilde{d}}(\upsilon-\upsilon_0)}{\sqrt{\tilde{b}}^3}\right)}{\sqrt{(\upsilon-\upsilon_0)^2+(\sigma-\sigma_0)^2}}\,\mathrm{d}\sigma\, e^{i\frac{k}{\tilde{d}\sqrt{\tilde{b}}}R\upsilon}\,\mathrm{d}\upsilon.
\end{aligned}$$

Defining $\tilde{d}_1 := 1/\tilde{d}\sqrt{\tilde{b}}$ and $\tilde{d}_2 := \tilde{c}/(2\tilde{d})$ leads to

$$W_j^{3.2} = \frac{1}{\tilde{d}\tilde{b}} \int\limits_{\frac{\psi_0-\epsilon}{\tilde{d}_1}}^{\frac{1}{\tilde{d}_1}} \tilde{\chi}_\epsilon^2\left(\tilde{d}_1(v-v_0)\right) \int\limits_{\tilde{d}_2 v}^{\tilde{d}_2 v + 2\pi\sqrt{\tilde{b}}^3} \frac{\tilde{\chi}_\epsilon^1\left(\frac{\sigma-\sigma_0-\tilde{d}_2(v-v_0)}{\sqrt{\tilde{b}}^3}\right)}{\sqrt{(v-v_0)^2+(\sigma-\sigma_0)^2}}\,\mathrm{d}\sigma\, e^{ik\tilde{d}_1 Rv}\,\mathrm{d}v. \tag{4.2.49}$$

Recall that ϵ was chosen in such a way that $\tilde{\chi}_\epsilon^1((\sigma-\sigma_0-\tilde{d}_2(v-v_0))/\sqrt{\tilde{b}}^3)$ is zero for σ equal to the boundaries of the domain of integration w.r.t. σ. Thus, integrating by parts w.r.t. σ leads to

$$\begin{aligned}
&\int\limits_{\tilde{d}_2 v}^{\tilde{d}_2 v + 2\pi\sqrt{\tilde{b}}^3} \frac{\tilde{\chi}_\epsilon^1\left(\frac{\sigma-\sigma_0-\tilde{d}_2(v-v_0)}{\sqrt{\tilde{b}}^3}\right)}{\sqrt{(v-v_0)^2+(\sigma-\sigma_0)^2}}\,\mathrm{d}\sigma \\
&\quad= \int\limits_{\tilde{d}_2 v}^{\tilde{d}_2 v + 2\pi\sqrt{\tilde{b}}^3} \tilde{\chi}_\epsilon^1\left(\frac{\sigma-\sigma_0-\tilde{d}_2(v-v_0)}{\sqrt{\tilde{b}}^3}\right) \partial_\sigma\left[\log\left(\sigma-\sigma_0+\sqrt{(v-v_0)^2+(\sigma-\sigma_0)^2}\right)\right]\mathrm{d}\sigma \\
&\quad= -\int\limits_{\tilde{d}_2 v}^{\tilde{d}_2 v + 2\pi\sqrt{\tilde{b}}^3} \frac{\left[\tilde{\chi}_\epsilon^1\right]'\left(\frac{\sigma-\sigma_0-\tilde{d}_2(v-v_0)}{\sqrt{\tilde{b}}^3}\right)}{\sqrt{\tilde{b}}^3} \log\left(\sigma-\sigma_0+\sqrt{(v-v_0)^2+(\sigma-\sigma_0)^2}\right)\mathrm{d}\sigma.
\end{aligned} \tag{4.2.50}$$

Note that the integrand of the integral on the right-hand side is uniformly bounded since $\left[\tilde{\chi}_\epsilon^1\right]'(\phi)$ is zero in a neighbourhood of $\phi = 0$. For the following, define

$$s(v,\sigma) := \sigma-\sigma_0+\sqrt{(v-v_0)^2+(\sigma-\sigma_0)^2}.$$

Taking into account that

$$\partial_v\left[\log s(v,\sigma)\right] = -(v-v_0)\,\partial_\sigma\left[\frac{1}{s(v,\sigma)}\right],$$

it can be concluded that (cf. (4.2.50))

$$\begin{aligned}
\partial_v\left[\int\limits_{\tilde{d}_2 v}^{\tilde{d}_2 v + 2\pi\sqrt{\tilde{b}}^3} \frac{\tilde{\chi}_\epsilon^1\left(\frac{\sigma-\sigma_0-\tilde{d}_2(v-v_0)}{\sqrt{\tilde{b}}^3}\right)}{\sqrt{(v-v_0)^2+(\sigma-\sigma_0)^2}}\,\mathrm{d}\sigma\right] &= -\partial_v\left[\int\limits_{\tilde{d}_2 v}^{\tilde{d}_2 v + 2\pi\sqrt{\tilde{b}}^3} \frac{\left[\tilde{\chi}_\epsilon^1\right]'\left(\frac{\sigma-\sigma_0-\tilde{d}_2(v-v_0)}{\sqrt{\tilde{b}}^3}\right)}{\sqrt{\tilde{b}}^3}\log s(v,\sigma)\,\mathrm{d}\sigma\right] \\
&= \frac{\tilde{d}_2}{\tilde{b}^3}\int\limits_{\tilde{d}_2 v}^{\tilde{d}_2 v + 2\pi\sqrt{\tilde{b}}^3} \left[\tilde{\chi}_\epsilon^1\right]''\left(\frac{\sigma-\sigma_0-\tilde{d}_2(v-v_0)}{\sqrt{\tilde{b}}^3}\right)\log s(v,\sigma)\,\mathrm{d}\sigma \\
&\quad +(v-v_0)\int\limits_{\tilde{d}_2 v}^{\tilde{d}_2 v + 2\pi\sqrt{\tilde{b}}^3} \frac{\left[\tilde{\chi}_\epsilon^1\right]'\left(\frac{\sigma-\sigma_0-\tilde{d}_2(v-v_0)}{\sqrt{\tilde{b}}^3}\right)}{\sqrt{\tilde{b}}^3}\,\partial_\sigma\left[\frac{1}{s(v,\sigma)}\right]\mathrm{d}\sigma.
\end{aligned}$$

Since $[\tilde{\chi}_\epsilon^1]'((\sigma-\sigma_0-\tilde{d}_2(v-v_0))/\sqrt{\tilde{b}}^3)$ is zero for σ equal to the boundaries of the domain of integration w.r.t. σ, integration by parts w.r.t. σ for the second integral on the right-hand side leads to

$$\partial_v\left[\int\limits_{\tilde{d}_2 v}^{\tilde{d}_2 v + 2\pi\sqrt{\tilde{b}}^3} \frac{\tilde{\chi}_\epsilon^1\left(\frac{\sigma-\sigma_0-\tilde{d}_2(v-v_0)}{\sqrt{\tilde{b}}^3}\right)}{\sqrt{(v-v_0)^2+(\sigma-\sigma_0)^2}}\,\mathrm{d}\sigma\right] = \frac{\tilde{d}_2}{\tilde{b}^3}\int\limits_{\tilde{d}_2 v}^{\tilde{d}_2 v + 2\pi\sqrt{\tilde{b}}^3} \left[\tilde{\chi}_\epsilon^1\right]''\left(\frac{\sigma-\sigma_0-\tilde{d}_2(v-v_0)}{\sqrt{\tilde{b}}^3}\right)\log s(v,\sigma)\,\mathrm{d}\sigma$$

$$- \frac{1}{\tilde{b}^3} \int\limits_{\tilde{d}_2 v}^{\tilde{d}_2 v + 2\pi\sqrt{\tilde{b}}^3} [\tilde{\chi}^1_\epsilon]'' \left(\frac{\sigma - \sigma_0 - \tilde{d}_2(v - v_0)}{\sqrt{\tilde{b}}^3} \right) \frac{v - v_0}{s(v,\sigma)} \,\mathrm{d}\sigma. \tag{4.2.51}$$

Note that all integrands on the right-hand side of (4.2.51) are uniformly bounded, since $\left[\tilde{\chi}^1_\epsilon\right]''(\phi)$ is also zero in a neighbourhood of $\phi = 0$.

With this in mind, integration by parts w.r.t. v is applied to integral $W^{3.2}_j$ (cf. (4.2.49)), where $\tilde{\chi}^2_\epsilon(\tilde{d}_1\,(v - v_0))$ is again zero at the boundaries of the domain of integration w.r.t. v. Hence, recalling that $[\tilde{\chi}^2_\epsilon]'(\psi) \equiv 0$ in a small neighbourhood of $\psi = 0$, (cf. (4.2.51))

$$\begin{aligned} W^{3.2}_j &= -\frac{1}{ikR\,\tilde{d}\tilde{b}} \int\limits_{\frac{\psi_0 - \epsilon}{\tilde{d}_1}}^{\frac{1}{\tilde{d}_1}} [\tilde{\chi}^2_\epsilon]' \left(\tilde{d}_1(v - v_0)\right) \int\limits_{\tilde{d}_2 v}^{\tilde{d}_2 v + 2\pi\sqrt{\tilde{b}}^3} \frac{\tilde{\chi}^1_\epsilon\left(\frac{\sigma - \sigma_0 - \tilde{d}_2(v - v_0)}{\sqrt{\tilde{b}}^3}\right)}{\sqrt{(v - v_0)^2 + (\sigma - \sigma_0)^2}} \,\mathrm{d}\sigma\, e^{ik\tilde{d}_1 R v}\,\mathrm{d}v \\ &\quad - \frac{1}{ikR\,\tilde{d}_1\tilde{d}\tilde{b}} \int\limits_{\frac{\psi_0 - \epsilon}{\tilde{d}_1}}^{\frac{1}{\tilde{d}_1}} \tilde{\chi}^2_\epsilon \left(\tilde{d}_1(v - v_0)\right) \partial_v \left[\int\limits_{\tilde{d}_2 v}^{\tilde{d}_2 v + 2\pi\sqrt{\tilde{b}}^3} \frac{\tilde{\chi}^1_\epsilon\left(\frac{\sigma - \sigma_0 - \tilde{d}_2(v - v_0)}{\sqrt{\tilde{b}}^3}\right)}{\sqrt{(v - v_0)^2 + (\sigma - \sigma_0)^2}} \,\mathrm{d}\sigma \right] e^{ik\tilde{d}_1 R v}\,\mathrm{d}v \\ &= o\left(\frac{1}{R}\right), \end{aligned}$$

since the remaining integrand is uniformly bounded on the domain of integration, which allows to apply the Riemann-Lebesgue lemma. Finally (cf. (4.2.35) and (4.2.48))

$$W^3_{1,j} = o\left(\frac{1}{R}\right). \tag{4.2.52}$$

4.2.4.2 Singularity in direction of asymptotics

It is now assumed that $km' = k\nu' = k' + \tilde{\omega}'_{\ell,j}$ (cf. Fig. 4.3(c)) and $\epsilon < \min\{\sin\alpha, 1 - \sin\alpha\}$ such that $n^r_z = \sqrt{1 - n'^2} > 0$ for all $n' \in \operatorname{supp}\chi_\epsilon\left(k(\,\cdot\,,\,\cdot\,)^\top - km'\right)$. In this subsection the two cases of $\ell = 1$ and $\ell = 2$ are examined separately, since in both cases the function $h_{\ell,j}(n', \sqrt{1 - n'^2})$ has a singularity at $n' = \nu' = m'$. For $\ell > 2$ the same techniques and arguments as for $W^1_{\ell,j}$ can be used to proof the asymptotic behaviour (compare with the beginning of Sect. 4.2.4.1)

$$W^3_{\ell,j} = 2\pi\, h_{\ell,j}(m')\, \frac{e^{ikR}}{ikR} + o\left(\frac{1}{R}\right), \qquad \ell = 3, 4. \tag{4.2.53}$$

For $\ell = 1, 2$ the same substitution as in Section 4.2.3 is applied. Thus, (cf. (4.2.8), (4.2.22), (4.2.23) and the first line of (4.2.21))

$$W^3_{\ell,j} = \int\limits_0^{2\pi} \int\limits_0^1 \chi_\epsilon\big(kn'(\psi,\phi) - k\nu'\big)\, h_{\ell,j}\big(n'(\psi,\phi)\big)\, e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi. \tag{4.2.54}$$

Estimate of $W^3_{1,j}$:

First $W^3_{1,j}$ is examined (cf. (4.2.34)).

$$W^3_{1,j} = \int\limits_0^{2\pi} \int\limits_0^1 \chi_\epsilon\big(kn'(\psi,\phi) - k\nu'\big)\, \frac{f_j(\psi,\phi)}{|n'(\psi,\phi) - \nu'|}\, e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi$$

This time the cut-off function is specified as $\chi_\epsilon(kn'(\psi,\phi)-k\nu')=\tilde{\chi}_\epsilon(\psi-1)$ with $\tilde{\chi}_\epsilon\equiv 1$ in a neighbourhood of zero, where $\tilde{\chi}_\epsilon\in C_0^\infty(\mathbb{R})$ is defined with the same or a smaller epsilon than before. Recall that $n'(1,\phi)=m'=\nu'$ for any $\phi\in[0,2\pi)$,

$$W_{1,j}^3=\int_0^{2\pi}\int_0^1\tilde{\chi}_\epsilon(\psi-1)\,\frac{f_j(\psi,\phi)}{|n'(\psi,\phi)-\nu'|}\,e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi. \tag{4.2.55}$$

For $\alpha\in[0,\pi/2)$ it is easily seen that (cf. (4.2.22))

$$\begin{aligned}n'(\psi,\phi)&=(\sin\alpha\,\psi+\cos\alpha\cos\phi\sqrt{1-\psi^2})\begin{pmatrix}\cos\beta\\ \sin\beta\end{pmatrix}+\sin\phi\sqrt{1-\psi^2}\begin{pmatrix}-\sin\beta\\ \cos\beta\end{pmatrix},\\ \nu'&=\sin\alpha\begin{pmatrix}\cos\beta\\ \sin\beta\end{pmatrix}\end{aligned}$$

and

$$\begin{aligned}|n'(\psi,\phi)-\nu'|^2&=\left[\sin\alpha\,(\psi-1)+\cos\alpha\cos\phi\,\sqrt{1-\psi^2}\right]^2+\sin^2\phi\,(1-\psi^2)\\
&=\sin^2\alpha\,(1-\psi)^2+2\sin\alpha\cos\alpha\cos\phi\,(\psi-1)\,\sqrt{1-\psi^2}\\
&\quad+\cos^2\alpha\cos^2\phi\,(1-\psi^2)+\sin^2\phi\,(1-\psi^2)\\
&=(1-\psi)\Big[\sin^2\alpha\,(1-\psi)-2\sin\alpha\cos\alpha\cos\phi\,\sqrt{1-\psi^2}\\
&\qquad+\cos^2\alpha\cos^2\phi\,(1+\psi)+\sin^2\phi\,(1+\psi)\Big]\\
&=(1-\psi)\Big[\sin^2\alpha\,(1-\psi)-2\sin\alpha\cos\alpha\cos\phi\,\sqrt{1-\psi^2}\\
&\qquad-\cos^2\alpha\cos^2\phi\,(1-\psi)+2\cos^2\alpha\cos^2\phi-\sin^2\phi\,(1-\psi)+2\sin^2\phi\Big]\\
&=(1-\psi)\Big[2\cos^2\alpha\cos^2\phi+2\sin^2\phi-2\sin\alpha\cos\alpha\cos\phi\,\sqrt{1-\psi^2}\\
&\qquad+(1-\psi)\,\left(\sin^2\alpha-\cos^2\alpha\cos^2\phi-\sin^2\phi\right)\Big]\\
&=(1-\psi)\Big[2\left(1-\sin^2\alpha\cos^2\phi\right)-2\sin\alpha\cos\alpha\cos\phi\,\sqrt{1-\psi^2}\\
&\qquad+(1-\psi)\,\left(\sin^2\alpha\cos^2\phi-\cos^2\alpha\right)\Big].\end{aligned} \tag{4.2.56}$$

Keeping this in mind, define

$$\begin{aligned}g_j(\psi,\phi)&:=\tilde{\chi}_\epsilon(\psi-1)\,f_j(\psi,\phi)\,\frac{\sqrt{1-\psi}}{|n'(\psi,\phi)-\nu'|}\\
&=\frac{\tilde{\chi}_\epsilon(\psi-1)\,f_j(\psi,\phi)}{\sqrt{2-2\sin^2\alpha\cos^2\phi-2\sin\alpha\cos\alpha\cos\phi\,\sqrt{1-\psi^2}+(1-\psi)\,\left(\sin^2\alpha\cos^2\phi-\cos^2\alpha\right)}},\end{aligned} \tag{4.2.57}$$

for which

Lemma 4.5. *There exists a continuous function $g_j^0(\phi)$ such that, for any $0\le\phi<2\pi$, the limit*

$$\lim_{\psi\to 1}\left[\partial_\psi\left[g_j(\psi,\phi)\right]-\frac{g_j^0(\phi)}{\sqrt{1-\psi}}\right]$$

exists and is uniformly bounded w.r.t. ϕ.

Proof. Note that $g_j(1,\phi)=f_j(1,\phi_0)/(\sqrt{2}\sqrt{1-\sin^2\alpha\cos^2\phi})<\infty$, since $f_j(1,\phi)=f_j(1,\phi_0)$ and $\sin^2\alpha\cos^2\phi<1$ for all $\phi\in[0,2\pi)$ and any fixed $\alpha\in\left[0,\frac{\pi}{2}\right)$. Furthermore the function $f_j(\psi,\phi)$

has the form (cf. (4.2.34) and (4.2.2))

$$\begin{aligned} f_j(\psi,\phi) &= c_h\,\big[n_z^r(\psi,\phi)\big]^n\, e^{-k\sqrt{1-\psi}\,\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}}\,\Big(D(\phi)+E(\phi)\,\psi\sqrt{1-\psi^2}+F(\phi)\,\psi^2\Big)\\ &= c_h\,\Big(\big[\cos\alpha\,\psi\big]^n + G(\psi,\phi) + \mathbb{1}_{[1,\infty)}(n)\,H(\phi)\,\psi^{n-1}\sqrt{1-\psi^2}\Big)\\ &\quad e^{-k\sqrt{1-\psi}\,\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}}\,\Big(D(\phi)+E(\phi)\,\psi\sqrt{1-\psi^2}+F(\phi)\,\psi^2\Big), \end{aligned} \tag{4.2.58}$$

where $A(\phi) := 2 - 2\sin^2\alpha\cos^2\phi$, $B(\phi) := \sin^2\alpha\cos^2\phi - \cos^2\alpha$, $C(\phi) := -2\sin\alpha\cos\alpha\cos\phi$ and

$$c_h := i\,\frac{\Delta k^2}{4\pi\epsilon_0}. \tag{4.2.59}$$

Similarly, the functions $D(\phi)$, $E(\phi)$ and $F(\phi)$ are second order polynomials of $\sin\phi$ and $\cos\phi$, defined such that (cf. (4.2.22) and (4.2.23))

$$D(\phi) + E(\phi)\psi\sqrt{1-\psi^2} + F(\phi)\psi^2 = \big(\vec{n}^r(\psi,\phi)\times\vec{e}^{\,0}\big)\times\vec{n}^r(\psi,\phi). \tag{4.2.60}$$

Moreover, by the binomial theorem (cf. Thm. C.12 and Eqn. (4.2.23))

$$\big[n_z^r(\psi,\phi)\big]^n = \sum_{m=0}^{n}\binom{n}{m}\big[\cos\alpha\,\psi\big]^{n-m}\Big[-\sin\alpha\cos\phi\sqrt{1-\psi^2}\Big]^m$$

such that

$$\begin{aligned} G(\psi,\phi) := G_n(\psi,\phi) &:= \sum_{m=2}^{n}\binom{n}{m}\big[\cos\alpha\,\psi\big]^{n-m}\Big[-\sin\alpha\cos\phi\sqrt{1-\psi^2}\Big]^m,\\ H(\phi) &:= -\frac{n!}{(n-1)!}\,\sin\alpha\,\cos\phi\,\big[\cos\alpha\big]^{n-1}. \end{aligned} \tag{4.2.61}$$

Here it is assumed that $G_n(\psi,\phi)\equiv 0$ for $n<2$. This shows that

$$\begin{aligned} \partial_\psi G(\psi,\phi) &= \sum_{m=2}^{n}\binom{n}{m}(n-m)\,\,[\cos\alpha]^{n-m}\,\,\psi^{n-m-1}\Big[-\sin\alpha\cos\phi\sqrt{1-\psi^2}\Big]^m\\ &\quad -\sum_{m=2}^{n}\binom{n}{m}m\,\big[\cos\alpha\,\psi\big]^{n-m}[-\sin\alpha\cos\phi]^m\,\,\psi\,\sqrt{1-\psi^2}^{\,m-2} \end{aligned}$$

and $G(\psi,\phi)/\sqrt{1-\psi}$ are uniformly bounded w.r.t. $(\psi,\phi)\in\operatorname{supp}\tilde\chi_\epsilon(\cdot-1)\times[0,2\pi]$ for any fixed n. It follows that (cf. (4.2.57))

$$\begin{aligned} \partial_\psi\,[g_j(\psi,\phi)] &= \frac{\tilde\chi_\epsilon'\big(\psi-1\big)\,f_j(\psi,\phi)+\tilde\chi_\epsilon\big(\psi-1\big)\,\partial_\psi\,[f_j(\psi,\phi)]}{\sqrt{2-2\sin^2\alpha\cos^2\phi-2\sin\alpha\cos\alpha\cos\phi\,\sqrt{1-\psi^2}+(1-\psi)\,\big(\sin^2\alpha\cos^2\phi-\cos^2\alpha\big)}}\\ &\quad-\frac{\frac{1}{2}\,\tilde\chi_\epsilon\big(\psi-1\big)\,f_j(\psi,\phi)\,\Big(2\sin\alpha\cos\alpha\cos\phi\,\frac{\psi}{\sqrt{1-\psi^2}}-\sin^2\alpha\cos^2\phi+\cos^2\alpha\Big)}{\sqrt{2-2\sin^2\alpha\cos^2\phi-2\sin\alpha\cos\alpha\cos\phi\,\sqrt{1-\psi^2}+(1-\psi)\,\big(\sin^2\alpha\cos^2\phi-\cos^2\alpha\big)}^{\,3}}, \end{aligned} \tag{4.2.62}$$

where

$$\begin{aligned} &\partial_\psi\,[f_j(\psi,\phi)]\\ &\quad= c_h\,\frac{k}{2}\left(\frac{\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}}{\sqrt{1-\psi}}+\frac{B(\phi)\,\sqrt{1-\psi}+\frac{C(\phi)}{\sqrt{1+\psi}}\,\psi}{\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}}\right)\\ &\qquad e^{-k\,\sqrt{1-\psi}\,\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}}\,\Big(D(\phi)+E(\phi)\,\psi\sqrt{1-\psi^2}+F(\phi)\,\psi^2\Big)\,\big[n_z^r(\psi,\phi)\big]^n \end{aligned}$$

$$+\, c_h\, e^{-k\sqrt{1-\psi}\,\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}} \left(E(\phi)\,\sqrt{1-\psi^2} - \frac{E(\phi)\,\psi^2}{\sqrt{1-\psi^2}} + 2F(\phi)\,\psi \right) \left[n_z^r(\psi,\phi)\right]^n$$
$$-\, c_h\, \mathbb{1}_{[1,\infty)}(n) \left(n\,\cos^n\alpha\,\psi^{n-1} + \partial_\psi G(\psi,\phi) + (n-1)\,H(\phi)\,\psi^{n-2}\sqrt{1-\psi^2} - H(\phi)\,\frac{\psi^n}{\sqrt{1-\psi^2}} \right)$$
$$e^{-k\sqrt{1-\psi}\,\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}} \left(D(\phi) + E(\phi)\,\psi\sqrt{1-\psi^2} + F(\phi)\,\psi^2 \right).$$

Collecting the terms in $\partial_\psi[f_j(\psi,\phi)]$ that contain $1/\sqrt{1-\psi}$,

$$\partial_\psi\left[f_j(\psi,\phi)\right] = \frac{f_j^s(\psi,\phi)}{\sqrt{1-\psi}} + f_j^r(\psi,\phi),$$

where

$$\begin{aligned} f_j^s(\psi,\phi) :=\,& c_h \left[\cos\alpha\,\psi\right]^n e^{-k\sqrt{1-\psi}\,\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}} \Bigg\{ -\frac{E(\phi)\,\psi^2}{\sqrt{1+\psi}} \\ &+ \frac{k}{2}\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}\left(D(\phi)+F(\phi)\,\psi^2\right)\Bigg\} \\ &+ c_h\,\mathbb{1}_{[1,\infty)}(n)\,H(\phi)\,\frac{\psi^n}{\sqrt{1+\psi}}\,e^{-k\sqrt{1-\psi}\,\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}}\left(D(\phi)+F(\phi)\,\psi^2\right) \end{aligned} \tag{4.2.63}$$

$$\begin{aligned} f_j^r(\psi,\phi) :=\,& c_h\,\frac{k}{2}\left[\cos\alpha\,\psi\right]^n E(\phi)\,\psi\sqrt{1+\psi}\,e^{-k\sqrt{1-\psi}\,\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}} \\ &\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}} \\ &+ c_h\left[\frac{G(\psi,\phi)}{\sqrt{1-\psi}} + \mathbb{1}_{[1,\infty)}(n)\,H(\phi)\,\psi^{n-1}\sqrt{1+\psi}\right] \\ &e^{-k\sqrt{1-\psi}\,\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}}\Bigg\{-\frac{E(\phi)\,\psi^2}{\sqrt{1+\psi}} \\ &+\frac{k}{2}\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}\left(D(\phi)+E(\phi)\,\psi\sqrt{1-\psi^2}+F(\phi)\,\psi^2\right)\Bigg\} \\ &+ c_h\left[n_z^r(\psi,\phi)\right]^n e^{-k\sqrt{1-\psi}\,\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}}\Bigg\{E(\phi)\,\sqrt{1-\psi^2}+2F(\phi)\,\psi \\ &+\frac{k}{2}\frac{B(\phi)\,\sqrt{1-\psi}+\frac{C(\phi)}{\sqrt{1+\psi}}\,\psi}{\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}}\left(D(\phi)+E(\phi)\,\psi\sqrt{1-\psi^2}+F(\phi)\,\psi^2\right)\Bigg\} \\ &- c_h\,\mathbb{1}_{[1,\infty)}(n)\left(n\,\cos^n\alpha\,\psi^{n-1}+\partial_\psi G(\psi,\phi)+(n-1)\,H(\phi)\,\psi^{n-2}\sqrt{1-\psi^2}\right) \\ &e^{-k\sqrt{1-\psi}\,\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}}\left(D(\phi)+E(\phi)\,\psi\sqrt{1-\psi^2}+F(\phi)\,\psi^2\right) \\ &+ c_h\,\mathbb{1}_{[1,\infty)}(n)\,H(\phi)\,E(\phi)\,\psi^{n+1}\,e^{-k\sqrt{1-\psi}\,\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}}. \end{aligned} \tag{4.2.64}$$

With this (cf. (4.2.62))

$$\partial_\psi\left[g_j(\psi,\phi)\right] = \frac{g_j^s(\psi,\phi)}{\sqrt{1-\psi}} + g_j^r(\psi,\phi), \tag{4.2.65}$$

where

$$g_j^s(\psi,\phi) := \frac{\tilde{\chi}_\epsilon(\psi-1)\,f_j^s(\psi,\phi)}{\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}} + \frac{\frac{1}{2}\tilde{\chi}_\epsilon(\psi-1)\,f_j(\psi,\phi)\,C(\phi)\,\frac{\psi}{\sqrt{1+\psi}}}{\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}^{\,3}}, \tag{4.2.66}$$

$$g_j^r(\psi,\phi) := \frac{\tilde{\chi}'_\epsilon\big(\psi-1\big)\,f_j(\psi,\phi)+\tilde{\chi}_\epsilon\big(\psi-1\big)\,f_j^r(\psi,\phi)}{\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}}+\frac{\frac{1}{2}\tilde{\chi}_\epsilon\big(\psi-1\big)\,f_j(\psi,\phi)\,B(\phi)}{\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}^{\,3}}.$$

In order to obtain the limit behaviour of $\partial_\psi\,[g_j(\psi,\phi)]$ at $\psi=1$ (cf. the subsequent (4.2.72)), the limit $\psi\to 1$ of the two functions $f_j^s(\psi,\phi)$ and $f_j^r(\psi,\phi)$ has to be evaluated. In view of (4.2.63) and (4.2.64),

$$\begin{aligned} f_j^0(\phi) &:= f_j^s(1,\phi) \qquad\qquad (4.2.67)\\ &= c_h\,\cos^n\alpha\left\{-\frac{E(\phi)}{\sqrt{2}}+\frac{k}{2}\sqrt{A(\phi)}\,\big(D(\phi)+F(\phi)\big)\right\}+c_h\,\mathbb{1}_{[1,\infty)}(n)\,\frac{H(\phi)}{\sqrt{2}}\,\big(D(\phi)+F(\phi)\big),\\ f_j^1(\phi) &:= f_j^r(1,\phi)\\ &= c_h\,\cos^n\alpha\left\{\frac{k}{\sqrt{2}}\,E(\phi)\,\sqrt{A(\phi)}+2F(\phi)+\frac{k\,C(\phi)}{2\sqrt{2}\,\sqrt{A(\phi)}}\,\big(D(\phi)+F(\phi)\big)\right\}\\ &\quad+c_h\,\mathbb{1}_{[1,\infty)}(n)\left\{\left[\frac{k}{\sqrt{2}}\,H(\phi)\,\sqrt{A(\phi)}-n\,\cos^n\alpha+\frac{n!}{2(n-2)!}\sin^2\alpha\cos^2\phi\,\big[\cos\alpha\big]^{n-2}\right]\right.\\ &\qquad\left.\Big(D(\phi)+F(\phi)\Big)\right\}. \end{aligned}$$

Similarly, for the functions $g_j^s(\psi,\phi)$ and $g_j^r(\psi,\phi)$,

$$g_j^0(\phi) := g_j^s(1,\phi) = \frac{f_j^0(\phi)}{\sqrt{2}\sqrt{1-\sin^2\alpha\cos^2\phi}}-\frac{f_j(1,\phi_0)\,\sin\alpha\cos\alpha\cos\phi}{4\sqrt{1-\sin^2\alpha\cos^2\phi}^{\,3}}, \qquad (4.2.68)$$

$$g_j^1(\phi) := g_j^r(1,\phi) = \frac{f_j^1(\phi)}{\sqrt{2}\sqrt{1-\sin^2\alpha\cos^2\phi}}-\frac{f_j(1,\phi_0)\,\left(\cos^2\alpha-\sin^2\alpha\cos^2\phi\right)}{4\sqrt{2}\,\sqrt{1-\sin^2\alpha\cos^2\phi}^{\,3}}. \qquad (4.2.69)$$

To evaluate the limit $\lim_{\psi\to 1}[\partial_\psi[g_j(\psi,\phi)]-g_j^0(\phi)/\sqrt{1-\psi}]$ using L'Hôpital's rule, it is necessary to take a closer look at the derivatives $\partial_\psi[f_j^s(\psi,\phi)]$ and $\partial_\psi[g_j^s(\psi,\phi)]$. For the first one (cf. (4.2.63)) a singularity $1/\sqrt{1-\psi}$ arises only in the terms where the exponential or $(A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2})^{1/2}$ is differentiated. Hence, it is easily shown that a function $F_j^s(\psi,\phi)$ exists that is uniformly bounded w.r.t. ψ in a neighbourhood of $\psi_0=1$, such that

$$\begin{aligned} \partial_\psi\big[f_j^s(\psi,\phi)\big] &= F_j^s(\psi,\phi)\\ &\quad+c_h\,\frac{k}{2}\big[\cos\alpha\,\psi\big]^n\,\frac{\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}}{\sqrt{1-\psi}}\\ &\quad\; e^{-k\sqrt{1-\psi}\,\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}}\left\{-\frac{E(\phi)\,\psi^2}{\sqrt{1+\psi}}\right.\\ &\qquad\left.+\frac{k}{2}\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}\,\Big(D(\phi)+F(\phi)\,\psi^2\Big)\right\}\\ &\quad+c_h\,\frac{k}{2}\,\mathbb{1}_{[1,\infty)}(n)\,H(\phi)\,\frac{\psi^n}{\sqrt{1+\psi}}\,\frac{\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}}{\sqrt{1-\psi}}\\ &\quad\; e^{-k\sqrt{1-\psi}\,\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}}\Big(D(\phi)+F(\phi)\,\psi^2\Big)\\ &\quad-c_h\,\frac{k}{4}\,\big[\cos\alpha\,\psi\big]^n\,e^{-k\sqrt{1-\psi}\,\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}}\\ &\quad\;\frac{C(\phi)\,\frac{\psi}{\sqrt{1-\psi^2}}}{\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}}\,\Big(D(\phi)+F(\phi)\,\psi^2\Big). \qquad (4.2.70) \end{aligned}$$

Similarly, a function $G_j^s(\psi,\phi)$, uniformly bounded w.r.t. ψ in a neighbourhood of $\psi_0 = 1$, can be found such that (cf. (4.2.66))

$$\partial_\psi\left[g_j^s(\psi,\phi)\right] = G_j^s(\psi,\phi) + \frac{\tilde{\chi}_\epsilon(\psi-1)\,\partial_\psi\left[f_j^s(\psi,\phi)\right]}{\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}} \tag{4.2.71}$$
$$+\frac{\tilde{\chi}_\epsilon(\psi-1)\,f_j^s(\psi,\phi)\,C(\phi)\,\frac{\psi}{\sqrt{1-\psi^2}}}{\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}^3}+\frac{\frac{3}{4}\,\tilde{\chi}_\epsilon(\psi-1)\,f_j(\psi,\phi)\,C(\phi)^2\,\frac{\psi^2}{(1+\psi)\sqrt{1-\psi}}}{\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}^5}.$$

Using L'Hôpital's rule, it can now be shown that (cf. (4.2.65))

$$\lim_{\psi\to 1}\left[\partial_\psi\left[g_j(\psi,\phi)\right]-\frac{g_j^0(\phi)}{\sqrt{1-\psi}}\right] = \lim_{\psi\to 1}\left[\frac{g_j^s(\psi,\phi)-g_j^0(\phi)}{\sqrt{1-\psi}}\right]+g_j^1(\phi)$$
$$= \lim_{\psi\to 1}\left[\partial_\psi\left[g_j^s(\psi,\phi)\right](-2)\sqrt{1-\psi}\right]+g_j^1(\phi).$$

Equation (4.2.71) thus implies that

$$\lim_{\psi\to 1}\left[\partial_\psi\left[g_j(\psi,\phi)\right]-\frac{g_j^0(\phi)}{\sqrt{1-\psi}}\right]$$
$$= g_j^1(\phi)-2\left\{\frac{\lim_{\psi\to 1}\left[\partial_\psi\left[f_j^s(\psi,\phi)\right]\sqrt{1-\psi}\right]}{\sqrt{A(\phi)}}+\frac{f_j^0(\phi)\,C(\phi)\,\frac{1}{\sqrt{2}}}{\sqrt{A(\phi)}^3}+\frac{\frac{3}{4}\,f_j(1,\phi)\,C(\phi)^2\,\frac{1}{2}}{\sqrt{A(\phi)}^5}\right\}.$$

Now, since $f_j(1,\phi) = f_j(1,\phi_0)$, (4.2.70), (4.2.67) and (4.2.58) yield

$$\lim_{\psi\to 1}\left[\partial_\psi\left[g_j(\psi,\phi)\right]-\frac{g_j^0(\phi)}{\sqrt{1-\psi}}\right]$$
$$= g_j^1(\phi)-2\Bigg[c_h\frac{k}{2}\cos^n\alpha\left\{-\frac{E(\phi)}{\sqrt{2}}+\frac{k}{2}\sqrt{A(\phi)}\Big(D(\phi)+F(\phi)\Big)\right\}$$
$$+c_h\frac{k}{2}\,\mathbb{1}_{[1,\infty)}(n)H(\phi)\frac{1}{\sqrt{2}}\Big(D(\phi)+F(\phi)\Big)$$
$$-c_h\frac{k}{4\sqrt{2}}\cos^n\alpha\frac{C(\phi)}{A(\phi)}\Big(D(\phi)+F(\phi)\Big)\Bigg]$$
$$-2\frac{C(\phi)}{\sqrt{A(\phi)}^3}\Bigg[c_h\cos^n\alpha\left\{-\frac{E(\phi)}{2}+\frac{k}{\sqrt{2}^3}\sqrt{A(\phi)}\Big(D(\phi)+F(\phi)\Big)\right\}$$
$$+c_h\,\mathbb{1}_{[1,\infty)}(n)H(\phi)\frac{1}{2}\Big(D(\phi)+F(\phi)\Big)\Bigg]$$
$$-\frac{3}{4}c_h\cos^n\alpha\frac{C(\phi)^2}{\sqrt{A(\phi)}^5}\Big(D(\phi)+F(\phi)\Big)$$
$$= g_j^1(\phi)+c_h\cos^n\alpha E(\phi)\left[\frac{k}{\sqrt{2}}+\frac{C(\phi)}{\sqrt{A(\phi)}^3}\right]$$
$$-c_h\cos^n\alpha\left[\frac{k^2}{2}\sqrt{A(\phi)}+\frac{k\,C(\phi)}{2\sqrt{2}\,A(\phi)}+\frac{3}{4}\frac{C(\phi)^2}{\sqrt{A(\phi)}^5}\right]\Big(D(\phi)+F(\phi)\Big)$$
$$-c_h\,\mathbb{1}_{[1,\infty)}(n)H(\phi)\left[\frac{k}{\sqrt{2}}+\frac{C(\phi)}{\sqrt{A(\phi)}^3}\right]\Big(D(\phi)+F(\phi)\Big), \tag{4.2.72}$$

which (cf. (4.2.69)) is uniformly bounded w.r.t. ϕ. ∎

Employing this lemma, $W^3_{1,j}$ (cf. (4.2.55) and (4.2.57)) is split into

$$W^3_{1,j} = W^{3.5}_j + W^{3.6}_j + W^{3.7}_j,$$

where

$$W^{3.5}_j := \int_0^{2\pi}\int_0^1 \frac{g_j(\psi,\phi) - g_j(1,\phi) + 2\,g^0_j(\phi)\,\sqrt{1-\psi}}{\sqrt{1-\psi}}\, e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi, \tag{4.2.73}$$

$$W^{3.6}_j := \int_0^{2\pi} g_j(1,\phi)\,\mathrm{d}\phi \int_0^1 \frac{e^{ikR\psi}}{\sqrt{1-\psi}}\,\mathrm{d}\psi, \tag{4.2.74}$$

and

$$W^{3.7}_j := -2\int_0^{2\pi} g^0_j(\phi)\,\mathrm{d}\phi \int_0^1 e^{ikR\psi}\,\mathrm{d}\psi = -2\int_0^{2\pi} g^0_j(\phi)\,\mathrm{d}\phi\,\frac{e^{ikR}-1}{ikR}. \tag{4.2.75}$$

Consider $W^{3.5}_j$ by applying integration by parts w.r.t. ψ. For this, note that by using L'Hôpital's rule once more, it can be shown that (cf. (4.2.65), (4.2.68) and (4.2.69))

$$\begin{aligned}
&\lim_{\psi\to 1}\left[\frac{g_j(\psi,\phi) - g_j(1,\phi) + 2\,g^0_j(\phi)\,\sqrt{1-\psi}}{1-\psi}\right] \\
&\qquad = \lim_{\psi\to 1} -\partial_\psi\left[g_j(\psi,\phi) - g_j(1,\phi) + 2\,g^0_j(\phi)\,\sqrt{1-\psi}\right] \\
&\qquad = \lim_{\psi\to 1} -\left[\partial_\psi\left[g_j(\psi,\phi)\right] - \frac{g^0_j(\phi)}{\sqrt{1-\psi}}\right]
\end{aligned}$$

is finite (cf. Lemma 4.5). Consequently,

$$\left|g_j(\psi,\phi) - g_j(1,\phi) + 2\,g^0_j(\phi)\,\sqrt{1-\psi}\right| \sim |1-\psi| \tag{4.2.76}$$

for $\psi \to 1$. Thus, keeping in mind that $g_j(0,\phi) = 0$ (cf. (4.2.57)) since $\tilde{\chi}_\epsilon(-1) = 0$, integration by parts w.r.t. ψ in (4.2.73) provides

$$\begin{aligned}
W^{3.5}_j = {}& \frac{1}{ikR}\int_0^{2\pi}\left[g_j(1,\phi) - 2\,g^0_j(\phi)\right]\mathrm{d}\phi \\
& - \frac{1}{ikR}\int_0^{2\pi}\int_0^1 \left\{\frac{\partial_\psi\left[g_j(\psi,\phi)\right] - \frac{g^0_j(\phi)}{\sqrt{1-\psi}}}{\sqrt{1-\psi}} + \frac{1}{2}\,\frac{g_j(\psi,\phi) - g_j(1,\phi) + 2\,g^0_j(\phi)\,\sqrt{1-\psi}}{\sqrt{1-\psi}^3}\right\} e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi,
\end{aligned}$$

where the integrand of the second integral on the right-hand side is absolutely integrable w.r.t. ψ and ϕ (cf. (4.2.72) and (4.2.76)). It follows that the Riemann-Lebesgue lemma can be applied, leading to

$$W^{3.5}_j = \frac{1}{ikR}\int_0^{2\pi}\left[g_j(1,\phi) - 2\,g^0_j(\phi)\right]\mathrm{d}\phi + o\left(\frac{1}{R}\right). \tag{4.2.77}$$

It remains to consider $W^{3.6}_j$ (cf. (4.2.74)). Using [32, Eqn. 16, p. 18 and 75] leads to

$$\begin{aligned}
\int_0^1 \frac{e^{ikR\psi}}{\sqrt{1-\psi}}\,\mathrm{d}\psi &= \sqrt{2\pi}\,\frac{\cos(kR)\,\tilde{C}(kR) + \sin(kR)\,\tilde{S}(kR)}{\sqrt{kR}} + i\sqrt{2\pi}\,\frac{\sin(kR)\,\tilde{C}(kR) - \cos(kR)\,\tilde{S}(kR)}{\sqrt{kR}} \\
&= \sqrt{\frac{2\pi}{k}}\,\left(\tilde{C}(kR) - i\tilde{S}(kR)\right)\,\frac{e^{ikR}}{\sqrt{R}},
\end{aligned}$$

where $\tilde{C}$ and $\tilde{S}$ are the Fresnel integrals. Furthermore, since (cf. [1, Eqns. 7.3.9 and 7.3.10, p. 88 and Eqns. 7.3.27 and 7.3.28, p. 89])

$$\tilde{C}(kR) \overset{R\to\infty}{\sim} \frac{1}{2} + \frac{\sin\left(\frac{\pi}{2}k^2R^2\right)}{\pi\, k\, R} + \mathcal{O}\left(\frac{1}{R^3}\right),$$
$$\tilde{S}(kR) \overset{R\to\infty}{\sim} \frac{1}{2} - \frac{\cos\left(\frac{\pi}{2}k^2R^2\right)}{\pi\, k\, R} + \mathcal{O}\left(\frac{1}{R^3}\right),$$

it follows that

$$\int\limits_0^1 \frac{e^{ikR\psi}}{\sqrt{1-\psi}}\,\mathrm{d}\psi = \sqrt{\pi}\,\frac{1-i}{\sqrt{2k}}\,\frac{e^{ikR}}{\sqrt{R}} + o\left(\frac{1}{R}\right).$$

Thus (cf. (4.2.77), (4.2.74) and (4.2.75))

$$\begin{aligned} W^3_{1,j} &= W^{3.5}_j + W^{3.6}_j + W^{3.7}_j \\ &= \frac{1}{ikR}\int\limits_0^{2\pi}\left[g_j(1,\phi) - 2\,g^0_j(\phi)\right]\,\mathrm{d}\phi + \sqrt{\pi}\int\limits_0^{2\pi} g_j(1,\phi)\,\mathrm{d}\phi\,\frac{1-i}{\sqrt{2k}}\,\frac{e^{ikR}}{\sqrt{R}} - 2\int\limits_0^{2\pi} g^0_j(\phi)\,\mathrm{d}\phi\,\frac{e^{ikR}-1}{ikR} + o\left(\frac{1}{R}\right) \\ &= \frac{1}{ikR}\int\limits_0^{2\pi} g_j(1,\phi)\,\mathrm{d}\phi + \sqrt{\pi}\int\limits_0^{2\pi} g_j(1,\phi)\,\mathrm{d}\phi\,\frac{1-i}{\sqrt{2k}}\,\frac{e^{ikR}}{\sqrt{R}} - 2\int\limits_0^{2\pi} g^0_j(\phi)\,\mathrm{d}\phi\,\frac{e^{ikR}}{ikR} + o\left(\frac{1}{R}\right). \end{aligned} \tag{4.2.78}$$

Using $f_j(1,\phi) = f_j(1,\phi_0)$ (cf. (4.2.34) and (4.2.22)), [1, Eqn. 17.2.6, p. 234] and (4.2.57) leads to

$$\begin{aligned} \int\limits_0^{2\pi} g_j(1,\phi)\,\mathrm{d}\phi &= \frac{f_j(1,\phi_0)}{\sqrt{2}}\int\limits_0^{2\pi}\frac{1}{\sqrt{1-\sin^2\alpha\cos^2\phi}}\,\mathrm{d}\phi = \sqrt{2}\,f_j(1,\phi_0)\int\limits_0^{\pi}\frac{1}{\sqrt{1-\sin^2\alpha\cos^2\phi}}\,\mathrm{d}\phi \\ &= \sqrt{2}\,f_j(1,\phi_0)\int\limits_0^{\pi}\frac{1}{\sqrt{1-\sin^2\alpha\sin^2\phi}}\,\mathrm{d}\phi \\ &= \sqrt{2}\,f_j(1,\phi_0)\,\tilde{F}(\pi\setminus\alpha), \end{aligned} \tag{4.2.79}$$

where $\tilde{F}$ denotes the elliptic integral of the first kind. For the last remaining integral $\int_0^{2\pi} g^0_j(\phi)\,\mathrm{d}\phi$, a closer look at (cf. (4.2.68), (4.2.67), (4.2.58) and (4.2.61))

$$\begin{aligned} g^0_j(\phi) &= \frac{f^0_j(\phi)}{\sqrt{2}\sqrt{1-\sin^2\alpha\cos^2\phi}} - \frac{f_j(1,\phi_0)\,\sin\alpha\cos\alpha\cos\phi}{4\sqrt{1-\sin^2\alpha\cos^2\phi}^3} \\ &= -\frac{c_h}{2}\,\frac{\cos^n\alpha\,E(\phi)}{\sqrt{1-\sin^2\alpha\cos^2\phi}} + c_h\,\frac{k}{2}\,\cos^n\alpha\,\Big(D(\phi)+F(\phi)\Big) \\ &\quad - \frac{c_h}{2}\,\frac{n!}{(n-1)!}\mathbb{1}_{[1,\infty)}(n)\,\big[\cos\alpha\big]^{n-1}\,\frac{\sin\alpha\,\cos\phi}{\sqrt{1-\sin^2\alpha\cos^2\phi}}\,\Big(D(\phi)+F(\phi)\Big) \\ &\quad - \frac{f_j(1,\phi_0)\,\sin\alpha\cos\alpha\cos\phi}{4\sqrt{1-\sin^2\alpha\cos^2\phi}^3} \end{aligned}$$

is necessary. Using (4.2.18), it is concluded that

$$\vec{n}^r(\psi,\phi) = \vec{v}_0(\alpha,\beta,\psi) + \cos\phi\,\vec{v}_1(\alpha,\beta,\sqrt{1-\psi^2}) + \sin\phi\,\vec{v}_2(\alpha,\beta,\sqrt{1-\psi^2}),$$

where $\vec{v}_0(\alpha,\beta,\psi)$, $\vec{v}_1(\alpha,\beta,\psi)$ and $\vec{v}_2(\alpha,\beta,\psi)$ are smooth vector valued functions. Moreover, equation (4.2.60) implies that $D(\phi)+F(\phi) = \big(\vec{m}\times\vec{e}^{\,0}\big)\times\vec{m}$. For the coefficient $E(\phi)$ of $\psi\sqrt{1-\psi^2}$ in (4.2.60), it is concluded that $E(\phi) = E_1\,\sin\phi + E_2\,\cos\phi$, with constants E_1 and E_2 only dependent on α, β and $\vec{e}^{\,0}$. Indeed, due to (4.2.18) the coefficient of $\cos^2\phi$ can arise only from those terms in $\big(\vec{v}_1\times\vec{e}^{\,0}\big)\times\vec{v}_1$, which do not contribute to the terms with factor $\cos\theta\sin\theta = \psi\sqrt{1-\psi^2}$. Similarly, the coefficients of $\sin^2\phi$ and 1 do not contribute to the terms with factor $\psi\sqrt{1-\psi^2}$, i.e., to $E(\phi)$.

Hence

$$\begin{aligned}\int_0^{2\pi} g_j^0(\phi)\,\mathrm{d}\phi = \int_0^{2\pi} \Bigg\{ &-\frac{c_h}{2}\,\frac{\cos^n\alpha\, E(\phi)}{\sqrt{1-\sin^2\alpha\cos^2\phi}} + c_h\,\frac{k}{2}\,\cos^n\alpha\ \left[\left(\vec{m}\times\vec{e}^{\,0}\right)\times\vec{m}\right] \\ &-\frac{c_h}{2}\,\frac{n!}{(n-1)!}\mathbb{1}_{[1,\infty)}(n)\left[\cos\alpha\right]^{n-1}\frac{\sin\alpha\,\cos\phi}{\sqrt{1-\sin^2\alpha\cos^2\phi}}\ \left[\left(\vec{m}\times\vec{e}^{\,0}\right)\times\vec{m}\right] \\ &-\frac{f_j(1,\phi_0)\,\sin\alpha\cos\alpha\cos\phi}{4\sqrt{1-\sin^2\alpha\cos^2\phi}^{\,3}}\Bigg\}\,\mathrm{d}\phi \\ = c_h\,\pi k\cos^n\alpha\ &\left[\left(\vec{m}\times\vec{e}^{\,0}\right)\times\vec{m}\right],\end{aligned}$$

since for any fixed $m\in\mathbb{R}$ and any c_1, c_2

$$\begin{aligned}\int_0^{2\pi}\frac{c_1\,\sin\phi + c_2\,\cos\phi}{\sqrt{1-\sin^2\alpha\cos^2\phi}^{\,m}}\,\mathrm{d}\phi &= \int_0^{\pi}\frac{c_1\,\sin\phi + c_2\,\cos\phi}{\sqrt{1-\sin^2\alpha\cos^2\phi}^{\,m}}\,\mathrm{d}\phi + \int_0^{\pi}\frac{c_1\,\sin(\phi+\pi) + c_2\,\cos(\phi+\pi)}{\sqrt{1-\sin^2\alpha\cos^2(\phi+\pi)}^{\,m}}\,\mathrm{d}\phi \\ &= \int_0^{\pi}\frac{c_1\,\sin\phi + c_2\,\cos\phi}{\sqrt{1-\sin^2\alpha\cos^2\phi}^{\,m}}\,\mathrm{d}\phi + \int_0^{\pi}\frac{-c_1\,\sin\phi - c_2\,\cos\phi}{\sqrt{1-\sin^2\alpha\cos^2\phi}^{\,m}}\,\mathrm{d}\phi \\ &= 0.\end{aligned}$$

Consequently, since (cf. (4.2.2) and (4.2.34))

$$f_j(1,\phi_0) = i\,\frac{\Delta\,k^2}{4\pi\epsilon_0}\,m_z^n\ \left[\left(\vec{m}\times\vec{e}^{\,0}\right)\times\vec{m}\right],$$

$m_z = \cos\alpha$ (cf. (4.2.17)) and in view of (4.2.59), (4.2.78) and (4.2.79)

$$\begin{aligned}W_{1,j}^3 &= \sqrt{2}\,f_j(1,\phi_0)\,\tilde{F}(\pi\setminus\alpha)\left(\frac{1}{ikR} + \sqrt{\pi}\,\frac{1-i}{\sqrt{2k}}\,\frac{e^{ikR}}{\sqrt{R}}\right) - i\,\frac{\Delta k^3}{2\epsilon_0}\,\cos^n\alpha\ \left[\left(\vec{m}\times\vec{e}^{\,0}\right)\times\vec{m}\right]\,\frac{e^{ikR}}{ikR} \\ &\quad + o\left(\frac{1}{R}\right) \\ &= i\,\frac{\Delta\,k^2}{4\pi\epsilon_0}\,\tilde{F}(\pi\setminus\alpha)\,m_z^n\ \left[\left(\vec{m}\times\vec{e}^{\,0}\right)\times\vec{m}\right]\left(\frac{\sqrt{2}}{ikR} + \sqrt{\pi}\,\frac{1-i}{\sqrt{k}}\,\frac{e^{ikR}}{\sqrt{R}}\right) \\ &\quad - i\,\frac{\Delta k^3}{2\epsilon_0}\,m_z^n\ \left[\left(\vec{m}\times\vec{e}^{\,0}\right)\times\vec{m}\right]\,\frac{e^{ikR}}{ikR} + o\left(\frac{1}{R}\right).\end{aligned} \tag{4.2.80}$$

Estimate of $W_{2,j}^3$:

Next $W_{2,j}^3$ is examined (cf. (4.2.54)).

$$W_{2,j}^3 = \int_0^{2\pi}\int_0^1 \chi_\epsilon\big(kn'(\psi,\phi) - k\nu'\big)\,h_{2,j}\big(n'(\psi,\phi)\big)\,e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi.$$

The cut-off function is defined the same way as in the case of $\ell = 1$. Recall that the modified Bessel function $K_0\big(k\,|n'-\nu'|\big)$ in $h_{2,j}\big(n'(\psi,\phi)\big)$ (cf. (4.2.3)) has a logarithmic singularity of the form $-\log\big(\frac{k}{2}\,|n'-\nu'|\big)$ (cf. [1, Eqn. 9.6.13, p. 119]), which, as seen above (cf. (4.2.56)), can be transformed to

$$\begin{aligned}\log\left(\frac{k}{2}\,|n'-\nu'|\right) = \frac{1}{2}\,\log(1-\psi) + \frac{1}{2}\,\log\Bigg[\frac{k^2}{4}\Big(&2 - 2\sin^2\alpha\cos^2\phi - 2\sin\alpha\cos\alpha\cos\phi\,\sqrt{1-\psi^2} \\ &+ (1-\psi)\left(\sin^2\alpha\cos^2\phi - \cos^2\alpha\right)\Big)\Bigg].\end{aligned} \tag{4.2.81}$$

Define (cf. (4.2.3))

$$h_j(\psi,\phi) := c_h k\, \tilde{\chi}_\epsilon(\psi-1)\sqrt{1-n'^2}^{\,n} \left[\left(\vec{n}^r \times \vec{e}^0\right) \times \vec{n}^r\right] K_0\left(k\,|n'-\nu'|\right)$$
$$+ c_h k\, m_z^n \left[\left(\vec{m} \times \vec{e}^0\right) \times \vec{m}\right] \frac{1}{2}\log\left(1-\psi\right),$$

where c_h is the same as in (4.2.59). With this and (cf. [1, Eqns. 9.6.13 and 9.6.12, p. 119] and (4.2.81))

$$\begin{aligned} K_0\left(k\,|n'-\nu'|\right) &= -\log\left(\frac{k}{2}\,|n'-\nu'|\right) - \tilde{\gamma} + \mathcal{O}\left(\log|n'-\nu'|\,|n'-\nu'|^2\right) \\ &= -\frac{1}{2}\log\left(1-\psi\right) - \tilde{\gamma} + \mathcal{O}\left(\log|n'-\nu'|\,|n'-\nu'|^2\right) \\ &\quad - \frac{1}{2}\log\Bigg[\frac{k^2}{4}\Big(2 - 2\sin^2\alpha\cos^2\phi - 2\sin\alpha\cos\alpha\cos\phi\sqrt{1-\psi^2} \\ &\qquad + (1-\psi)\left(\sin^2\alpha\cos^2\phi - \cos^2\alpha\right)\Big)\Bigg], \end{aligned} \tag{4.2.82}$$

where $\tilde{\gamma}$ is Euler's constant, it follows that

$$h_j(1,\phi) := \lim_{\psi\nearrow 1} h_j(\psi,\phi) = -c_h k\, m_z^n \left[\left(\vec{m} \times \vec{e}^0\right) \times \vec{m}\right] \left\{\tilde{\gamma} + \frac{1}{2}\log\left[\frac{k^2}{2}\left(1-\sin^2\alpha\cos^2\phi\right)\right]\right\}.$$

Similar to $W^3_{1,j}$, the integral $W^3_{2,j}$ is split as

$$W^3_{2,j} = W^{3,8}_j + W^{3,9}_j, \tag{4.2.83}$$

where

$$W^{3,8}_j := \int_0^{2\pi}\int_0^1 h_j(\psi,\phi)\, e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi$$

and

$$W^{3,9}_j := -c_h k\,\pi\, m_z^n \left[\left(\vec{m} \times \vec{e}^0\right) \times \vec{m}\right] \int_0^1 \log(1-\psi)\, e^{ikR\psi}\,\mathrm{d}\psi. \tag{4.2.84}$$

Once more, integration by parts w.r.t. ψ is applied to examine the asymptotic behaviour of $W^{3,8}_j$. Recalling that $\tilde{\chi}_\epsilon(-1) = 0$,

$$\begin{aligned} W^{3,8}_j &= -c_h k\, m_z^n \left[\left(\vec{m} \times \vec{e}^0\right) \times \vec{m}\right] \int_0^{2\pi} \left\{\tilde{\gamma} + \frac{1}{2}\log\left(\frac{k^2}{2}\right) + \frac{1}{2}\log\left(1-\sin^2\alpha\cos^2\phi\right)\right\}\mathrm{d}\phi\, \frac{e^{ikR}}{ikR} \\ &\quad - \frac{1}{ikR}\int_0^{2\pi}\int_0^1 \partial_\psi\left[h_j(\psi,\phi)\right] e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi. \end{aligned} \tag{4.2.85}$$

To show that the last integral on the right-hand side tends to zero with order $o(1/R)$, it is necessary to show that $\partial_\psi[h_j(\psi,\phi)]$ is absolutely integrable w.r.t. $\psi \in [0,1]$. Consider (cf. [1, Eqn. 9.6.27, p. 120] and (4.2.30))

$$\begin{aligned} \partial_\psi\left[h_j(\psi,\phi)\right] &= c_h k\, \tilde{\chi}'_\epsilon(\psi-1)\sqrt{1-n'^2}^{\,n} \left[\left(\vec{n}^r \times \vec{e}^0\right) \times \vec{n}^r\right] K_0\left(k\,|n'-\nu'|\right) \\ &\quad + c_h k\, \tilde{\chi}_\epsilon(\psi-1)\partial_\psi\left[n'(\psi,\phi)\right] \cdot \nabla_{n'}\left[\sqrt{1-n'^2}^{\,n} \left[\left(\vec{n}^r \times \vec{e}^0\right) \times \vec{n}^r\right]\right] K_0\left(k\,|n'-\nu'|\right) \\ &\quad - c_h k\, \tilde{\chi}_\epsilon(\psi-1)\sqrt{1-n'^2}^{\,n} \left[\left(\vec{n}^r \times \vec{e}^0\right) \times \vec{n}^r\right] k\,\partial_\psi\left[\,|n'-\nu'|\,\right] K_1\left(k\,|n'-\nu'|\right) \\ &\quad - c_h \frac{k}{2}\, m_z^n \left[\left(\vec{m} \times \vec{e}^0\right) \times \vec{m}\right] \frac{1}{1-\psi}. \end{aligned} \tag{4.2.86}$$

Recall that $\tilde{\chi}_\epsilon$ was defined in such a way that $\tilde{\chi}_\epsilon' \equiv 0$ in a neighbourhood of zero. Consequently the first term on the right-hand side of (4.2.86) is uniformly bounded w.r.t. $\psi \in [0,1]$ and thus absolutely integrable. The second term, on the other hand, is absolutely bounded for $\psi \in [0,1]$ by the integrable function (cf. (4.2.82))

$$c\left(1+\frac{1}{\sqrt{1-\psi}}+\frac{\log(1-\psi)}{\sqrt{1-\psi}}\right),$$

since $\nabla_{n'}[\sqrt{1-n'^2}^{\,n}\ [(\vec{n}^r\times\vec{e}^{\,0})\times\vec{n}^r]]$ is uniformly bounded w.r.t. ψ and ϕ. Indeed, $n_z^r(\psi,\phi)=\sqrt{1-n'(\psi,\phi)^2}>0$ for all $\psi\in\operatorname{supp}\tilde{\chi}_\epsilon$. It remains to consider the last two terms in (4.2.86). For this the series expansion of K_1 is needed (cf. [1, Eqns. 9.6.11 and 9.6.10, p. 119] and [1, Eqn. 6.3.2, p. 79])

$$K_1\left(k\,|n'-\nu'|\right)=\frac{1}{k\,|n'-\nu'|}+\frac{1}{4}\left[2\log\left(\frac{k}{2}\,|n'-\nu'|\right)+2\tilde{\gamma}-1\right]k\,|n'-\nu'|+o\left(|n'-\nu'|^2\right), \quad (4.2.87)$$

as well as the derivative (cf. (4.2.56))

$$\begin{aligned}\partial_\psi\left[\,|n'-\nu'|\,\right]&=-\frac{1}{2}\frac{\sqrt{2-2\sin^2\alpha\cos^2\phi-2\sin\alpha\cos\alpha\cos\phi\sqrt{1-\psi^2}+(1-\psi)\left(\sin^2\alpha\cos^2\phi-\cos^2\alpha\right)}}{\sqrt{1-\psi}}\\&\quad+\frac{1}{2}\frac{2\sin\alpha\cos\alpha\cos\phi\,\frac{\psi}{\sqrt{1+\psi}}-\sqrt{1-\psi}\left(\sin^2\alpha\cos^2\phi-\cos^2\alpha\right)}{\sqrt{2-2\sin^2\alpha\cos^2\phi-2\sin\alpha\cos\alpha\cos\phi\sqrt{1-\psi^2}+(1-\psi)\left(\sin^2\alpha\cos^2\phi-\cos^2\alpha\right)}}\\&=-\frac{1}{2}\frac{|n'-\nu'|}{1-\psi}\\&\quad+\frac{1}{2}\frac{2\sin\alpha\cos\alpha\cos\phi\,\frac{\psi}{\sqrt{1+\psi}}-\sqrt{1-\psi}\left(\sin^2\alpha\cos^2\phi-\cos^2\alpha\right)}{\sqrt{2-2\sin^2\alpha\cos^2\phi-2\sin\alpha\cos\alpha\cos\phi\sqrt{1-\psi^2}+(1-\psi)\left(\sin^2\alpha\cos^2\phi-\cos^2\alpha\right)}},\end{aligned} \quad (4.2.88)$$

where the last denominator is bounded. Indeed, $\sqrt{1-\psi}$ is the singular factor in the term $|n'(\psi,\phi)-\nu'|$ (cf. (4.2.56)) in the neighbourhood that is not cut-off by the factor $\tilde{\chi}_\epsilon(\psi-1)$, while the denominator equals $|n'(\psi,\phi)-\nu'|/\sqrt{1-\psi}$. Since the last two terms on the right-hand side of (4.2.86) are bounded for any $\psi\in[0,1)$, it remains to examine the limit $\psi\nearrow 1$ of the two, by using (4.2.87) and (4.2.88). For $\psi\nearrow 1$, this leads to

$$\begin{aligned}&-c_hk\,\tilde{\chi}_\epsilon(\psi-1)\sqrt{1-n'^2}^{\,n}\ \left[\left(\vec{n}^r\times\vec{e}^{\,0}\right)\times\vec{n}^r\right]\,k\,\partial_\psi\left[\,|n'-\nu'|\,\right]K_1\left(k\,|n'-\nu'|\right)\\&-c_h\frac{k}{2}\,m_z^n\ \left[\left(\vec{m}\times\vec{e}^{\,0}\right)\times\vec{m}\right]\,\frac{1}{1-\psi}\\&\qquad\sim-c_h\frac{k}{2}\,m_z^n\ \left[\left(\vec{m}\times\vec{e}^{\,0}\right)\times\vec{m}\right]\left\{\frac{1}{1-\psi}+2k\,\partial_\psi\left[\,|n'-\nu'|\,\right]K_1\left(k\,|n'-\nu'|\right)\right\}\\&\qquad=-c_h\frac{k}{2}\,m_z^n\ \left[\left(\vec{m}\times\vec{e}^{\,0}\right)\times\vec{m}\right]\left\{\mathcal{O}\left(\frac{1}{\sqrt{1-\psi}}\right)+\mathcal{O}\left(|\log(1-\psi)|\right)+\mathcal{O}\left(1\right)+\mathcal{O}\left(|\sqrt{1-\psi}|\right)\right\},\end{aligned}$$

where $\lim_{\psi\nearrow 1}\sqrt{1-n'(\psi,\phi)^2}=\lim_{\psi\nearrow 1}n_z^r(\psi,\phi)=m_z$. Thus $\partial_\psi[h_j(\psi,\phi)]$ (cf. (4.2.86)) is absolutely integrable w.r.t. $\psi\in[0,1]$. Furthermore, using the Riemann-Lebesgue lemma, this shows that the integral w.r.t. ψ on the right-hand side of (4.2.85) converges to zero with the order $o(1)$ for $R\to\infty$. Since the integral w.r.t. ψ is also uniformly bounded w.r.t. R and ϕ, Lebesgue's theorem can be applied to show that this convergence order also holds for the integral w.r.t. ϕ. Hence

$$\begin{aligned}W_j^{3,8}&=-c_hk\,m_z^n\ \left[\left(\vec{m}\times\vec{e}^{\,0}\right)\times\vec{m}\right]\int_0^{2\pi}\left\{\tilde{\gamma}+\frac{1}{2}\log\left(\frac{k^2}{2}\right)+\frac{1}{2}\log\left(1-\sin^2\alpha\cos^2\phi\right)\right\}\mathrm{d}\phi\,\frac{e^{ikR}}{ikR}+o\left(\frac{1}{R}\right)\\&=-c_hk\,m_z^n\ \left[\left(\vec{m}\times\vec{e}^{\,0}\right)\times\vec{m}\right]\left\{2\pi\tilde{\gamma}+\pi\log\left(\frac{k^2}{2}\right)+\int_0^{\pi}\log\left(1-\sin^2\alpha\cos^2\phi\right)\mathrm{d}\phi\right\}\frac{e^{ikR}}{ikR}+o\left(\frac{1}{R}\right).\end{aligned} \quad (4.2.89)$$

Claim 4.1. The remaining integral can be evaluated as

$$\int_0^\pi \log\left(1 - \sin^2\alpha\cos^2\phi\right)\,\mathrm{d}\phi = 4\pi\log\left(\cos\frac{\alpha}{2}\right). \tag{4.2.90}$$

Proof. It is easily seen that (4.2.90) holds true for $\alpha = 0$. Thus, if the derivatives w.r.t. α of the two sides of (4.2.90) are equal, then (4.2.90) follows. Applying the derivative w.r.t. α to (4.2.90) leads to

$$-2\sin\alpha\cos\alpha\int_0^\pi \frac{\cos^2\phi}{1-\sin^2\alpha\cos^2\phi}\,\mathrm{d}\phi = -2\pi\tan\left(\frac{\alpha}{2}\right). \tag{4.2.91}$$

To evaluate the integral on the left-hand side of (4.2.91), $\tan(\phi/2)$ is substituted by u, with which

$$\begin{aligned}\cos\phi = \cos\left(2\,\frac{\phi}{2}\right) &= \cos^2\left(\frac{\phi}{2}\right) - \sin^2\left(\frac{\phi}{2}\right)\\ &= \frac{\cos^2\left(\frac{\phi}{2}\right)-\sin^2\left(\frac{\phi}{2}\right)}{\cos^2\left(\frac{\phi}{2}\right)+\sin^2\left(\frac{\phi}{2}\right)} = \frac{1-\tan^2\left(\frac{\phi}{2}\right)}{1+\tan^2\left(\frac{\phi}{2}\right)} = \frac{1-u^2}{1+u^2}\end{aligned}$$

and

$$\mathrm{d}u = \frac{1}{2}\frac{1}{\cos^2\left(\frac{\phi}{2}\right)}\,\mathrm{d}\phi, \qquad \mathrm{d}\phi = 2\cos^2\left(\frac{\phi}{2}\right)\mathrm{d}u = 2\frac{\cos^2\left(\frac{\phi}{2}\right)}{\cos^2\left(\frac{\phi}{2}\right)+\sin^2\left(\frac{\phi}{2}\right)}\,\mathrm{d}u = \frac{2}{1+u^2}\,\mathrm{d}u.$$

This leads to

$$-\int_0^\infty \frac{4\sin\alpha\cos\alpha\left(\frac{1-u^2}{1+u^2}\right)^2}{(1+u^2)\left[1-\sin^2\alpha\left(\frac{1-u^2}{1+u^2}\right)^2\right]}\,\mathrm{d}u = -\int_0^\infty \frac{4\sin\alpha\cos\alpha\,(1-u^2)^2}{(1+u^2)\left[(1+u^2)^2-\sin^2\alpha(1-u^2)^2\right]}\,\mathrm{d}u.$$

Furthermore, it is easily confirmed that

$$(1+u^2)^2 - \sin^2\alpha(1-u^2)^2 = (1-\sin^2\alpha)(u_0^2+u^2)\left(\frac{1}{u_0^2}+u^2\right),$$

where $u_0 := \sqrt{(1-\sin\alpha)/(1+\sin\alpha)}$. Using this for a partial fraction decomposition it can be shown that

$$\begin{aligned}&-4\sin\alpha\cos\alpha\int_0^\infty \frac{\left(\frac{1-u^2}{1+u^2}\right)^2}{(1+u^2)\left[1-\sin^2\alpha\left(\frac{1-u^2}{1+u^2}\right)^2\right]}\,\mathrm{d}u\\ &= -\frac{4\sin\alpha\cos\alpha}{1-\sin^2\alpha}\int_0^\infty \frac{(1-u^2)^2}{(1+u^2)\,(u_0^2+u^2)\left(\frac{1}{u_0^2}+u^2\right)}\,\mathrm{d}u\\ &= -\frac{4\sin\alpha\cos\alpha}{1-\sin^2\alpha}\int_0^\infty \Bigg\{-\frac{4u_0^2}{(1-u_0^2)^2}\,\frac{1}{1+u^2} + u_0^2\,\frac{(1+u_0^2)^2}{(1-u_0^2)(1-u_0^4)}\,\frac{1}{u_0^2+u^2}\\ &\qquad\qquad + \frac{(1+u_0^2)^2}{(1-u_0^2)(1-u_0^4)}\,\frac{1}{\frac{1}{u_0^2}+u^2}\Bigg\}\,\mathrm{d}u\\ &= -\frac{4\sin\alpha\cos\alpha}{1-\sin^2\alpha}\left\{-\frac{4u_0^2}{(1-u_0^2)^2}\,\frac{\pi}{2} + u_0^2\,\frac{(1+u_0^2)^2}{(1-u_0^2)(1-u_0^4)}\,\frac{1}{u_0}\,\frac{\pi}{2} + \frac{(1+u_0^2)^2}{(1-u_0^2)(1-u_0^4)}\,u_0\,\frac{\pi}{2}\right\}\\ &= -4\pi\tan\alpha\left\{-\frac{2u_0^2}{(1-u_0^2)^2} + u_0\,\frac{1+u_0^2}{1-u_0^2}\,\frac{1+u_0^2}{1-u_0^4}\right\}\end{aligned}$$

$$
\begin{aligned}
&= -4\pi \tan\alpha \left\{ \frac{-2\frac{1-\sin\alpha}{1+\sin\alpha}}{4\frac{\sin^2\alpha}{(1+\sin\alpha)^2}} + \sqrt{\frac{1-\sin\alpha}{1+\sin\alpha}}\,\frac{1}{\sin\alpha}\,\frac{1+\sin\alpha}{2\sin\alpha} \right\} \\
&= -4\pi \tan\alpha \left\{ \frac{1}{2}\frac{\cos\alpha}{\sin^2\alpha}(1-\cos\alpha) \right\} \\
&= -2\pi \frac{1-\cos\alpha}{\sin\alpha} \\
&= -2\pi \tan\left(\frac{\alpha}{2}\right),
\end{aligned}
$$

which proves equation (4.2.91) and thus (4.2.90). ■

Hence, (cf. (4.2.89))

$$
W_j^{3,8} = -c_h k\, m_z^n \left[\left(\vec{m} \times \vec{e}^{\,0}\right) \times \vec{m} \right] \left\{ 2\pi\tilde{\gamma} + \pi \log\left(\frac{k^2}{2}\right) + 4\pi \log\left(\cos\frac{\alpha}{2}\right) \right\} \frac{e^{ikR}}{ikR} + o\left(\frac{1}{R}\right). \tag{4.2.92}
$$

Finally, consider $W_j^{3,9}$ (cf. (4.2.84)) using [32, Eqn. 116, p. 28 and 83]

$$
\begin{aligned}
W_j^{3,9} &= -c_h k\, \pi\, m_z^n \left[\left(\vec{m} \times \vec{e}^{\,0}\right) \times \vec{m} \right] \int_0^1 \log(1-\psi)\, e^{ikR\psi}\, \mathrm{d}\psi \\
&= -c_h k\, \pi\, m_z^n \left[\left(\vec{n}^r \times \vec{e}^{\,0}\right) \times \vec{n}^r \right] \left[\mathrm{Ci}(kR) - \tilde{\gamma} - \log(kR) - i\,\mathrm{Si}(kR) \right] \frac{e^{ikR}}{ikR}.
\end{aligned}
$$

Moreover, since (cf. [1, Eqns. 5.2.8, 5.2.9, 5.2.34 and 5.2.35, p. 60 and 61])

$$
\mathrm{Ci}(kR) \overset{R\to\infty}{\sim} \mathcal{O}\left(\frac{1}{R}\right), \qquad \mathrm{Si}(kR) \overset{R\to\infty}{\sim} \frac{\pi}{2} + \mathcal{O}\left(\frac{1}{R}\right),
$$

it follows that

$$
W_j^{3,9} = c_h k\, \pi\, m_z^n \left[\left(\vec{n}^r \times \vec{e}^{\,0}\right) \times \vec{n}^r \right] \left[\tilde{\gamma} + \log(kR) + i\frac{\pi}{2} \right] \frac{e^{ikR}}{ikR} + o\left(\frac{1}{R}\right)
$$

and (cf. (4.2.83), (4.2.92) and (4.2.59))

$$
\begin{aligned}
W_{2,j}^3 &= W_j^{3,8} + W_j^{3,9} \\
&= -c_h k\, \pi\, m_z^n \left[\left(\vec{m} \times \vec{e}^{\,0}\right) \times \vec{m} \right] \left\{ 2\tilde{\gamma} + \log\left(\frac{k^2}{2}\right) + 4 \log\left(\cos\frac{\alpha}{2}\right) \right\} \frac{e^{ikR}}{ikR} \\
&\quad + c_h k\, \pi\, m_z^n \left[\left(\vec{n}^r \times \vec{e}^{\,0}\right) \times \vec{n}^r \right] \left[\tilde{\gamma} + \log(kR) + i\frac{\pi}{2} \right] \frac{e^{ikR}}{ikR} + o\left(\frac{1}{R}\right) \\
&= i\,\frac{\Delta\, k^3}{4\,\epsilon_0}\, m_z^n \left[\left(\vec{m} \times \vec{e}^{\,0}\right) \times \vec{m} \right] \left[\log R - \tilde{\gamma} - \log\left(\frac{k}{2}\right) - 4\log\left(\cos\frac{\alpha}{2}\right) + i\frac{\pi}{2} \right] \frac{e^{ikR}}{ikR} + o\left(\frac{1}{R}\right)
\end{aligned} \tag{4.2.93}
$$

4.2.4.3 Singularity outside unit disc

Next, the case that $|k+\tilde{\omega}'_{\ell,j}|/k > 1$ is considered. For this purpose, the substitution to polar coordinates, used in the first line of (4.2.9), leads to (cf. (4.2.8))

$$
W_{\ell,j}^3 = \int_{\phi_0-\pi}^{\phi_0+\pi} \int_1^\infty \chi_\epsilon(k\rho n_0' - k\nu')\, \frac{\tilde{f}_{\ell,j}(\rho n_0')}{|\rho n_0' - \nu'|}\, \frac{\rho}{\sqrt{1-\rho^2}}\, e^{ik\rho R n_0' \cdot m'}\, e^{-kR m_z \sqrt{\rho^2-1}}\, \mathrm{d}\rho\, \mathrm{d}\phi,
$$

where (cf. (4.2.2)–(4.2.5))

$$
\tilde{f}_{\ell,j}(\rho n_0') := h_{\ell,j}(\rho n_0')\; |\rho n_0' - \nu'|\,, \qquad \ell = 1, \ldots, 4
$$

is uniformly bounded w.r.t. ρ and ϕ on compact sets. Note that, since the support of the cut-off function $(\rho, n_0') \mapsto \chi_\epsilon(k\rho n_0' - k\nu')$ is located completely outside the unit circle around zero, there exists a constant $\delta > 0$ such that $\sqrt{\rho^2 - 1} \geq \delta$ for all $k\rho n_0' - k\nu' \in \operatorname{supp}\chi_\epsilon$. Thus, for $R \geq 1$,

$$\left|W^3_{\ell,j}\right| \leq \frac{c}{\delta} \int_{\phi_0-\pi}^{\phi_0+\pi} \int_1^\infty \frac{|\chi_\epsilon(k\rho n_0' - k\nu')|}{|\rho n_0' - \nu'|} \,\mathrm{d}\rho\,\mathrm{d}\phi\, e^{-kRm_z\delta} = o\left(\frac{1}{R}\right), \tag{4.2.94}$$

since $|\rho n_0' - \nu'|^{-1}$ is locally integrable w.r.t. ρ and ϕ.

4.2.4.4 The three cases together

Finally, combining (4.2.33), (4.2.52), (4.2.53), (4.2.80), (4.2.93) and (4.2.94),

$$\begin{aligned}
W^3_{\ell,j} &= \mathbb{1}_{k'+\tilde\omega'_{\ell,j}}(km') \left\{ \delta_{1\ell}\, W^3_{1,j} + \delta_{2\ell}\, W^3_{2,j} + 2\pi \Big[\delta_{3\ell}\, h_{3,j}(m') + \delta_{4\ell}\, h_{4,j}(m')\Big] \frac{e^{ikR}}{ikR} \right\} + o\left(\frac{1}{R}\right)\\
&= \mathbb{1}_{k'+\tilde\omega'_{\ell,j}}(km') \Bigg\{ i\,\delta_{1\ell}\, \frac{\Delta\, k^2}{4\pi\epsilon_0}\, m_z^n\, \tilde F(\pi\setminus\alpha)\, \left[\left(\vec m \times \vec e^{\,0}\right) \times \vec m\right] \left(\frac{\sqrt2}{ikR} + \sqrt{\pi}\frac{1-i}{\sqrt{k}}\,\frac{e^{ikR}}{\sqrt{R}} \right)\\
&\quad - i\,\delta_{1\ell}\, \frac{\Delta k^3}{2\epsilon_0}\, m_z^n\, \left[\left(\vec m \times \vec e^{\,0}\right) \times \vec m\right] \frac{e^{ikR}}{ikR}\\
&\quad + i\,\delta_{2\ell}\, \frac{\Delta\, k^3}{4\,\epsilon_0}\, m_z^n\, \left[\left(\vec m \times \vec e^{\,0}\right) \times \vec m\right] \left[\log R - \tilde\gamma - \log\left(\frac{k}{2}\right) - 4\log\left(\cos\frac{\alpha}{2}\right) + i\frac{\pi}{2}\right] \frac{e^{ikR}}{ikR}\\
&\quad + 2\pi \Big[\delta_{3\ell}\, h_{3,j}(m') + \delta_{4\ell}\, h_{4,j}(m')\Big] \frac{e^{ikR}}{ikR} \Bigg\} + o\left(\frac{1}{R}\right),
\end{aligned} \tag{4.2.95}$$

no matter if the point n' with $kn' = k' + \tilde\omega'_{\ell,j}$ is located inside or outside the unit circle and where $\delta_{m\ell}$ is defined as the Kronecker delta.

In conclusion this shows that (cf. (4.2.6), (4.2.15), (4.2.32) and (4.2.95))

$$\begin{aligned}
&\int_{\mathbb{R}^2} \frac{h_{\ell,j}(n')}{n_z^r}\, e^{ik\vec n^r\cdot\vec x}\,\mathrm{d}n'\\
&\quad = W^1_{\ell,j} + W^2_{\ell,j} + W^3_{\ell,j}\\
&\quad = 2\pi\, \mathbb{1}_{\{1,2\}}(\ell) \left(1 - \mathbb{1}_{k'+\tilde\omega'_{\ell,j}}(km')\right) h_{\ell,j}(m')\, \frac{e^{ikR}}{ikR} + 2\pi\, \mathbb{1}_{\{3,4\}}(\ell)\, h_{\ell,j}(m')\, \frac{e^{ikR}}{ikR}\\
&\qquad + i\,\delta_{1\ell}\, \mathbb{1}_{k'+\tilde\omega'_{1,j}}(km')\, \frac{\Delta\, k^2}{4\pi\epsilon_0}\, m_z^n\, \tilde F(\pi\setminus\alpha)\, \left[\left(\vec m \times \vec e^{\,0}\right) \times \vec m\right] \left(\frac{\sqrt2}{ikR} + \sqrt{\pi}\frac{1-i}{\sqrt{k}}\,\frac{e^{ikR}}{\sqrt{R}} \right)\\
&\qquad - i\,\delta_{1\ell}\, \mathbb{1}_{k'+\tilde\omega'_{1,j}}(km')\, \frac{\Delta k^3}{2\epsilon_0}\, m_z^n\, \left[\left(\vec m \times \vec e^{\,0}\right) \times \vec m\right] \frac{e^{ikR}}{ikR}\\
&\qquad + i\,\delta_{2\ell}\, \mathbb{1}_{k'+\tilde\omega'_{2,j}}(km')\, \frac{\Delta\, k^3}{4\,\epsilon_0}\, m_z^n\, \left[\left(\vec m \times \vec e^{\,0}\right) \times \vec m\right]\\
&\qquad\qquad \left[\log R - \tilde\gamma - \log\left(\frac{k}{2}\right) - 4\log\left(\cos\frac{\alpha}{2}\right) + i\frac{\pi}{2}\right] \frac{e^{ikR}}{ikR} + o\left(\frac{1}{R}\right).
\end{aligned}$$

This gives the asymptotics of one term in (4.2.1). From the uniform and absolute convergence of the summation in (4.2.1) (cf. Thm. 3.1), it is obvious that the asymptotic limit and the summation in (4.2.1) can be interchanged.

Finally the formulas for E_ℓ, for $\ell = 1, \ldots, 4$,

$$E_\ell = \sum_{n\in\mathbb{N}_0} \sum_{j\in\mathbb{Z}} \Bigg\{ 2\pi\, \mathbb{1}_{\{1,2\}}(\ell) \int_0^1 \tilde\lambda^n_{\ell,j}\, \frac{(-ik\zeta)^n}{n!}\,\mathrm{d}\zeta \left(1 - \mathbb{1}_{k'+\tilde\omega'_{\ell,j}}(km')\right) h_{\ell,j}(m')\, \frac{e^{ikR}}{ikR}$$

$$
\begin{aligned}
&+ 2\pi\, \mathbb{1}_{\{3,4\}}(\ell) \int_0^1 \tilde{\lambda}^n_{\ell,j}\, \frac{(-ik\zeta)^n}{n!}\, h_{\ell,j}(m')\, \mathrm{d}\zeta\, \frac{e^{ikR}}{ikR} \\
&+ i\,\delta_{1\ell}\, \mathbb{1}_{k'+\tilde{\omega}'_{1,j}}(km')\, \frac{\Delta\, k^2}{4\pi\epsilon_0}\, \tilde{F}(\pi\setminus\alpha)\, m_z^n \int_0^1 \tilde{\lambda}^n_{\ell,j}\, \frac{(-ik\zeta)^n}{n!}\, \mathrm{d}\zeta\, \left[(\vec{m}\times\vec{e}^{\,0})\times\vec{m}\right] \left(\frac{\sqrt{2}}{ikR} + \sqrt{\pi}\frac{1-i}{\sqrt{k}}\, \frac{e^{ikR}}{\sqrt{R}}\right) \\
&- i\,\delta_{1\ell}\, \mathbb{1}_{k'+\tilde{\omega}'_{1,j}}(km')\, \frac{\Delta k^3}{2\epsilon_0}\, m_z^n \int_0^1 \tilde{\lambda}^n_{\ell,j}\, \frac{(-ik\zeta)^n}{n!}\, \mathrm{d}\zeta\, \left[(\vec{m}\times\vec{e}^{\,0})\times\vec{m}\right] \frac{e^{ikR}}{ikR} \\
&+ i\,\delta_{2\ell}\, \mathbb{1}_{k'+\tilde{\omega}'_{2,j}}(km')\, \frac{\Delta\, k^3}{4\,\epsilon_0}\, m_z^n \int_0^1 \tilde{\lambda}^n_{\ell,j}\, \frac{(-ik\zeta)^n}{n!}\, \mathrm{d}\zeta\, \left[(\vec{m}\times\vec{e}^{\,0})\times\vec{m}\right] \\
&\qquad\qquad \left[\log R - \tilde{\gamma} - \log\left(\frac{k}{2}\right) - 4\log\left(\cos\frac{\alpha}{2}\right) + i\frac{\pi}{2}\right] \frac{e^{ikR}}{ikR} \Bigg\} + o\left(\frac{1}{R}\right)
\end{aligned}
\tag{4.2.96}
$$

are obtained, assuming that both (3.3.41) and $|k' + \tilde{\omega}'_{\ell,j}| \neq k$, for $\ell = 1,\ldots,4$ and all $j \in \mathbb{Z}$, are satisfied. The far-field asymptotics of E_ℓ for $\ell = 1,\ldots,4$ in the case that $|k' + \tilde{\omega}'_{\ell,j}| = k$ is derived in the appendix in Chapter B. These examinations are quite lengthy, since additional care has to be taken concerning the occurring singularities of the integrands. Apart from that, the approach is very similar to the one used to obtain (4.2.96).

Hence, with (4.2.96), (3.1.2)–(3.1.4) and Theorem B.1 with Equation (4.2.1) it can be shown that Equation (4.1.1) in Theorem 4.1 holds. Indeed, Equation (4.1.1) can be obtained by separating the different orders of decay w.r.t. R in (3.1.3), (3.1.4), (4.2.96) and (B.1.2). To be precise, Equations (3.1.3) and (3.1.4) consist of non-decaying plane waves, while radial decay e^{ikR}/R appears in the first, second, fifth and seventh line of (4.2.96), as well as in the first term of (B.1.2). Apart from these decay orders, the second term of (B.1.2) is a 'plane wave' decaying with $1/R$, in the fourth line of (4.2.96) the radial decay orders $1/R$ and $e^{ikR}/\sqrt{R}$ arise and the seventh line of (4.2.96) shows the usual radial decay tempered by a logarithm, i.e. $\log R\, e^{ikR}/R$. For E_1 this leads to (cf. (4.2.2), (B.1.1) and (B.1.2))

$$
\begin{aligned}
E_1 = \sum_{n\in\mathbb{N}_0}\sum_{j\in\mathbb{Z}} \Bigg\{ &2\pi \int_0^1 \tilde{\lambda}^n_{1,j}\, \frac{(-ik\zeta)^n}{n!}\, \mathrm{d}\zeta \left(1 - \mathbb{1}_{k'+\tilde{\omega}'_{1,j}}(km')\right) h_{1,j}(m')\, \frac{e^{ikR}}{ikR} \\
&+ i\, \mathbb{1}_{k'+\tilde{\omega}'_{1,j}}(km')\, \frac{\Delta\, k^2}{4\pi\epsilon_0}\, \tilde{F}(\pi\setminus\alpha)\, m_z^n \int_0^1 \tilde{\lambda}^n_{1,j}\, \frac{(-ik\zeta)^n}{n!}\, \mathrm{d}\zeta \\
&\qquad \left[(\vec{m}\times\vec{e}^{\,0})\times\vec{m}\right] \left(\frac{\sqrt{2}}{ikR} + \sqrt{\pi}\frac{1-i}{\sqrt{k}}\, \frac{e^{ikR}}{\sqrt{R}}\right) \\
&- i\, \mathbb{1}_{k'+\tilde{\omega}'_{1,j}}(km')\, \frac{\Delta k^3}{2\epsilon_0}\, m_z^n \int_0^1 \tilde{\lambda}^n_{1,j}\, \frac{(-ik\zeta)^n}{n!}\, \mathrm{d}\zeta\, \left[(\vec{m}\times\vec{e}^{\,0})\times\vec{m}\right] \frac{e^{ikR}}{ikR} \Bigg\} \\
+ \sum_{n\in\mathbb{N}_0}\sum_{j\in\mathbb{Z}} \Bigg\{ &\mathbb{1}_k(|k' + \tilde{\omega}'_{1,j}|) \int_0^1 \tilde{\lambda}^n_{1,j}\, \frac{(-ik\zeta)^n}{n!}\, \mathrm{d}\zeta \Bigg[2\pi\, h_{1,j}(m')\, \frac{e^{ikR}}{ikR} \\
&+ \mathbb{1}_0(n)\, 2\pi\, f_{1,j,n}\left(\frac{k' + \tilde{\omega}'_{1,j}}{k}, 0\right) \frac{e^{iR(k'+\tilde{\omega}'_{1,j})\cdot m'}}{kRm_z} \Bigg] \Bigg\} + o\left(\frac{1}{R}\right) \\
= \frac{\Delta\, k^3}{2\epsilon_0} &\sum_{n\in\mathbb{N}_0}\sum_{j\in\mathbb{Z}} \int_0^1 \tilde{\lambda}^n_{1,j}\, \frac{(-ikm_z\zeta)^n}{n!}\, \tilde{h}_{1,j,n}(\vec{m},\zeta)\, \mathrm{d}\zeta\, \left[(\vec{m}\times\vec{e}^{\,0})\times\vec{m}\right] \frac{e^{ikR}}{kR} \\
+ \frac{\Delta\, k^2}{4\pi\epsilon_0} &\mathcal{H}_1(\vec{m})\, \left[(\vec{m}\times\vec{e}^{\,0})\times\vec{m}\right] \left(\frac{1}{kR} + \sqrt{\pi}\,\frac{1+i}{\sqrt{2}}\, \frac{e^{ikR}}{\sqrt{kR}}\right)
\end{aligned}
$$

$$+ i \, \frac{\Delta k^2}{2\epsilon_0} \sum_{\substack{j\in\mathbb{Z} \\ |k'+\tilde{\omega}'_{1,j}|=k}} \int_0^1 \tilde{\lambda}^0_{1,j}(\zeta)\, \mathrm{d}\zeta \left[\left(\left(\frac{k'+\tilde{\omega}'_{1,j}}{k}, 0 \right)^\top \times \vec{e}^{\,0} \right) \times \left(\frac{k'+\tilde{\omega}'_{1,j}}{k}, 0 \right)^\top \right] \frac{e^{iR(k'+\tilde{\omega}'_{1,j})\cdot m'}}{kRm_z}$$

where

$$\mathcal{H}_1(\vec{m}) := \sqrt{2}\, \tilde{F}(\pi \setminus \alpha) \sum_{n\in\mathbb{N}_0} \sum_{\substack{j\in\mathbb{Z} \\ \tilde{\omega}'_{1,j}=km'-k'}} \int_0^1 \tilde{\lambda}^n_{1,j}(\zeta)\, \frac{(-ikm_z\,\zeta)^n}{n!}\, \mathrm{d}\zeta.$$

and where the indicator functions $\mathbb{1}$ in line 1,2,4 and 5 were transformed to a condition to the sum w.r.t. j in the last line or to a case in the function $\tilde{h}_{1,j,n}$, defined as

$$\tilde{h}_{1,j,n}(\vec{m},\zeta) := \begin{cases} \frac{e^{-\left|km'-(k'+\tilde{\omega}'_{1,j})\right|}}{\left|km'-(k'+\tilde{\omega}'_{1,j})\right|} & \text{if } m' \neq \frac{k'+\tilde{\omega}'_{1,j}}{k} \\ -1 & \text{if } m' = \frac{k'+\tilde{\omega}'_{1,j}}{k} \end{cases}.$$

Similarly, for $\ell = 2$ and with $\cos\alpha = m_z$ and $4\log(\cos(\alpha/2)) = \log(1/4\,(1+\cos\alpha)^2)$, (cf. (4.2.3) and (B.1.2))

$$\begin{aligned} E_2 = \sum_{n\in\mathbb{N}_0} \sum_{j\in\mathbb{Z}} \Bigg\{ & 2\pi \int_0^1 \tilde{\lambda}^n_{2,j}\, \frac{(-ik\zeta)^n}{n!}\, \mathrm{d}\zeta \left(1 - \mathbb{1}_{k'+\tilde{\omega}'_{2,j}}(km')\right) h_{2,j}(m')\, \frac{e^{ikR}}{ikR} \\ & + i\, \mathbb{1}_{k'+\tilde{\omega}'_{2,j}}(km')\, \frac{\Delta k^3}{4\,\epsilon_0}\, m_z^n \int_0^1 \tilde{\lambda}^n_{2,j}\, \frac{(-ik\zeta)^n}{n!}\, \mathrm{d}\zeta\, \left[\left(\vec{m} \times \vec{e}^{\,0}\right) \times \vec{m} \right] \\ & \left[\log R - \tilde{\gamma} - \log\left(\frac{k}{2}\right) - 4\log\left(\cos\frac{\alpha}{2}\right) + i\frac{\pi}{2} \right] \frac{e^{ikR}}{ikR} \Bigg\} \\ & + \sum_{n\in\mathbb{N}_0} \sum_{j\in\mathbb{Z}} \mathbb{1}_k(|k'+\tilde{\omega}'_{2,j}|) \int_0^1 \tilde{\lambda}^n_{2,j}\, \frac{(-ik\zeta)^n}{n!}\, \mathrm{d}\zeta\, 2\pi\, h_{2,j}(m')\, \frac{e^{ikR}}{ikR} + o\left(\frac{1}{R}\right) \\ = & \frac{\Delta k^3}{2\epsilon_0} \sum_{n\in\mathbb{N}_0} \sum_{j\in\mathbb{Z}} \int_0^1 \tilde{\lambda}^n_{2,j}\, \frac{(-ikm_z\zeta)^n}{n!}\, \tilde{h}_{2,j,n}(\vec{m},\zeta)\, \mathrm{d}\zeta\, \left[\left(\vec{m}\times\vec{e}^{\,0}\right)\times\vec{m} \right] \frac{e^{ikR}}{kR} \\ & + \frac{\Delta k^3}{4\epsilon_0}\, \mathcal{H}_2(\vec{m})\, \left[\left(\vec{m}\times\vec{e}^{\,0}\right)\times\vec{m} \right] \frac{\log R}{kR}\, e^{ikR} + o\left(\frac{1}{R}\right), \end{aligned}$$

where

$$\mathcal{H}_2(\vec{m}) := \sum_{n\in\mathbb{N}_0} \sum_{\substack{j\in\mathbb{Z} \\ \tilde{\omega}'_{2,j}=km'-k'}} \int_0^1 \tilde{\lambda}^n_{2,j}(\zeta)\, \frac{(-ikm_z\,\zeta)^n}{n!}\, \mathrm{d}\zeta$$

and

$$\tilde{h}_{2,j,n}(\vec{m},\zeta) := \begin{cases} K_0\left(\left|km' - (k'+\tilde{\omega}'_{2,j})\right|\right) & \text{if } m' \neq \frac{k'+\tilde{\omega}'_{2,j}}{k} \\ -\frac{1}{2}\left[\tilde{\gamma} + \log\left(\frac{k}{8}\,(1+m_z)^2\right) - i\frac{\pi}{2}\right] & \text{if } m' = \frac{k'+\tilde{\omega}'_{2,j}}{k} \end{cases}.$$

At last, for $\ell = 3, 4$, (cf. (4.2.4), (4.2.5) and (B.1.2))

$$\begin{aligned} E_\ell = & \sum_{n\in\mathbb{N}_0} \sum_{j\in\mathbb{Z}} 2\pi \int_0^1 \tilde{\lambda}^n_{\ell,j}\, \frac{(-ik\zeta)^n}{n!}\, h_{\ell,j}(m')\, \mathrm{d}\zeta\, \frac{e^{ikR}}{ikR} \\ & + \sum_{n\in\mathbb{N}_0} \sum_{j\in\mathbb{Z}} \mathbb{1}_k(|k'+\tilde{\omega}'_{\ell,j}|) \int_0^1 \tilde{\lambda}^n_{\ell,j}\, \frac{(-ik\zeta)^n}{n!}\, \mathrm{d}\zeta\, 2\pi\, h_{\ell,j}(m')\, \frac{e^{ikR}}{ikR} + o\left(\frac{1}{R}\right) \end{aligned}$$

$$= \frac{\Delta k^3}{2\epsilon_0} \sum_{n\in\mathbb{N}_0} \sum_{j\in\mathbb{Z}} \int_0^1 \tilde{\lambda}_{\ell,j}^n \frac{(-ikm_z\zeta)^n}{n!} \tilde{h}_{\ell,j,n}(\vec{m},\zeta)\,\mathrm{d}\zeta\ \left[\left(\vec{m}\times\vec{e}^{\,0}\right)\times\vec{m}\right] \frac{e^{ikR}}{kR} + o\left(\frac{1}{R}\right),$$

where

$$\tilde{h}_{\ell,j,n}(\vec{m},\zeta) := \begin{cases} e^{-\left|km'-(k'+\tilde{\omega}'_{3,j})\right|} & \text{if } \ell = 3 \\ \frac{1}{2\pi}\int_{\mathbb{R}^2} \tilde{g}_n(\eta',\zeta)\, e^{-i\eta'\cdot(km'-k')}\,\mathrm{d}\eta' & \text{if } \ell = 4 \end{cases}.$$

Subtracting these formulas for E_1 to E_4 and Equation (3.1.4) for E_0 from E_Q (cf. (3.1.2) and (3.1.3)) easily leads to (4.1.1), which concludes the proof of Theorem 4.1.

4.3 Reduced wave mode in specular reflection

In this subsection it will be shown that the results in Section II.E.1 of Stearns [36] can be derived rigorously in the sense of Born approximation for interface functions in $\mathcal{A}\cap L_Q^\infty$. To be precise, it will be proven that the wave mode of the plane wave reflected in specular direction can be represented as the wave mode for reflection at an ideal interface multiplied by a correction factor. Indeed this factor can be given explicitly. Note that this is shown for fields in the sense of Born approximation.

Theorem 4.6 (Reduced specularly reflected wave mode)**.** *Assuming an interface function $f \in \mathcal{A}\cap L_Q^\infty$, the wave mode of the reflected plane wave in specular direction $\vec{k}^r = (k_x, k_y, -k_z)^\top$, in the above defined sense of Born approximation, is*

$$\frac{\Delta}{4\epsilon_0\, k_z^2}\, \hat{w}(-2k_z)\ \left[\left(\vec{k}^r \times \vec{e}^{\,0}\right)\times\vec{k}^r\right] e^{i\vec{k}^r\cdot\vec{x}} + \mathcal{O}\left(\left[\frac{\Delta k^2}{k_z^2}\right]^2\right), \tag{4.3.1}$$

where

$$\hat{w}(-2k_z) := \int_{-\frac{h}{2}}^{\frac{h}{2}} \partial_\zeta\left[\lim_{R\to\infty}\frac{1}{4R^2}\int_{-R}^{R}\int_{-R}^{R} \mathbb{1}_{[f(\eta'),\infty)}(\zeta)\,\mathrm{d}\eta_x\,\mathrm{d}\eta_y\right] e^{-i2|k_z|\zeta}\,\mathrm{d}\zeta. \tag{4.3.2}$$

Remark 4.7. *In the case of an ideal surface with $f = f_Q \equiv 0$, the function $\hat{w} = \hat{w}_Q$ is the Fourier transform of $\partial_\zeta \mathbb{1}_{[0,\infty)} = \delta$, i.e., $\hat{w}_Q \equiv 1$. Consequently, Eqn. (4.3.1) shows that the specularly reflected plane-wave mode for a general rough surface is that of the reflected plane-wave mode of the ideal planar surface multiplied by the attenuation factor $\hat{w}(-2k_z)$. Thus, the efficiency of that mode is attenuated by the factor $[\hat{w}(-2k_z)]^2$, where $|\hat{w}(-2k_z)|$ is less or equal to one. Indeed,*

$$|\hat{w}(-2k_z)| = \left|\int_{-\frac{h}{2}}^{\infty} e^{-i2|k_z|\zeta}\,\mathrm{d}p(\zeta)\right| \le p(\infty) - p(-h/2) = 1$$

with the monotonically increasing function $p(\zeta) := \lim_{R\to\infty} 1/(4R^2)\int_{-R}^{R}\int_{-R}^{R}\mathbb{1}_{[f(\eta'),\infty)}(\zeta)\,\mathrm{d}\eta_x\,\mathrm{d}\eta_y$ satisfying $p(\infty) = 1$ and $p(-h/2) = 0$.

Remark 4.8. *Applying the formula for the Fourier transform of a derivative to Eqn. (4.3.2) and subtracting $\hat{w}_Q(-2k_z) \equiv 1$, there holds*

$$\hat{w}(-2k_z) = 1 + i2|k_z| \int_{-\frac{h}{2}}^{\frac{h}{2}} \left[\lim_{R\to\infty}\frac{1}{4R^2}\int_{-R}^{R}\int_{-R}^{R}\left(\mathbb{1}_{[f(\eta'),\infty)}(\zeta) - \mathbb{1}_{[0,\infty)}(\zeta)\right)\mathrm{d}\eta_x\,\mathrm{d}\eta_y\right] e^{-i2|k_z|\zeta}\,\mathrm{d}\zeta.$$

This provides a way to define $\hat{w}$ by classical integration.

Proof. By examining Equation (3.1.4) and the definition of $\vec{\omega}_j$ it is easily seen that a plane wave in specular direction coincides with $\tilde{\omega}'_{0,j} = (0,0)^\top$. Moreover, by notation, there is a unique $j = j_0$ such that $\tilde{\omega}'_{0,j} = (0,0)^\top$. Note that the corresponding $\tilde{\lambda}^n_{0,j_0}$ is the mean value of $f_n(\eta') = f^{n+1}(\eta')\, e^{ik_z\zeta\, f(\eta')}$. To be precise, it can be represented as (cf. (3.3.15) and (3.3.16))

$$\begin{aligned}
\tilde{\lambda}^n_{0,j_0} &= \lim_{R\to\infty} \frac{1}{4R^2} \int_{-R}^{R}\int_{-R}^{R} f^{n+1}(\eta')\, e^{ik_z\zeta\, f(\eta')}\, \mathrm{d}\eta_x\, \mathrm{d}\eta_y \\
&= \lim_{R\to\infty} \frac{1}{4R^2} \int_{-R}^{R}\int_{-R}^{R} \left\{ \sum_{\ell=0}^{3} \left[\frac{1}{\sqrt{1+|\eta'|^2}^{\,\ell}} \sum_{j\in\mathbb{Z}} \tilde{\lambda}^n_{\ell,j}\, e^{i\tilde{\omega}'_{\ell,j}\cdot\eta'} \right] + \tilde{g}_n(\eta',\zeta) \right\} \mathrm{d}\eta_x\, \mathrm{d}\eta_y. \qquad (4.3.3)
\end{aligned}$$

Indeed, the mean value of all decaying parts of f_n can be bounded by

$$\begin{aligned}
&\lim_{R\to\infty} \left| \sum_{\ell=1}^{3} \frac{1}{4R^2} \int_{-R}^{R}\int_{-R}^{R} \frac{1}{\sqrt{1+|\eta'|^2}^{\,\ell}} \sum_{j\in\mathbb{Z}} \tilde{\lambda}^n_{\ell,j}\, e^{i\tilde{\omega}'_{\ell,j}\cdot\eta'}\, \mathrm{d}\eta_x\, \mathrm{d}\eta_y + \frac{1}{4R^2} \int_{-R}^{R}\int_{-R}^{R} \tilde{g}_n(\eta',\zeta)\, \mathrm{d}\eta_x\, \mathrm{d}\eta_y \right| \\
&\quad\le \lim_{R\to\infty} \sum_{\ell=1}^{3} \frac{1}{4R^2} \int_{-R}^{R}\int_{-R}^{R} \frac{1}{\sqrt{1+|\eta'|^2}^{\,\ell}}\, \mathrm{d}\eta_x\, \mathrm{d}\eta_y \sum_{j\in\mathbb{Z}} \left|\tilde{\lambda}^n_{\ell,j}\right| + \frac{1}{4R^2} \int_{-R}^{R}\int_{-R}^{R} |\tilde{g}_n(\eta',\zeta)|\, \mathrm{d}\eta_x\, \mathrm{d}\eta_y \\
&\quad\le \lim_{R\to\infty} \sum_{\ell=1}^{3} \frac{1}{4R^2} \int_{-R}^{R}\int_{-R}^{R} \frac{1}{\sqrt{1+|\eta'|^2}^{\,\ell}}\, \mathrm{d}\eta_x\, \mathrm{d}\eta_y \sum_{j\in\mathbb{Z}} \left|\tilde{\lambda}^n_{\ell,j}\right| + \frac{\|\tilde{g}_n(\,\cdot\,,\zeta)\|_{4,\infty}}{4R^2} \int_{-R}^{R}\int_{-R}^{R} \frac{1}{\left(1+|\eta'|^2\right)^2}\, \mathrm{d}\eta_x\, \mathrm{d}\eta_y \\
&\quad\le \lim_{R\to\infty} \frac{\|f_n\|_{\mathcal{A}}}{4R^2} \int_{-R}^{R}\int_{-R}^{R} \frac{1}{\sqrt{1+|\eta'|^2}}\, \mathrm{d}\eta_x\, \mathrm{d}\eta_y
\end{aligned}$$

for any fixed $\zeta \in [0,1]$. Substituting $u' = \eta'/R$, with $u' = (u_x, u_y)^\top$, then leads to

$$\begin{aligned}
&\lim_{R\to\infty} \left| \sum_{\ell=1}^{3} \frac{1}{4R^2} \int_{-R}^{R}\int_{-R}^{R} \frac{1}{\sqrt{1+|\eta'|^2}^{\,\ell}} \sum_{j\in\mathbb{Z}} \tilde{\lambda}^n_{\ell,j}\, e^{i\tilde{\omega}'_{\ell,j}\cdot\eta'}\, \mathrm{d}\eta_x\, \mathrm{d}\eta_y + \frac{1}{4R^2} \int_{-R}^{R}\int_{-R}^{R} \tilde{g}_n(\eta',\zeta)\, \mathrm{d}\eta_x\, \mathrm{d}\eta_y \right| \\
&\quad\le \lim_{R\to\infty} \frac{\|f_n\|_{\mathcal{A}}}{4} \int_{-1}^{1}\int_{-1}^{1} \frac{1}{\sqrt{1+R^2\,|u'|^2}}\, \mathrm{d}u_x\, \mathrm{d}u_y \\
&\quad= 0
\end{aligned}$$

and (cf. (4.3.3))

$$\lim_{R\to\infty} \frac{1}{4R^2} \int_{-R}^{R}\int_{-R}^{R} f_n(\eta')\, \mathrm{d}\eta_x\, \mathrm{d}\eta_y = \lim_{R\to\infty} \frac{1}{4R^2} \int_{-R}^{R}\int_{-R}^{R} \sum_{j\in\mathbb{Z}} \tilde{\lambda}^n_{\ell,j}\, e^{i\tilde{\omega}'_{\ell,j}\cdot\eta'}\, \mathrm{d}\eta_x\, \mathrm{d}\eta_y$$

Additionally, since the sum exists absolutely, it can be evaluated after the integration. Moreover, for $\tilde{\omega}'_{0,j} \ne (0,0)^\top$ the summands in the sum w.r.t. j are periodic with a mean of zero. Thus Equation (4.3.3) follows.

With this, the specular part $\vec{E}^s$ of $\vec{E}^r$ (cf. (3.1.2) and (3.1.4)) minus the summand $\vec{E}_{\mathcal{Q}}$ (cf. (3.1.3)), corresponding to the reflection at an ideal interface, is examined. Replacing $\tilde{\lambda}^n_{0,j_0}$ (cf. (4.3.3)) leads to

$$\vec{E}^s_0(\vec{x}) := -i\,\frac{\Delta}{2\epsilon_0} \sum_{n\in\mathbb{N}_0} \int_0^1 \tilde{\lambda}^n_{0,j_0}\, \frac{(-i\zeta)^n}{n!}\, \mathrm{d}\zeta \ \left[\left(\vec{k}^r \times \vec{e}^{\,0}\right) \times \vec{k}^r \right] |k_z|^{n-1}\, e^{i\vec{k}^r\cdot\vec{x}}$$

$$= -i\,\frac{\Delta}{2\epsilon_0}\sum_{n\in\mathbb{N}_0}\int_0^1 \lim_{R\to\infty}\frac{1}{4R^2}\int_{-R}^{R}\int_{-R}^{R} f^{n+1}(\eta')\,e^{ik_z\zeta\,f(\eta')}\,\mathrm{d}\eta_x\,\mathrm{d}\eta_y\,\frac{(-i\zeta)^n}{n!}\,\mathrm{d}\zeta\,|k_z|^{n-1}$$
$$\left[\left(\vec{k}^r\times\vec{e}^{\,0}\right)\times\vec{k}^r\right]e^{i\vec{k}^r\cdot\vec{x}}.$$

Applying Lebesgue's theorem for an infinite sum (integration with a discrete measure), it is easily seen that

$$\lim_{R\to\infty}\sum_{n\in\mathbb{N}_0}\int_0^1\frac{1}{4R^2}\int_{-R}^{R}\int_{-R}^{R} f^{n+1}(\eta')\,e^{ik_z\zeta\,f(\eta')}\,\mathrm{d}\eta_x\,\mathrm{d}\eta_y\,\frac{(-i\zeta)^n}{n!}\,\mathrm{d}\zeta\,|k_z|^{n-1}$$
$$= \sum_{n\in\mathbb{N}_0}\lim_{R\to\infty}\int_0^1\frac{1}{4R^2}\int_{-R}^{R}\int_{-R}^{R} f^{n+1}(\eta')\,e^{ik_z\zeta\,f(\eta')}\,\mathrm{d}\eta_x\,\mathrm{d}\eta_y\,\frac{(-i\zeta)^n}{n!}\,\mathrm{d}\zeta\,|k_z|^{n-1},$$

since, with $\|f\|_\infty < h < \infty$,

$$\left|\int_0^1\frac{1}{4R^2}\int_{-R}^{R}\int_{-R}^{R} f^{n+1}(\eta')\,e^{ik_z\zeta\,f(\eta')}\,\mathrm{d}\eta_x\,\mathrm{d}\eta_y\,\frac{(-i\zeta)^n}{n!}\,\mathrm{d}\zeta\,|k_z|^{n-1}\right| \le \int_0^1\frac{1}{4R^2}\int_{-R}^{R}\int_{-R}^{R} h^{n+1}\,\mathrm{d}\eta_x\,\mathrm{d}\eta_y\,\frac{|k_z|^{n-1}}{n!}\,\mathrm{d}\zeta$$
$$= \frac{h^{n+1}|k_z|^{n-1}}{n!},$$

which is absolutely summable w.r.t. n. Consequently,

$$\vec{E}_0^s(\vec{x}) = -i\,\frac{\Delta}{2\epsilon_0}\lim_{R\to\infty}\frac{1}{4R^2}\int_{-R}^{R}\int_{-R}^{R}\int_0^1\sum_{n\in\mathbb{N}_0}\frac{(-i|k_z|\zeta\,f(\eta'))^n}{n!}\,e^{ik_z\zeta\,f(\eta')}\,\mathrm{d}\zeta\,\frac{f(\eta')}{|k_z|}\,\mathrm{d}\eta_x\,\mathrm{d}\eta_y\left[\left(\vec{k}^r\times\vec{e}^{\,0}\right)\times\vec{k}^r\right]e^{i\vec{k}^r\cdot\vec{x}}$$
$$= -i\,\frac{\Delta}{2\epsilon_0}\lim_{R\to\infty}\frac{1}{4R^2}\int_{-R}^{R}\int_{-R}^{R}\int_0^1 e^{-i2|k_z|\zeta\,f(\eta')}\,\mathrm{d}\zeta\,\frac{f(\eta')}{|k_z|}\,\mathrm{d}\eta_x\,\mathrm{d}\eta_y\left[\left(\vec{k}^r\times\vec{e}^{\,0}\right)\times\vec{k}^r\right]e^{i\vec{k}^r\cdot\vec{x}}, \tag{4.3.4}$$

since $k_z < 0$. Note that

$$\int_0^1 e^{-i2|k_z|\zeta\,f(\eta')}\,\mathrm{d}\zeta\,f(\eta') = \int_0^{f(\eta')} e^{-i2|k_z|\zeta}\,\mathrm{d}\zeta = \int_{-\frac{h}{2}}^{\frac{h}{2}} \mathbb{1}_{[0,f(\eta')]}(\zeta)\,e^{-i2|k_z|\zeta}\,\mathrm{d}\zeta.$$

Applying this to the right-hand side of (4.3.4) and using Fubini's theorem leads to

$$\vec{E}_0^s(\vec{x}) = -i\,\frac{\Delta}{2\epsilon_0}\lim_{R\to\infty}\int_{-\frac{h}{2}}^{\frac{h}{2}}\frac{1}{4R^2}\int_{-R}^{R}\int_{-R}^{R}\mathbb{1}_{[0,f(\eta')]}(\zeta)\,\mathrm{d}\eta_x\,\mathrm{d}\eta_y\,e^{-i2|k_z|\zeta}\,\mathrm{d}\zeta\,\frac{\left[\left(\vec{k}^r\times\vec{e}^{\,0}\right)\times\vec{k}^r\right]}{|k_z|}\,e^{i\vec{k}^r\cdot\vec{x}}. \tag{4.3.5}$$

The next step is to evaluate the limit w.r.t. R. To do so, note that the integral $\mu(f,\zeta,R) := \int_{-R}^{R}\int_{-R}^{R}\mathbb{1}_{[0,f(\eta')]}(\zeta)\,\mathrm{d}\eta_x\,\mathrm{d}\eta_y$ is a measure for the set of points $\eta'\in[-R,R]^2$ for which $|\zeta| \le \operatorname{sgn}\zeta\, f(\eta')$ (cf. Fig. 4.4). With this in mind, it is easily seen that

$$\left|\frac{\mu(f,\zeta,R)}{4R^2}\right| \le \frac{1}{4R^2}\int_{-R}^{R}\int_{-R}^{R}\left|\mathbb{1}_{[0,f(\eta')]}(\zeta)\right|\,\mathrm{d}\eta_x\,\mathrm{d}\eta_y \le \frac{1}{4R^2}\int_{-R}^{R}\int_{-R}^{R} 1\,\mathrm{d}\eta_x\,\mathrm{d}\eta_y = 1,$$

for any ζ. The last expression is integrable w.r.t. ζ over the compact domain of integration $[-h/2, h/2]$. Lebesgue's theorem thus shows that the limit w.r.t. R in (4.3.5) can be evaluated before the integration

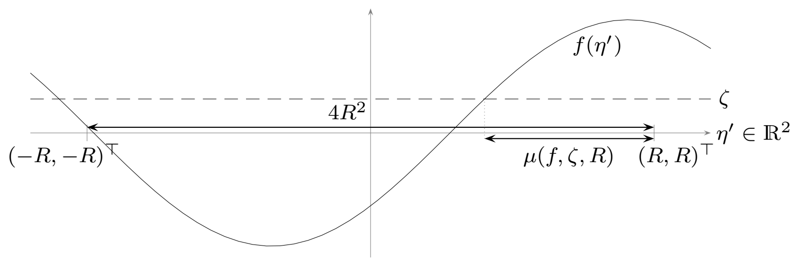


Figure 4.4: Symbolic visualisation of measure $\mu(f,\zeta,R)$

w.r.t. ζ. Moreover, note that this limit is zero for $|\zeta| > h/2 \geq |f(\eta')|$. Hence the domain of integration w.r.t. ζ in (4.3.5) can be extended to $\mathbb{R}$. The integral can then be interpreted as a Fourier transform and

$$\begin{aligned}\vec{E}_0^s(\vec{x}) &= -i\,\frac{\Delta}{2\epsilon_0|k_z|}\int\limits_{\mathbb{R}}\lim_{R\to\infty}\frac{\mu(f,\zeta,R)}{4R^2}\,e^{-i2|k_z|\zeta}\,\mathrm{d}\zeta\,\left[\left(\vec{k}^r\times\vec{e}^{\,0}\right)\times\vec{k}^r\right]\,e^{i\vec{k}^r\cdot\vec{x}}\\ &= -\frac{\Delta}{4\epsilon_0|k_z|^2}\int\limits_{\mathbb{R}}\partial_\zeta\left[\lim_{R\to\infty}\frac{\mu(f,\zeta,R)}{4R^2}\right]e^{-i2|k_z|\zeta}\,\mathrm{d}\zeta\,\left[\left(\vec{k}^r\times\vec{e}^{\,0}\right)\times\vec{k}^r\right]\,e^{i\vec{k}^r\cdot\vec{x}}.\end{aligned}\tag{4.3.6}$$

In correspondence with [36, Equation (12)] define

$$\begin{aligned}p(\zeta) &:= \lim_{R\to\infty}\frac{1}{4R^2}\int\limits_{-R}^{R}\int\limits_{-R}^{R}\mathbb{1}_{[f(\eta'),\infty)}(\zeta)\,\mathrm{d}\eta_x\,\mathrm{d}\eta_y,\\ p_{\mathcal{Q}}(\zeta) &:= \lim_{R\to\infty}\frac{1}{4R^2}\int\limits_{-R}^{R}\int\limits_{-R}^{R}\mathbb{1}_{[0,\infty)}(\zeta)\,\mathrm{d}\eta_x\,\mathrm{d}\eta_y = \mathbb{1}_{[0,\infty)}(\zeta).\end{aligned}$$

It is easily confirmed that $\lim_{R\to\infty}\mu(f,\zeta,R)/(4R^2) = p_{\mathcal{Q}}(\zeta) - p(\zeta)$ and that the Fourier transform $\int_{\mathbb{R}} p'_{\mathcal{Q}}(\zeta)\,e^{-i2|k_z|\zeta}\,\mathrm{d}\zeta$ is equal to one, by using results for generalised Fourier transforms. Furthermore, it can be shown that $\operatorname{supp}(p') \subseteq [-h/2, h/2]$. Thus, separately applying the integral w.r.t. ζ in (4.3.6) to p' and $p'_{\mathcal{Q}}$ is well defined and leads to

$$\vec{E}_0^s(\vec{x}) = \frac{\Delta}{4\epsilon_0|k_z|^2}\hat{w}(-2k_z)\,\left[\left(\vec{k}^r\times\vec{e}^{\,0}\right)\times\vec{k}^r\right]\,e^{i\vec{k}^r\cdot\vec{x}} - \frac{\Delta}{4\epsilon_0|k_z|^2}\left[\left(\vec{k}^r\times\vec{e}^{\,0}\right)\times\vec{k}^r\right]\,e^{i\vec{k}^r\cdot\vec{x}},\tag{4.3.7}$$

where $\hat{w}(-2k_z) := \int_{\mathbb{R}} p'(\zeta)\,e^{-i2|k_z|\zeta}\,\mathrm{d}\zeta$. On the other hand, the subsequent Lemma 4.9 states that the second summand in (4.3.7) is an approximation of the field $\vec{E}^r_{\mathcal{Q}}(\vec{x})$ (cf. (3.1.3)) reflected from an ideal interface. Thus, since (4.3.7) is a formula for the plane-wave part of the field reflected in specular direction minus an approximation of the reflected field for an ideal interface ($\vec{E}_0^s = \vec{E}^s - \vec{E}^r_{\mathcal{Q}}$), it follows that the plane wave part is equal to (cf. subsequent (4.3.8))

$$\vec{E}^s(\vec{x}) = \vec{E}_0^s(\vec{x}) + \vec{E}^r_{\mathcal{Q}}(\vec{x}) = \frac{\Delta}{4\epsilon_0|k_z|^2}\hat{w}(-2k_z)\,\left[\left(\vec{k}^r\times\vec{e}^{\,0}\right)\times\vec{k}^r\right]\,e^{i\vec{k}^r\cdot\vec{x}} + \mathcal{O}\left(\left[\frac{\Delta k^2}{k_z^2}\right]^2\right),$$

which is equal to [36, Equation (42)]. ■

For the proof of Theorem 4.6 the following lemma was used.

Lemma 4.9. *Assume an ideal interface, defined by the graph of the function $f_{\mathcal{Q}} \equiv 0$, is illuminated by an incoming plane wave as described in Subsection 2.1. The reflected field is then given by*

$$\vec{E}^r_{\mathcal{Q}}(\vec{x}) = \frac{\Delta}{4\epsilon_0 k_z^2}\left[\left(\vec{k}^r\times\vec{e}^{\,0}\right)\times\vec{k}^r\right]\,e^{i\vec{k}^r\cdot\vec{x}} + \mathcal{O}\left(\left[\frac{k^2\Delta}{k_z^2}\right]^2\right).\tag{4.3.8}$$

Proof. The field reflected by an ideal interface is determined by Fresnel's formulas. To be precise, for some constant polarisation $\vec{e}^0$, (cf. (A.3.2))

$$\vec{E}^r_Q(\vec{x}) = \left\{ \frac{k_z + \sqrt{\tilde{k}^2 - |k'|^2}}{k_z - \sqrt{\tilde{k}^2 - |k'|^2}} \, \nu^r_{TE}(\vec{k}, \vec{e}^0) \, \vec{e}^1_{TE}(\vec{k}) - \frac{\tilde{k}^2 k_z + k^2 \sqrt{\tilde{k}^2 - |k'|^2}}{\tilde{k}^2 k_z - k^2 \sqrt{\tilde{k}^2 - |k'|^2}} \, \nu^r_{TM}(\vec{k}, \vec{e}^0) \, \vec{e}^1_{TM}(\vec{k}) \right\} e^{i\vec{k}^r \cdot \vec{x}}, \tag{4.3.9}$$

where $\tilde{k} = \sqrt{\mu_0 \epsilon'_0}\omega$, $k_z < 0$,

$$\nu^r_{TE}(\vec{k}, \vec{e}^0) := \frac{k_y e^0_x - k_x e^0_y}{|k'|}, \qquad \vec{e}^1_{TE}(\vec{k}) := \frac{1}{|k'|} \begin{pmatrix} k_y \\ -k_x \\ 0 \end{pmatrix},$$

$$\nu^r_{TM}(\vec{k}, \vec{e}^0) := \frac{k_z (k_x e^0_x + k_y e^0_y) - |k'|^2 \, e^0_z}{k \, |k'|}, \qquad \vec{e}^1_{TM}(\vec{k}) := \frac{1}{k \, |k'|} \begin{pmatrix} k_x k_z \\ k_y k_z \\ |k'|^2 \end{pmatrix}. \tag{4.3.10}$$

Here, the symbols $\vec{e}^1_{TE}(\vec{k})$ and $\vec{e}^1_{TM}(\vec{k})$ identify the polarisation directions of the reflected field, when an ideal interface is illuminated by a TE- or TM-polarised plane wave. Thus, $\vec{E}^r_Q(\vec{x})$ is a convex combination of the reflected fields resulting from these two polarisation states. To obtain (4.3.8), it is thus sufficient to study the asymptotic behaviour in the case of these two polarisations. This is done by considering the asymptotic behaviour of the two quotients in (4.3.9) for $\epsilon'_0 \to \epsilon_0$, or equivalently $\Delta \to 0$. To be precise, some terms are split off from these quotients and it will be shown that the remaining terms decay with the order $\mathcal{O}([k^2\Delta/k_z^2]^2)$, while the split off terms are relevant for the asymptotics. These decomposed terms are then plugged into (4.3.9) to replace the quotients. At the end, it will be shown that this representation can be reduced to (4.3.8) for $\epsilon'_0 \to \epsilon_0$.

First, the case of TE-polarisation is considered. Since $k^2 = |k'|^2 + k_z^2$, $k_z < 0$, $k^2 = \mu_0 \epsilon_0 \omega^2$ and $\tilde{k}^2 = \mu_0 \epsilon'_0 \omega^2$, it is easily seen that

$$\frac{k_z + \sqrt{\tilde{k}^2 - |k'|^2}}{k_z - \sqrt{\tilde{k}^2 - |k'|^2}} = -\frac{-|k_z| + \sqrt{\tilde{k}^2 - |k'|^2}}{|k_z| + \sqrt{\tilde{k}^2 - |k'|^2}} = -\frac{\tilde{k}^2 - k^2}{\left[|k_z| + \sqrt{\tilde{k}^2 - |k'|^2}\right]^2} = \frac{k^2 \Delta}{\epsilon_0 \left[|k_z| + \sqrt{\tilde{k}^2 - |k'|^2}\right]^2}$$
$$= \frac{k^2 \Delta}{4\epsilon_0 k_z^2} \left\{ 1 + \frac{4k_z^2}{\left[|k_z| + \sqrt{\tilde{k}^2 - |k'|^2}\right]^2} - 1 \right\},$$

where

$$\frac{4k_z^2}{\left[|k_z| + \sqrt{\tilde{k}^2 - |k'|^2}\right]^2} - 1 = \frac{4k_z^2 - \left[|k_z| + \sqrt{\tilde{k}^2 - |k'|^2}\right]^2}{\left[|k_z| + \sqrt{\tilde{k}^2 - |k'|^2}\right]^2}$$
$$= \left[2|k_z| - |k_z| - \sqrt{\tilde{k}^2 - |k'|^2}\right] \frac{2|k_z| + |k_z| + \sqrt{\tilde{k}^2 - |k'|^2}}{\left[|k_z| + \sqrt{\tilde{k}^2 - |k'|^2}\right]^2}$$
$$= \left[k_z^2 - \sqrt{\tilde{k}^2 - |k'|^2}^2\right] \frac{3|k_z| + \sqrt{\tilde{k}^2 - |k'|^2}}{\left[|k_z| + \sqrt{\tilde{k}^2 - |k'|^2}\right]^3}$$
$$= \left[k^2 - \tilde{k}^2\right] \frac{3|k_z| + \sqrt{\tilde{k}^2 - |k'|^2}}{\left[|k_z| + \sqrt{\tilde{k}^2 - |k'|^2}\right]^3} = \frac{k^2 \Delta}{\epsilon_0} \frac{3|k_z| + \sqrt{\tilde{k}^2 - |k'|^2}}{\left[|k_z| + \sqrt{\tilde{k}^2 - |k'|^2}\right]^3}.$$

Note that

$$\lim_{\epsilon_0'\to\epsilon_0} \frac{k_z^2}{\epsilon_0} \frac{3|k_z| + \sqrt{\tilde{k}^2 - |k'|^2}}{\left[|k_z| + \sqrt{\tilde{k}^2 - |k'|^2}\right]^3} = \frac{k_z^2}{\epsilon_0} \frac{3|k_z| + \sqrt{k^2 - |k'|^2}}{\left[|k_z| + \sqrt{k^2 - |k'|^2}\right]^3} = \frac{k_z^2}{\epsilon_0} \frac{4\,|k_z|}{[2\,|k_z|]^3} = \frac{1}{2\epsilon_0}$$

is finite, such that

$$\frac{4k_z^2}{\left[|k_z| + \sqrt{\tilde{k}^2 - |k'|^2}\right]^2} - 1 = \mathcal{O}\left(\frac{k^2\Delta}{k_z^2}\right)$$

and

$$\frac{k_z + \sqrt{\tilde{k}^2 - |k'|^2}}{k_z - \sqrt{\tilde{k}^2 - |k'|^2}} = \frac{k^2\Delta}{4\epsilon_0 k_z^2} + \mathcal{O}\left(\left[\frac{k^2\Delta}{k_z^2}\right]^2\right). \tag{4.3.11}$$

Similarly, in the TM case, (cf. (4.3.9))

$$\begin{aligned}
\frac{\tilde{k}^2 k_z + k^2\sqrt{\tilde{k}^2-|k'|^2}}{\tilde{k}^2 k_z - k^2\sqrt{\tilde{k}^2-|k'|^2}} &= -\frac{-\tilde{k}^2|k_z| + k^2\sqrt{\tilde{k}^2-|k'|^2}}{\tilde{k}^2|k_z| + k^2\sqrt{\tilde{k}^2-|k'|^2}} = -\frac{-\tilde{k}^4 k_z^2 + k^4\left(\tilde{k}^2-|k'|^2\right)}{\left[\tilde{k}^2|k_z| + k^2\sqrt{\tilde{k}^2-|k'|^2}\right]^2} \\
&= -\frac{-\tilde{k}^4\left(k^2-|k'|^2\right) + k^4\left(\tilde{k}^2-|k'|^2\right)}{\left[\tilde{k}^2|k_z| + k^2\sqrt{\tilde{k}^2-|k'|^2}\right]^2} = -\frac{\left(k^4-\tilde{k}^4\right)\left(k^2-|k'|^2\right) - k^4\left(k^2-\tilde{k}^2\right)}{\left[\tilde{k}^2|k_z| + k^2\sqrt{\tilde{k}^2-|k'|^2}\right]^2} \\
&= -\left(k^2-\tilde{k}^2\right)\frac{k_z^2\left(k^2+\tilde{k}^2\right) - k^4}{\left[\tilde{k}^2|k_z| + k^2\sqrt{\tilde{k}^2-|k'|^2}\right]^2} = -\frac{k^2\Delta}{\epsilon_0}\frac{k_z^2\left(k^2+\tilde{k}^2\right) - k^4}{\left[\tilde{k}^2|k_z| + k^2\sqrt{\tilde{k}^2-|k'|^2}\right]^2} \\
&= -\frac{k^2\Delta}{4\epsilon_0 k_z^2}\left[2\frac{k_z^2}{k^2} - 1\right] - \frac{k^2\Delta}{\epsilon_0}\left\{\frac{k_z^2\left(k^2+\tilde{k}^2\right) - k^4}{\left[\tilde{k}^2|k_z| + k^2\sqrt{\tilde{k}^2-|k'|^2}\right]^2} - \frac{2\frac{k_z^2}{k^2} - 1}{4k_z^2}\right\},
\end{aligned} \tag{4.3.12}$$

where

$$\begin{aligned}
\frac{k_z^2\left(k^2+\tilde{k}^2\right) - k^4}{\left[\tilde{k}^2|k_z| + k^2\sqrt{\tilde{k}^2-|k'|^2}\right]^2} - \frac{2\frac{k_z^2}{k^2} - 1}{4k_z^2} &= \frac{k_z^2\left(k^2+\tilde{k}^2\right) - k^4}{\left[\tilde{k}^2|k_z| + k^2\sqrt{\tilde{k}^2-|k'|^2}\right]^2} - \frac{k^2\left(k_z^2 - |k'|^2\right)}{4k^4 k_z^2} \\
&= \left(k_z^2\left(k^2+\tilde{k}^2\right) - k^4\right)\left[\frac{1}{\left[\tilde{k}^2|k_z| + k^2\sqrt{\tilde{k}^2-|k'|^2}\right]^2} - \frac{1}{4k^4 k_z^2}\right] \\
&\quad + \frac{1}{4k^4 k_z^2}\left[k_z^2\left(k^2+\tilde{k}^2\right) - k^4 - k^2\left(k_z^2 - |k'|^2\right)\right]
\end{aligned} \tag{4.3.13}$$

and

$$k_z^2\left(k^2+\tilde{k}^2\right) - k^4 - k^2\left(k_z^2 - |k'|^2\right) = k_z^2\tilde{k}^2 - k^2\,|k'|^2 - k^2 k_z^2 + k^2\,|k'|^2 = -\frac{k_z^2 k^2\Delta}{\epsilon_0}. \tag{4.3.14}$$

Furthermore, in the first summand on the right-hand side of (4.3.13),

$$\frac{1}{\left[\tilde{k}^2|k_z| + k^2\sqrt{\tilde{k}^2 - |k'|^2}\right]^2} - \frac{1}{4k^4k_z^2} = \frac{4k^4k_z^2 - \left[\tilde{k}^2|k_z| + k^2\sqrt{\tilde{k}^2 - |k'|^2}\right]^2}{4k^4k_z^2\left[\tilde{k}^2|k_z| + k^2\sqrt{\tilde{k}^2 - |k'|^2}\right]^2} \tag{4.3.15}$$
$$= \left[2k^2|k_z| - \tilde{k}^2|k_z| - k^2\sqrt{\tilde{k}^2 - |k'|^2}\right] \frac{2k^2|k_z| + \tilde{k}^2|k_z| + k^2\sqrt{\tilde{k}^2 - |k'|^2}}{4k^4k_z^2\left[\tilde{k}^2|k_z| + k^2\sqrt{\tilde{k}^2 - |k'|^2}\right]^2},$$

with

$$\begin{aligned}
2k^2|k_z| - \tilde{k}^2|k_z| - k^2\sqrt{\tilde{k}^2 - |k'|^2} &= \frac{\left[2k^2 - \tilde{k}^2\right]^2 k_z^2 - k^4\left(\tilde{k}^2 - |k'|^2\right)}{2k^2|k_z| - \tilde{k}^2|k_z| + k^2\sqrt{\tilde{k}^2 - |k'|^2}} \\
&= \frac{4k^2k_z^2\left(k^2 - \tilde{k}^2\right) + \tilde{k}^4k_z^2 - \tilde{k}^2k^4 + k^4\,|k'|^2}{2k^2|k_z| - \tilde{k}^2|k_z| + k^2\sqrt{\tilde{k}^2 - |k'|^2}} \\
&= \frac{4k^2k_z^2\left(k^2 - \tilde{k}^2\right) + \tilde{k}^4k^2 - \tilde{k}^4\,|k'|^2 - \tilde{k}^2k^4 + k^4\,|k'|^2}{2k^2|k_z| - \tilde{k}^2|k_z| + k^2\sqrt{\tilde{k}^2 - |k'|^2}} \\
&= \left(k^2 - \tilde{k}^2\right)\frac{4k^2k_z^2 - \tilde{k}^2k^2 + |k'|^2\left(k^2 + \tilde{k}^2\right)}{2k^2|k_z| - \tilde{k}^2|k_z| + k^2\sqrt{\tilde{k}^2 - |k'|^2}} \\
&= \frac{k^2\Delta}{\epsilon_0}\,\frac{4k^2k_z^2 - \tilde{k}^2k^2 + |k'|^2\left(k^2 + \tilde{k}^2\right)}{2k^2|k_z| - \tilde{k}^2|k_z| + k^2\sqrt{\tilde{k}^2 - |k'|^2}}.
\end{aligned}$$

Using this together with (4.3.15), (4.3.14) and (4.3.13), it is easily seen that

$$\begin{aligned}
&\lim_{\epsilon_0' \to \epsilon_0} \frac{k_z^4}{k^2\,\epsilon_0\,\Delta}\left\{\frac{k_z^2\left(k^2 + \tilde{k}^2\right) - k^4}{\left[\tilde{k}^2|k_z| + k^2\sqrt{\tilde{k}^2 - |k'|^2}\right]^2} - \frac{2\frac{k_z^2}{k^2} - 1}{4k_z^2}\right\} \\
&= \lim_{\epsilon_0' \to \epsilon_0} \frac{k_z^4}{k^2\,\epsilon_0\,\Delta}\left\{-\frac{\Delta}{4\epsilon_0 k^2}\right. \\
&\quad \left. + \left(k_z^2\left(k^2 + \tilde{k}^2\right) - k^4\right)\frac{k^2\Delta}{\epsilon_0}\,\frac{4k^2k_z^2 - \tilde{k}^2k^2 + |k'|^2\left(k^2 + \tilde{k}^2\right)}{2k^2|k_z| - \tilde{k}^2|k_z| + k^2\sqrt{\tilde{k}^2 - |k'|^2}}\,\frac{2k^2|k_z| + \tilde{k}^2|k_z| + k^2\sqrt{\tilde{k}^2 - |k'|^2}}{4k^4k_z^2\left[\tilde{k}^2|k_z| + k^2\sqrt{\tilde{k}^2 - |k'|^2}\right]^2}\right\} \\
&= -\frac{k_z^4}{4\epsilon_0^2k^4} + \frac{k_z^4}{\epsilon_0^2}\,k^2\left(2k_z^2 - k^2\right)\frac{4k^2k_z^2 - k^4 + 2k^2|k'|^2}{2k^2|k_z|}\,\frac{4\,k^2|k_z|}{16\,k^8k_z^4} \\
&= -\frac{k_z^4}{4\epsilon_0^2k^4} + \frac{1}{8\epsilon_0^2k^4}\left(2k_z^2 - k^2\right)\left(4k_z^2 - k^2 + 2|k'|^2\right) = -\frac{k_z^4}{4\epsilon_0^2k^4} + \frac{4k_z^4 - k^4}{8\epsilon_0^2k^4} = \frac{2k_z^4 - k^4}{8\epsilon_0^2k^4}
\end{aligned}$$

is finite. It follows that

$$\frac{\tilde{k}^2k_z + k^2\sqrt{\tilde{k}^2 - |k'|^2}}{\tilde{k}^2k_z - k^2\sqrt{\tilde{k}^2 - |k'|^2}} = -\frac{k^2\Delta}{4\epsilon_0k_z^2}\left[2\frac{k_z^2}{k^2} - 1\right] + \mathcal{O}\left(\left[\frac{k^2\Delta}{k_z^2}\right]^2\right) \tag{4.3.16}$$

for $\epsilon_0' \to \epsilon_0$, such that with (4.3.11) and (4.3.9)

$$\vec{E}^r_Q(\vec{x}) = \frac{k^2\Delta}{4\epsilon_0 k_z^2} \left\{ \nu^r_{TE}(\vec{k},\vec{e}^{\,0})\, \vec{e}^{\,1}_{TE}(\vec{k}) + \left[2\frac{k_z^2}{k^2} - 1\right] \nu^r_{TM}(\vec{k},\vec{e}^{\,0})\, \vec{e}^{\,1}_{TM}(\vec{k}) \right\} e^{i\vec{k}^r\cdot\vec{x}} + \mathcal{O}\left(\left[\frac{k^2\Delta}{k_z^2}\right]^2 \right). \tag{4.3.17}$$

Note that since $\vec{k}^r$ is orthogonal to $\vec{e}^{\,0}_{TE}(\vec{k}) = (k_y, -k_x, 0)^\top / |k'|$ (cf. (A.1.1)), there holds

$$\left(\vec{k}^r \times \vec{e}^{\,0}_{TE}(\vec{k})\right) \times \vec{k}^r = -\left(\vec{k}^r \cdot \vec{e}^{\,0}_{TE}(\vec{k})\right) \vec{k}^r + k^2 \vec{e}^{\,0}_{TE}(\vec{k}) = k^2 \vec{e}^{\,0}_{TE}(\vec{k}) = k^2 \vec{e}^{\,1}_{TE}(\vec{k}). \tag{4.3.18}$$

Similarly, since $\vec{k}$ is orthogonal to $\vec{e}^{\,0}_{TM}(\vec{k}) = -(k_x k_z, k_y k_z, -|k'|^2)^\top / (k|k'|)$ (cf. (A.2.2)), $\vec{k}^r \cdot \vec{e}^{\,0}_{TM}(\vec{k}) = -2k_z\, [e^0_{TM}]_z$ and

$$\begin{aligned}
\left(\vec{k}^r \times \vec{e}^{\,0}_{TM}(\vec{k})\right) \times \vec{k}^r &= -\left(\vec{k}^r \cdot \vec{e}^{\,0}_{TM}(\vec{k})\right) \vec{k}^r + k^2\, \vec{e}^{\,0}_{TM}(\vec{k}) = 2\frac{k_z\,|k'|}{k} \begin{pmatrix} k_x \\ k_y \\ -k_z \end{pmatrix} - \frac{k^2}{k\,|k'|} \begin{pmatrix} k_x k_z \\ k_y k_z \\ -|k'|^2 \end{pmatrix} \\
&= - \begin{pmatrix} \left[-2\,|k'|^2 + k^2\right] \frac{1}{k|k'|} k_x k_z \\ \left[-2\,|k'|^2 + k^2\right] \frac{1}{k|k'|} k_y k_z \\ \left[2k_z^2 - k^2\right] \frac{|k'|^2}{k|k'|} \end{pmatrix} = -\left[2k_z^2 - k^2\right] \frac{1}{k\,|k'|} \begin{pmatrix} k_x k_z \\ k_y k_z \\ |k'|^2 \end{pmatrix} \\
&= -k^2 \left[2\frac{k_z^2}{k^2} - 1\right] \vec{e}^{\,1}_{TM}(\vec{k}).
\end{aligned} \tag{4.3.19}$$

Moreover, the polarisation vector $\vec{e}^{\,0}$ can be represented as a convex combination of the polarisation vectors in the TE and TM case, i.e. $\vec{e}^{\,0} = \nu^r_{TE}(\vec{k},\vec{e}^{\,0})\, \vec{e}^{\,0}_{TE}(\vec{k}) - \nu^r_{TM}(\vec{k},\vec{e}^{\,0})\, \vec{e}^{\,0}_{TM}(\vec{k})$ (cf. (A.3.1) and (4.3.10)). Consequently, (cf. (4.3.18) and (4.3.19))

$$\begin{aligned}
\left(\vec{k}^r \times \vec{e}^{\,0}\right) \times \vec{k}^r &= \nu^r_{TE}(\vec{k},\vec{e}^{\,0}) \left[\left(\vec{k}^r \times \vec{e}^{\,0}_{TE}(\vec{k})\right) \times \vec{k}^r\right] - \nu^r_{TM}(\vec{k},\vec{e}^{\,0}) \left[\left(\vec{k}^r \times \vec{e}^{\,0}_{TM}(\vec{k})\right) \times \vec{k}^r\right] \\
&= k^2 \left\{ \nu^r_{TE}(\vec{k},\vec{e}^{\,0})\, \vec{e}^{\,1}_{TE}(\vec{k}) - \left[2\frac{k_z^2}{k^2} - 1\right] \nu^r_{TM}(\vec{k},\vec{e}^{\,0})\, \vec{e}^{\,1}_{TM}(\vec{k}) \right\}
\end{aligned}$$

such that (cf. (4.3.17))

$$\vec{E}^r_Q(\vec{x}) = \frac{\Delta}{4\epsilon_0 k_z^2} \left[\left(\vec{k}^r \times \vec{e}^{\,0}\right) \times \vec{k}^r\right] e^{i\vec{k}^r\cdot\vec{x}} + \mathcal{O}\left(\left[\frac{k^2\Delta}{k_z^2}\right]^2 \right),$$

proving the statement of the lemma. ∎

4.4 The special case of a sinusoidal grating

In this section Formula (4.1.1) is compared with the one derived by Stearns [36] for the simple case of a specific sinusoidal grating in the case of classical diffraction (incident direction $\vec{k}$ orthogonal to grooves of periodic grating). In the first subsection a simplified version of Formula (4.1.1) for a specific sinusoidal grating will be derived. This formula is then compared with that of Stearns in the second subsection.

4.4.1 Applied far-field formula

Assume an interface function $f \in \mathcal{A} \cap L^\infty_Q$, with

$$f(x') := \lambda_{0,-1}\, e^{i\omega'_{0,-1}\cdot x'} + \lambda_{0,1}\, e^{i\omega'_{0,1}\cdot x'} = \frac{h}{2} \cos x. \tag{4.4.1}$$

It follows that

$$\begin{aligned}
\lambda_{0,-1} &= \frac{h}{4}, & \omega'_{0,-1} &= \begin{pmatrix} -1 \\ 0 \end{pmatrix}, \\
\lambda_{0,1} &= \frac{h}{4}, & \omega'_{0,1} &= \begin{pmatrix} 1 \\ 0 \end{pmatrix}.
\end{aligned} \tag{4.4.2}$$

To evaluate the second line of (4.1.1) it is necessary to determine the values of $\tilde{\lambda}^n_{0,j}$ and $\tilde{\omega}'_{0,j}$ for the interface (4.4.1). To do so, consider the formulas (3.3.17) and (3.3.18). Note that for f defined by (4.4.1), the index set $\mathbb{Z}$ in (3.3.17) and (3.3.18) is reduced to $\{-1, 1\}$. Thus (cf. (4.4.2))

$$\tilde{\omega}'_{0,j} = \begin{pmatrix} j \\ 0 \end{pmatrix}$$

for $j \in \mathbb{Z}$. Consequently, (cf. the definition of $\vec{\omega}_j$ after (3.3.65))

$$\vec{\omega}_j = \begin{pmatrix} k_x + j \\ k_y \\ \sqrt{k^2 - (k_x + j)^2 - k_y^2} \end{pmatrix}.$$

From now on classical diffraction will be assumed, meaning that $k_y = 0$, which leads to

$$\vec{\omega}_j = \begin{pmatrix} k_x + j \\ 0 \\ \sqrt{k^2 - (k_x + j)^2} \end{pmatrix}. \tag{4.4.3}$$

The factor $\tilde{\lambda}^n_{0,j}$ can be transformed to (cf. (3.3.18))

$$\begin{aligned}
\tilde{\lambda}^n_{0,j} &= \sum_{\substack{\tilde{m}=\max\{n+1,|j|\} \\ \tilde{m}+j \equiv 0 \bmod 2}}^{\infty} (ik_z\zeta)^{\tilde{m}-n-1} \frac{\tilde{m}!}{(\tilde{m}-n-1)!} \frac{h^{\tilde{m}}}{4^{\tilde{m}} \left(\frac{\tilde{m}-j}{2}\right)! \left(\frac{\tilde{m}+j}{2}\right)!} \\
&= \sum_{\substack{\tilde{m}=\max\{0,|j|-n-1\} \\ \tilde{m}+n+1+j \equiv 0 \bmod 2}}^{\infty} (ik_z\zeta)^{\tilde{m}} \frac{(\tilde{m}+n+1)!}{\tilde{m}!} \frac{h^{\tilde{m}+n+1}}{4^{(\tilde{m}+n+1)} \left(\frac{\tilde{m}+n+1-j}{2}\right)! \left(\frac{\tilde{m}+n+1+j}{2}\right)!}.
\end{aligned}$$

Indeed, the sum w.r.t. m_∞ (here $m_\infty = (m_1, m_{-1})$) in (3.3.24) reduces to the sum over all pairs $(m_{-1}, m_1) \in \mathbb{N}_0^2$, where $m_1 + m_{-1} = \tilde{m}$ and $m_1 - m_{-1} = j$, such that $m_1\omega'_{0,1} + m_{-1}\omega'_{0,-1} = \tilde{\omega}'_{0,j}$. Note that this is a linear system of two linear independent equations for two variables, with the unique solution $m_{-1} = (\tilde{m} - j)/2$ and $m_1 = (\tilde{m} + j)/2$. Moreover, $m_{-1}, m_1 \in \mathbb{N}_0$ implies that $\tilde{m} + j$ has to be even and that $\tilde{m} \geq |j|$. Thus (cf. (3.3.23), (3.3.24) and (3.3.21))

$$\tilde{\lambda}^n_{0,j} = \sum_{\tilde{m}\in\mathbb{N}_0} \sum_{\substack{m_\infty \in J_{\tilde{m}}: \\ \bar{\omega}'_0(m_\infty) = \tilde{\omega}'_{0,j}}} \tilde{\lambda}^n_0(\tilde{m}, m_\infty) = \sum_{\substack{\tilde{m}=\max\{0,|j|-n-1\} \\ \tilde{m}+n+1+j \equiv 0 \bmod 2}}^{\infty} \bar{\lambda}^n_{0,\tilde{m}} \left(\frac{\tilde{m}+j}{2}, \frac{\tilde{m}-j}{2} \right).$$

It follows that (cf. (4.1.1))

$$\begin{aligned}
\vec{E}^r(\vec{x}) = -i\frac{\Delta}{2\epsilon_0} \sum_{n\in\mathbb{N}_0} \sum_{j\in\mathbb{Z}} \sum_{\substack{\tilde{m}=\max\{0,|j|-n-1\} \\ \tilde{m}+n+1+j \equiv 0 \bmod 2}}^{\infty} \Bigg\{ & \frac{(-i)^n}{n!} \int_0^1 \zeta^{n+\tilde{m}} \, \mathrm{d}\zeta \, (ik_z)^{\tilde{m}} \frac{(\tilde{m}+n+1)!}{\tilde{m}!} \\
& \frac{h^{\tilde{m}+n+1} \left[(\vec{\omega}_j \times \vec{e}^{\,0}) \times \vec{\omega}_j \right] \left(\omega_z^j\right)^{n-1}}{4^{(\tilde{m}+n+1)} \left(\frac{\tilde{m}+n+1-j}{2}\right)! \left(\frac{\tilde{m}+n+1+j}{2}\right)!} e^{i\vec{\omega}_j\cdot\vec{x}} \Bigg\} + \vec{E}^r_Q(\vec{x})
\end{aligned}$$

$$= -i\,\frac{\Delta}{2\epsilon_0}\sum_{n\in\mathbb{N}_0}\sum_{j\in\mathbb{Z}}\sum_{\substack{\tilde m=\max\{0,|j|-n-1\}\\ \tilde m+n+1+j\equiv 0 \bmod 2}}^{\infty}\Bigg\{\frac{(-i)^n}{n!}\,(ik_z)^{\tilde m}\,\frac{(\tilde m+n)!}{\tilde m!}$$
$$\frac{h^{\tilde m+n+1}\left[\left(\vec\omega_j\times\vec e^{\,0}\right)\times\vec\omega_j\right]\,\left(\omega_z^j\right)^{n-1}}{4^{(\tilde m+n+1)}\,\left(\frac{\tilde m+n+1-j}{2}\right)!\,\left(\frac{\tilde m+n+1+j}{2}\right)!}\,e^{i\vec\omega_j\cdot\vec x}\Bigg\}+\vec E^r_{\mathcal{Q}}(\vec x). \tag{4.4.4}$$

Note that three functions F_j, G and H_j can be defined such that

$$S_0 := i\frac{2\epsilon_0}{\Delta}\left[\vec E^r(\vec x)-\vec E^r_{\mathcal{Q}}(\vec x)\right]=\sum_{j\in\mathbb{Z}}\sum_{n\in\mathbb{N}_0}\sum_{\substack{\tilde m=\max\{0,|j|-n-1\}\\ \tilde m+n+1+j\equiv 0 \bmod 2}}^{\infty}F_j(\tilde m+n)\,G(\tilde m)\,H_j(n),$$

with

$$\begin{aligned}
F_j(\tilde m+n) &:= \frac{(\tilde m+n)!\,h^{\tilde m+n+1}}{4^{(\tilde m+n+1)}\,\left(\frac{\tilde m+n+1-j}{2}\right)!\,\left(\frac{\tilde m+n+1+j}{2}\right)!},\\
G(\tilde m) &:= \frac{(ik_z)^{\tilde m}}{\tilde m!},\\
H_j(n) &:= \frac{(-i)^n}{n!}\,\left[\left(\vec\omega_j\times\vec e^{\,0}\right)\times\vec\omega_j\right]\,\left(\omega_z^j\right)^{n-1}e^{i\vec\omega_j\cdot\vec x}.
\end{aligned}$$

For the absolutely converging sum in S_0 there holds

$$S_0 = S_1 + S_2, \tag{4.4.5}$$

where

$$\begin{aligned}
S_1 &:= \sum_{j\in\mathbb{Z}}\sum_{n=0}^{|j|-1}\sum_{\substack{\tilde m=|j|-n-1\\ \tilde m+n+1+j\equiv 0 \bmod 2}}^{\infty}F_j(\tilde m+n)\,G(\tilde m)\,H_j(n)\\
&= \sum_{j\in\mathbb{Z}\setminus\{0\}}\sum_{n=0}^{|j|-1}\sum_{\substack{\tilde m=|j|-n-1\\ \tilde m+n+1+j\equiv 0 \bmod 2}}^{\infty}F_j(\tilde m+n)\,G(\tilde m)\,H_j(n),\\
S_2 &:= \sum_{j\in\mathbb{Z}}\sum_{n=|j|}^{\infty}\sum_{\substack{\tilde m=0\\ \tilde m+n+1+j\equiv 0 \bmod 2}}^{\infty}F_j(\tilde m+n)\,G(\tilde m)\,H_j(n).
\end{aligned}$$

To switch the order of summation in the absolute convergent sums w.r.t. n and $\tilde m$ in S_1, the variable $\tilde m$ is substituted by $m-n-1$ such that

$$\begin{aligned}
S_1 &= \sum_{j\in\mathbb{Z}\setminus\{0\}}\sum_{n=0}^{|j|-1}\sum_{\substack{m=|j|\\ m+j\equiv 0 \bmod 2}}^{\infty}F_j(m-1)\,G(m-n-1)\,H_j(n)\\
&= \sum_{j\in\mathbb{Z}\setminus\{0\}}\sum_{\substack{m=|j|\\ m+j\equiv 0 \bmod 2}}^{\infty}\sum_{n=0}^{|j|-1}F_j(m-1)\,G(m-n-1)\,H_j(n).
\end{aligned}$$

Here, n is substituted by $m-\tilde m-1$, leading to

$$\begin{aligned}
S_1 &= \sum_{j\in\mathbb{Z}\setminus\{0\}}\sum_{\substack{m=|j|\\ m+j\equiv 0 \bmod 2}}^{\infty}\sum_{\tilde m=m-|j|}^{m-1}F_j(m-1)\,G(\tilde m)\,H_j(m-\tilde m-1)\\
&= \sum_{j\in\mathbb{Z}\setminus\{0\}}\sum_{\substack{n=|j|\\ n+j\equiv 0 \bmod 2}}^{\infty}\sum_{\tilde m=n-|j|}^{n-1}F_j(n-1)\,G(\tilde m)\,H_j(n-\tilde m-1).
\end{aligned} \tag{4.4.6}$$

Similarly in S_2, substituting $\tilde{m}$ by $m-n-1$, where $m := \tilde{m}+n+1 \geq |j|+1$, gives

$$\begin{aligned}
S_2 &= \sum_{j\in\mathbb{Z}} \sum_{n=|j|}^{\infty} \sum_{\substack{m=n+1 \\ m+j\equiv 0 \bmod 2}}^{\infty} F_j(m-1)\, G(m-n-1)\, H_j(n) \\
&= \sum_{j\in\mathbb{Z}} \sum_{n=|j|}^{\infty} \sum_{\substack{m=|j|+1 \\ m+j\equiv 0 \bmod 2 \\ m\geq n+1}}^{\infty} F_j(m-1)\, G(m-n-1)\, H_j(n) \\
&= \sum_{j\in\mathbb{Z}} \sum_{\substack{m=|j|+1 \\ m+j\equiv 0 \bmod 2}}^{\infty} \sum_{\substack{n=|j| \\ n\leq m-1}}^{\infty} F_j(m-1)\, G(m-n-1)\, H_j(n) \\
&= \sum_{j\in\mathbb{Z}} \sum_{\substack{m=|j|+1 \\ m+j\equiv 0 \bmod 2}}^{\infty} \sum_{n=|j|}^{m-1} F_j(m-1)\, G(m-n-1)\, H_j(n).
\end{aligned}$$

Substituting, once more, n by $m-\tilde{m}-1$,

$$\begin{aligned}
S_2 &= \sum_{j\in\mathbb{Z}} \sum_{\substack{m=|j|+1 \\ m+j\equiv 0 \bmod 2}}^{\infty} \sum_{\tilde{m}=0}^{m-|j|-1} F_j(m-1)\, G(\tilde{m})\, H_j(m-\tilde{m}-1) \\
&= \sum_{j\in\mathbb{Z}} \sum_{\substack{n=|j|+1 \\ n+j\equiv 0 \bmod 2}}^{\infty} \sum_{\tilde{m}=0}^{n-|j|-1} F_j(n-1)\, G(\tilde{m})\, H_j(n-\tilde{m}-1). \qquad (4.4.7)
\end{aligned}$$

Consequently, (cf. (4.4.5), (4.4.6) and (4.4.7))

$$\begin{aligned}
S_0 = &\sum_{j\in\mathbb{Z}\setminus\{0\}} \sum_{\substack{n=|j| \\ n+j\equiv 0 \bmod 2}}^{\infty} \sum_{\tilde{m}=n-|j|}^{n-1} F_j(n-1)\, G(\tilde{m})\, H_j(n-\tilde{m}-1) \\
&+ \sum_{j\in\mathbb{Z}} \sum_{\substack{n=|j|+1 \\ n+j\equiv 0 \bmod 2}}^{\infty} \sum_{\tilde{m}=0}^{n-|j|-1} F_j(n-1)\, G(\tilde{m})\, H_j(n-\tilde{m}-1) \\
= &\sum_{j\in\mathbb{Z}\setminus\{0\}} \sum_{\substack{n=|j|+1 \\ n+j\equiv 0 \bmod 2}}^{\infty} \sum_{\tilde{m}=n-|j|}^{n-1} F_j(n-1)\, G(\tilde{m})\, H_j(n-\tilde{m}-1) \\
&+ \sum_{j\in\mathbb{Z}\setminus\{0\}} \sum_{\tilde{m}=0}^{|j|-1} F_j(|j|-1)\, G(\tilde{m})\, H_j(|j|-\tilde{m}-1) \\
&+ \sum_{j\in\mathbb{Z}\setminus\{0\}} \sum_{\substack{n=|j|+1 \\ n+j\equiv 0 \bmod 2}}^{\infty} \sum_{\tilde{m}=0}^{n-|j|-1} F_j(n-1)\, G(\tilde{m})\, H_j(n-\tilde{m}-1) \\
&+ \sum_{\substack{n=1 \\ n\equiv 0 \bmod 2}}^{\infty} \sum_{\tilde{m}=0}^{n-1} F_0(n-1)\, G(\tilde{m})\, H_0(n-\tilde{m}-1).
\end{aligned}$$

The first and the third line on the right-hand side of the last equation can obviously be combined, leading to

$$
\begin{aligned}
S_0 = &\sum_{j\in\mathbb{Z}\setminus\{0\}} \sum_{\substack{n=|j|+1\\ n+j\equiv 0 \bmod 2}}^{\infty} \sum_{\tilde{m}=0}^{n-1} F_j(n-1)\, G(\tilde{m})\, H_j(n-\tilde{m}-1) \\
&+ \sum_{j\in\mathbb{Z}\setminus\{0\}} \sum_{\tilde{m}=0}^{|j|-1} F_j(|j|-1)\, G(\tilde{m})\, H_j(|j|-\tilde{m}-1) \\
&+ \sum_{\substack{n=1\\ n\equiv 0 \bmod 2}}^{\infty} \sum_{\tilde{m}=0}^{n-1} F_0(n-1)\, G(\tilde{m})\, H_0(n-\tilde{m}-1) \\
= &\sum_{j\in\mathbb{Z}\setminus\{0\}} \sum_{\substack{n=|j|\\ n+j\equiv 0 \bmod 2}}^{\infty} \sum_{\tilde{m}=0}^{n-1} F_j(n-1)\, G(\tilde{m})\, H_j(n-\tilde{m}-1) \\
&+ \sum_{\substack{n=1\\ n\equiv 0 \bmod 2}}^{\infty} \sum_{\tilde{m}=0}^{n-1} F_0(n-1)\, G(\tilde{m})\, H_0(n-\tilde{m}-1),
\end{aligned}
\tag{4.4.8}
$$

where the first and second line are merged into the fourth line. Thus, in view of the absolute convergence in (3.1.4), the equations (4.4.4) and (4.4.8) imply

$$
\begin{aligned}
\vec{E}^r(\vec{x}) = &-i\,\frac{\Delta}{2\epsilon_0} \sum_{j\in\mathbb{Z}\setminus\{0\}} \sum_{\substack{n=|j|\\ n+j\equiv 0 \bmod 2}}^{\infty} \sum_{\tilde{m}=0}^{n-1} \Bigg\{ \frac{(-i)^{(n-\tilde{m}-1)}}{(n-\tilde{m}-1)!}\, (ik_z)^{\tilde{m}}\, \frac{(n-1)!}{\tilde{m}!} \\
&\qquad \frac{h^n \left[\left(\vec{\omega}_j \times \vec{e}^{\,0}\right) \times \vec{\omega}_j\right] \left(\omega_z^j\right)^{n-\tilde{m}-2}}{4^n \left(\frac{n-j}{2}\right)!\, \left(\frac{n+j}{2}\right)!}\, e^{i\vec{\omega}_j\cdot\vec{x}} \Bigg\} \\
&- i\,\frac{\Delta}{2\epsilon_0} \sum_{\substack{n=1\\ n\equiv 0 \bmod 2}}^{\infty} \sum_{\tilde{m}=0}^{n-1} \frac{(-i)^{(n-\tilde{m}-1)}}{(n-\tilde{m}-1)!}\, (ik_z)^{\tilde{m}}\, \frac{(n-1)!}{\tilde{m}!}\, \frac{h^n \left[\left(\vec{\omega}_0 \times \vec{e}^{\,0}\right) \times \vec{\omega}_0\right] \left(\omega_z^0\right)^{n-\tilde{m}-2}}{4^n \left[\left(\frac{n}{2}\right)!\right]^2}\, e^{i\vec{\omega}_0\cdot\vec{x}} \\
&+ \vec{E}^r_{\mathcal{Q}}(\vec{x}) \\
= &-i\,\frac{\Delta}{2\epsilon_0} \sum_{j\in\mathbb{Z}\setminus\{0\}} \sum_{\substack{n=|j|\\ n+j\equiv 0 \bmod 2}}^{\infty} \sum_{\tilde{m}=0}^{n-1} \frac{(-i)^{(n-1)}\, h^n (n-1)!\, (-k_z)^{\tilde{m}}}{4^n\, \tilde{m}!\, (n-\tilde{m}-1)!} \left(\omega_z^j\right)^{n-\tilde{m}-2} \frac{\left[\left(\vec{\omega}_j \times \vec{e}^{\,0}\right) \times \vec{\omega}_j\right]}{\left(\frac{n-j}{2}\right)!\, \left(\frac{n+j}{2}\right)!}\, e^{i\vec{\omega}_j\cdot\vec{x}} \\
&- i\,\frac{\Delta}{2\epsilon_0} \sum_{\substack{n=1\\ n\equiv 0 \bmod 2}}^{\infty} \sum_{\tilde{m}=0}^{n-1} \frac{(-i)^{(n-1)}\, h^n (n-1)!}{4^n\, \tilde{m}!\, (n-\tilde{m}-1)!}\, (-k_z)^{n-2}\, \frac{\left[\left(\vec{k}^r \times \vec{e}^{\,0}\right) \times \vec{k}^r\right]}{\left[\left(\frac{n}{2}\right)!\right]^2}\, e^{i\vec{k}^r\cdot\vec{x}} \\
&+ \vec{E}^r_{\mathcal{Q}}(\vec{x}),
\end{aligned}
\tag{4.4.9}
$$

where $\vec{k}^r = \vec{\omega}_0 = (k_x, 0, -k_z)$ for $k_y = 0$ and $k_z < 0$.

4.4.2 Near-field formula of Stearns

According to Stearns (cf. [36, Eqn. (19), p. 494])

$$
\vec{E}^r(\vec{x}) = \frac{\Delta k^2}{8\pi^2\epsilon_0} \int\limits_{\mathbb{R}^2} \frac{\hat{g}(k\vec{n}^r - \vec{k})}{n_z^r(n_z^r - n_z^0)} \left[\left(\vec{n}^r \times \vec{e}^{\,0}\right) \times \vec{n}^r\right] e^{ik\vec{n}^r\cdot\vec{x}}\, \mathrm{d}n',
$$

where $\vec{n}^r := \left(n_x, n_y, \sqrt{1-n'^2}\right)^\top$, $n' := (n_x, n_y)^\top$, $n'^2 := n_x^2 + n_y^2$, $n_z^0 := \frac{k_z}{k}$ and where

$$
\hat{g}(\vec{s}) := \mathcal{F}(g)(\vec{s}),
$$

for $g(\vec{x}) := \delta\left(z - \frac{h}{2}\cos x\right)$, is defined in a generalised sense (cf. (2.3.9)). Formally applying the Fourier transform to g and using the power series of the exponential function leads to

$$\begin{aligned}
\hat{g}(\vec{s}) &:= \int_{\mathbb{R}^3} g(\vec{x})\, e^{-i\vec{s}\cdot\vec{x}}\, \mathrm{d}\vec{x} = \int_{\mathbb{R}^2}\int_{\mathbb{R}} \delta(z - \frac{h}{2}\cos x)\, e^{-is_z z}\, \mathrm{d}z\, e^{-is'\cdot x'}\, \mathrm{d}x' = \int_{\mathbb{R}^2} e^{-i\frac{h}{2}\, s_z \cos x}\, e^{-is'\cdot x'}\, \mathrm{d}x' \\
&= 2\pi\, \delta(s_y) \int_{\mathbb{R}} e^{-i\frac{h}{2}\, s_z\, \cos x}\, e^{-is_x\, x}\, \mathrm{d}x = 2\pi\, \delta(s_y) \sum_{n\in\mathbb{N}_0} \frac{\left(-i\frac{h}{2}\, s_z\right)^n}{n!} \int_{\mathbb{R}} \cos^n x\, e^{-is_x\, x}\, \mathrm{d}x,
\end{aligned}$$

where, using the binomial theorem,

$$\begin{aligned}
\int_{\mathbb{R}} \cos^n x\, e^{-is_x\, x}\, \mathrm{d}x &= \frac{1}{2^n}\int_{\mathbb{R}} \left(e^{ix} + e^{-ix}\right)^n\, e^{-is_x\, x}\, \mathrm{d}x \\
&= \frac{1}{2^n}\sum_{m=0}^{n} \frac{n!}{m!\,(n-m)!} \int_{\mathbb{R}} e^{i(2m-n)\,x}\, e^{-is_x\, x}\, \mathrm{d}x \\
&= \frac{2\pi}{2^n}\sum_{m=0}^{n} \frac{n!}{m!\,(n-m)!}\, \delta(s_x + n - 2m).
\end{aligned}$$

Hence,

$$\hat{g}(\vec{s}) := 4\pi^2\, \delta(s_y) \sum_{n\in\mathbb{N}_0} \frac{(-ihs_z)^n}{4^n} \sum_{m=0}^{n} \frac{1}{m!\,(n-m)!}\, \delta(s_x + n - 2m)$$

and the occurring sums are absolutely convergent in the sense of distributions, i.e. when tested with a smooth function $\varphi \in C_0^\infty(\mathbb{R}^3)$. It can now be shown that

$$\vec{E}^r(\vec{x}) = \frac{\Delta k}{2\epsilon_0} \sum_{n\in\mathbb{N}_0}\sum_{m=0}^{n} \frac{(-ih)^n (kw_z^{n,m} - k_z)^n}{4^n\, m!\,(n-m)!} \frac{\left[\left(\vec{w}^{n,m} \times \vec{e}^{\,0}\right) \times \vec{w}^{n,m}\right]}{w_z^{n,m}\,(kw_z^{n,m} - k_z)}\, e^{ik\vec{w}^{n,m}\cdot\vec{x}},$$

where $\vec{w}^{n,m} := (k_x/k + (2m-n)/k,\ k_y/k,\ w_z^{n,m})^\top$ and $w_z^{n,m} := \sqrt{1 - [k_x/k + (2m-n)/k]^2 - [k_y/k]^2}$ with $k_y = 0$. Note that to get the correct power of k, the formula

$$\int_{\mathbb{R}^2} \delta(kn_x - k_x + n - 2m)\, \delta(kn_y)\, \varphi(n')\, \mathrm{d}n' = \frac{1}{k^2}\int_{\mathbb{R}^2} \delta(n_x)\, \delta(n_y)\, \varphi\left(\frac{1}{k}\left[n_x + k_x - n + 2m\right], \frac{1}{k}n_y\right)\, \mathrm{d}n'$$

has been used. Splitting off the summand with $n = 0$ and applying the binomial theorem to $(kw_z^{n,m} - k_z)^{n-1}$ the formula can be rearranged to get

$$\begin{aligned}
\vec{E}^r(\vec{x}) &= \frac{\Delta k}{2\epsilon_0} \sum_{n\in\mathbb{N}_0}\sum_{m=0}^{n} \frac{(-ih)^n (kw_z^{n,m} - k_z)^{n-1}}{4^n\, m!\,(n-m)!} \frac{\left[\left(\vec{w}^{n,m} \times \vec{e}^{\,0}\right) \times \vec{w}^{n,m}\right]}{w_z^{n,m}}\, e^{ik\vec{w}^{n,m}\cdot\vec{x}} \\
&= \frac{\Delta k}{2\epsilon_0} \sum_{n\in\mathbb{N}}\sum_{m=0}^{n} \frac{(-ih)^n (kw_z^{n,m} - k_z)^{n-1}}{4^n\, m!\,(n-m)!} \frac{\left[\left(\vec{w}^{n,m} \times \vec{e}^{\,0}\right) \times \vec{w}^{n,m}\right]}{w_z^{n,m}}\, e^{ik\vec{w}^{n,m}\cdot\vec{x}} \\
&\quad + \frac{\Delta k}{2\epsilon_0} \frac{\left[\left(\vec{w}^{0,0} \times \vec{e}^{\,0}\right) \times \vec{w}^{0,0}\right]}{w_z^{0,0}\,(kw_z^{0,0} - k_z)}\, e^{ik\vec{w}^{0,0}\cdot\vec{x}} \\
&= \frac{\Delta k^2}{2\epsilon_0} \sum_{n\in\mathbb{N}}\sum_{m=0}^{n}\sum_{\tilde{m}=0}^{n-1} \frac{(-ih)^n\,(n-1)!\,(-k_z)^{\tilde{m}}}{4^n\,\tilde{m}!\,(n-1-\tilde{m})!} [kw_z^{n,m}]^{n-1-\tilde{m}}\, \frac{\left[\left(\vec{w}^{n,m} \times \vec{e}^{\,0}\right) \times \vec{w}^{n,m}\right]}{kw_z^{n,m}\, m!\,(n-m)!}\, e^{ik\vec{w}^{n,m}\cdot\vec{x}} \\
&\quad + \frac{\Delta k}{2\epsilon_0} \frac{\left[\left(\vec{n}_0^r \times \vec{e}^{\,0}\right) \times \vec{n}_0^r\right]}{-n_z^0\,(-kn_z^0 - k_z)}\, e^{ik\vec{n}_0^r\cdot\vec{x}}
\end{aligned}$$

$$= \frac{\Delta k^2}{2\epsilon_0} \sum_{n\in\mathbb{N}} \sum_{m=0}^{n} \sum_{\tilde{m}=0}^{n-1} \frac{(-ih)^n\,(n-1)!\,(-k_z)^{\tilde{m}}}{4^n\,\tilde{m}!\,(n-\tilde{m}-1)!}\,[kw_z^{n,m}]^{n-\tilde{m}-2}\,\frac{\left[\left(\vec{w}^{n,m}\times\vec{e}^{\,0}\right)\times\vec{w}^{n,m}\right]}{m!\,(n-m)!}\,e^{ik\vec{w}^{n,m}\cdot\vec{x}}$$
$$+\frac{\Delta k}{2\epsilon_0}\,\frac{\left[\left(\vec{n}_0^r\times\vec{e}^{\,0}\right)\times\vec{n}_0^r\right]}{n_z^0\,(kn_z^0+k_z)}\,e^{ik\vec{n}_0^r\cdot\vec{x}},$$

where $\vec{w}^{0,0} = \vec{n}_0^r$ and $w_z^{0,0} = -n_z^0$ since $n_z^0 < 0$. To further transform the term, it is used that the summands w.r.t. n and m can be sorted w.r.t. $2m-n$. To be precise, for any fixed j, the summands for all pairs (n,m) where $2m-n=j$ are collected and added. Afterwards the sum over all these partial sums is evaluated. Since $2m-n$ can take the value of every integer number, the sum over all partial sums corresponds to the sum over all $j\in\mathbb{Z}$. For convenience, define

$$F(2m-n,n) := \sum_{\tilde{m}=0}^{n-1} \frac{(-k_z)^{\tilde{m}}}{\tilde{m}!\,(n-\tilde{m}-1)!}\,[kw_z^{n,m}]^{n-\tilde{m}-2}\left[\left(\vec{w}^{n,m}\times\vec{e}^{\,0}\right)\times\vec{w}^{n,m}\right]e^{ik\vec{w}^{n,m}\cdot\vec{x}},$$
$$G(n) := \frac{(-ih)^n\,(n-1)!}{4^n}.$$

Consequently,

$$\sum_{n\in\mathbb{N}}\sum_{m=0}^{n}\frac{F(2m-n,n)\,G(n)}{m!\,(n-m)!} = \sum_{j\in\mathbb{Z}}\sum_{n\in\mathbb{N}}\sum_{\substack{m=0\\2m-n=j}}^{n}\frac{F(j,n)\,G(n)}{m!\,(n-m)!}$$
$$= \sum_{j\in\mathbb{Z}}\sum_{\substack{n=\max\{|j|,1\}\\n+j\equiv 0 \bmod 2}}^{\infty}\frac{F(j,n)\,G(n)}{\left(\frac{n+j}{2}\right)!\left(\frac{n-j}{2}\right)!}$$
$$= \sum_{j\in\mathbb{Z}\setminus\{0\}}\sum_{\substack{n=|j|\\n+j\equiv 0 \bmod 2}}^{\infty}\frac{F(j,n)\,G(n)}{\left(\frac{n+j}{2}\right)!\left(\frac{n-j}{2}\right)!}$$
$$+\sum_{\substack{n=1\\n\equiv 0 \bmod 2}}^{\infty}\frac{F(0,n)\,G(n)}{\left[\left(\frac{n}{2}\right)!\right]^2}.$$

Keeping in mind that $\vec{w}^{n,m} = (k_x/k + (2m-n)/k,\,0,\,\sqrt{1-[k_x/k+(2m-n)/k]^2})^\top$ for $j=2m-n$ is equal to $1/k\,(k_x+j,0,\sqrt{k^2-(k_x+j)^2})^\top = 1/k\,\vec{\omega}_j$ (cf. (4.4.3)), this leads to

$$\vec{E}^r(\vec{x}) = \frac{\Delta k^2}{2\epsilon_0}\sum_{j\in\mathbb{Z}\setminus\{0\}}\sum_{\substack{n=|j|\\n+j\equiv 0 \bmod 2}}^{\infty}\sum_{\tilde{m}=0}^{n-1}\frac{(-ih)^n\,(n-1)!\,(-k_z)^{\tilde{m}}}{4^n\,\tilde{m}!\,(n-\tilde{m}-1)!}\left(\omega_z^j\right)^{n-\tilde{m}-2}\frac{\frac{1}{k^2}\left[\left(\vec{\omega}_j\times\vec{e}^{\,0}\right)\times\vec{\omega}_j\right]}{\left(\frac{n-j}{2}\right)!\,\left(\frac{n+j}{2}\right)!}\,e^{i\vec{\omega}_j\cdot\vec{x}}$$
$$+\frac{\Delta k^2}{2\epsilon_0}\sum_{\substack{n=1\\n\equiv 0 \bmod 2}}^{\infty}\sum_{\tilde{m}=0}^{n-1}\frac{(-ih)^n\,(n-1)!\,(-k_z)^{\tilde{m}}}{4^n\,\tilde{m}!\,(n-\tilde{m}-1)!}\left(\omega_z^0\right)^{n-\tilde{m}-2}\frac{\frac{1}{k^2}\left[\left(\vec{\omega}_0\times\vec{e}^{\,0}\right)\times\vec{\omega}_0\right]}{\left[\left(\frac{n}{2}\right)!\right]^2}\,e^{i\vec{\omega}_0\cdot\vec{x}}$$
$$+\frac{\Delta k}{2\,\epsilon_0}\,\frac{\left[\left(\vec{n}_0^r\times\vec{e}^{\,0}\right)\times\vec{n}_0^r\right]}{n_z^0\,(kn_z^0+k_z)}\,e^{ik\vec{n}_0^r\cdot\vec{x}}$$
$$= -i\,\frac{\Delta}{2\epsilon_0}\sum_{j\in\mathbb{Z}\setminus\{0\}}\sum_{\substack{n=|j|\\n+j\equiv 0 \bmod 2}}^{\infty}\sum_{\tilde{m}=0}^{n-1}\frac{(-i)^{n-1}h^n\,(n-1)!\,(-k_z)^{\tilde{m}}}{4^n\,\tilde{m}!\,(n-\tilde{m}-1)!}\left(\omega_z^j\right)^{n-\tilde{m}-2}\frac{\left[\left(\vec{\omega}_j\times\vec{e}^{\,0}\right)\times\vec{\omega}_j\right]}{\left(\frac{n-j}{2}\right)!\,\left(\frac{n+j}{2}\right)!}\,e^{i\vec{\omega}_j\cdot\vec{x}}$$
$$-\,i\,\frac{\Delta}{2\epsilon_0}\sum_{\substack{n=1\\n\equiv 0 \bmod 2}}^{\infty}\sum_{\tilde{m}=0}^{n-1}\frac{(-i)^{n-1}h^n\,(n-1)!}{4^n\,\tilde{m}!\,(n-\tilde{m}-1)!}\,(-k_z)^{n-2}\,\frac{\left[\left(\vec{k}^r\times\vec{e}^{\,0}\right)\times\vec{k}^r\right]}{\left[\left(\frac{n}{2}\right)!\right]^2}\,e^{i\vec{k}^r\cdot\vec{x}}$$
$$+\frac{\Delta}{4\,\epsilon_0[n_z^0]^2}\left[\left(\vec{n}_0^r\times\vec{e}^{\,0}\right)\times\vec{n}_0^r\right]e^{ik\vec{n}_0^r\cdot\vec{x}} \qquad (4.4.10)$$

for $k_z = k\vec{n}_z^0$, where $\vec{k}^r$ is defined as at the end of Section 4.4.1. Moreover, Lemma 4.9 states that (cf. Eqn. (36) in [36] for $\vec{e}^* \cdot \vec{n}_0^r = 0$)

$$\frac{\Delta}{4\,\epsilon_0 [n_z^0]^2}\,\left[\left(\vec{n}_0^r \times \vec{e}^0\right) \times \vec{n}_0^r\right]\,e^{ik\vec{n}_0^r \cdot \vec{x}} = \frac{\Delta}{4\,\epsilon_0 k_z^2}\,\left[\left(\vec{k}^r \times \vec{e}^0\right) \times \vec{k}^r\right]\,e^{i\vec{k}^r \cdot \vec{x}} = \vec{E}_Q^r(\vec{x}) + \mathcal{O}\left(\left[\frac{k^2\Delta}{k_z^2}\right]^2\right).$$

Thus the two equations (4.4.9) and (4.4.10) are asymptotically the same for $k^2\Delta/k_z^2 \ll 1$.

Chapter 5

The transmitted far field

The preceding three Chapters 2–4 only showed how the far-field formula in the sense of the Born approximation can be derived for the reflected field. Naturally this can also be done for the transmitted field. For now it will be assumed that ϵ_0', the dielectric constant of the material below the interface, is real valued and thus that the corresponding material is non-absorbing. The case of an absorbing lower material is discussed in Remark 5.2.

In the non-absorbing case, it can be shown that

Theorem 5.1 (The transmitted far field). *Assume the interface is the graph of a function $f \in \mathcal{A} \cap L_Q^\infty$ as described in Remark 3.4 that satisfies condition (3.3.41). Furthermore, suppose this interface is illuminated by an incoming plane wave as described in Subsection 2.1. Then the far-field asymptotics of the transmitted polarised electric field for $z < -\max\{2\|f\|_{\mathcal{A}}, 2\|f\|_\infty\}$ in the sense of the Born approximation is*

$$
\begin{aligned}
\vec{E}^t(R\vec{m}) = {} & t(\vec{k},\vec{e}^{\,0})\,\frac{e^{ikR\vec{n}_0^t\cdot\vec{m}}}{|k'|^2} \\
& + i\,\frac{\Delta}{2\epsilon_0'}\sum_{n\in\mathbb{N}_0}\sum_{\substack{j\in\mathbb{Z}\\ |k'+\tilde{\omega}_{0,j}'|<\tilde{k}}}\int_0^1 \tilde{\lambda}_{0,j}^n(\zeta)\frac{(-i\zeta)^n}{n!}\,\mathrm{d}\zeta\;\left[\left(\vec{\omega}_j^t\times\vec{e}^{\,0}\right)\times\vec{\omega}_j^t\right]\,\left(\tilde{\omega}_z^j\right)^{n-1}\,e^{iR\vec{\omega}_j^t\cdot\vec{m}} \\
& + \frac{\Delta\,\tilde{k}^3}{2\epsilon_0'}\,\tilde{\mathcal{H}}(\vec{m})\,\left[\left(\vec{m}\times\vec{e}^{\,0}\right)\times\vec{m}\right]\,\frac{e^{i\tilde{k}R}}{\tilde{k}R} \\
& + i\,\frac{\Delta}{2\epsilon_0'}\sum_{\substack{j\in\mathbb{Z}\\ |k'+\tilde{\omega}_{1,j}'|=\tilde{k}}}\int_0^1 \tilde{\lambda}_{1,j}^0(\zeta)\,\mathrm{d}\zeta\,\left[\left((k'+\tilde{\omega}_{1,j}',0)^\top\times\vec{e}^{\,0}\right)\times(k'+\tilde{\omega}_{1,j}',0)^\top\right]\,\frac{e^{iR(k'+\tilde{\omega}_{1,j}')\cdot m'}}{\tilde{k}Rm_z} \\
& + \frac{\Delta\,\tilde{k}^2}{4\pi\epsilon_0'}\,\tilde{\mathcal{H}}_1(\vec{m})\,\left[\left(\vec{m}\times\vec{e}^{\,0}\right)\times\vec{m}\right]\left(\frac{1}{\tilde{k}R}+\sqrt{i\pi}\,\frac{e^{i\tilde{k}R}}{\sqrt{\tilde{k}R}}\right) \\
& + \frac{\Delta\,\tilde{k}^3}{4\epsilon_0'}\,\tilde{\mathcal{H}}_2(\vec{m})\,\left[\left(\vec{m}\times\vec{e}^{\,0}\right)\times\vec{m}\right]\,\frac{\log R}{\tilde{k}R}\,e^{i\tilde{k}R}+o\left(\frac{1}{R}\right),
\end{aligned}
\tag{5.1}
$$

where $m_z < 0$, $\tilde{k} := \sqrt{\mu_0\epsilon_0'}\omega$, $\epsilon_0' \ge 0$, $\vec{n}_0^t := (n_x^0, n_y^0, n_z^t)^\top$, $n_z^t := -\sqrt{\tilde{k}^2-|k'|^2}/\tilde{k}$, $\vec{\omega}_j^t := (k'+\tilde{\omega}_{0,j}', \tilde{\omega}_z^j)^\top$, $\tilde{\omega}_z^j := -\sqrt{\tilde{k}^2-|k'+\tilde{\omega}_{0,j}'|^2}$,

$$
\tilde{\mathcal{H}}(\vec{m}) := \sum_{n\in\mathbb{N}_0}\sum_{j\in\mathbb{Z}}\sum_{\ell=1}^4\int_0^1 \tilde{\lambda}_{\ell,j}^n(\zeta)\,\frac{(-i\tilde{k}m_z\,\zeta)^n}{n!}\,h_{\ell,j,n}^t(\vec{m},\zeta)\,\mathrm{d}\zeta,
$$

$$\tilde{\mathcal{H}}_1(\vec{m}) := \sqrt{2}\,\tilde{F}(\pi \setminus \alpha) \sum_{n\in\mathbb{N}_0} \sum_{\substack{j\in\mathbb{Z} \\ \tilde{\omega}'_{1,j}=\tilde{k}m'-k'}} \int_0^1 \tilde{\lambda}^n_{1,j}(\zeta)\, \frac{(-i\tilde{k}m_z\,\zeta)^n}{n!}\,\mathrm{d}\zeta,$$

$$\tilde{\mathcal{H}}_2(\vec{m}) := \sum_{n\in\mathbb{N}_0} \sum_{\substack{j\in\mathbb{Z} \\ \tilde{\omega}'_{2,j}=\tilde{k}m'-k'}} \int_0^1 \tilde{\lambda}^n_{2,j}(\zeta)\, \frac{(-i\tilde{k}m_z\,\zeta)^n}{n!}\,\mathrm{d}\zeta,$$

and where $\tilde{\lambda}^n_{\ell,j}$, $\tilde{\omega}_{\ell,j}$ and $\tilde{g}_n$ are defined in Lemma 3.9. The term $\tilde{F}$ denotes the elliptic integral of the first kind,

$$h^t_{\ell,j,n}(\vec{m},\zeta) := \begin{cases} \frac{e^{-\left|\tilde{k}m'-(k'+\tilde{\omega}'_{1,j})\right|}}{\left|\tilde{k}m'-(k'+\tilde{\omega}'_{1,j})\right|} & \text{if } \ell=1 \text{ and } m' \neq \frac{k'+\tilde{\omega}'_{1,j}}{\tilde{k}} \\ -1 & \text{if } \ell=1 \text{ and } m' = \frac{k'+\tilde{\omega}'_{1,j}}{\tilde{k}} \\ K_0\left(\left|\tilde{k}m'-(k'+\tilde{\omega}'_{2,j})\right|\right) & \text{if } \ell=2 \text{ and } m' \neq \frac{k'+\tilde{\omega}'_{2,j}}{\tilde{k}} \\ -\frac{1}{2}\left[\tilde{\gamma}+\log\left(\frac{\tilde{k}}{8}\,(1+m_z)^2\right)-i\frac{\pi}{2}\right] & \text{if } \ell=2 \text{ and } m' = \frac{k'+\tilde{\omega}'_{2,j}}{\tilde{k}} \\ e^{-\left|\tilde{k}m'-(k'+\tilde{\omega}'_{3,j})\right|} & \text{if } \ell=3 \\ \frac{1}{2\pi}\int_{\mathbb{R}^2} \tilde{g}_n(\eta',\zeta)\, e^{-i\eta'\cdot\left(\tilde{k}m'-k'\right)}\,\mathrm{d}\eta' & \text{if } \ell=4 \end{cases}$$

and

$$t(\vec{k},\vec{e}^{\,0}) := \left\{ 2\frac{k_y e^0_x - k_x e^0_y}{k_z - \sqrt{\tilde{k}^2-|k'|^2}} \begin{pmatrix} k_y \\ -k_x \\ 0 \end{pmatrix} + 2\frac{k_z(k_x e^0_x + k_y e^0_y) - |k'|^2\, e^0_z}{\tilde{k}^2 k_z - k^2\sqrt{\tilde{k}^2-|k'|^2}} \begin{pmatrix} -k_x\sqrt{\tilde{k}^2-|k'|^2} \\ -k_y\sqrt{\tilde{k}^2-|k'|^2} \\ -|k'|^2 \end{pmatrix} \right\} k_z. \quad (5.2)$$

To prove this, all the derivations from Chapter 2 to 4 and those in Chapter B in the appendix would have to be repeated for the transmitted field. On the other hand, these derivations are very similar to those for the reflected field. The main differences are changed constants and signs. As a consequence, the proof for the transmitted field will only be outlined by highlighting the differences to the proof for the reflected far field.

The first step is again to derive an inhomogeneous vector Helmholtz equation (cf. (2.2.3)), the solution of which will now describe the total field below the interface. As before, the limiting absorption principle is applied. But this time an imaginary part is added to the real valued dielectric constant ϵ'_0 of the material below the interface. This is done in such a way that a small τ is added to the third component of the wave vector of specular transmission $\vec{k}^t := (k', k^t_z)^\top$ with $k^t_z := -(\tilde{k}^2 - |k'|^2)^{1/2}$, i.e. $\vec{k}^t_\tau := (k', k^t_{z,\tau})^\top$ with $k^t_{z,\tau} := k^t_z + i\tau$. Here and in the following, the term 'specular transmission direction' is used to describe the propagation direction corresponding to the transmitted plane wave $\vec{E}^t_Q$, which results from diffraction at an ideal plane.

Defining $\tilde{\epsilon}_\tau := \epsilon'_0 - \tau^2/(\mu_0\omega^2) + i2\tau k^t_z/(\mu_0\omega^2)$ ensures that $\tilde{k}^2_\tau := \vec{k}^t_\tau \cdot \vec{k}^t_\tau = \mu_0\tilde{\epsilon}_\tau\omega^2$ with $\operatorname{Im}\tilde{\epsilon}_\tau > 0$. With this, Maxwell's equations (2.2.1) and (2.2.2) are used to show that

$$\nabla^2\vec{\mathcal{D}} - \mu_0\tilde{\epsilon}_\tau\partial_t^2\vec{\mathcal{D}} = -\nabla\times\nabla\times\left(\vec{\mathcal{D}} - \tilde{\epsilon}_\tau\vec{\mathcal{E}}\right) + \tilde{\epsilon}_\tau\partial_t\nabla\times\left(\vec{\mathcal{B}} - \mu_0\vec{\mathcal{H}}\right)$$

and for the assumed time-independent amplitude factors that

$$\left(\nabla^2 + \tilde{k}^2_\tau\right)\vec{D} = -\nabla\times\nabla\times\left(\vec{D} - \tilde{\epsilon}_\tau\vec{E}\right).$$

For any $\vec{x}$ below the interface, described by the graph of a function $f \in L^\infty(\mathbb{R}^2)$, i.e. $z < f(x')$, the total displacement field $\vec{D}(\vec{x})$ is equal to $\tilde{\varepsilon}_\tau(\vec{x})\vec{E}(\vec{x})$, where

$$\tilde{\varepsilon}_\tau(\vec{x}) := \begin{cases} \epsilon_0 & \text{if } z > f(x') \\ \tilde{\epsilon}_\tau & \text{if } z < f(x') \end{cases}.$$

Moreover, the total electric and displacement fields below the interface are equal to the transmitted electric and displacement fields, respectively, such that $\vec{D} = \vec{D}^t$, $\vec{E} = \vec{E}^t$ and

$$\left(\nabla^2 + \tilde{k}_\tau^2\right) \vec{D}^t = -\nabla \times \left[\nabla \times \left(\tilde{\alpha}\, \vec{E}^t\right)\right],$$

where $\tilde{\alpha}(\vec{x}) := \tilde{\varepsilon}_\tau(\vec{x}) - \tilde{\epsilon}_\tau$. At this point, the Born approximation is applied to this equation. Since the low contrast case is assumed, the non-specular scattered field is very small compared to the field transmitted in specular direction. In this sense almost all the energy of the incident field $\vec{E}^0 = \vec{e}^{\,0}\, e^{i\vec{k}\cdot\vec{x}}$ is transmitted, such that $\vec{E}^t \sim \vec{E}^0$ and similar to the transformations in Section 2.3 a new vector Helmholtz equation

$$\left(\nabla^2 + \tilde{k}_\tau^2\right) \vec{D}^t = -\nabla \times \left[\nabla \times \left(\tilde{\alpha}\, \vec{E}^0\right)\right] \tag{5.3}$$

is obtained. Note that the approximation $\vec{E}^t \sim \vec{E}^0$ holds only at the material interface. Further away from the interface, i.e. in negative z-direction in the lower material, the difference of the two fields $\vec{E}^t$ and $\vec{E}^0$ would increase. However, since $\tilde{\alpha}(\vec{x})$ is supported above the interface, this has no influence on the presented Born approximation (5.3). Again, the same equation can also be formulated for the special case of an ideal interface $f_Q \equiv 0$ and the corresponding $\tilde{\alpha}_Q$ and $\vec{D}_Q^t$, such that by defining $\tilde{\alpha}_d := \tilde{\alpha} - \tilde{\alpha}_Q$ and $\vec{D}_d^t := \vec{D}^t - D_Q^t$, (cf. the transformation leading to (2.3.5))

$$\left(\nabla^2 + \tilde{k}_\tau^2\right) \vec{D}_d^t = -\nabla \times \left[\nabla \times \left(\tilde{\alpha}_d\, \vec{E}^0\right)\right] \tag{5.4}$$

in the sense of the Born approximation. Similar to the reflected case, for the remainder of this thesis the term 'Born approximation' will refer to the approximation applied to reach Equation (5.4) for the transmitted field.

As for (2.3.5) the Fourier transform is applied to both sides of this equation, which is then resolved w.r.t. the Fourier transform of the transmitted field. Afterwards the generalised inverse Fourier transform is applied and some of the occurring integrals are represented as Cauchy principal value integrals at infinity to switch the order of integration (cf. transformations leading to (3.2.4)). Following the same path for (5.4) gives

$$\begin{aligned}&\left\langle \vec{D}_d^t(\vec{x}), \varphi(\vec{x}) \right\rangle \\ &\quad= \frac{1}{(2\pi)^3} \lim_{\tilde{r}\to\infty} \lim_{r,R\to\infty} \int_{\mathbb{R}^3} \bar{\varphi}(\vec{x}) \int_{B_2(r)} \int_{-R}^{R} \int_{C_3(\tilde{r})} \tilde{\alpha}_d(\vec{\eta})\, e^{-i\vec{\eta}\cdot(\vec{s}-\vec{k})}\, \mathrm{d}\vec{\eta}\, \frac{\left[\left(\vec{s} \times \vec{e}^{\,0}\right) \times \vec{s}\right]}{s_z^2 - \tilde{\xi}_\tau^2}\, e^{i\vec{s}\cdot\vec{x}}\, \mathrm{d}s_z\, \mathrm{d}s'\, \mathrm{d}\vec{x},\end{aligned}$$

where $\tilde{\xi}_\tau := -\sqrt{\tilde{k}_\tau^2 - |s'|^2}$, with $\operatorname{Im} \tilde{\xi}_\tau < 0$ by definition of the chosen branch cut at the end of Section 3.2.2. The integral w.r.t. s_z can again be integrated analytically by employing the residue theorem. Similar to Section 3.2.3 it can be shown that with $\hat{\alpha}_{\tilde{r}}^t := \mathcal{F}(\tilde{\alpha}_d(\vec{\eta})\, \mathbb{1}_{C_3(\tilde{r})}(\vec{\eta}))$,

$$\lim_{R\to\infty} \int_{-R}^{R} \hat{\alpha}_{\tilde{r}}^t(\vec{s} - \vec{k})\, \frac{\left[\left(\vec{s} \times \vec{e}^{\,0}\right) \times \vec{s}\right]}{s_z^2 - \tilde{\xi}_\tau^2}\, e^{is_z z}\, \mathrm{d}s_z = -\pi i\, \hat{\alpha}_{\tilde{r}}\big(\vec{s}_{\tilde{\xi}_\tau} - \vec{k}\big)\, \frac{\left[\left(\vec{s}_{\tilde{\xi}_\tau} \times \vec{e}^{\,0}\right) \times \vec{s}_{\xi_\tau}\right]}{\tilde{\xi}_\tau}\, e^{i\tilde{\xi}_\tau z}.$$

This is shown using the same approach as in Section 3.2.3, but by replacing the curve C_R with the clockwise oriented curve $C_{-R} := \{z \in \mathbb{C} : \operatorname{Im} z \le 0, |z| = R\}$ such that the singularity point enclosed by the path $[-R, R] \cup C_{-R}$ is at $w = \tilde{\xi}_\tau$. With this, the same estimates as before can be used, since again $z \sin\phi$ and $(z/2 - f(\eta'))\sin\phi$ are positive for $z < -h$ (transmitted case) and $\phi \in [\pi, 2\pi]$ (from parametrisation $R\, e^{i\phi}$ of curve C_{-R}). Similarly, the term $(z - \zeta\, f(\eta')) \operatorname{Im} \tilde{\xi}_\tau$ is again positive for $\zeta \in [0, 1]$ and $z < -h$, and $\lim_{|s'|\to\infty} \operatorname{Im} \tilde{\xi}_\tau < 0$, which was used to show that the constant $c_4(\tilde{r})$ (cf. (3.2.11)) is finite. It follows that (cf. (3.2.14))

$$\left\langle \vec{D}_d^t(\vec{x}), \varphi(\vec{x}) \right\rangle = -\frac{i}{8\pi^2} \lim_{\tilde{r}\to\infty} \lim_{r\to\infty} \int_{\mathbb{R}^3} \bar{\varphi}(\vec{x}) \int_{B_2(r)} \hat{\alpha}_{\tilde{r}}\big(\vec{s}_{\tilde{\xi}_\tau} - \vec{k}\big)\, \frac{\left[\left(\vec{s}_{\tilde{\xi}_\tau} \times \vec{e}^{\,0}\right) \times \vec{s}_{\xi_\tau}\right]}{\tilde{\xi}_\tau}\, e^{i\vec{s}_{\tilde{\xi}_\tau}\cdot\vec{x}}\, \mathrm{d}s'\, \mathrm{d}\vec{x}$$

if $\varphi(\vec{x}) \equiv 0$ for $z \geq -h$. With the same arguments for the estimates as above, an estimate very similar to (3.2.15) can be shown, such that Lebesgue's theorem can be used to evaluate the limit w.r.t. r before the integration w.r.t. $\vec{x}$, giving (cf. (3.2.16))

$$\left\langle \vec{D}_d^t(\vec{x}), \varphi(\vec{x}) \right\rangle = -\frac{i}{8\pi^2} \lim_{\tilde{r}\to\infty} \int_{\mathbb{R}^3} \bar{\varphi}(\vec{x}) \int_{\mathbb{R}^2} \hat{\alpha}_{\tilde{r}}\big(\vec{s}_{\tilde{\xi}_\tau} - \vec{k}\big)\, \frac{\left[\left(\vec{s}_{\tilde{\xi}_\tau} \times \vec{e}^{\,0}\right) \times \vec{s}_{\tilde{\xi}_\tau}\right]}{\tilde{\xi}_\tau}\, e^{i\vec{s}_{\tilde{\xi}_\tau}\cdot\vec{x}}\, \mathrm{d}s'\, \mathrm{d}\vec{x}$$

if $\varphi(\vec{x}) \equiv 0$ for $z \geq -h$.

To resolve the remaining limits w.r.t. $\tilde{r}$ and τ the approach from Section 3.3 is applied almost identically. The space of interface functions is again restricted to functions $f \in \mathcal{A} \cap L^\infty_Q$ and it is then shown that the limits w.r.t. $\tilde{r}$ and τ exist for such interfaces. Afterwards, these limits are evaluated explicitly. With this, the transformations and estimates in Section 3.3 also hold for the formulas of the transmitted field, since, similar to $e^{i\xi_\tau z}$ for $z > h$, the term $e^{i\tilde{\xi}_\tau z}$ decays exponentially for $z < -h$ as $|s'|$ tends to infinity. At last, a formula for the transmitted field below the interface region is obtained, (cf. (3.3.65))

$$\begin{aligned}
\vec{D}_d^t(\vec{x}) &= \epsilon_0'\, \vec{E}_d^t(\vec{x}) = \epsilon_0' \left(\vec{E}^t(\vec{x}) - \vec{E}_Q^t(\vec{x})\right) \\
&= i\,\frac{\Delta}{2} \sum_{n\in\mathbb{N}_0} \sum_{j\in\mathbb{Z}} \int_0^1 \tilde{\lambda}_{0,j}^n(\zeta) \frac{(-i\zeta)^n}{n!}\, \mathrm{d}\zeta\, \left[\left(\vec{\omega}_j^t \times \vec{e}^{\,0}\right) \times \vec{\omega}_j^t\right] \left(\tilde{\omega}_z^j\right)^{n-1} e^{i\vec{\omega}_j^t\cdot\vec{x}} \\
&\quad + i\,\frac{\Delta}{4\pi} \sum_{n\in\mathbb{N}_0} \sum_{j\in\mathbb{Z}} \int_0^1 \tilde{\lambda}_{1,j}^n(\zeta) \frac{(-i\zeta)^n}{n!}\, \mathrm{d}\zeta \int_{\mathbb{R}^2} \left\{ \tilde{\xi}^{n-1}\, \frac{e^{-\left|s'-(k'+\tilde{\omega}_{1,j}')\right|}}{\left|s'-(k'+\tilde{\omega}_{1,j}')\right|} \left[\left(\vec{s}_{\tilde{\xi}} \times \vec{e}^{\,0}\right) \times \vec{s}_{\tilde{\xi}}\right] e^{i\vec{s}_{\tilde{\xi}}\cdot\vec{x}} \right\} \mathrm{d}s' \\
&\quad + i\,\frac{\Delta}{4\pi} \sum_{n\in\mathbb{N}_0} \sum_{j\in\mathbb{Z}} \int_0^1 \tilde{\lambda}_{2,j}^n(\zeta) \frac{(-i\zeta)^n}{n!}\, \mathrm{d}\zeta \int_{\mathbb{R}^2} \left\{ \tilde{\xi}^{n-1}\, K_0\left(\left|s'-(k'+\tilde{\omega}_{2,j}')\right|\right) \left[\left(\vec{s}_{\tilde{\xi}} \times \vec{e}^{\,0}\right) \times \vec{s}_{\tilde{\xi}}\right] e^{i\vec{s}_{\tilde{\xi}}\cdot\vec{x}} \right\} \mathrm{d}s' \\
&\quad + i\,\frac{\Delta}{4\pi} \sum_{n\in\mathbb{N}_0} \sum_{j\in\mathbb{Z}} \int_0^1 \tilde{\lambda}_{3,j}^n(\zeta) \frac{(-i\zeta)^n}{n!}\, \mathrm{d}\zeta \int_{\mathbb{R}^2} \left\{ \tilde{\xi}^{n-1}\, e^{-\left|s'-(k'+\tilde{\omega}_{3,j}')\right|} \left[\left(\vec{s}_{\tilde{\xi}} \times \vec{e}^{\,0}\right) \times \vec{s}_{\tilde{\xi}}\right] e^{i\vec{s}_{\tilde{\xi}}\cdot\vec{x}} \right\} \mathrm{d}s' \\
&\quad + i\,\frac{\Delta}{8\pi^2} \sum_{n\in\mathbb{N}_0} \int_0^1 \frac{(-i\zeta)^n}{n!} \int_{\mathbb{R}^2} \left\{ \tilde{\xi}^{n-1} \int_{\mathbb{R}^2} \tilde{g}_n(\eta',\zeta)\, e^{-i\eta'\cdot(s'-k')}\, \mathrm{d}\eta' \left[\left(\vec{s}_{\tilde{\xi}} \times \vec{e}^{\,0}\right) \times \vec{s}_{\tilde{\xi}}\right] e^{i\vec{s}_{\tilde{\xi}}\cdot\vec{x}} \right\} \mathrm{d}s'\, \mathrm{d}\zeta
\end{aligned} \tag{5.5}$$

for $z < -h$, with $\tilde{\xi} := -\sqrt{\tilde{k}^2 - |s'|^2}$. Thus, using (A.3.3) in the appendix,

$$\vec{E}^t(\vec{x}) = \vec{E}_d^t(\vec{x}) + t(\vec{k}, \vec{e}^{\,0})\, \frac{e^{i\vec{k}^t\cdot\vec{x}}}{|k'|^2}. \tag{5.6}$$

Remark 5.2. *It is not hard to show that the same formula is obtained if* $\mathrm{Im}(\epsilon_0') > 0$*, except that* $\tilde{k}$ *as well* $\tilde{\xi}$ *will also be complex valued and that* $\tilde{\omega}_z^j$ *is complex valued for all* $s' \in \mathbb{R}^2$*. This makes the evaluation of the far-field asymptotics significantly easier. Indeed, all the terms in (5.5) will decay exponentially as* $R := \|\vec{x}\|$ *tends to infinity. In the first term on the right-hand side this is easily seen since the imaginary part of* $\tilde{\omega}_z^j = -(\tilde{k}^2 - |k' + \tilde{\omega}_{0,j}'|^2)^{1/2}$ *is negative for all possible* $\tilde{\omega}_{0,j}'$ *and* k'*, such that* $|e^{iR\tilde{\omega}_z^j m_z}| = e^{-R\,\mathrm{Im}(\tilde{\omega}_z^j)\, m_z}$ *decays exponentially for* $m_z := z/R < -h$ *and* $R \to \infty$*. Similarly, for the remaining terms* $\int_{\mathbb{R}^2} F(s')\, e^{i\vec{s}_{\tilde{\xi}}\cdot\vec{x}}\, \mathrm{d}s'$ *in (5.5), where* $F(s')$ *is a locally integrable function with polynomial growth at infinity, this is just as easily seen. To be precise, since* $\mathrm{Im}\,\tilde{\xi} = -\mathrm{Im}(\tilde{k}^2 - |s'|^2)^{1/2} < -c < 0$ *and* $\mathrm{Im}\,\tilde{\xi} \sim -|s'|$*, for* $|s'| \to \infty$*, it follows that the integral*

$$\left| \int_{\mathbb{R}^2} F(s')\, e^{i\vec{s}_{\tilde{\xi}}\cdot\vec{x}}\, \mathrm{d}s' \right| \leq \int_{\mathbb{R}^2} |F(s')|\, e^{-\frac{1}{2}\,\mathrm{Im}\,\tilde{\xi}\, m_z}\, \mathrm{d}s'\, e^{-\frac{R}{2} c\, |m_z|}$$

is well defined and decays exponentially for $m_z < 0$ and $R > 1$ as R tends to infinity.

Note the similarities of (5.6) to the reflected field (3.1.2). As a consequence of these similarities, it is not hard, but very lengthy, to check that all estimates made in Chapters 4 and B to determine the reflected far field also hold for this formula for the transmitted field, keeping in mind that $e^{i\tilde{\xi}\, z}$ decays exponentially as $|s'|$ tends to infinity for $z < -h$. At last, this gives the formula for the transmitted far field presented in Theorem 5.1.

Based on this formula for the transmitted far field, a result similar to Theorem 4.6 can be proven.

Theorem 5.3 (Reduced specularly transmitted wave mode)**.** *Assuming the scattering interface as the graph of a function $f \in \mathcal{A} \cap L^\infty_{\mathcal{Q}}$, the wave mode of the transmitted plane wave in specular direction $\vec{k}^t = (k_x, k_y, k_z^t)^\top$ in the sense of Born approximation is*

$$\vec{E}^s(\vec{x}) = \left(1 + \frac{k^2\,\Delta}{4\epsilon_0\,k_z^2}\right) \hat{w}(k_z^t - k_z)\, \frac{\left[(\vec{k}^t \times \vec{e}^{\,0}) \times \vec{k}^t\right]}{\tilde{k}^2}\, e^{i\vec{k}^t\cdot\vec{x}} + \mathcal{O}\left(\left[\frac{\Delta k^2}{k_z^2}\right]^2\right)$$

for $z < -h$, where $k_z^t := -\sqrt{\tilde{k}^2 - |k'|^2}$ and

$$\hat{w}(k_z^t - k_z) := \int\limits_{-\frac{h}{2}}^{\frac{h}{2}} \partial_\zeta \left[\lim_{R\to\infty} \frac{1}{4R^2} \int\limits_{-R}^{R}\int\limits_{-R}^{R} \mathbb{1}_{[f(\eta'),\infty)}(\zeta)\, \mathrm{d}\eta_x\, \mathrm{d}\eta_y\right] e^{-i(k_z^t - k_z)\,\zeta}\, \mathrm{d}\zeta.$$

Proof. The proof of this theorem is very similar to that of Theorem 4.6. Note that the specular transmitted plane-wave component of (5.1) again corresponds to the index j_0 defined in the latter proof, such that (cf. (4.3.3))

$$\begin{aligned}\tilde{\lambda}^n_{0,j_0} &= \lim_{R\to\infty} \frac{1}{4R^2} \int\limits_{-R}^{R}\int\limits_{-R}^{R} f^{n+1}(\eta')\, e^{ik_z\zeta\, f(\eta')}\, \mathrm{d}\eta_x\, \mathrm{d}\eta_y \\ &= \lim_{R\to\infty} \frac{1}{4R^2} \int\limits_{-R}^{R}\int\limits_{-R}^{R} \left\{ \sum_{\ell=0}^{3} \left[\frac{1}{\sqrt{1+|\eta'|^2}^{\,\ell}} \sum_{j\in\mathbb{Z}} \tilde{\lambda}^n_{\ell,j}\, e^{i\tilde{\omega}'_{\ell,j}\cdot\eta'}\right] + \tilde{g}_n(\eta',\zeta) \right\} \mathrm{d}\eta_x\, \mathrm{d}\eta_y.\end{aligned}$$

With this, the same transformations that led to the first line of (4.3.4), give

$$\begin{aligned}\vec{E}^s_0(\vec{x}) &= i\,\frac{\Delta}{2\epsilon_0'} \lim_{R\to\infty} \frac{1}{4R^2} \int\limits_{-R}^{R}\int\limits_{-R}^{R}\int\limits_{0}^{1} \sum_{n\in\mathbb{N}_0} \frac{(-ik_z^t\,\zeta\, f(\eta'))^n}{n!}\, e^{ik_z\zeta\, f(\eta')}\, \mathrm{d}\zeta\, \frac{f(\eta')}{k_z^t}\, \mathrm{d}\eta_x\, \mathrm{d}\eta_y \left[\left(\vec{k}^t \times \vec{e}^{\,0}\right) \times \vec{k}^t\right] e^{i\vec{k}^t\cdot\vec{x}} \\ &= i\,\frac{\Delta}{2\epsilon_0'\,k_z^t} \lim_{R\to\infty} \frac{1}{4R^2} \int\limits_{-R}^{R}\int\limits_{-R}^{R}\int\limits_{0}^{1} e^{-i(k_z^t - k_z)\,\zeta\, f(\eta')}\, \mathrm{d}\zeta\, f(\eta')\, \mathrm{d}\eta_x\, \mathrm{d}\eta_y \left[\left(\vec{k}^t \times \vec{e}^{\,0}\right) \times \vec{k}^t\right] e^{i\vec{k}^t\cdot\vec{x}},\end{aligned}$$

for $z < -h$. Continuing along the lines of the proof of Theorem 4.6 then easily leads to

$$\begin{aligned}\vec{E}^s_0(\vec{x}) &= i\,\frac{\Delta}{2\epsilon_0'\,k_z^t} \int\limits_{\mathbb{R}} \lim_{R\to\infty} \frac{\mu(f,\zeta,R)}{4R^2}\, e^{-i(k_z^t - k_z)\,\zeta}\, \mathrm{d}\zeta \left[\left(\vec{k}^t \times \vec{e}^{\,0}\right) \times \vec{k}^t\right] e^{i\vec{k}^t\cdot\vec{x}} \\ &= -\frac{\Delta}{2\epsilon_0'\,k_z^t\,(k_z^t - k_z)} \left(\hat{w}(k_z^t - k_z) - 1\right) \left[\left(\vec{k}^t \times \vec{e}^{\,0}\right) \times \vec{k}^t\right] e^{i\vec{k}^t\cdot\vec{x}}.\end{aligned} \tag{5.7}$$

On the other hand,

$$-\frac{\Delta}{2\epsilon_0'\,k_z^t\,(k_z^t - k_z)} = \frac{\mu_0(\epsilon_0 - \epsilon_0')\omega^2}{2\mu_0\epsilon_0'\omega^2\,k_z^t\,(k_z - k_z^t)} = \frac{k^2 - \tilde{k}^2}{2\tilde{k}^2\,k_z^t\,(k_z - k_z^t)} = \frac{|k'|^2 + k_z^2 - |k'|^2 - [k_z^t]^2}{2\tilde{k}^2\,k_z^t\,(k_z - k_z^t)}$$

$$
\begin{aligned}
&= \frac{k_z^2 - [k_z^t]^2}{2\tilde{k}^2\, k_z^t\, (k_z - k_z^t)} = \frac{k_z + k_z^t}{2\tilde{k}^2\, k_z^t} = \frac{1}{\tilde{k}^2} + \frac{1}{2k_z^t}\,\frac{k_z - k_z^t}{\tilde{k}^2} \\
&= \frac{1}{\tilde{k}^2} + \frac{1}{2k_z^t}\,\frac{k_z^2 - [k_z^t]^2}{\tilde{k}^2\,(k_z + k_z^t)} = \frac{1}{\tilde{k}^2} + \frac{\Delta}{2\epsilon_0'\, k_z}\,\frac{k_z}{k_z^t\,(k_z + k_z^t)} \\
&= \frac{1}{\tilde{k}^2} + \frac{\Delta}{4\epsilon_0'\, k_z^2} + \frac{\Delta}{2\epsilon_0'}\left[\frac{1}{k_z^t\,(k_z + k_z^t)} - \frac{1}{2k_z^2}\right],
\end{aligned}
$$

where

$$
\begin{aligned}
\frac{1}{k_z^t\,(k_z + k_z^t)} - \frac{1}{2k_z^2} &= \frac{2k_z^2 - k_z^t\, k_z - [k_z^t]^2}{2k_z^2\, k_z^t\,(k_z + k_z^t)} = \frac{k_z^2 - k_z^t\, k_z + k_z^2 - [k_z^t]^2}{2k_z^2\, k_z^t\,(k_z + k_z^t)} \\
&= \frac{k_z - k_z^t}{2k_z\, k_z^t\,(k_z + k_z^t)} + \frac{k^2 - \tilde{k}^2}{2k_z^2\, k_z^t\,(k_z + k_z^t)} = \frac{k_z^2 - [k_z^t]^2}{2k_z\, k_z^t\,(k_z + k_z^t)^2} + \frac{\Delta\, k^2}{2\epsilon_0\, k_z^2\, k_z^t\,(k_z + k_z^t)} \\
&= \frac{\Delta\, k^2}{2\epsilon_0\, k_z\, k_z^t\,(k_z + k_z^t)^2} + \frac{\Delta\, k^2}{2\epsilon_0\, k_z^2\, k_z^t\,(k_z + k_z^t)} \qquad (5.8)
\end{aligned}
$$

such that

$$
\frac{\Delta}{2\epsilon_0'}\left[\frac{1}{k_z^t\,(k_z + k_z^t)} - \frac{1}{2k_z^2}\right] = \mathcal{O}\left(\left[\frac{\Delta\, k^2}{k_z^2}\right]^2\right)
$$

and

$$
\begin{aligned}
-\frac{\Delta}{2\epsilon_0'\, k_z^t\,(k_z^t - k_z)} &= \frac{1}{\tilde{k}^2}\left(1 + \frac{\Delta\,\tilde{k}^2}{4\epsilon_0'\, k_z^2}\right) + \mathcal{O}\left(\left[\frac{\Delta\, k^2}{k_z^2}\right]^2\right) \\
&= \frac{1}{\tilde{k}^2}\left(1 + \frac{\Delta\, k^2}{4\epsilon_0\, k_z^2}\right) + \mathcal{O}\left(\left[\frac{\Delta\, k^2}{k_z^2}\right]^2\right).
\end{aligned}
$$

With this, it follows that (cf. (5.7))

$$
\begin{aligned}
\vec{E}_0^s(\vec{x}) = {}& \frac{1}{\tilde{k}^2}\left(1 + \frac{\Delta\, k^2}{4\epsilon_0\, k_z^2}\right)\hat{w}(k_z^t - k_z)\left[\left(\vec{k}^t \times \vec{e}^{\,0}\right)\times \vec{k}^t\right] e^{i\vec{k}^t\cdot\vec{x}} - \frac{1}{\tilde{k}^2}\left(1 + \frac{\Delta\, k^2}{4\epsilon_0\, k_z^2}\right)\left[\left(\vec{k}^t \times \vec{e}^{\,0}\right)\times \vec{k}^t\right] e^{i\vec{k}^t\cdot\vec{x}} \\
&+ \mathcal{O}\left(\left[\frac{\Delta\, k^2}{k_z^2}\right]^2\right)
\end{aligned}
$$

for $z < -h$. Moreover, using the subsequent Lemma 5.5,

$$
\vec{E}^s(\vec{x}) = \vec{E}_0^s(\vec{x}) + \vec{E}_Q^t(\vec{x}) = \frac{1}{\tilde{k}^2}\left(1 + \frac{\Delta\, k^2}{4\epsilon_0\, k_z^2}\right)\hat{w}(k_z^t - k_z)\left[\left(\vec{k}^t \times \vec{e}^{\,0}\right)\times \vec{k}^t\right] e^{i\vec{k}^t\cdot\vec{x}} + \mathcal{O}\left(\left[\frac{\Delta\, k^2}{k_z^2}\right]^2\right)
$$

for $z < -h$, concluding the proof of the theorem. ■

Remark 5.4. *It is easily shown that the Remarks 4.7 and 4.8 also hold for the transmitted field, if* $\hat{w}(-2k_z)$ *is replaced by* $\hat{w}(k_z^t - k_z)$*. Moreover, the result of Theorem 5.3 coincides with the conclusion by Stearns (cf. [36, second line of Eqn. (42)]).*

To prove Theorem 5.3 it was used that

Lemma 5.5. *Assume an ideal interface, defined by the graph of a function* $f_Q \equiv 0$*, is illuminated by an incoming plane wave as described in Subsection 2.1. The transmitted field is then given by*

$$
\vec{E}_Q^t(\vec{x}) = \frac{1}{\tilde{k}^2}\left(1 + \frac{\Delta\, k^2}{4\epsilon_0\, k_z^2}\right)\left[\left(\vec{k}^t \times \vec{e}^{\,0}\right)\times \vec{k}^t\right] e^{i\vec{k}^t\cdot\vec{x}} + \mathcal{O}\left(\left[\frac{k^2\Delta}{k_z^2}\right]^2\right).
$$

Proof. In view of (A.3.3) in the appendix,

$$\vec{E}^t_Q(\vec{x}) = \left\{ \frac{2k_z}{k_z + k^t_z}\, \nu_{TE}\, \vec{e}^{\,t}_{TE} + \frac{2kk_z}{\tilde{k}^2 k_z + k^2 k^t_z}\, \nu_{TM}\, \vec{e}^{\,t}_{TM} \right\} e^{i\vec{k}^t\cdot\vec{x}},$$

where

$$\nu_{TE} := \frac{k_y e^0_x - k_x e^0_y}{|k'|}, \qquad \vec{e}^{\,t}_{TE} := \frac{1}{|k'|} \begin{pmatrix} k_y \\ -k_x \\ 0 \end{pmatrix},$$

$$\nu_{TM} := -\frac{k_z(k_x e^0_x + k_y e^0_y) - |k'|^2\, e^0_z}{k\,|k'|}, \qquad \vec{e}^{\,t}_{TM} := -\frac{1}{|k'|} \begin{pmatrix} k_x\, k^t_z \\ k_y\, k^t_z \\ -|k'|^2 \end{pmatrix}.$$

Moreover, using (4.3.11) and (4.3.16), it is easily seen that

$$\frac{2k_z}{k_z + k^t_z} = 1 + \frac{k_z - k^t_z}{k_z + k^t_z} = 1 + \frac{k^2\Delta}{4\epsilon_0 k^2_z} + \mathcal{O}\left(\left[\frac{k^2\Delta}{k^2_z}\right]^2\right)$$

$$\tilde{k}^2\, \frac{2k_z}{\tilde{k}^2 k_z + k^2 k^t_z} = 1 + \frac{\tilde{k}^2 k_z + k^2\sqrt{\tilde{k}^2 - |k'|^2}}{\tilde{k}^2 k_z - k^2\sqrt{\tilde{k}^2 - |k'|^2}} = 1 - \frac{k^2\Delta}{4\epsilon_0 k^2_z}\left[2\frac{k^2_z}{k^2} - 1\right] + \mathcal{O}\left(\left[\frac{k^2\Delta}{k^2_z}\right]^2\right),$$

such that

$$\vec{E}^t_Q(\vec{x}) = \frac{1}{\tilde{k}^2}\left\{ \left(1 + \frac{k^2\Delta}{4\epsilon_0 k^2_z}\right) \nu_{TE}\, \tilde{k}^2\, \vec{e}^{\,t}_{TE} + k\left(1 - \frac{k^2\Delta}{4\epsilon_0 k^2_z}\left[2\frac{k^2_z}{k^2} - 1\right]\right) \nu_{TM}\, \vec{e}^{\,t}_{TM} \right\} e^{i\vec{k}^t\cdot\vec{x}} + \mathcal{O}\left(\left[\frac{k^2\Delta}{k^2_z}\right]^2\right). \tag{5.9}$$

Furthermore, it is easily seen that (cf. (A.1.1) and (A.1.6))

$$\left(\vec{k}^t \times \vec{e}^{\,0}_{TE}\right) \times \vec{k}^t = -\left(\vec{k}^t \cdot \vec{e}^{\,0}_{TE}\right) \vec{k}^t + \tilde{k}^2\, \vec{e}^{\,0}_{TE} = \tilde{k}^2\, \vec{e}^{\,0}_{TE} = \tilde{k}^2\, \vec{e}^{\,t}_{TE}. \tag{5.10}$$

It is harder to show a similar result for the TM-case. Consider (cf. (A.2.2) and (A.2.6))

$$\begin{aligned}
\left(\vec{k}^t \times \vec{e}^{\,0}_{TM}\right) \times \vec{k}^t &= -\left(\vec{k}^t \cdot \vec{e}^{\,0}_{TM}\right) \vec{k}^t + \tilde{k}^2\, \vec{e}^{\,0}_{TM} \\
&= \frac{1}{k\,|k'|}\left[k^2_x\, k_z + k^2_y\, k_z - k^t_z\, |k'|^2\right] \begin{pmatrix} k_x \\ k_y \\ k^t_z \end{pmatrix} - \frac{\tilde{k}^2}{k\,|k'|} \begin{pmatrix} k_x\, k_z \\ k_y\, k_z \\ -|k'|^2 \end{pmatrix} \\
&= -\frac{1}{k\,|k'|} \begin{pmatrix} \left[-|k'|^2 \frac{k_z - k^t_z}{k^t_z} + \frac{\tilde{k}^2\, k_z}{k^t_z}\right] k_x\, k^t_z \\ \left[-|k'|^2 \frac{k_z - k^t_z}{k^t_z} + \frac{\tilde{k}^2\, k_z}{k^t_z}\right] k_y\, k^t_z \\ \left[(k_z - k^t_z)\, k^t_z + \tilde{k}^2\right] (-|k'|^2) \end{pmatrix} \\
&= \frac{1}{k}\left[|k'|^2 + k_z\, k^t_z\right] \vec{e}^{\,t}_{TM} = \frac{1}{k}\left[k^2 - k^2_z + k_z\, k^t_z\right] \vec{e}^{\,t}_{TM}.
\end{aligned}$$

With this,

$$\left(1 + \frac{k^2\Delta}{4\epsilon_0 k^2_z}\right)\left[\left(\vec{k}^t \times \vec{e}^{\,0}_{TM}\right) \times \vec{k}^t\right] = k\left(1 + \frac{k^2\Delta}{4\epsilon_0 k^2_z}\right) \vec{e}^{\,t}_{TM} - \frac{k_z}{k}\left(1 + \frac{k^2\Delta}{4\epsilon_0 k^2_z}\right) (k_z - k^t_z)\, \vec{e}^{\,t}_{TM},$$

where

$$k_z - k^t_z = \frac{k^2 - \tilde{k}^2}{k_z + k^t_z} = \frac{\Delta\, k^2}{\epsilon_0\,(k_z + k^t_z)} = \frac{\Delta\, k^2}{2\epsilon_0\, k_z} + \frac{\Delta\, k^2}{\epsilon_0}\left[\frac{1}{(k_z + k^t_z)} - \frac{1}{2k_z}\right].$$

Similarly to (5.8), it is easily shown that

$$\frac{1}{(k_z+k_z^t)}-\frac{1}{2k_z}=\frac{\Delta\,k^2}{2\epsilon_0\,k_z\,(k_z+k_z^t)^2}$$

such that

$$k_z-k_z^t=\frac{\Delta\,k^2}{2\epsilon_0\,k_z}+\mathcal{O}\left(\left[\frac{k^2\Delta}{k_z^2}\right]^2\right)$$

and

$$\begin{aligned}\left(1+\frac{k^2\Delta}{4\epsilon_0 k_z^2}\right)\left[\left(\vec{k}^t\times\vec{e}^{\,0}_{TM}\right)\times\vec{k}^t\right]&=k\left(1+\frac{k^2\Delta}{4\epsilon_0 k_z^2}\right)\vec{e}^{\,t}_{TM}-\frac{\Delta\,k}{2\epsilon_0}\,\vec{e}^{\,t}_{TM}+\mathcal{O}\left(\left[\frac{k^2\Delta}{k_z^2}\right]^2\right)\\&=k\left(1-\frac{k^2\Delta}{4\epsilon_0 k_z^2}\left[2\frac{k_z^2}{k^2}-1\right]\right)\vec{e}^{\,t}_{TM}+\mathcal{O}\left(\left[\frac{k^2\Delta}{k_z^2}\right]^2\right).\end{aligned}\tag{5.11}$$

Consequently, since $\vec{e}^{\,0}=\nu_{TE}\,\vec{e}^{\,0}_{TE}+\nu_{TM}\,\vec{e}^{\,0}_{TM}$ (cf. (A.3.1), (5.10) and (5.11)),

$$\begin{aligned}&\left(1+\frac{k^2\Delta}{4\epsilon_0 k_z^2}\right)\nu_{TE}\,\tilde{k}^2\,\vec{e}^{\,t}_{TE}+k\left(1-\frac{k^2\Delta}{4\epsilon_0 k_z^2}\left[2\frac{k_z^2}{k^2}-1\right]\right)\nu_{TM}\,\vec{e}^{\,t}_{TM}\\&\qquad=\left(1+\frac{k^2\Delta}{4\epsilon_0 k_z^2}\right)\left\{\nu_{TE}\left[\left(\vec{k}^t\times\vec{e}^{\,0}_{TE}\right)\times\vec{k}^t\right]+\nu_{TM}\left[\left(\vec{k}^t\times\vec{e}^{\,0}_{TM}\right)\times\vec{k}^t\right]\right\}+\mathcal{O}\left(\left[\frac{k^2\Delta}{k_z^2}\right]^2\right)\\&\qquad=\left(1+\frac{k^2\Delta}{4\epsilon_0 k_z^2}\right)\left[\left(\vec{k}^t\times\vec{e}^{\,0}\right)\times\vec{k}^t\right]+\mathcal{O}\left(\left[\frac{k^2\Delta}{k_z^2}\right]^2\right)\end{aligned}$$

and (cf. (5.9))

$$\vec{E}^t_{\mathcal{Q}}(\vec{x})=\frac{1}{\tilde{k}^2}\left(1+\frac{k^2\Delta}{4\epsilon_0 k_z^2}\right)\left[\left(\vec{k}^t\times\vec{e}^{\,0}\right)\times\vec{k}^t\right]e^{i\vec{k}^t\cdot\vec{x}}+\mathcal{O}\left(\left[\frac{k^2\Delta}{k_z^2}\right]^2\right).$$

■

Chapter 6

A numerical example

In this chapter, an application of the far-field formulas (4.1.1) and (5.1) will be shown for the simple example of a non-decaying interface from $\mathcal{A} \cap L^\infty_{\mathbb{Q}}$. The interface, or more precisely its amplitude factors, are constructed in such a way that the height of the interface at every point is a realisation of a Gaussian distribution with mean zero and a given variance. Moreover, the heights at any two points of the interface will be correlated according to a given correlation function. At the end, numerical results will be presented and discussed shortly.

For simplicity, in the context of this chapter, the set of interface functions considered is restricted to a subset of $\mathcal{A}$. To be precise, an interface function $f \in \mathcal{A}$ (cf. (3.3.1)) is supposed to consist only of the almost periodic part (index $\ell = 0$), leading to $f(\eta') = \sum_{j\in\mathbb{Z}} \lambda_j \, e^{i\omega'_j\cdot\eta'}$. Moreover, to actually calculate the field, the infinite sum w.r.t. j is restricted to a finite one. At last, to further simplify the calculations, it is assumed that the spatial frequencies ω'_j are chosen from an equidistant mesh, i.e. $\omega'_j = \omega\,\ell'$, with a small fixed $\omega \in \mathbb{R}$ and $\ell' \in \mathbb{Z}^2$.

Under these restrictions, the following theorem is shown.

Theorem 6.1. *For any interface function*

$$f(\eta') = \sum_{\ell'\in\mathcal{I}} \lambda_{\ell'} \, e^{i\omega\,\ell'\cdot\eta'}, \tag{6.1}$$

from $\mathcal{A}$ (cf. (3.3.1)) with a finite subset $\mathcal{I}$ of $\mathbb{Z}^2$, the reflected and transmitted far fields can be calculated as

$$\begin{aligned}
\vec{e}^{\,*}\cdot \vec{E}^r(\vec{x}) \sim {} & -i\,\frac{\Delta}{2\epsilon_0} \sum_{\substack{\ell'\in\mathbb{Z}^2\\ |k'+\omega\,\ell'|\le k}} \sum_{n=0}^{N}\sum_{m=0}^{M} \frac{(-i)^n (ik_z)^m}{m!\,n!\,(n+m+1)}\, \lambda_{\ell'}^{(n+m+1)} \big[\omega_z^{\ell'}\big]^{n-1}\, \vec{e}^{\,*}\cdot \big[\big(\vec{\omega}_{\ell'}\times\vec{e}^{\,0}\big)\times\vec{\omega}_{\ell'}\big]\; e^{ik\vec{\omega}_{\ell'}\cdot\vec{x}} \\
& + r(\vec{k},\vec{e}^{\,0},\vec{e}^{\,*})\,\frac{e^{ik\vec{n}_0^{\,r}\cdot\vec{x}}}{|k'|^2} + E^r_{N,M}(\vec{x}), \\
\vec{e}^{\,*}\cdot \vec{E}^t(\vec{x}) \sim {} & i\,\frac{\Delta}{2\epsilon'_0} \sum_{\substack{\ell'\in\mathbb{Z}^2\\ |k'+\omega\,\ell'|\le \tilde{k}}} \sum_{n=0}^{\tilde{N}}\sum_{m=0}^{\tilde{M}} \frac{(-i)^n (ik_z)^m}{m!\,n!\,(n+m+1)}\, \lambda_{\ell'}^{(n+m+1)} \big[\tilde{\omega}_z^{\ell'}\big]^{n-1}\, \vec{e}^{\,*}\cdot \big[\big(\vec{\omega}^t_{\ell'}\times\vec{e}^{\,0}\big)\times\vec{\omega}^t_{\ell'}\big]\; e^{i\tilde{k}\vec{\omega}^t_{\ell'}\cdot\vec{x}} \\
& + t(\vec{k},\vec{e}^{\,0},\vec{e}^{\,*})\,\frac{e^{i\tilde{k}\vec{n}_0^{\,t}\cdot\vec{x}}}{|k'|^2} + E^t_{\tilde{N},\tilde{M}}(\vec{x}),
\end{aligned}$$

where the functions $r(\vec{k},\vec{e}^{\,0},\vec{e}^{\,*})$ and $t(\vec{k},\vec{e}^{\,0},\vec{e}^{\,*})$ are defined by the Formulas (3.1.9) and (5.2), and where $\lambda_{\ell'}^{(n+m+1)}$ is defined such that (6.4) *holds. The terms $E^r_{N,M}(\vec{x})$ and $E^t_{\tilde{N},\tilde{M}}(\vec{x})$ are defined as the remainder of the truncated sums w.r.t. n and m, i.e. the sums from $N+1$, $M+1$, $\tilde{N}+1$ and $\tilde{M}+1$ to infinity. Under the assumption that $N+1 > 2(k\,\|f\|_{\mathcal{A}} - 1)$, $M > 2(|k_z|\,\|f\|_{\mathcal{A}} - 1)$, $\tilde{N} > 2\,\tilde{k}\,\|f\|_{\mathcal{A}} - 1$*

and $\tilde{M} = M > 2\left(|k_z|\,\|k\|_{\mathcal{A}} - 1\right)$, *these truncation error terms are bounded by*

$$\left\|E^r_{N,M}(\vec{x})\right\| \leq \frac{2}{\omega_0}\left(\sum_{n=0}^{N}\frac{(k\,\|f\|_{\mathcal{A}})^{n+1}}{(n+1)!}\right)\frac{(k_z\,\|f\|_{\mathcal{A}})^{M+1}}{(M+1)!} + \frac{2}{\omega_0}\frac{(k\,\|f\|_{\mathcal{A}})^{N+2}}{(N+2)!}\,e^{k_z\,\|f\|_{\mathcal{A}}},$$

$$\left\|E^t_{\tilde{N},\tilde{M}}(\vec{x})\right\| \leq \frac{2}{\tilde{\omega}_0}\left(\sum_{n=0}^{\tilde{N}}\frac{(\tilde{k}\,\|f\|_{\mathcal{A}})^{n+1}}{(n+1)!}\right)\frac{(k_z\,\|f\|_{\mathcal{A}})^{\tilde{M}+1}}{(\tilde{M}+1)!} + \frac{2}{\tilde{\omega}_0}\frac{(\tilde{k}\,\|f\|_{\mathcal{A}})^{\tilde{N}+2}}{(\tilde{N}+2)!}\,e^{k_z\,\|f\|_{\mathcal{A}}},$$

where

$$\omega_0 := \min\Big\{\sqrt{k^2 - |k' + \omega\,\ell'|^2}/k : \ \ell' \in \mathbb{Z}^2 \text{ s.t. } k > |k' + \omega\,\ell'|\Big\}, \tag{6.2}$$

$$\tilde{\omega}_0 := \min\Big\{\sqrt{\tilde{k}^2 - |k' + \omega\,\ell'|^2}/\tilde{k} : \ \ell' \in \mathbb{Z}^2 \text{ s.t. } \tilde{k} > |k' + \omega\,\ell'|\Big\}.$$

Proof. First consider the reflected field. For the given subset of non-decaying interface functions f (cf. (6.1)) from $\mathcal{A}\cap L^\infty_{\mathcal{Q}}$, the proof of Lemma 3.9 and the subsequent transformations leading to Theorem 3.1 easily reveal that the reflected far-field formula (4.1.1) reduces to only its first two lines, i.e.

$$\vec{e}^{*}\!\cdot \vec{E}^r(R\vec{m}) = r(\vec{k},\vec{e}^{\,0},\vec{e}^{\,*})\,\frac{e^{ikR\vec{n}^r_0\cdot\vec{m}}}{|k'|^2} \tag{6.3}$$
$$- i\,\frac{\Delta}{2\epsilon_0}\sum_{n\in\mathbb{N}_0}\ \sum_{\substack{j\in\mathbb{Z}\\ |k'+\tilde{\omega}'_{0,j}|<k}}\ \int_0^1 \tilde{\lambda}^n_{0,j}(\zeta)\frac{(-i\zeta)^n}{n!}\,\mathrm{d}\zeta\ \ \vec{e}^{\,*}\cdot\left[\left(\vec{\omega}^{\,j}_z\times\vec{e}^{\,0}\right)\times\vec{\omega}^{\,j}_z\right]\ \left(\omega^j_z\right)^{n-1}\ e^{iR\vec{\omega}^{\,j}_z\cdot\vec{m}}.$$

By choosing the spatial frequencies ω'_j of f from an equidistant mesh, it is possible to simplify the calculation of the amplitude factors $\tilde{\lambda}^n_{0,j}(\zeta)$. Recall that the sum w.r.t. j results from Lemma 3.9. Comparing Formula (3.3.16) with (3.3.15) for f defined above,

$$[f(\eta')]^{n+1}\ e^{ik_z\zeta\,f(\eta')} = \sum_{j\in\mathbb{Z}}\tilde{\lambda}^n_{0,j}\,e^{i\tilde{\omega}'_{0,j}\cdot\eta'} = \sum_{m\in\mathbb{N}_0}\frac{(ik_z\zeta)^m}{m!}\,[f(\eta')]^{m+n+1} = \sum_{m\in\mathbb{N}_0}\frac{(ik_z\zeta)^m}{m!}\sum_{\ell'\in\mathbb{Z}^2}\lambda^{(n+m+1)}_{\ell'}\,e^{i\omega\,\ell'\cdot\eta'},$$

where $\lambda^{(n+m+1)}_{\ell'}$ is defined such that

$$[f(\eta')]^{m+n+1} = \left[\sum_{\ell'\in\mathcal{I}}\lambda_{\ell'}\,e^{i\omega\,\ell'\cdot\eta'}\right]^{m+n+1} = \sum_{\ell'\in\mathbb{Z}^2}\lambda^{(n+m+1)}_{\ell'}\,e^{i\omega\,\ell'\cdot\eta'}. \tag{6.4}$$

Thus, the sum w.r.t. j in (6.3) is replaced by the two sums w.r.t. m and ℓ', the summand $\tilde{\lambda}^n_{0,j}(\zeta)$ is replaced by $(ik_z\zeta)^m/m!\ \lambda^{(n+m+1)}_{\ell'}$ and $\tilde{\omega}'_{0,j}$ by $\omega\,\ell'$. Hence, defining $\omega^{\ell'}_z := \sqrt{k^2 - |k' + \omega\,\ell'|^2}$ and $\vec{\omega}_{\ell'} := (k' + \omega\,\ell', \omega^{\ell'}_z)^\top$,

$$\vec{e}^{*}\!\cdot \vec{E}^r(R\vec{m}) = r(\vec{k},\vec{e}^{\,0},\vec{e}^{\,*})\,\frac{e^{ikR\vec{n}^r_0\cdot\vec{m}}}{|k'|^2}$$
$$- i\,\frac{\Delta}{2\epsilon_0}\sum_{n\in\mathbb{N}_0}\sum_{m\in\mathbb{N}_0}\Bigg\{$$
$$\sum_{\substack{\ell'\in\mathbb{Z}^2\\ |k'+\omega\,\ell|<k}}\int_0^1\frac{(ik_z\zeta)^m\,(-i\zeta)^n}{m!\,n!}\,\mathrm{d}\zeta\,\lambda^{(n+m+1)}_{\ell'}\ \ \vec{e}^{\,*}\cdot\left[\left(\vec{\omega}_{\ell'}\times\vec{e}^{\,0}\right)\times\vec{\omega}_{\ell'}\right]\ \left[\omega^{\ell'}_z\right]^{n-1} e^{iR\vec{\omega}_{\ell'}\cdot\vec{m}}\Bigg\}$$
$$= r(\vec{k},\vec{e}^{\,0},\vec{e}^{\,*})\,\frac{e^{ikR\vec{n}_0^{\,r}\cdot\vec{m}}}{|k'|^2} \tag{6.5}$$
$$- i\,\frac{\Delta}{2\epsilon_0}\sum_{n\in\mathbb{N}_0}\sum_{m\in\mathbb{N}_0}\frac{(-i)^n(ik_z)^m}{m!\,n!\,(n+m+1)}\sum_{\substack{\ell'\in\mathbb{Z}^2\\ |k'+\omega\,\ell'|<k}}\lambda^{(n+m+1)}_{\ell'}\left[\omega^{\ell'}_z\right]^{n-1}\vec{e}^{\,*}\!\cdot\left[\left(\vec{\omega}_{\ell'}\times\vec{e}^{\,0}\right)\times\vec{\omega}_{\ell'}\right]e^{iR\vec{\omega}_{\ell'}\cdot\vec{m}}.$$

Note, that using the convolution operator '$*$'

$$\left(\sum_{\ell'\in\mathbb{Z}^2}\lambda_{\ell'}^{(s_1)}\,e^{i\omega\,\ell'\cdot\eta'}\right)\left(\sum_{\ell'\in\mathbb{Z}^2}\lambda_{\ell'}^{(s_2)}\,e^{i\omega\,\ell'\cdot\eta'}\right)=\sum_{\ell'\in\mathbb{Z}^2}\left[\lambda^{(s_1)}*\lambda^{(s_2)}\right]_{\ell'}e^{i\omega\,\ell'\cdot\eta'}=\sum_{\ell'\in\mathbb{Z}^2}\lambda_{\ell'}^{(s_1+s_2)}\,e^{i\omega\,\ell'\cdot\eta'},$$

which allows to calculate $\lambda_{\ell'}^{(n+m+1)}$ relatively easy by successively applying discrete convolution algorithms.

Using this, all values in Formula (6.5) can be calculated and it only remains to evaluate the formula to obtain the reflected far field. Naturally the sums over n and m in (6.5) have to be truncated to be evaluated. To control the error of such a cut-off, an error bound has to be found. The error of truncating the sums after N and M steps is

$$\begin{aligned}\left\|E^r_{N,M}(\vec{x})\right\|=\Bigg\|&\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\frac{(-i)^n(ik_z)^m}{m!\,n!\,(n+m+1)}\sum_{\substack{\ell'\in\mathbb{Z}^2\\|k'+\omega\,\ell'|<k}}\lambda_{\ell'}^{(n+m+1)}\left[\omega_z^{\ell'}\right]^{n-1}\vec{e}^{\,*}\cdot\left[\left(\vec{\omega}_{\ell'}\times\vec{e}^{\,0}\right)\times\vec{\omega}_{\ell'}\right]\\&-\sum_{n=0}^{N}\sum_{m=0}^{M}\frac{(-i)^n(ik_z)^m}{m!\,n!\,(n+m+1)}\sum_{\substack{\ell'\in\mathbb{Z}^2\\|k'+\omega\,\ell'|<k}}\lambda_{\ell'}^{(n+m+1)}\left[\omega_z^{\ell'}\right]^{n-1}\vec{e}^{\,*}\cdot\left[\left(\vec{\omega}_{\ell'}\times\vec{e}^{\,0}\right)\times\vec{\omega}_{\ell'}\right]\Bigg\|.\end{aligned}$$

First note that $\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}a_{n,m}-\sum_{n=0}^{N}\sum_{m=0}^{M}a_{n,m}=\sum_{n=0}^{N}\sum_{m=M+1}^{\infty}a_{n,m}+\sum_{n=N+1}^{\infty}\sum_{m=0}^{\infty}a_{n,m}$ for some absolutely summable sequence $(a_{n,m})_{(n,m)^\top\in\mathbb{N}^2}$. Furthermore,

$$\begin{aligned}&\left\|\frac{(-i)^n(ik_z)^m}{m!\,n!\,(n+m+1)}\sum_{\substack{\ell'\in\mathbb{Z}^2\\|k'+\omega\,\ell'|<k}}\lambda_{\ell'}^{(n+m+1)}\left[\omega_z^{\ell'}\right]^{n-1}\vec{e}^{\,*}\cdot\left[\left(\vec{\omega}_{\ell'}\times\vec{e}^{\,0}\right)\times\vec{\omega}_{\ell'}\right]\right\|\\&\qquad\le\frac{k_z^m\,k^2}{m!\,n!\,(n+m+1)}\sum_{\substack{\ell'\in\mathbb{Z}^2\\|k'+\omega\,\ell'|<k}}\left|\lambda_{\ell'}^{(n+m+1)}\right|\left|\omega_z^{\ell'}\right|^{n-1}.\end{aligned}$$

Observe that the set $\{\ell'\in\mathbb{Z}^2|\,|k'+\omega\,\ell'|<k\}$ is finite. This shows that the positive constant $\omega_0<1$, defined as the smallest real value of $\sqrt{k^2-|k'+\omega\,\ell'|}/k$ for all $\ell'\in\mathbb{Z}^2$ (cf. (6.2)), is well defined and that $|\omega_z^{\ell'}|\ge k\omega_0$ such that $|\omega_z^{\ell'}|^{n-1}\le k^{n-1}/\omega_0$, since $|\omega_z^{\ell'}|\le\|\vec{\omega}_{\ell'}\|=k$. Moreover, since

$$\sum_{\substack{\ell'\in\mathbb{Z}^2\\|k'+\omega\ell'|<k}}\left|\lambda_{\ell'}^{(n+m+1)}\right|\le\sum_{\ell'\in\mathbb{Z}^2}\left|\lambda_{\ell'}^{(n+m+1)}\right|=\left\|f^{(n+m+1)}\right\|_{\mathcal{A}},$$

the Banach algebra properties of $\mathcal{A}$ prove that

$$\sum_{\substack{\ell'\in\mathbb{Z}^2\\|k'+\omega\ell'|<k}}\left|\lambda_{\ell'}^{(n+m+1)}\right|\le\|f\|_{\mathcal{A}}^{(n+m+1)}.$$

Altogether,

$$\begin{aligned}&\left\|\frac{(-i)^n(ik_z)^m}{m!\,n!\,(n+m+1)}\sum_{\substack{\ell'\in\mathbb{Z}^2\\|k'+\omega\,\ell'|<k}}\lambda_{\ell'}^{(n+m+1)}\left[\omega_z^{\ell'}\right]^{n-1}\vec{e}^{\,*}\cdot\left[\left(\vec{\omega}_{\ell'}\times\vec{e}^{\,0}\right)\times\vec{\omega}_{\ell'}\right]\right\|\\&\qquad\le\frac{1}{\omega_0}\frac{k_z^m\,k^{n+1}}{m!\,(n+1)!}\,\|f\|^{n+m+1}\end{aligned}$$

and

$$\begin{aligned}&\left\|E^r_{N,M}(\vec{x})\right\|\\&\quad\le\frac{1}{\omega_0}\left(\sum_{n=0}^{N}\frac{(k\,\|f\|_{\mathcal{A}})^{n+1}}{(n+1)!}\right)\left(\sum_{m=M+1}^{\infty}\frac{(|k_z|\,\|f\|_{\mathcal{A}})^m}{m!}\right)+\frac{1}{\omega_0}\left(\sum_{n=N+1}^{\infty}\frac{(k\,\|f\|_{\mathcal{A}})^{n+1}}{(n+1)!}\right)\left(\sum_{m=0}^{\infty}\frac{(|k_z|\,\|f\|_{\mathcal{A}})^m}{m!}\right).\end{aligned}$$

This can be further bounded using standard estimates for the approximation error of the exponential function. To be precise, for e^a and an arbitrary $a \in \mathbb{R}$,

$$e^a - \sum_{n=0}^{N} \frac{a^n}{n!} = \frac{a^{N+1}}{(N+1)!}\, r_N(a),$$

where $|r_N(a)| < 2$ if $N > 2(|a|-1)$. Indeed, for $N > 2(|a|-1)$ and thus $|a|/(N+2) < 1/2$, it is easily seen that

$$\begin{aligned}\left| e^a - \sum_{n=0}^{N} \frac{a^n}{n!} \right| &\leq \sum_{n=N+1}^{\infty} \frac{|a|^n}{n!} = \frac{|a|^{N+1}}{(N+1)!} \sum_{n=0}^{\infty} |a|^n \frac{(N+1)!}{(N+1+n)!} \leq \frac{|a|^{N+1}}{(N+1)!} \sum_{n=0}^{\infty} \left(\frac{|a|}{N+2} \right)^n \\ &\leq \frac{|a|^{N+1}}{(N+1)!} \sum_{n=0}^{\infty} \frac{1}{2^n} = 2 \frac{|a|^{N+1}}{(N+1)!},\end{aligned}$$

since

$$\frac{(N+1)!}{(N+1+n)!} = \frac{1}{\prod_{\iota=0}^{n-1} (N+2+\iota)} \leq \frac{1}{\prod_{\iota=0}^{n-1} (N+2)} = \frac{1}{(N+2)^n}.$$

Hence, assuming N and M sufficiently large, i.e. $N+1 > 2(k\,\|f\|_{\mathcal{A}} - 1)$ and $M > 2(|k_z|\,\|f\|_{\mathcal{A}} - 1)$,

$$\left\| E^r_{N,M}(\vec{x}) \right\| \leq \frac{2}{\omega_0} \left(\sum_{n=0}^{N} \frac{(k\,\|f\|_{\mathcal{A}})^{n+1}}{(n+1)!} \right) \frac{(k_z\,\|f\|_{\mathcal{A}})^{M+1}}{(M+1)!} + \frac{2}{\omega_0} \frac{(k\,\|f\|_{\mathcal{A}})^{N+2}}{(N+2)!}\, e^{k_z\,\|f\|_{\mathcal{A}}}.$$

At last, using this bound to determine sufficiently large N and M to get a small error in the reflected electric field,

$$\begin{aligned}\vec{e}^{\,*}\cdot\, \vec{E}^r(\vec{x}) \sim{}& r(\vec{k}, \vec{e}^{\,0}, \vec{e}^{\,*})\, \frac{e^{ik\vec{n}_0^{\,r}\cdot\vec{x}}}{|k'|^2} \\ &- i\, \frac{\Delta}{2\epsilon_0} \sum_{\substack{\ell' \in \mathbb{Z}^2 \\ |k'+\omega\,\ell'| \leq k}} \sum_{n=0}^{N} \sum_{m=0}^{M} \frac{(-i)^n (ik_z)^m}{m!\, n!\, (n+m+1)}\, \lambda_{\ell'}^{(n+m+1)} \left[\omega_z^{\ell'}\right]^{n-1} \vec{e}^{\,*}\cdot \left[(\vec{\omega}_{\ell'} \times \vec{e}^{\,0}) \times \vec{\omega}_{\ell'} \right]\, e^{ik\vec{\omega}_{\ell'}\cdot\vec{x}}\end{aligned} \tag{6.6}$$

for $N, M \to \infty$.

Starting with the first two lines of (5.1), the same approach can be used to get the formula and corresponding error estimate for the transmitted field in Theorem 6.1. ∎

To get an interface (6.1), for which these formulas can be used to calculate the resulting field, a set $\mathcal{I}$ was created containing a finite number of randomly chosen indices ℓ'. Of course, to get a real valued function f the negative indices $-\ell'$ are also added to $\mathcal{I}$, i.e. $\mathcal{I} = \mathcal{I}_+ \cup \mathcal{I}_-$, where the ℓ' in $\mathcal{I}_+$ are chosen randomly and their negatives are collected in $\mathcal{I}_-$. It is well known that if the length of the corrugations in the rough surface is much smaller than the wavelength, the light 'sees' only the averaged surface. In view of this, it can be assumed that the corrugation lengths $2\pi/|\omega\,\ell'|$ of the surface are larger than a small constant times the wavelength. This restricts the range when choosing the finite number of indices ℓ'. To get the corresponding complex valued amplitudes $\lambda_{\ell'}$ it is possible to simply choose them independently and according to a uniform random distribution. The downside of this approach is that it creates a random surfaces with no specific correlation function. Another way to define the interface function is as follows.

Definition 6.2. *Let for a given correlation function $\sigma^2 e^{-(|\eta_1'-\eta_2'|/c_l)^{2\alpha}}$, where σ is the standard deviation of the random effect, c_l the correlation length and α a constant quantifying the roughness, the interface function f be defined as*

$$f(\eta') := \frac{\omega\, L}{\pi\sigma\,\sqrt{2|\mathcal{I}|}} \sum_{\ell' \in \mathcal{I}} \sqrt{G_\alpha(\omega\,\ell')}\, \left(h_{r,\ell'} + i\, h_{i,\ell'}\right) e^{i\omega\,\ell'\cdot\eta'}, \tag{6.7}$$

with

$$G_\alpha(s') := \sigma^2 \int_{\mathbb{R}^2} e^{-(|x'|/c_l)^{2\alpha}} e^{-is'\cdot x'}\,\mathrm{d}x'. \tag{6.8}$$

Here the value $|\mathcal{I}| = |\mathcal{I}_+| + |\mathcal{I}_-| = 2\,|\mathcal{I}_+|$, where $\mathcal{I}_+$ is the set of indices chosen uniformly, independent and identically distributed from a finite set $\mathcal{L}_+ := \{-L, -L+1, \ldots, L-1\}^2 \subset \mathbb{Z}^2$ for some fixed positive $L \in \mathbb{N}$. The set $\mathcal{I}_-$ is defined as $\{\ell' \in \{-L+1, \ldots, L-1, L\}^2 : -\ell' \in \mathcal{I}_+\}$ such that $\mathcal{I} := \mathcal{I}_+ \cup \mathcal{I}_-$. Similarly to the indices in $\mathcal{I}_+$, the values $h_{r,\ell'}$ and $h_{i,\ell'}$ for $\ell' \in \mathcal{I}_+$ are realisations of independent and identically distributed random numbers. These random numbers are Gaussian with standard deviation σ and mean zero. By defining $h_{r,\ell'} := h_{r,-\ell'}$ and $h_{i,\ell'} := -h_{i,-\ell'}$ for all $\ell' \in \mathcal{I}_-$ it is ensured that f is a real valued function. The Fourier transform G_α in (6.7) *is called the power spectrum density and it is shown in [28] that it can be evaluated explicitly for $\alpha = 1/2$ and $\alpha = 1$ (cf. [33, Eqns. (2.6) and (2.7), p. 14]). Indeed,*

$$G_{\frac{1}{2}}(s') = \frac{2\pi\,\sigma^2 c_l^2}{\sqrt{1+(c_l|s'|)^2}^3}, \qquad G_1(s') = \pi\,\sigma^2 c_l^2\, e^{-\left(\frac{c_l|s'|}{2}\right)^2}.$$

For such interface functions, there holds

Proposition 6.3. *The graph of a function f defined as in* (6.7) *describes a surface that has a correlation function* $\mathrm{Corr}(\eta_1', \eta_2')$ *that approximates $\sigma^2 e^{-(|\eta_1'-\eta_2'|/c_l)^{2\alpha}}$. For all fixed compact sets $\mathtt{E} \subset \mathbb{R}^2$ and if $\eta_1' - \eta_2' \in \mathtt{E}$, the approximation* $\mathrm{Corr}(\eta_1', \eta_2')$ *tends to the desired correlation function for ω tending to zero and ωL tending to infinity.*

Proof. For similarly defined one-dimensional random surfaces something comparable is shown in [24, Appendix Chapter A].

Note, that f is defined with the help of two multivariate random variables. Firstly, a fixed number $|\mathcal{I}_+|$ of indices ℓ' are chosen randomly from the set $\mathcal{L}_+ = \{-L, -L+1, \ldots, L-1\}^2$. This can be represented by a selection function $S_{\ell'} : \mathcal{L} \mapsto \{0, 1\}$, which is one if ℓ' is one of the randomly selected indices in $\mathcal{I}_+$ and zero otherwise. With this (cf. (6.7)) and $\mathcal{L} := \{-L, -L+1, \ldots, L-1, L\}^2$,

$$f_{(S_{\ell'},H)}(\eta') = \frac{\omega\,L}{\pi\sigma\,\sqrt{2|\mathcal{I}|}} \sum_{\ell' \in \mathcal{L}} (S_{\ell'} + S_{-\ell'})\,\sqrt{G_\alpha(\omega\,\ell')}\,\big(h_{r,\ell'} + i\,h_{i,\ell'}\big)\,e^{i\omega\,\ell'\cdot\eta'}. \tag{6.9}$$

In this sense $S_{\ell'}$ can be identified by a $4L^2$-dimensional discrete random variable that takes values from $\{0,1\}^{4L^2}$ where exactly $|\mathcal{I}_+|$ values are one, i.e. $|S_{\ell'}| := \sum_{\ell' \in \mathcal{L}_+} S_{\ell'} = |\mathcal{I}_+|$. In contrast, the $8L^2$-dimensional random variable $H := ((h_{r,\ell'})_{\ell' \in \mathcal{L}_+}, (h_{i,\ell'})_{\ell' \in \mathcal{L}_+})$ is continuous and takes values from $\mathbb{R}^{8L^2}$.

To calculate the correlation function of the heights at two given points η_1' and η_2', the expected value of the product of the random function at the two points is calculated, i.e.

$$\begin{aligned}
\mathrm{Corr}(\eta_1', \eta_2') &:= E(f_{(S_{\ell'},H)}(\eta_1') f_{(S_{\ell'},H)}(\eta_2')) \\
&:= \sum_{\substack{S_{\ell'} \in \{0,1\}^{4L^2} \\ |S_{\ell'}| = |\mathcal{I}_+|}} \int_{\mathbb{R}^{8L^2}} f_{(S_{\ell'},H)}(\eta_1')\,\overline{f_{(S_{\ell'},H)}(\eta_2')}\,p(S_{\ell'}, H)\,\mathrm{d}H,
\end{aligned}$$

where $p(S_{\ell'}, H)$ is the corresponding joint probability density function. Since the random variables are chosen independently, the joint density function is equal to the product of the density functions of the single random variables. To be precise,

$$p(S_{\ell'}, H) = p(S_{\ell'}) \prod_{\hat{\ell}' \in \mathcal{L}_+} p(h_{r,\hat{\ell}'})\,p(h_{i,\hat{\ell}'})$$

such that

$$\mathrm{Corr}(\eta_1',\eta_2') = \frac{\omega^2 L^2}{4\pi^2\sigma^2\,|\mathcal{I}_+|} \sum_{\substack{S_{\ell'}\in\{0,1\}^{4L^2}\\ |S_{\ell'}|=|\mathcal{I}_+|}} \int_{\mathbb{R}^{8L^2}} \Bigg\{ \Bigg[\sum_{\ell_1'\in\mathcal{L}} \big(S_{\ell_1'}+S_{-\ell_1'}\big)\sqrt{G_\alpha(\omega\,\ell_1')}\,\big(h_{r,\ell_1'}+i\,h_{i,\ell_1'}\big)e^{i\omega\,\ell_1'\cdot\eta_1'}\Bigg] \overline{\Bigg[\sum_{\ell_2'\in\mathcal{L}} \big(S_{\ell_2'}+S_{-\ell_2'}\big)\sqrt{G_\alpha(\omega\,\ell_2')}\,\big(h_{r,\ell_2'}+i\,h_{i,\ell_2'}\big)e^{i\omega\,\ell_2'\cdot\eta_2'}\Bigg]}\; p(S_{\ell'})\prod_{\hat\ell'\in\mathcal{L}_+} p(h_{r,\hat\ell'})\,p(h_{i,\hat\ell'})\Bigg\}\,\mathrm{d}H.$$

Moreover, for any fixed realisation $S_{\ell'}$ the summations over ℓ' consists only of the indices ℓ' from $\mathcal{I}_+$ and $\mathcal{I}_-$, leading for $j=1,2$ to

$$\begin{aligned}
&\sum_{\ell_j'\in\mathcal{L}} \Big(S_{\ell_j'}+S_{-\ell_j'}\Big)\sqrt{G_\alpha(\omega\,\ell_j')}\,\big(h_{r,\ell_j'}+i\,h_{i,\ell_j'}\big)e^{i\omega\,\ell_j'\cdot\eta_j'}\\
&\quad= \sum_{\ell_j'\in\mathcal{I}_+} \sqrt{G_\alpha(\omega\,\ell_j')}\,\big(h_{r,\ell_j'}+i\,h_{i,\ell_j'}\big)e^{i\omega\,\ell_j'\cdot\eta_j'} + \sum_{\ell_j'\in\mathcal{I}_-} \sqrt{G_\alpha(\omega\,\ell_j')}\,\big(h_{r,\ell_j'}+i\,h_{i,\ell_j'}\big)e^{i\omega\,\ell_j'\cdot\eta_j'}\\
&\quad= \sum_{\ell_j'\in\mathcal{I}_+} \sqrt{G_\alpha(\omega\,\ell_j')}\,\big(h_{r,\ell_j'}+i\,h_{i,\ell_j'}\big)e^{i\omega\,\ell_j'\cdot\eta_j'} + \sum_{\ell_j'\in\mathcal{I}_+} \sqrt{G_\alpha(\omega\,\ell_j')}\,\big(h_{r,\ell_j'}-i\,h_{i,\ell_j'}\big)e^{-i\omega\,\ell_j'\cdot\eta_j'},
\end{aligned}$$

where it was used that $G_\alpha(-\omega\ell') = G_\alpha(\omega\ell')$ (cf. (6.8)) and that $h_{r,\ell'} = h_{r,-\ell'}$ and $h_{i,\ell'} = -h_{i,-\ell'}$ for all $\ell'\in\mathcal{I}_-$. Thus,

$$\begin{aligned}
\mathrm{Corr}(\eta_1',\eta_2') = \frac{\omega^2 L^2}{4\pi^2\sigma^2\,|\mathcal{I}_+|} &\sum_{\substack{S_{\ell'}\in\{0,1\}^{4L^2}\\ |S_{\ell'}|=|\mathcal{I}_+|}} \sum_{\ell_1'\in\mathcal{I}_+}\sum_{\ell_2'\in\mathcal{I}_+} \sqrt{G_\alpha(\omega\,\ell_1')}\sqrt{G_\alpha(\omega\,\ell_2')}\Bigg\{\\
&\int_{\mathbb{R}^{8L^2}} \big(h^1_{r,\ell_1'}+i\,h^1_{i,\ell_1'}\big)\big(h^2_{r,\ell_2'}-i\,h^2_{i,\ell_2'}\big)\prod_{\hat\ell'\in\mathcal{L}_+} p(h_{r,\hat\ell'})\,p(h_{i,\hat\ell'})\,\mathrm{d}H\; e^{i\omega(\ell_1'\cdot\eta_1'-\ell_2'\cdot\eta_2')}\\
&+\int_{\mathbb{R}^{8L^2}} \big(h^1_{r,\ell_1'}-i\,h^1_{i,\ell_1'}\big)\big(h^2_{r,\ell_2'}-i\,h^2_{i,\ell_2'}\big)\prod_{\hat\ell'\in\mathcal{L}_+} p(h_{r,\hat\ell'})\,p(h_{i,\hat\ell'})\,\mathrm{d}H\; e^{-i\omega(\ell_1'\cdot\eta_1'+\ell_2'\cdot\eta_2')}\\
&+\int_{\mathbb{R}^{8L^2}} \big(h^1_{r,\ell_1'}+i\,h^1_{i,\ell_1'}\big)\big(h^2_{r,\ell_2'}+i\,h^2_{i,\ell_2'}\big)\prod_{\hat\ell'\in\mathcal{L}_+} p(h_{r,\hat\ell'})\,p(h_{i,\hat\ell'})\,\mathrm{d}H\; e^{i\omega(\ell_1'\cdot\eta_1'+\ell_2'\cdot\eta_2')}\\
&+\int_{\mathbb{R}^{8L^2}} \big(h^1_{r,\ell_1'}-i\,h^1_{i,\ell_1'}\big)\big(h^2_{r,\ell_2'}+i\,h^2_{i,\ell_2'}\big)\prod_{\hat\ell'\in\mathcal{L}_+} p(h_{r,\hat\ell'})\,p(h_{i,\hat\ell'})\,\mathrm{d}H\; e^{-i\omega(\ell_1'\cdot\eta_1'-\ell_2'\cdot\eta_2')}\Bigg\}\,p(S_{\ell'}).
\end{aligned}$$

Note that the mean integrals w.r.t. H correspond to the correlation of the random variables $h_{r,\ell_j'}$ and $h_{i,\ell_j'}$ for all $\ell_j'\in\mathcal{L}$ and $j=1,2$. As mentioned before, the random variables are independent and Gaussian distributed with constant zero mean and variance σ^2, such that the means of

$$\begin{aligned}
\big(h_{r,\ell_1'}+i\,h_{i,\ell_1'}\big)\big(h_{r,\ell_2'}-i\,h_{i,\ell_2'}\big) &= h_{r,\ell_1'}\,h_{r,\ell_2'}+h_{i,\ell_1'}\,h_{i,\ell_2'}+i\big(h_{i,\ell_1'}\,h_{r,\ell_2'}-h_{r,\ell_1'}\,h_{i,\ell_2'}\big),\\
\big(h_{r,\ell_1'}-i\,h_{i,\ell_1'}\big)\big(h_{r,\ell_2'}-i\,h_{i,\ell_2'}\big) &= h_{r,\ell_1'}\,h_{r,\ell_2'}-h_{i,\ell_1'}\,h_{i,\ell_2'}-i\big(h_{i,\ell_1'}\,h_{r,\ell_2'}+h_{r,\ell_1'}\,h_{i,\ell_2'}\big),\\
\big(h_{r,\ell_1'}+i\,h_{i,\ell_1'}\big)\big(h_{r,\ell_2'}+i\,h_{i,\ell_2'}\big) &= h_{r,\ell_1'}\,h_{r,\ell_2'}-h_{i,\ell_1'}\,h_{i,\ell_2'}+i\big(h_{i,\ell_1'}\,h_{r,\ell_2'}+h_{r,\ell_1'}\,h_{i,\ell_2'}\big),\\
\big(h_{r,\ell_1'}-i\,h_{i,\ell_1'}\big)\big(h_{r,\ell_2'}+i\,h_{i,\ell_2'}\big) &= h_{r,\ell_1'}\,h_{r,\ell_2'}+h_{i,\ell_1'}\,h_{i,\ell_2'}-i\big(h_{i,\ell_1'}\,h_{r,\ell_2'}-h_{r,\ell_1'}\,h_{i,\ell_2'}\big)
\end{aligned}$$

are zero for all $\hat\ell'\notin\mathcal{I}_+$, all $\ell_1'\neq\ell_2'$ and all $\ell_1'=\ell_2'=\hat\ell'$ in the second and third line, where the covariance $\sigma^2-\sigma^2=0$ is obtained both times. Only the means of the first and last line can be non-zero, i.e. $2\sigma^2$, and even then only in the cases of $\ell_1' = \ell_2' = \hat{\ell}'$. Consequently,

$$\mathrm{Corr}(\eta_1', \eta_2') = \frac{\omega^2 L^2}{2\pi^2 |\mathcal{I}_+|} \sum_{\substack{S_{\ell'} \in \{0,1\}^{4L^2} \\ |S_{\ell'}| = |\mathcal{I}_+|}} \left\{ \sum_{\ell' \in \mathcal{I}_+} G_\alpha(\omega\, \ell')\, e^{i\omega \ell' \cdot (\eta_1' - \eta_2')} + \sum_{\ell' \in \mathcal{I}_+} G_\alpha(\omega\, \ell')\, e^{-i\omega \ell' \cdot (\eta_1' - \eta_2')} \right\} p(S_{\ell'}). \tag{6.10}$$

Note that since the indices ℓ' in $\mathcal{I}_+$ are chosen uniformly, identically and independently distributed, the sums

$$\frac{4L^2}{|\mathcal{I}_+|} \sum_{\ell' \in \mathcal{I}_+} G_\alpha(\omega\, \ell')\, e^{i\omega \ell' \cdot (\eta_1' - \eta_2')}, \qquad \frac{4L^2}{|\mathcal{I}_+|} \sum_{\ell' \in \mathcal{I}_+} G_\alpha(\omega\, \ell')\, e^{-i\omega \ell' \cdot (\eta_1' - \eta_2')}$$

are Monte-Carlo approximations of the full sums

$$\sum_{\ell' \in \mathcal{L}_+} G_\alpha(\omega\, \ell')\, e^{i\omega \ell' \cdot (\eta_1' - \eta_2')}, \qquad \sum_{\ell' \in \mathcal{L}_+} G_\alpha(\omega\, \ell')\, e^{-i\omega \ell' \cdot (\eta_1' - \eta_2')},$$

respectively. It follows that the expected values of these sums in (6.10) are equal to these full sums, giving

$$\mathrm{Corr}(\eta_1', \eta_2') = \frac{\omega^2}{8\pi^2} \sum_{\ell' \in \mathcal{L}_+} G_\alpha(\omega\, \ell')\, e^{i\omega \ell' \cdot (\eta_1' - \eta_2')} + \frac{\omega^2}{8\pi^2} \sum_{\ell' \in \mathcal{L}_+} G_\alpha(\omega\, \ell')\, e^{-i\omega \ell' \cdot (\eta_1' - \eta_2')}. \tag{6.11}$$

Recalling the definition $\mathcal{L}_+ = \{-L, -L+1, \ldots, L-1\}^2$ it is then apparent that these sums are Riemann sums approximating the integral

$$\int_{[-\omega L, \omega L]^2} G_\alpha(s')\, e^{\pm i s' \cdot (\eta_1' - \eta_2')}\, \mathrm{d}s'.$$

To be precise, the domain of integration $[-\omega L, \omega L]^2$ is split into $4L^2$ squares of equal size ω^2. The integral over one such square $[\omega \ell_x, \omega(\ell_x + 1)] \times [\omega \ell_y, \omega(\ell_y + 1)]$ is then approximated by the cuboid with the square as base and the height equal to the function value of $G_\alpha(s')\, e^{\pm i s' \cdot (\eta_1' - \eta_2')}$ at $s' = \omega(\ell_x, \ell_y)^\top$. Since $G_\alpha(-s) = G_\alpha(s)$ it follows that

$$\begin{aligned} \mathrm{Corr}(\eta_1', \eta_2') &\approx \frac{1}{8\pi^2} \int_{[-\omega L, \omega L]^2} G_\alpha(s')\, e^{i s' \cdot (\eta_1' - \eta_2')}\, \mathrm{d}s' + \frac{1}{8\pi^2} \int_{[-\omega L, \omega L]^2} G_\alpha(s')\, e^{-i s' \cdot (\eta_1' - \eta_2')}\, \mathrm{d}s' \\ &= \frac{1}{4\pi^2} \int_{[-\omega L, \omega L]^2} G_\alpha(s')\, e^{i s' \cdot (\eta_1' - \eta_2')}\, \mathrm{d}s'. \end{aligned} \tag{6.12}$$

Moreover, for $c_l, \alpha > 0$ the kernel of the Fourier transform G_α (cf. (6.8)) is absolutely integrable such that the Riemann-Lebesgue lemma gives that $G_\alpha(s')$ tends to zero for $|s'| \to \infty$. Hence, the truncated integral on the right-hand side of (6.12) is an approximation of the integral over the entire $\mathbb{R}^2$, i.e. (cf. (6.8))

$$\mathrm{Corr}(\eta_1', \eta_2') \approx \frac{1}{4\pi^2} \int_{\mathbb{R}^2} G_\alpha(s')\, e^{i s' \cdot (\eta_1' - \eta_2')}\, \mathrm{d}s' = \left(\mathcal{F}^{-1} G_\alpha\right)(\eta_1' - \eta_2') = \sigma^2 e^{-(|\eta_1' - \eta_2'|/c_l)^{2\alpha}}. \tag{6.13}$$

Note that this last approximation is better in the case of $\alpha = 1$, where G_α decays exponentially, while G_α decays much slower for $\alpha = 1/2$. This shows that the function f in Definition 6.2 approximately has the given correlation function $\sigma^2 e^{-(|\eta_1' - \eta_2'|/c_l)^{2\alpha}}$.

It remains to consider the validity of these approximations. It is easily seen that (6.11) is a periodic function w.r.t. $\eta_1' - \eta_2'$, while, according to the Riemann-Lebesgue lemma, (6.12) decays to zero as $|\eta_1' - \eta_2'|$ tends to infinity. Consequently, (6.11) can only tend uniformly to (6.12) for decreasing ω, if

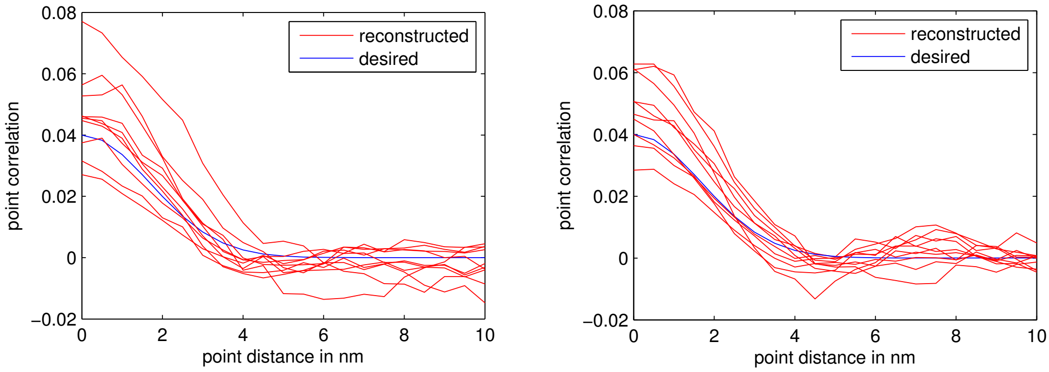


Figure 6.1: Desired and reconstructed auto-correlation functions for 10 interface realisations and 100 (left) and 1000 (right) randomly chosen spatial frequencies

the difference $\eta_1' - \eta_2'$ is restricted to a compact set. In this sense, the function (6.11) tends to (6.12) weakly, i.e. when testing with functions from $C_0^\infty(\mathbb{R}^2)$. Integral (6.12) on the other hand converges uniformly w.r.t. $\eta_1' - \eta_2'$ to (6.13) as L tends to infinity, since G_α is absolutely integrable. Indeed,

$$\left| \int_{\mathbb{R}^2} G_\alpha(s')\, e^{is'\cdot(\eta_1'-\eta_2')}\, \mathrm{d}s' - \int_{[-\omega L,\omega L]^2} G_\alpha(s')\, e^{is'\cdot(\eta_1'-\eta_2')}\, \mathrm{d}s' \right| = \left| \int_{\mathbb{R}^2\setminus[-\omega L,\omega L]^2} G_\alpha(s')\, e^{is'\cdot(\eta_1'-\eta_2')}\, \mathrm{d}s' \right|$$
$$\leq \int_{\mathbb{R}^2\setminus[-\omega L,\omega L]^2} |G_\alpha(s')|\, \mathrm{d}s'$$

tends to zero as L tends to infinity. ■

Remark 6.4. *Using the same approach as in the proof of Proposition 6.3 it is also easily shown that the given mean height μ of zero and height variance σ^2 are approximated by the mean μ_f and variance $\sigma_f^2 = \mathrm{Corr}(\eta', \eta')$ of the function f.*

An example of such an interface is shown in Figure 6.2. Moreover, Figure 6.1 confirms that the interface is correlated according to the auto-correlation function $\sigma^2 e^{-(|\eta'|/c_l)^{2\alpha}}$ (here: $\alpha = 1$). The two plots in the figure show the desired auto-correlation function (blue) depending on the distance of the points of the interface and the reconstructed auto-correlation functions (red) for ten realisations of the interface. The latter are calculated by randomly choosing a finite number of point pairs (η_1', η_2') with fixed distance $r = |\eta_1' - \eta_2'|$ and calculating the correlation for the corresponding pairs of interface heights $(f(\eta_1'), f(\eta_2'))$ for an interface realisation f. This is repeated for different distances r to get the approximated correlation function for one realisation. Note that all field calculations in this chapter were done for interface realisations where 100 spatial frequencies were chosen randomly. The right picture in Figure 6.1 shows that the behaviour of the correlation function of the interface realisations can be slightly improved by increasing the number of randomly chosen frequencies, or in this sense, the number of basis functions for the interface. Naturally, this will also increase the computational cost since the matrix $\lambda_{\ell'}$, for all $\ell' \in [-L, L]^2 \supset \mathcal{I}$, will have more non-zero entries, which will negatively affect fast convolution algorithms used to calculate the factors $\lambda_{\ell'}^{(n)}$.

Using the derived far-field formula (6.6), the efficiencies of the propagating plane waves (all ℓ' where $|k' + \omega\,\ell'| < k$) can be calculated (cf. Fig. 6.3(a)). They can be considered as discrete approximate values for the density function of the scattered power. Recall (cf. [36, Equ. (24)]) that this density is the differential power dP^{sc} scattered into a solid angle $d\Omega$ with direction $\vec{m} = (m_x, m_y, m_z)^\top$, i.e. (cf. [13, Eqn. (1.36), p. 9])

$$\frac{dP^{sc}}{d\Omega} := \frac{\|\vec{E}^{sc}(\vec{m})\|^2}{\|\vec{E}^0\|^2}.$$

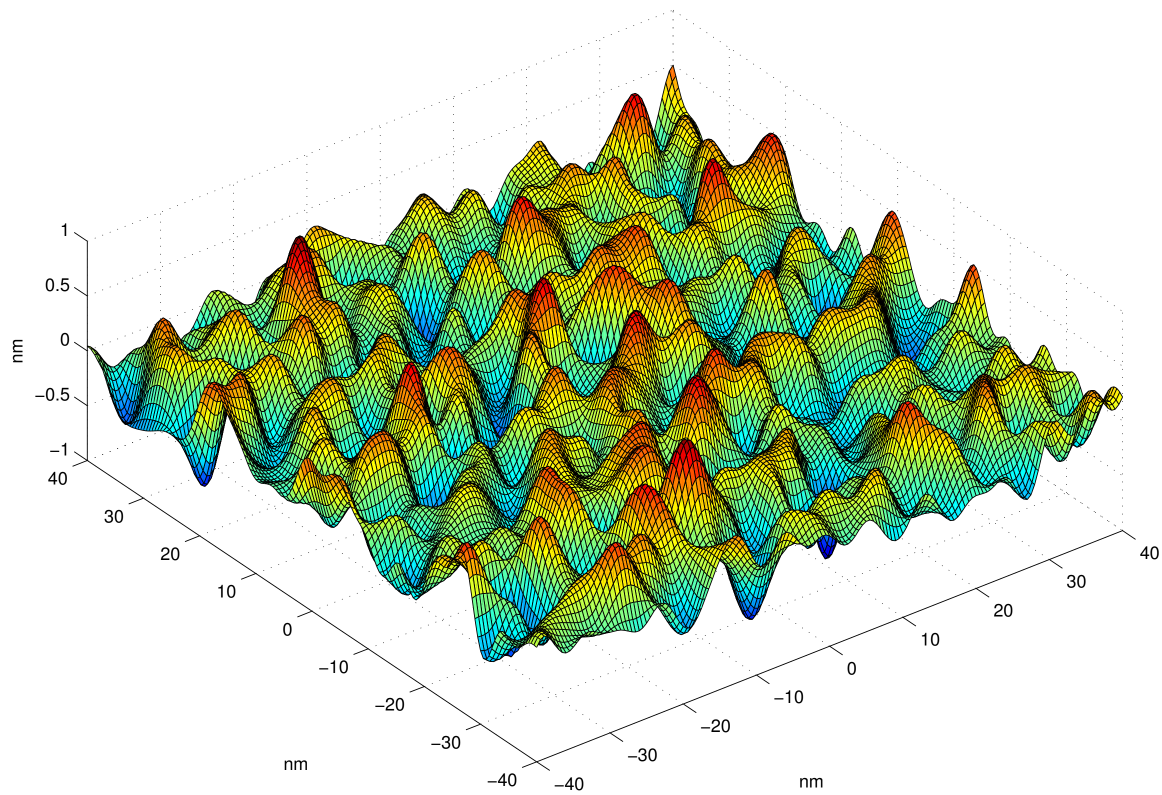


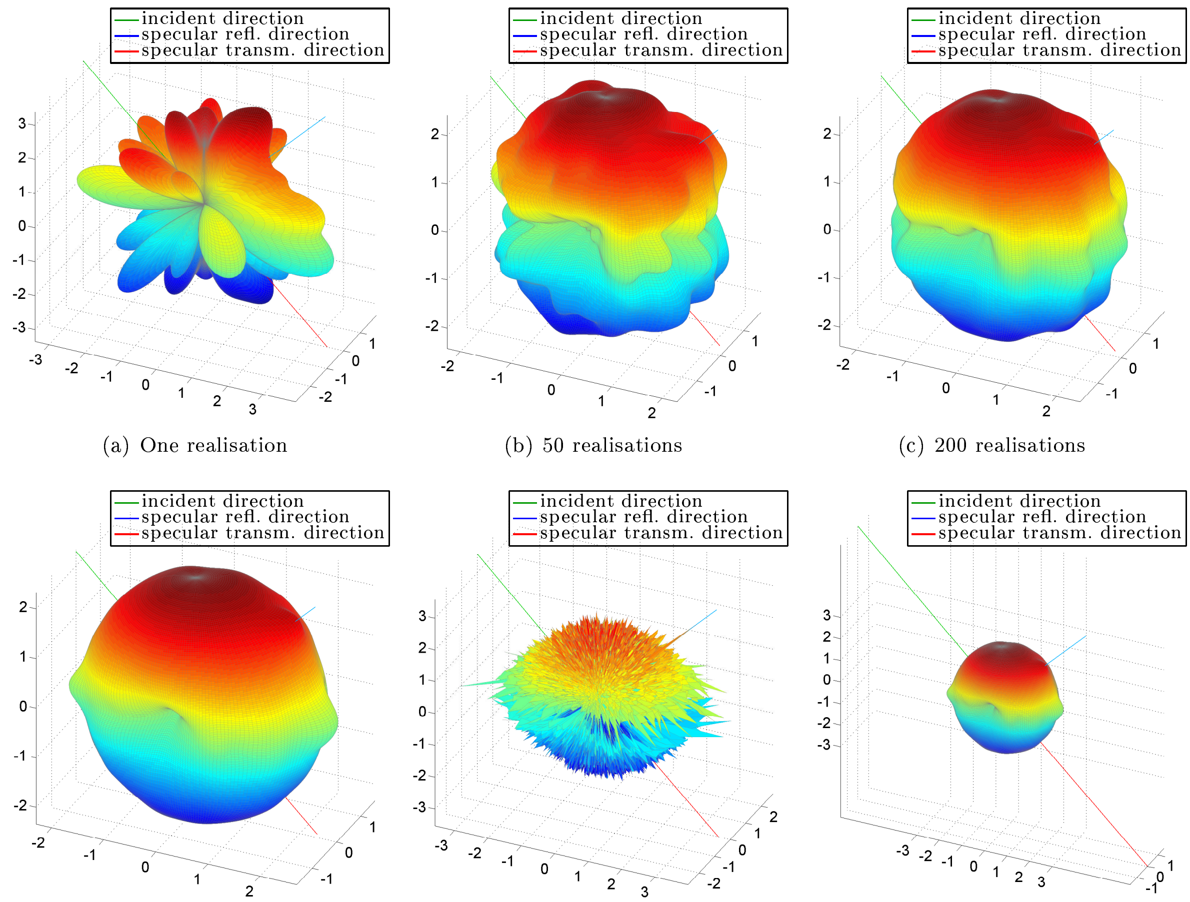
Figure 6.2: An interface realisation from $\mathcal{A} \cap L^\infty_Q$ with 100 randomly chosen spatial frequencies, a correlation length of 2.4 nm and a standard deviation for the height of 0.2 nm

The plane wave efficiencies displayed in Figure 6.3, on the other hand, are defined as

$$E(\vec{m}) := \frac{\|\vec{E}^{sc}(\vec{m})\|^2}{\|\vec{E}^0\|^2} \frac{k\,|m_z|}{|k_z|}.$$

Note that $dP^{sc}/d\Omega$ is the portion of the incident energy scattered into direction $\vec{m}$, i.e. the energy passing through a reference area orthogonal to $\vec{m}$. The efficiency $E(\vec{m})$, on the other hand, is the portion of $dP^{sc}/d\Omega$ passing through a reference area parallel to the x-y-plane. The plots in Figures 6.3 and 6.5 are to be understood as follows. The distance of every plotted surface point from the origin corresponds to the differential power dP^{sc} scattered into the solid angle $d\Omega$.

Knowing that the width of the illuminating beam is much larger than the wavelength, the actually observable density function of the scattered power can be simulated as the average over many realisations of such a simple rough interface. Indeed, in many practical applications the random interface is assumed to be ergodic. This means that it is irrelevant whether the statistical average is taken over many different parts of one realisation of the interface or over many different realisations at one point of the interface (cf. [33, Sect. 2.1.7(c)]). Applying the latter, the power average is computed in a classical Monte-Carlo manner and is presented in Figures 6.3(b) to 6.3(d) in a logarithmic scale, where, instead of $dP^r/d\Omega$, either the value $9 + \log_{10}(dP^r/d\Omega)$ is plotted, if the value is positive, or zero is plotted otherwise. Such a scaling was chosen, since, depending on the direction, drastic differences in the order of magnitude of $dP^r/d\Omega$ can be observed. Naturally, a logarithmic scaling resolves this problem. However, since $dP^r/d\Omega < 1$, it follows that $\log_{10}(dP^r/d\Omega) < 0$, which can not be used as a radial component in spherical coordinates for the desired plots. Adding an arbitrary constant (here: 9) and setting all resulting negative values to zero resolves this problem and results in a logarithmic plot dominated by the highest values of $dP^r/d\Omega$, while ignoring the smallest values. In addition to this rescaling, all the surfaces in Figure 6.3, except that of Figure 6.3(e), are smoothened by convoluting the radial components of the surface with a scaled density function of the Gaussian normal distribution. To be



(a) One realisation

(b) 50 realisations

(c) 200 realisations

(d) 2000 realisations

(e) 2000 realisations without smoothening

(f) 2000 realisations with specular efficiencies for full field

Figure 6.3: Approximated power density averaged over 1, 50, 200 and 2000 realisations of the interface function: spatial frequencies for the interfaces with norm between zero and fixed upper bound (the length of the lines representing the incident and specular directions in Figure (a)–(e) do not represent the incident or deflected power in these directions; in Figure (f), the length of these lines represents the power of the total field $\vec{E}_d^{sc} + \vec{E}_{\mathcal{Q}}^{sc}$ deflected in the specular directions)

precise, let the $E(\vec{m}_j)$, for a finite number of $j \in \mathbb{N}$, be the calculated efficiencies. Then, the radial function

$$R(\vec{n}) := \frac{1}{2\pi\, s^2 \left[1 - e^{-\frac{2}{s^2}}\right]} \int_{\{\vec{m}\in\mathbb{R}^2:\|\vec{m}\|=1\}} e^{-\frac{\|\vec{n}-\vec{m}\|^2}{s^2}} \sum_j E(\vec{m}_j)\, \delta_{\vec{m}_j}(\vec{m})\, \mathrm{d}\vec{m},$$

where s (here: $1/10$) defines the smoothening radius, is used for the smoothened surfaces in the Figures 6.3 and 6.5 to define the distance of the surface from the origin for every direction $\vec{n}$. Using the coordinate transformation (4.2.22) to spherical coordinates, where $\vec{n}$ is the polar axis, the function $R(\vec{n})$ can be simplified to

$$R(\vec{n}) = \sum_j \frac{E(\vec{m}_j)}{2\pi\, s^2 \left[1 - e^{-\frac{2}{s^2}}\right]} e^{\frac{\vec{n}\cdot\vec{m}-1}{s^2}}.$$

The choice of the scaling constant $1/(2\pi\, s^2[1 - e^{-2/s^2}])$ ensures that

$$\frac{1}{2\pi\, s^2 \left[1 - e^{-\frac{2}{s^2}}\right]} \int_{\{\vec{m}\in\mathbb{R}^2:\|\vec{m}\|=1\}} e^{-\frac{\|\vec{n}-\vec{m}\|^2}{s^2}}\, \mathrm{d}\vec{m} = 1.$$

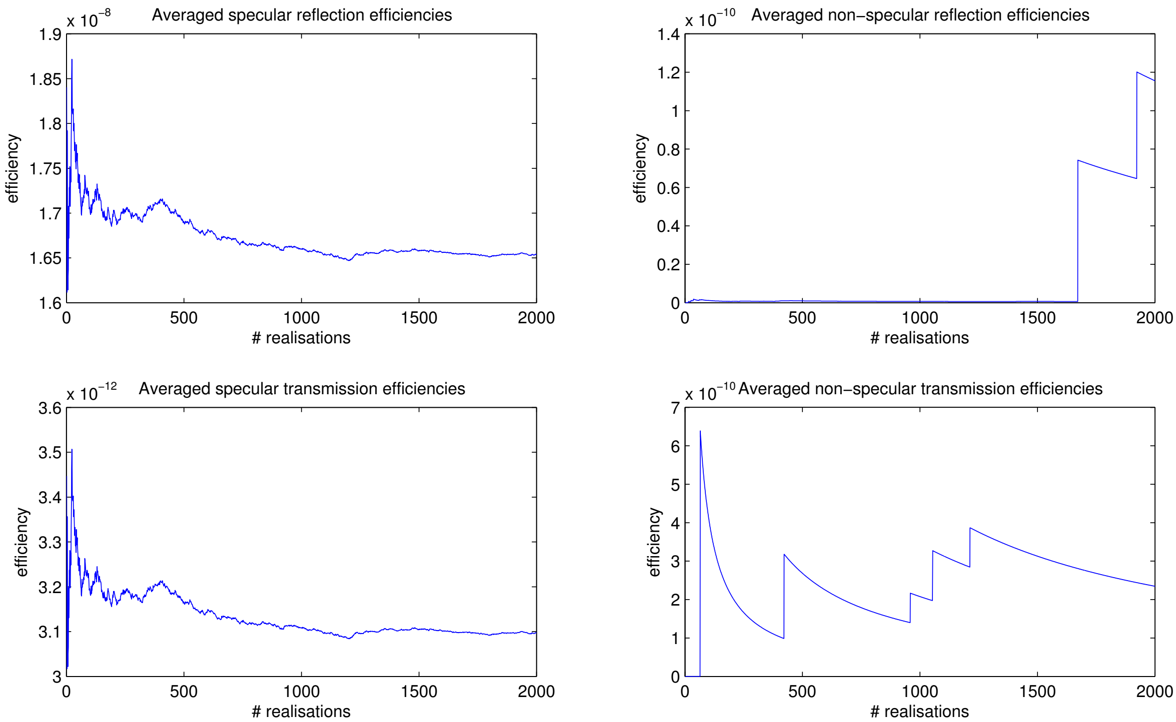


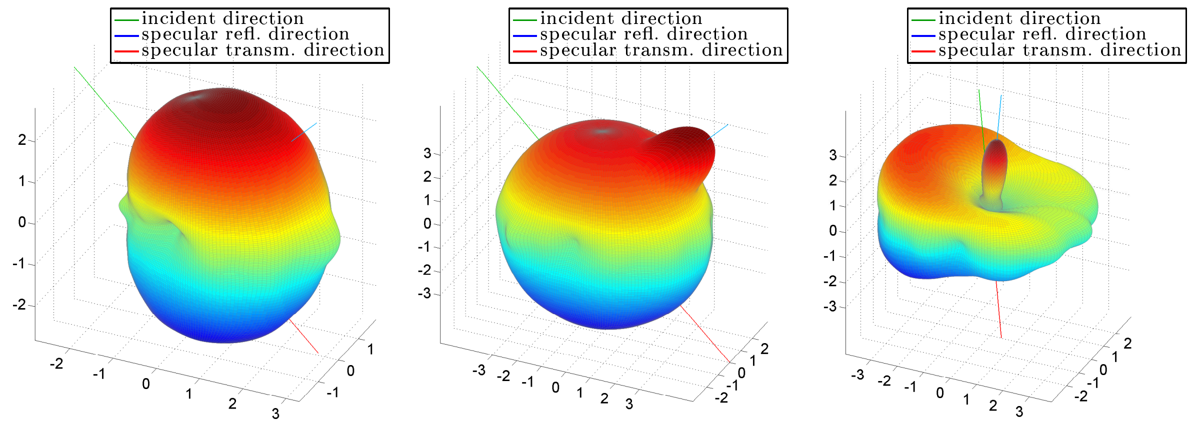
Figure 6.4: Simulated averaged efficiency for fixed specular (left) and arbitrary non-specular (right) directions as a function on the number of Monte-Carlo realisations

The smoothening is done to obtain surfaces, which represent the actual power density more closely, by removing the discrete nature of the calculated efficiencies, which can still be observed, even after averaging over 2000 realisations (cf. Fig. 6.3(e)). The mentioned discrete nature of the efficiencies is the result of choosing a finite number of spatial frequencies from a equidistant mesh to create the random surface realisations.

Note, that the plots in Figure 6.3 only show the averaged power for the difference field $\vec{E}_d^{sc}$ without the field $\vec{E}_Q^{sc}$ scattered at an ideal interface. This is done since the portion of the power refracted into the specular directions, especially the transmitted one, is much larger such that even the chosen logarithmic scaling can not resolve both orders of magnitude at once. Indeed, for 2000 realisations, the maximum differential power $dP^r/d\Omega$ of the difference field is $1.65 \cdot 10^{-8}$, while that for the specular refracted directions in the case of an ideal interface is $1.82 \cdot 10^{-4}$ (reflected) and 0.99981 (transmitted). This is visualised in Figure 6.3(f). This figure shows the same plot as Figure 6.3(d), except that the lengths of the lines representing the incident and specular directions, now correspond to the power of the incident field $\vec{E}^0$ and the efficiencies of the total field $\vec{E}_d^{sc} + \vec{E}_Q^{sc}$ in the specular directions. When studying the first four plots of Figure 6.3 it is apparent that, as one would expect, the surface smoothens with an increasing number of realisation. An interesting fact, when studying the averaged power of the difference field for this example, is that it seemingly converges much faster in the specular directions than in other directions. This is visualised in Figure 6.4 by plotting the averaged power in dependence of the number of realisations. The curves on the left side show the behaviour for the specular directions (reflected and transmitted), while the plots on the right side show the same for arbitrarily chosen directions other than the specular directions.

The following parameters and material constants were used for calculating the fields resulting in Figure 6.3.

- Incidence wavelength λ: 13.664 nm
- Dielectric constants ϵ_0: 1
- Lower dielectric constant ϵ_0': 0.97349584
- Magnetic permeability μ_0: 1



(a) Correlation length c_l of 5 nm (b) Standard deviation σ of 2 nm (c) Finite bound for spatial frequencies

Figure 6.5: Power density averaged over 2000 realisations of the interface function, where only one interface parameter of the original set was changed respectively – Left: Increased correlation length c_l, Middle: Increased standard deviation of interface heights, Right: spatial frequencies with norm between fixed positive lower and upper bound

- Incidence wave vector $\vec{k}$: $k\,(1/\sqrt{2}, 0, -1/\sqrt{2})^\top$
- Incidence polarisation $\vec{e}^{\,0}$: $(0, -1, 0)^\top$ (TE-polarisation, cf. (A.1.1))
- Step-size of spatial interface frequencies ω: $4\pi/1500$
- Upper bound for spatial frequencies: $|\omega\,\ell'| \leq 2\pi/5$ (or equivalently a lower bound for spatial wavelength or corrugation length of 5 nm)
- Roughness constant α: 1
- Correlation length c_l: 2.4 nm
- Standard deviation of the interface height σ: 0.2 nm

Note that all the presented plots as well as the underlying calculations have been done using Matlab.

Figure 6.5 shows the effect if parameters are changed or if structure is added to the random interfaces. For the first plot, the correlation length was more than doubled (now: 5 nm). In contrast, for the plot in the middle the correlation length was left at 2.4 nm, but the standard deviation was increased to the tenfold, i.e. to 2 nm. In both plots, these changes of the parameters defining the random behaviour of the interfaces have visible effects on the power density. For the rightmost plot in Figure 6.5, an upper bound for the corrugation length, or equivalently a positive lower bound for the spatial frequencies ($|\omega\,\ell'| \geq 2\pi/15$), of the rough surface is employed. This was not the case in the example above, where the corrugation length was unbounded, since any spatial frequency close to zero was permitted. Comparing the plot with Figure 6.3(d), a jump in the density function is observed for directions of a fixed angle to the specular reflection or transmission direction. For directions closer to these directions the density is remarkably smaller. This is plausible, since even for sinusoidal gratings with such an upper bound for the corrugation length, there is no light, apart from the specular reflected or transmitted modes, propagating into a cone around the specular direction.

Remark 6.5. *Since the change of parameters has a visible influence on the power density, it is conceivable to also consider the inverse problem, i.e. deriving the interface parameters from the measurement of the power density. Naturally, to do so, the scattered field has to be measured very precisely in all directions, not just the discrete refraction modes usually measured, e.g. for gratings. That such precise measurements are possible was, for example, shown by Hakko et al. [19]. In their work, they measured the weak scattered field in directions between the main refraction modes. This weak background scattered field is caused by imperfections of the grating, i.e. roughness.*

Chapter 7

Summary and perspective

In this thesis, Born approximation was used to derive explicit formulas (cf. Thms. 4.1 and 5.1) for the far field resulting from a plane wave scattered at a rough interface. This approach is heavily based on work by Stearns [36]. To rigorously prove the obtained formulas, slight changes to Stearns' approach were necessary. Firstly, the problem was solved in the sense of a modified limiting absorption principle by assuming materials that absorb energy of waves travelling away from the interface. Secondly the scattered field was not calculated directly, but instead the difference of this wanted field and the scattered field resulting from ideal planar surface was calculated. The latter was easily obtained by applying the well-known Fresnel formulas such that the wanted scattered field could be obtained by adding this formula to the solution for the difference field.

To apply the Born approximation it was assumed that the dielectric constants of the two materials separated by the interface are very close to each other (low contrast). Furthermore, it was assumed that the interface is defined by the graph of functions from a specific class (cf. Eqn. (3.3.1)), containing almost periodic functions as well as almost periodic functions modulated by radial functions decaying at infinity. For these interface functions the far-field formula for the reflected field were proven in detail, while the proof for the transmitted far-field formula was only sketched by presenting the few differences to the proof of the reflected field.

To derive the reflected far-field formula, the inhomogeneous vector Helmholtz equation was formulated in the sense of a modified limiting absorption principle. Afterwards, the equation was adapted using Born approximation by manipulating the right-hand side. This new equation could now be solved applying generalised Fourier transforms, leading to an approximate integral representation of the reflected field. The occurring integrals were represented as Cauchy principal integrals at infinity to change the order of integration and one of them was evaluated explicitly by employing the residue theorem. Assuming the above described class of interfaces, the remaining limits were evaluated. It was also shown that the obtained formulas are asymptotically identical (small contrast) to the results by Stearns, when comparing the reduced efficiencies in specular direction and the plane wave amplitudes for scattering at a sinusoidal grating.

To illustrate how the presented far-field formulas may be applied, a simple example where the interface was defined by purely non-decaying, i.e. containing no decaying parts, and highly oscillatory biperiodic functions was introduced. Especially the second restriction led to a simplified setting, allowing the use of discrete convolution algorithms to efficiently calculate the plane-wave amplitudes of the scattered field. Additionally, an error bound for truncating the infinite sums in the far-field formulas was derived. With this it was possible to implement a fast evaluation of a discrete approximation of the scattered power density, which in turn made it possible to make a statistical analysis of the latter using a simple Monte-Carlo approach. To be precise, the power density distribution was calculated for many interface realisations and averaged. These averaged efficiencies correspond to efficiencies observable by experimental physicist, since an illuminating beam in practice is much larger than the length of the surface corrugations, leading to an averaging over many interface realisations. Furthermore, to create more 'realistic' interface realisations, they were constructed in such a way that they satisfy a given correlation function.

One of the next steps, when analysing scattering at rough surfaces in this manner, could be to extend the presented class of interface functions. This applies in particular to the almost periodic part. At present this could be considered as a discrete representation of a random process. Indeed, Yaglom [41] proves that most stationary random processes occurring in nature possess a well defined spectral representation similar to the Fourier transform for integrable deterministic functions. To be precise, in the one-dimensional case, a random process $X(t)$ can be represented by

$$X(t) = \int\limits_{\mathbb{R}} e^{ist} \, \mathrm{d}Z(s), \tag{7.1}$$

where $Z(s)$ is another random process and the integral is defined as a Stieltjes integral, i.e.

$$\int\limits_{\mathbb{R}} e^{ist} \, \mathrm{d}Z(s) = \lim_{\substack{a \to -\infty \\ b \to +\infty}} \; \lim_{\max |s_n - s_{n-1}| \to 0} \sum_{n=1}^{N} e^{i\bar{s}_n t} \big[Z(s_n) - Z(s_{n-1}) \big],$$

where $a = s_0, s_1, \ldots, s_N = b$ is a partition of the interval $[a, b]$ and $\bar{s}_n$ an arbitrary point in (s_{n-1}, s_n). If the density function p_Z of Z exists (e.g. Gaussian distribution), the spectral representation (7.1) reduces to the usual Lebesgue integral, i.e.

$$X(t) = \int\limits_{\mathbb{R}} p_Z(s) \, e^{ist} \, \mathrm{d}s.$$

Using such a spectral representation (7.1), the class $\mathcal{A}$ (cf. (3.3.1)) of interface functions may be extended by replacing the almost periodic sums $\sum_{j \in \mathbb{Z}} \lambda_{\ell,j} \, e^{i\omega'_{\ell,j} \cdot \eta'}$ with (7.1). Naturally, a corresponding formula of (7.1) for the 2D case has to be formulated. By applying similar arguments and proofs as for the 'discrete' case, it may now be possible to deduce similar explicit formulas describing the scattered far field as a statistical distribution and not just as the field for a single interface realisation, as it is the case with the result presented in this thesis. The first step toward such a far-field distribution function, would be to once again consider realisations of the random interfaces, now defined with the spectral representation (7.1) instead of almost periodic functions. However, the analysis to obtain a corresponding far-field formula may necessitate the introduction of additional restrictions to the interface, incident field or materials. The next step would be to analyse the stochastic properties of these newly obtained formulas, i.e. the mean, variance, higher moments and distributions, as well as the correlation of the power densities in different scattering directions. Again it may be required to impose additional restrictions to the problem class.

Appendix A

Reflection at an ideal interface

In this chapter, the classical solutions for a plane wave deflected at an ideal planar surface $\mathcal{Q}$ will be derived. It is assumed that the incoming plane wave is as described in Subsection 2.1 with a wave vector $\vec{k}$. Furthermore, w.l.o.g. $\mathcal{Q}$ is assumed to be the x-y-plane. Thus $\vec{e}_3 := (0,0,1)^\top$ is the normal of $\mathcal{Q}$. Two polarisation states are distinguished. For the TE case, the polarisation vector $\vec{e}^{\,0}_{TE}$ is supposed to be in the x-y-plane. In the TM case the corresponding polarisation vector $\vec{e}^{\,0}_{TM}$ is supposed to be orthogonal to $\vec{e}^{\,0}_{TE}$ and $\vec{k}$. The two polarisation states will be examined in the first two sections. In the final section of this chapter, the formula for the deflected wave in case of an arbitrary constant polarisation $\vec{e}^{\,0}$, which can be represented as a linear combination of $\vec{e}^{\,0}_{TE}$ and $\vec{e}^{\,0}_{TM}$, will be considered. Note that the results of this chapter are well known. The main purpose of this chapter is to introduce the notation used in the context of the present thesis.

A.1 TE polarisation

In the TE case, the polarisation vector $\vec{e}^{\,0}_{TE}$ takes the form

$$\vec{e}^{\,0}_{TE} = \frac{1}{|k'|}\begin{pmatrix} k_y \\ -k_x \\ 0 \end{pmatrix}, \tag{A.1.1}$$

since $\vec{e}^{\,0}_{TE}$ must be orthogonal to the propagation direction $\vec{k}$ and of norm one. Naturally, this is not unique. This is especially true in the case of normal incidence, i.e. $\vec{k} = k\,(0,0,-1)^\top$, where (A.1.1) is not well defined. In the case of non-normal incidence, both $\vec{e}^{\,0}_{TE}$ as in (A.1.1) and its negative are possible polarisations. The given definition is chosen arbitrarily. In the normal case, all unit vectors parallel to the x-y-plane are possible. Here, $\vec{e}^{\,0}_{TE}$ is defined as $(1,0,0)^\top$. The case of non-normal incidence is considered first. The scattered electric field is now determined by the classical jump conditions

$$\left[\vec{E}\times\vec{e}_3\right]_{\mathcal{Q}} = 0, \qquad\qquad \left[\vec{H}\times\vec{e}_3\right]_{\mathcal{Q}} = 0,$$

i.e., by the equations (cf. [23, Eqn. (7.37), p. 304])

$$\left(\vec{e}^{\,0}_{TE} + \vec{e}^{\,r}_{TE} - \vec{e}^{\,t}_{TE}\right)\times\vec{e}_3 = 0, \tag{A.1.2}$$

$$\left(\vec{k}\times\vec{e}^{\,0}_{TE} + \vec{k}^{\,r}\times\vec{e}^{\,r}_{TE} - \vec{k}^{\,t}\times\vec{e}^{\,t}_{TE}\right)\times\vec{e}_3 = 0, \tag{A.1.3}$$

where $\vec{k}^{\,r} := (k', -k_z)^\top$, with $k' := (k_x, k_y)^\top$, and $\vec{k}^{\,t} := (k', k^t_z)$, with $k^t_z := -\sqrt{\tilde{k}^2 - |k'|^2}$ and $\tilde{k} := \sqrt{\mu_0\epsilon_0'}\omega$, are the wave vectors of the reflected and transmitted plane wave modes, respectively. The symbols $\vec{e}^{\,r}_{TE}$ and $\vec{e}^{\,t}_{TE}$ identify the complex valued polarisation vectors of these modes, such that

$$\vec{E}^r_{TE} = \vec{e}^{\,r}_{TE}\, e^{i\vec{k}^r\cdot\vec{x}}, \qquad\qquad \vec{E}^t_{TE} = \vec{e}^{\,t}_{TE}\, e^{i\vec{k}^t\cdot\vec{x}}.$$

Note that $\vec{e}^{\,r}_{TE}$ and $\vec{e}^{\,t}_{TE}$ are parallel to $\vec{e}^{\,0}_{TE}$. The orthogonality of $\vec{e}_3$ with $\vec{e}^{\,0}_{TE}$, $\vec{e}^{\,r}_{TE}$, $\vec{e}^{\,t}_{TE}$ implies that $(\vec{k}\times\vec{e}^{\,j}_{TE})\times\vec{e}_3 = -\vec{e}_3\cdot\vec{k}\,\vec{e}^{\,j}_{TE} = -k_z\vec{e}^{\,j}_{TE}$ for $j=0,r,t$. Hence, equation (A.1.3) simplifies to

$$-k_z\,\vec{e}^{\,0}_{TE} - k_z^r\,\vec{e}^{\,r}_{TE} + k_z^t\,\vec{e}^{\,t}_{TE} = 0. \tag{A.1.4}$$

On the other hand, for the polarisation vectors in the x-y-plane, equation (A.1.2) leads to $\vec{e}^{\,0}_{TE}+\vec{e}^{\,r}_{TE}-\vec{e}^{\,t}_{TE}=0$. Substituting $\vec{e}^{\,t}_{TE}=\vec{e}^{\,0}_{TE}+\vec{e}^{\,r}_{TE}$ into (A.1.4) gives

$$\vec{e}^{\,r}_{TE} = -\frac{k_z^t-k_z}{k_z^t-k_z^r}\,\vec{e}^{\,0}_{TE} = \frac{k_z+\sqrt{\tilde{k}^2-|k'|^2}}{k_z-\sqrt{\tilde{k}^2-|k'|^2}}\,\vec{e}^{\,0}_{TE} = \frac{k_z+\sqrt{\tilde{k}^2-|k'|^2}}{k_z-\sqrt{\tilde{k}^2-|k'|^2}}\,\frac{1}{|k'|}\begin{pmatrix} k_y\\ -k_x\\ 0\end{pmatrix}, \tag{A.1.5}$$

$$\vec{e}^{\,t}_{TE} = \vec{e}^{\,0}_{TE}+\vec{e}^{\,r}_{TE} = 2\frac{k_z}{k_z-\sqrt{\tilde{k}^2-|k'|^2}}\,\frac{1}{|k'|}\begin{pmatrix} k_y\\ -k_x\\ 0\end{pmatrix} \tag{A.1.6}$$

for $\vec{k}\neq k\,(0,0,-1)^\top$ and otherwise

$$\vec{e}^{\,r}_{TE} = \frac{k-\tilde{k}}{k+\tilde{k}}\begin{pmatrix}1\\0\\0\end{pmatrix}, \qquad \vec{e}^{\,t}_{TE} = 2\frac{k}{k+\tilde{k}}\begin{pmatrix}1\\0\\0\end{pmatrix}.$$

A.2 TM polarisation

As before, it is necessary to specify the unit vector $\vec{e}^{\,0}_{TM}$. Since the vector is contained in the incident plane, it has to be a linear combination of $\vec{k}$ and $\vec{e}_3$ such that $\vec{e}^{\,0}_{TM}\cdot\vec{k}=0$. Hence, a constant $\nu\in\mathbb{R}$ is to be determined such that $\vec{e}^{\,0}_{TM}$ is a multiple of $\vec{k}+\nu\,\vec{e}_3$ and $\vec{e}^{\,0}_{TM}\cdot\vec{k}=0$. Taking the scalar product of $\vec{e}^{\,0}_{TM}$ by $\vec{k}$ leads to $\nu=-k^2/k_z$ and, by an additional normalisation with

$$\begin{aligned}\left\|\vec{k}+\nu\,\vec{e}_3\right\|^2 &= \left\|\vec{k}-\frac{k^2}{k_z}\,\vec{e}_3\right\|^2 = \frac{1}{k_z^2}\,\left\|(k_zk_x,k_zk_y,-|k'|^2)^\top\right\|^2 = \frac{1}{k_z^2}\,\left[k_z^2(k_x^2+k_y^2)+(k_x^2+k_y^2)^2\right] \\ &= \frac{k^2\,|k'|^2}{k_z^2},\end{aligned} \tag{A.2.1}$$

to

$$\vec{e}^{\,0}_{TM} = \frac{1}{\left\|\vec{k}+\nu\,\vec{e}_3\right\|}\left(\vec{k}+\nu\,\vec{e}_3\right) = -\frac{k_z}{k\,|k'|}\left(\vec{k}+\nu\,\vec{e}_3\right) = -\frac{1}{k\,|k'|}\begin{pmatrix}k_xk_z\\ k_yk_z\\ -|k'|^2\end{pmatrix}. \tag{A.2.2}$$

Similar to the TE case, (A.2.2) is not well defined for normal incidence, i.e. $\vec{k}=(0,0,-1)^\top$. In this case, $\vec{e}^{\,0}_{TM}$ is, for definiteness, defined as $(0,1,0)^\top$. Note that this definition also satisfies the condition for the TE polarisation above, such that the same approach can be used to show that

$$\vec{e}^{\,r}_{TM} = \frac{k-\tilde{k}}{k+\tilde{k}}\begin{pmatrix}0\\1\\0\end{pmatrix}, \qquad \vec{e}^{\,t}_{TM} = 2\frac{k}{k+\tilde{k}}\begin{pmatrix}0\\1\\0\end{pmatrix},$$

for $\vec{k}=k\,(0,0,-1)^\top$.

In the case of $\vec{k}\neq k\,(0,0,-1)^\top$, the approach that led to (A.2.2) can also be used to easily show that the unit vectors $\vec{e}^{\,r}_0$ and $\vec{e}^{\,t}_0$, with $\vec{e}^{\,r}_{TM}=\nu_r\,\vec{e}^{\,r}_0$ and $\vec{e}^{\,t}_{TM}=\nu_t\,\vec{e}^{\,t}_0$, can be represented as

$$\vec{e}^{\,r}_0 = -\frac{1}{k\,|k'|}\begin{pmatrix}k_xk_z\\ k_yk_z\\ |k'|^2\end{pmatrix}, \qquad \vec{e}^{\,t}_0 = -\frac{1}{\tilde{k}\,|k'|}\begin{pmatrix}-k_x\sqrt{\tilde{k}^2-|k'|^2}\\ -k_y\sqrt{\tilde{k}^2-|k'|^2}\\ -|k'|^2\end{pmatrix}. \tag{A.2.3}$$

Similarly to the TE polarisation, the electric field is described by two jump equations, i.e.

$$\left[\epsilon\, \vec{E} \cdot \vec{e}_3\right]_{\mathcal{Q}} = 0, \qquad \left[\vec{E} \times \vec{e}_3\right]_{\mathcal{Q}} = 0,$$

or more precisely (cf. [23, Eqn. (7.37), p. 304])

$$\begin{aligned} \left[\epsilon_0 \left(\vec{e}^{\,0}_{TM} + \nu_r\, \vec{e}^{\,r}_0\right) - \epsilon_0'\, \nu_t\, \vec{e}^{\,t}_0\right] \cdot \vec{e}_3 &= 0, \\ \left(\vec{e}^{\,0}_{TM} + \nu_r\, \vec{e}^{\,r}_0 - \nu_t\, \vec{e}^{\,t}_0\right) \times \vec{e}_3 &= 0. \end{aligned} \tag{A.2.4}$$

The first equation shows that

$$\nu_t = \frac{\epsilon_0}{\epsilon_0'} \frac{\left[\vec{e}^{\,0}_{TM}\right]_z + \nu_r \left[\vec{e}^{\,r}_0\right]_z}{\left[\vec{e}^{\,t}_0\right]_z} = \frac{k^2}{\tilde{k}^2} \frac{\frac{|k'|^2}{k|k'|} - \nu_r \frac{|k'|^2}{k|k'|}}{\frac{|k'|^2}{\tilde{k}|k'|}} = \frac{k}{\tilde{k}} \left(1 - \nu_r\right),$$

while evaluating the cross product in (A.2.4) leads to

$$\begin{aligned} &\left(\vec{e}^{\,0}_{TM} + \nu_r\, \vec{e}^{\,r}_0 - \nu_t\, \vec{e}^{\,t}_0\right) \times \vec{e}_3 \\ &= -\frac{1}{k\,|k'|} \begin{pmatrix} k_y k_z \\ -k_x k_z \\ 0 \end{pmatrix} - \frac{\nu_r}{k\,|k'|} \begin{pmatrix} k_y k_z \\ -k_x k_z \\ 0 \end{pmatrix} + \frac{\nu_t}{\tilde{k}\,|k'|} \begin{pmatrix} -k_y \sqrt{\tilde{k}^2 - |k'|^2} \\ k_x \sqrt{\tilde{k}^2 - |k'|^2} \\ 0 \end{pmatrix} = 0. \end{aligned}$$

Obviously, the first and the second component of this vector valued equation are linear dependent, while the third component is always satisfied. Thus, considering only the first component w.l.o.g. by replacing ν_t with $k/\tilde{k}\,(1-\nu_r)$ and dividing by $k_y/|k'|$, there follows

$$\frac{k_z}{k} + \nu_r \frac{k_z}{k} + \frac{k}{\tilde{k}^2} \left(1 - \nu_r\right) \sqrt{\tilde{k}^2 - |k'|^2} = 0.$$

Hence,

$$\begin{aligned} \nu_r &= -\frac{\tilde{k}^2 k_z + k^2 \sqrt{\tilde{k}^2 - |k'|^2}}{\tilde{k}^2 k_z - k^2 \sqrt{\tilde{k}^2 - |k'|^2}}, \\ \vec{e}^{\,r}_{TM} &= -\frac{\tilde{k}^2 k_z + k^2 \sqrt{\tilde{k}^2 - |k'|^2}}{\tilde{k}^2 k_z - k^2 \sqrt{\tilde{k}^2 - |k'|^2}} \frac{1}{k\,|k'|} \begin{pmatrix} -k_x k_z \\ -k_y k_z \\ -|k'|^2 \end{pmatrix} \end{aligned} \tag{A.2.5}$$

for $\vec{k} \neq k\,(0,0,-1)^\top$ and (cf. (A.2.3))

$$\vec{e}^{\,t}_{TM} = \frac{k}{\tilde{k}} \left(1 - \nu_r\right) \vec{e}^{\,t}_0 = -2 \frac{k\, k_z}{\tilde{k}^2 k_z - k^2 \sqrt{\tilde{k}^2 - |k'|^2}} \frac{1}{|k'|} \begin{pmatrix} -k_x \sqrt{\tilde{k}^2 - |k'|^2} \\ -k_y \sqrt{\tilde{k}^2 - |k'|^2} \\ -|k'|^2 \end{pmatrix} \tag{A.2.6}$$

for $\vec{k} \neq k\,(0,0,-1)^\top$.

A.3 General polarisation

For a general polarisation, $\vec{e}^{\,0}$ is a linear combination of the TE and TM vector, i.e.

$$\vec{e}^{\,0} = \left(\vec{e}^{\,0} \cdot \vec{e}^{\,0}_{TE}\right) \vec{e}^{\,0}_{TE} + \left(\vec{e}^{\,0} \cdot \vec{e}^{\,0}_{TM}\right) \vec{e}^{\,0}_{TM}, \tag{A.3.1}$$

where

$$\vec{e}^{\,0} \cdot \vec{e}^{\,0}_{TE} = \frac{k_y e^0_x - k_x e^0_y}{|k'|}, \qquad \vec{e}^{\,0} \cdot \vec{e}^{\,0}_{TM} = -\frac{k_z (k_x e^0_x + k_y e^0_y) - |k'|^2 e^0_z}{k\,|k'|}$$

for $\vec{k} \neq k\,(0,0,-1)^\top$ and otherwise

$$\vec{e}^{\,0} \cdot \vec{e}^{\,0}_{TE} = e^0_x, \qquad \vec{e}^{\,0} \cdot \vec{e}^{\,0}_{TM} = e^0_y.$$

Consequently, the formulas (A.1.5) and (A.2.5) imply

$$\begin{aligned} \vec{E}^r(\vec{x}) = \Bigg\{ & \frac{k_z + \sqrt{\tilde{k}^2 - |k'|^2}}{k_z - \sqrt{\tilde{k}^2 - |k'|^2}} \left(k_y e^0_x - k_x e^0_y\right) \begin{pmatrix} k_y \\ -k_x \\ 0 \end{pmatrix} \\ & + \frac{\tilde{k}^2 k_z + k^2 \sqrt{\tilde{k}^2 - |k'|^2}}{\tilde{k}^2 k_z - k^2 \sqrt{\tilde{k}^2 - |k'|^2}} \, \frac{k_z (k_x e^0_x + k_y e^0_y) - |k'|^2 \, e^0_z}{k^2} \begin{pmatrix} -k_x k_z \\ -k_y k_z \\ -|k'|^2 \end{pmatrix} \Bigg\} \frac{e^{i\vec{k}^r \cdot \vec{x}}}{|k'|^2} \end{aligned} \tag{A.3.2}$$

for $\vec{k} \neq k\,(0,0,-1)^\top$, while (A.1.6) and (A.2.6) imply

$$\begin{aligned} \vec{E}^t(\vec{x}) = \Bigg\{ & 2 \frac{k_y e^0_x - k_x e^0_y}{k_z - \sqrt{\tilde{k}^2 - |k'|^2}} \begin{pmatrix} k_y \\ -k_x \\ 0 \end{pmatrix} \\ & + 2 \frac{k_z (k_x e^0_x + k_y e^0_y) - |k'|^2 \, e^0_z}{\tilde{k}^2 k_z - k^2 \sqrt{\tilde{k}^2 - |k'|^2}} \begin{pmatrix} -k_x \sqrt{\tilde{k}^2 - |k'|^2} \\ -k_y \sqrt{\tilde{k}^2 - |k'|^2} \\ -|k'|^2 \end{pmatrix} \Bigg\} \frac{k_z}{|k'|^2} \, e^{i\vec{k}^t \cdot \vec{x}} \end{aligned} \tag{A.3.3}$$

for $\vec{k} \neq k\,(0,0,-1)^\top$. In the case of $\vec{k} = k\,(0,0,-1)^\top$, it is easily shown that

$$\vec{E}^r(\vec{x}) = \frac{k - \tilde{k}}{k + \tilde{k}} \, \vec{e}^{\,0} \, e^{i\vec{k}^r \cdot \vec{x}}, \qquad \vec{E}^t(\vec{x}) = 2 \frac{k}{k + \tilde{k}} \, \vec{e}^{\,0} \, e^{i\vec{k}^t \cdot \vec{x}}.$$

Appendix B

Asymptotics for the case of all singularities on the unit circle

B.1 The formula

This chapter of the appendix deals exclusively with deriving the far-field asymptotics of Equation (4.2.6) (cf. (4.2.1)) in the cases that $|k' + \tilde{\omega}'_{\ell,j}| = k$ for $\ell = 1, \dots, 4$. In these cases the point of the weak singularity of $h_{\ell,j,n}(n')$ is located on the singularity manifold of $1/n_z^r = 1/\sqrt{1 - n'^2}$. For convenience, define $\nu' := (k' + \tilde{\omega}'_{\ell,j})/k$ for $\ell = 1, \dots, 4$ and

$$f_{\ell,j}(n', n_z^r) := f_{\ell,j,n}(n', n_z^r) := h_{\ell,j,n}(n') \; |n' - \nu'| \tag{B.1.1}$$

for $\ell = 1, \dots, 4$, where $\sqrt{1 - n'^2}$ in $h_{\ell,j}$ is identified by n_z^r.

Theorem B.1. *Assuming that $|\nu'| = 1$ and $\vec{x} = R\vec{m}$ with $\|\vec{m}\| = 1$ and $m_z > 0$,*

$$\begin{aligned}\mathcal{J} &:= \int\limits_{\mathbb{R}^2} \frac{f_{\ell,j}(n', n_z^r)}{|n' - \nu'|} \, \frac{1}{\sqrt{1 - n'^2}} \, e^{ikR\vec{n}^r \cdot \vec{m}} \, \mathrm{d}n' \\ &= 2\pi \, h_{\ell,j}(m') \, \frac{e^{ikR}}{ikR} + \mathbb{1}_{(1,0)}(\ell, n) \, 2\pi \, f_{\ell,j,n}(\nu', 0) \, \frac{e^{ikR\nu' \cdot m'}}{kRm_z} + o\left(\frac{1}{R}\right)\end{aligned} \tag{B.1.2}$$

as R tends to infinity for any fixed $\ell = 1, \dots, 4$ and $n \in \mathbb{N}_0$.

The proof of the theorem is split into several parts, distributed over the following sections and subsections. In Section B.2 an important lemma for the proof is presented and the domain of integration of $\mathcal{J}$ (cf. (4.2.6)) is split according to plane-wave and evanescent modes. The asymptotic behaviour of the integrals with these reduced domains of integration is determined in Sections B.3 and B.4.

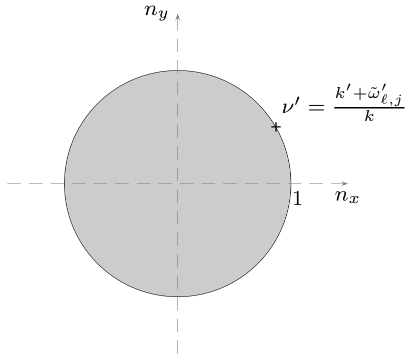
B.2 Splitting the integral

To prove Theorem B.1, the following lemma will be necessary.

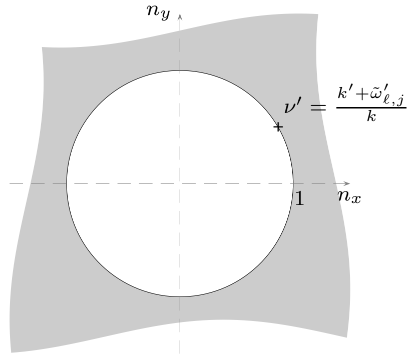
Lemma B.2. *Assuming the function $f_{\ell,j}(n', n_z^r)$ is defined as in (B.1.1), then $f_{\ell,j}(n', n_z^r)$ is finite at any point $(n', n_z^r)^\top \in \mathbb{R}^3$ for all $\ell = 1, \dots, 4$. Moreover, its partial derivatives are bounded for $\ell = 1, 3, 4$ and have at most a logarithmic singularity for $\ell = 2$ at the point $(n', n_z^r)^\top = (\nu', \sqrt{1 - |n'|^2})^\top$.*

Proof. Recall that (cf. (4.2.2) and (4.2.3))

$$\begin{aligned}f_{1,j}(n', n_z^r) &= i \, \frac{\Delta \, k^2}{4\pi\epsilon_0} \, [n_z^r]^n \, e^{-|kn' - k\nu'|} \; \left[\left(\vec{n}^r \times \vec{e}^0 \right) \times \vec{n}^r \right], \\ f_{2,j}(n', n_z^r) &= i \, \frac{\Delta \, k^3}{4\pi\epsilon_0} \, [n_z^r]^n K_0 \left(|kn' - k\nu'| \right) |n' - \nu'| \; \left[\left(\vec{n}^r \times \vec{e}^0 \right) \times \vec{n}^r \right].\end{aligned} \tag{B.2.1}$$



(a) $\mathcal{J}_1$ for $|\nu'| = 1$



(b) $\mathcal{J}_2$ for $|\nu'| = 1$

Figure B.1: Domains of integration of $\mathcal{J}_1$ and $\mathcal{J}_2$

Since the modified Bessel function $n' \mapsto K_0(|kn' - k\nu'|)$ has a logarithmic singularity at $n' = \nu'$, it is easily seen that both functions $f_{1,j}$ and $f_{2,j}$ are bounded for any $(n', n_z^r) \in \mathbb{R}^3$. Moreover, the gradient w.r.t. n' of $f_{\ell,j}(n', n_z^r)$ for $\ell = 1, 3, 4$ is bounded, whereas the gradient of $f_{2,j}(n', n_z^r)$ has a logarithmic singularity at $n' = \nu'$. To be precise, with $\vec{n}^r = (n', n_z^r)^\top$, (cf. [1, Eqn. 9.6.27, p. 120])

$$\begin{aligned}
\nabla_{n'} f_{1,j}(n', n_z^r) &= -i\,\frac{\Delta\, k^3}{4\pi\epsilon_0}\,[n_z^r]^n\,\frac{n'-\nu'}{|n'-\nu'|}\,e^{-|kn'-k\nu'|}\,\left[\left(\vec{n}^r \times \vec{e}^{\,0}\right) \times \vec{n}^r\right] \\
&\quad + i\,\frac{\Delta\, k^2}{4\pi\epsilon_0}\,[n_z^r]^n\,e^{-|kn'-k\nu'|}\,\nabla_{n'}\left[\left(\vec{n}^r \times \vec{e}^{\,0}\right) \times \vec{n}^r\right], \qquad \text{(B.2.2)} \\
\nabla_{n'} f_{2,j}(n', n_z^r) &= -i\,\frac{\Delta\, k^4}{4\pi\epsilon_0}\,[n_z^r]^n\,\frac{n'-\nu'}{|n'-\nu'|} K_1\left(|kn'-k\nu'|\right)\,|n'-\nu'|\,\left[\left(\vec{n}^r \times \vec{e}^{\,0}\right) \times \vec{n}^r\right] \\
&\quad + i\,\frac{\Delta\, k^3}{4\pi\epsilon_0}\,[n_z^r]^n K_0\left(|kn'-k\nu'|\right)\,\frac{n'-\nu'}{|n'-\nu'|}\,\left[\left(\vec{n}^r \times \vec{e}^{\,0}\right) \times \vec{n}^r\right] \\
&\quad + i\,\frac{\Delta\, k^3}{4\pi\epsilon_0}\,[n_z^r]^n K_0\left(|kn'-k\nu'|\right)\,|n'-\nu'|\,\nabla_{n'}\left[\left(\vec{n}^r \times \vec{e}^{\,0}\right) \times \vec{n}^r\right], \qquad \text{(B.2.3)}
\end{aligned}$$

where $K_1\left(|kn'-k\nu'|\right)|n'-\nu'|$ (cf. [1, Eqn. 9.6.11 with Eqn. 9.6.10, p. 119]) and $(n'-\nu')/|n'-\nu'|$ are bounded at $n' = \nu'$ and the term $(\vec{n}^r \times \vec{e}^{\,0}) \times \vec{n}^r$ is a polynomial of order two of n' and n_z^r. Thus all terms in (B.2.2) and (B.2.3), except the second line on the right-hand side of (B.2.3) where K_0 has a logarithmic singularity at zero, are bounded. Similarly, it is also not hard to show that $f_{\ell,j}(n', n_z^r)$ and $\nabla_{n'} f_{\ell,j}(n', n_z^r)$ for $\ell = 3, 4$ are bounded at $n' = \nu$, keeping in mind that $\|\tilde{g}_n(\,\cdot\,,\zeta)\|_{4,\infty} < \infty$ for any fixed $\zeta \in [0,1]$. The partial derivatives w.r.t. n_z are also bounded, since n_z only occurs as an argument of polynomials in $f_{\ell,j}$, $\ell = 1, \ldots, 4$. ∎

The remainder of Chapter B will be used to prove the asymptotic behaviour of $\mathcal{J}$, stated in Theorem B.1. The first step is to switch to polar coordinates (ρ, ϕ) and to split the area of integration $\mathbb{R}^2$ into the unit disc and its complement. This is a natural split, since the exponent of $e^{ikRm_z\sqrt{1-n'^2}}$ is purely imaginary for all n' on the unit disc and real valued and negative for all n' outside the unit disc. This corresponds to integrating over all plane waves and evanescent modes, respectively. Applying this coordinate transformation and split of the area of integration,

$$\begin{aligned}
\mathcal{J} &= \int_{\phi_0-\pi}^{\phi_0+\pi} \int_0^\infty \frac{f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2})}{|\rho n_0' - \nu'|}\, e^{ik\rho R n_0'\cdot m'}\, \frac{\rho}{\sqrt{1-\rho^2}}\, e^{ikRm_z\sqrt{1-\rho^2}}\, \mathrm{d}\rho\, \mathrm{d}\phi \\
&= \mathcal{J}_1 + \mathcal{J}_2, \qquad \text{(B.2.4)}
\end{aligned}$$

where $n_0' := (\cos\phi, \sin\phi)^\top$, ϕ_0 is defined such that $\nu' = (\cos\phi_0, \sin\phi_0)^\top$ and (cf. Figure B.1)

$$\mathcal{J}_1 := \int_{\phi_0-\pi}^{\phi_0+\pi} \int_0^1 \frac{f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2})}{|\rho n_0' - \nu'|}\, e^{ik\rho R n_0'\cdot m'}\, \frac{\rho}{\sqrt{1-\rho^2}}\, e^{ikRm_z\sqrt{1-\rho^2}}\, \mathrm{d}\rho\, \mathrm{d}\phi \qquad \text{(B.2.5)}$$

$$\mathcal{J}_2 := -i \int\limits_{\phi_0-\pi}^{\phi_0+\pi} \int\limits_{1}^{\infty} \frac{f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2})}{|\rho n_0' - \nu'|} \, e^{ik\rho R n_0' \cdot m'} \, \frac{\rho}{\sqrt{\rho^2-1}} \, e^{-kRm_z\sqrt{\rho^2-1}} \, \mathrm{d}\rho \, \mathrm{d}\phi. \tag{B.2.6}$$

The asymptotic behaviour of these two integrals will be determined in Sections B.3 and B.4.

B.3 Integrating over evanescent modes

To examine the asymptotic behaviour of the outer integral $\mathcal{J}_2$, it is necessary to take a closer look at the occurring singularity in (B.2.6). Note that here the norm of the difference of the two vectors $\rho n_0'$ and ν' can be separated into differences of the radii and the angles. Indeed,

$$\begin{aligned} |\rho n_0' - \nu'|^2 &= (\rho n_0' - \nu') \cdot (\rho n_0' - \nu') = (\rho n_0' - n_0' + n_0' - \nu') \cdot (\rho n_0' - n_0' + n_0' - \nu') \\ &= (\rho-1)^2 \, |n_0'|^2 + 2(\rho-1)\, \vec{n}_0' \cdot (n_0' - \nu') + |n_0' - \nu'|^2 \\ &= (\rho-1)^2 + 2(\rho-1)\, \vec{n}_0' \cdot (n_0' - \nu') + |n_0' - \nu'|^2 , \end{aligned}$$

where

$$\begin{aligned} |n_0' - \nu'|^2 &= (\cos\phi - \cos\phi_0)^2 + (\sin\phi - \sin\phi_0)^2 = 2 - 2\big(\cos\phi\cos\phi_0 + \sin\phi\sin\phi_0\big) \\ &= 2\big(1 - \cos(\phi-\phi_0)\big) = 4\sin^2\left(\frac{\phi-\phi_0}{2}\right) \end{aligned} \tag{B.3.1}$$

and

$$\begin{aligned} \vec{n}_0' \cdot (n_0' - \nu') &= \cos\phi\,(\cos\phi - \cos\phi_0) + \sin\phi\,(\sin\phi - \sin\phi_0) = 1 - \big(\cos\phi\cos\phi_0 + \sin\phi\sin\phi_0\big) \\ &= 1 - \cos(\phi - \phi_0) = 2\sin^2\left(\frac{\phi-\phi_0}{2}\right). \end{aligned} \tag{B.3.2}$$

Thus,

$$\begin{aligned} |\rho n_0' - \nu'|^2 &= (\rho-1)^2 + 4(\rho-1)\, \sin^2\left(\frac{\phi-\phi_0}{2}\right) + 4\sin^2\left(\frac{\phi-\phi_0}{2}\right) \\ &= (\rho-1)^2 + 4\,\rho\, \sin^2\left(\frac{\phi-\phi_0}{2}\right). \end{aligned} \tag{B.3.3}$$

The corresponding Taylor expansion w.r.t. ρ and ϕ leads to

$$|\rho n_0' - \nu'|^2 = (\rho-1)^2 + (\phi-\phi_0)^2 + (\rho-1)\,(\phi-\phi_0)^2 + \rho\,\mathcal{O}\big((\phi-\phi_0)^4\big). \tag{B.3.4}$$

With this, the outer integral (B.2.6) is split into

$$\mathcal{J}_2 = -i\big\{J_1 + J_2 + J_3 + J_4 + J_5\big\}, \tag{B.3.5}$$

where

$$\begin{aligned} J_1 := \int\limits_{\phi_0-\pi}^{\phi_0+\pi} \int\limits_{1}^{\infty} \Bigg\{ & f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2}) \left(\frac{1}{|\rho n_0' - \nu'|} - \frac{1}{\sqrt{(\rho-1)^2 + (\phi-\phi_0)^2}} \right) e^{ik\rho R n_0' \cdot m'} \\ & \frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}} \Bigg\} \mathrm{d}\rho\,\mathrm{d}\phi \end{aligned} \tag{B.3.6}$$

$$J_2 := \int\limits_{\phi_0-\pi}^{\phi_0+\pi} \int\limits_{1}^{\infty} \frac{f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2}) - f_{\ell,j}(\nu', 0)}{\sqrt{(\rho-1)^2 + (\phi-\phi_0)^2}} \, e^{ikRn_0'\cdot m'} \Big[e^{ik(\rho-1)Rn_0'\cdot m'} - 1 \Big] \frac{\rho}{\sqrt{\rho^2-1}} \, e^{-kRm_z\sqrt{\rho^2-1}} \, \mathrm{d}\rho\,\mathrm{d}\phi, \tag{B.3.7}$$

$$J_3 := \int_{\phi_0-\pi}^{\phi_0+\pi} \int_{1}^{\infty} \frac{f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2}) - f_{\ell,j}(\nu',0)}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\, e^{ikRn_0'\cdot m'} \frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}}\, \mathrm{d}\rho\, \mathrm{d}\phi, \tag{B.3.8}$$

$$J_4 := f_{\ell,j}(\nu',0) \int_{\phi_0-\pi}^{\phi_0+\pi} \int_{1}^{\infty} \frac{\left[e^{ik(\rho-1)Rn_0'\cdot m'} - 1\right]}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\, e^{ikRn_0'\cdot m'} \frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}}\, \mathrm{d}\rho\, \mathrm{d}\phi, \tag{B.3.9}$$

$$J_5 := f_{\ell,j}(\nu',0) \int_{\phi_0-\pi}^{\phi_0+\pi} \int_{1}^{\infty} \frac{1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\, e^{ikRn_0'\cdot m'} \frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}}\, \mathrm{d}\rho\, \mathrm{d}\phi. \tag{B.3.10}$$

Note that the integrals J_2 and J_4 are only non-trivial for $m' \neq (0,0)^\top$. Hence, for the following sections, it will be assumed that $m' \neq (0,0)^\top$. The asymptotic behaviour of J_1, J_3 and J_5 in the case of $m' = (0,0)^\top$ will be examined separately in Section B.3.2. In view of Lemma B.2 it is also easily seen that the constant $f_{\ell,j}(\nu',0)$ is finite. Moreover, taking a closer look at (B.1.1) with (4.2.2)–(4.2.5), it follows that $f_{\ell,j}(\nu',0) = 0$ for $\ell = 2,3,4$. Consequently, it is enough to examine the asymptotic behaviour of J_4 and J_5 for $\ell = 1$. Similarly in Section B.4 for the inner integral $\mathcal{J}_1$, the asymptotic behaviour of integrals that are multiplied with $f_{\ell,j}(\nu',0)$ will be examined. For these integrals the examinations will also be reduced to the case of $\ell = 1$.

B.3.1 Oblique reflection

B.3.1.1 J_1

To derive the asymptotic behaviour of J_1 it is necessary to show that the integrand is absolutely integrable. Consider the difference of the quotients in J_1 using the Taylor expansion (B.3.4),

$$\begin{aligned}
&\frac{1}{|\rho n_0' - \nu'|} - \frac{1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}} \\
&\quad = \frac{(\rho-1)^2+(\phi-\phi_0)^2 - |\rho n_0' - \nu'|^2}{|\rho n_0' - \nu'|\, \sqrt{(\rho-1)^2+(\phi-\phi_0)^2}\left(|\rho n_0' - \nu'| + \sqrt{(\rho-1)^2+(\phi-\phi_0)^2}\right)} \\
&\quad = -\frac{(\rho-1)\,(\phi-\phi_0)^2 + \rho\,\mathcal{O}\left((\phi-\phi_0)^4\right)}{|\rho n_0' - \nu'|\, \sqrt{(\rho-1)^2+(\phi-\phi_0)^2}\left(|\rho n_0' - \nu'| + \sqrt{(\rho-1)^2+(\phi-\phi_0)^2}\right)}.
\end{aligned}$$

Using this and substituting $(\rho-1, \phi-\phi_0)^\top$ with $r\,(\cos\gamma, \sin\gamma)^\top$ it is easily seen that

$$\lim_{r\to 0} \frac{1}{|\rho n_0' - \nu'|} - \frac{1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}} = \frac{1}{2}\,\cos\gamma\,\sin^2\gamma \tag{B.3.11}$$

is uniformly bounded by $1/2$ for all $\gamma \in [0,2\pi]$. Lemma 4.4 thus proves that the difference of quotients in (B.3.11) is uniformly bounded in a neighbourhood of $\rho n_0' = \nu'$. It follows that the integrand of J_1 is absolutely integrable, since only the weakly singular term $1/\sqrt{\rho^2-1}$ is locally unbounded, while the term $e^{-kRm_z\sqrt{\rho^2-1}}$ ensures exponential decay for ρ tending to infinity. To get an exponential function depending on m' but independent of ρ, the integral is split into

$$J_1 = J_{1.1} + J_{1.2}, \tag{B.3.12}$$

where

$$\begin{aligned}
J_{1.1} := \int_{\phi_0-\pi}^{\phi_0+\pi} \int_{1}^{\infty} \Bigg\{ & f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2}) \left(\frac{1}{|\rho n_0' - \nu'|} - \frac{1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\right) e^{ikRn_0'\cdot m'} \\
& \frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}} \Bigg\}\, \mathrm{d}\rho\, \mathrm{d}\phi,
\end{aligned}$$

$$J_{1.2} := \int_{\phi_0-\pi}^{\phi_0+\pi} \int_1^\infty \Bigg\{ f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2}) \left(\frac{1}{|\rho n_0' - \nu'|} - \frac{1}{\sqrt{(\rho-1)^2 + (\phi-\phi_0)^2}} \right) e^{ikRn_0'\cdot m'}$$
$$\left[e^{ik(\rho-1)Rn_0'\cdot m'} - 1 \right] \frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}} \Bigg\} \,\mathrm{d}\rho\,\mathrm{d}\phi \tag{B.3.13}$$

B.3.1.1.1 $J_{1.1}$

Integral $J_{1.1}$ is examined using integration by parts w.r.t. ρ, leading to

$$\begin{aligned} J_{1.1} = &-\frac{1}{kRm_z} \int_{\phi_0-\pi}^{\phi_0+\pi} \int_1^\infty \Bigg\{ f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2}) \left(\frac{1}{|\rho n_0' - \nu'|} - \frac{1}{\sqrt{(\rho-1)^2 + (\phi-\phi_0)^2}} \right) e^{ikRn_0'\cdot m'} \\ &\qquad \partial_\rho \left[e^{-kRm_z\sqrt{\rho^2-1}} \right] \Bigg\} \,\mathrm{d}\rho\,\mathrm{d}\phi \\ = &\frac{1}{kRm_z} \int_{\phi_0-\pi}^{\phi_0+\pi} f_{\ell,j}(n_0', 0) \left(\frac{1}{|n_0' - \nu'|} - \frac{1}{|\phi-\phi_0|} \right) e^{ikRn_0'\cdot m'} \,\mathrm{d}\phi \\ &+ \frac{1}{kRm_z} \int_{\phi_0-\pi}^{\phi_0+\pi} \int_1^\infty \Bigg\{ \partial_\rho \left[f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2}) \left(\frac{1}{|\rho n_0' - \nu'|} - \frac{1}{\sqrt{(\rho-1)^2 + (\phi-\phi_0)^2}} \right) \right] e^{ikRn_0'\cdot m'} \\ &\qquad e^{-kRm_z\sqrt{\rho^2-1}} \Bigg\} \,\mathrm{d}\rho\,\mathrm{d}\phi. \end{aligned} \tag{B.3.14}$$

First it will be shown that the first integral on the right hand side of (B.3.14) decays faster than $1/R$ as R tends to infinity. Defining ϕ_1 such that $m' = (\cos\phi_1, \sin\phi_1)^\top$, $\psi_0 := \phi_0 - \phi_1$ and substituting $\phi - \phi_1$ by ψ gives

$$\frac{1}{kRm_z} \int_{\psi_0-\pi}^{\psi_0+\pi} f_{\ell,j}\big(n_0'(\psi+\phi_1), 0\big) \left(\frac{1}{|n_0'(\psi+\phi_1) - \nu'|} - \frac{1}{|\psi-\psi_0|} \right) e^{ikR|m'|\cos\psi} \,\mathrm{d}\psi. \tag{B.3.15}$$

To estimate the asymptotic behaviour of this integral the following lemma is applied

Lemma B.3. *For any function $g \in L^\infty$, any constant $r \in \mathbb{R}$ and a positive constant $b \in \mathbb{R}$,*

$$\lim_{R\to\infty} \int_{\psi_0-\pi}^{\psi_0+\pi} g(\psi) \left[1 + r\log|\psi-\psi_0|\right] e^{ibR\cos\psi} \,\mathrm{d}\psi = 0.$$

Proof. To prove this, it is the goal to apply the Riemann-Lebesgue lemma. To do so $\cos\psi$ has to be substituted by a new variable t, for which the domain of integration has to split into parts where $\cos\psi$ is strictly monotonic.

Define l_0 as the unique integer such that $\psi_0 - \pi \le l_0\pi < \psi_0$ and

$$\begin{aligned} \mathrm{Arccos}_1 : \big[\cos(\psi_0-\pi), \cos(\ell_0\pi)\big] &\to \big[\psi_0-\pi, \ell_0\pi\big] \\ t &\mapsto \mathrm{Arccos}_1(t), \\ \mathrm{Arccos}_2 : \big[\cos(\ell_0\pi), \cos\big((\ell_0+1)\pi\big)\big] &\to \big(\ell_0\pi, (\ell_0+1)\pi\big] \\ t &\mapsto \mathrm{Arccos}_2(t), \\ \mathrm{Arccos}_3 : \big[\cos\big((\ell_0+1)\pi\big), \cos(\psi_0+\pi\big] &\to \big((\ell_0+1)\pi, \psi_0+\pi\big] \\ t &\mapsto \mathrm{Arccos}_3(t), \end{aligned}$$

such that $\cos(\mathrm{Arccos}_j(t)) = t$ for $j = 1, 2, 3$. This then leads to

$$\int_{\psi_0-\pi}^{\psi_0+\pi} g(\psi)\left[1 + r\log|\psi-\psi_0|\right] e^{ibR\cos\psi}\,\mathrm{d}\psi$$

$$= \int_{\psi_0-\pi}^{\ell_0\pi} g(\psi)\left[1 + r\log|\psi-\psi_0|\right] e^{ibR\cos\psi}\,\mathrm{d}\psi + \int_{\ell_0\pi}^{(\ell_0+1)\pi} g(\psi)\left[1 + r\log|\psi-\psi_0|\right] e^{ibR\cos\psi}\,\mathrm{d}\psi$$
$$+ \int_{(\ell_0+1)\pi}^{\psi_0+\pi} g(\psi)\left[1 + r\log|\psi-\psi_0|\right] e^{ibR\cos\psi}\,\mathrm{d}\psi$$
$$= \mathrm{sgn}(\sin\psi_0) \int_{-\cos\psi_0}^{(-1)^{\ell_0}} g\big(\mathrm{Arccos}_1(t)\big)\left[1 + r\log\big|\mathrm{Arccos}_1(t)-\psi_0\big|\right]\frac{1}{\sqrt{1-t^2}}\,e^{ikRt}\,\mathrm{d}t$$
$$- \mathrm{sgn}(\sin\psi_0) \int_{(-1)^{\ell_0}}^{(-1)^{\ell_0+1}} g\big(\mathrm{Arccos}_2(t)\big)\left[1 + r\log\big|\mathrm{Arccos}_2(t)-\psi_0\big|\right]\frac{1}{\sqrt{1-t^2}}\,e^{ikRt}\,\mathrm{d}t$$
$$+ \mathrm{sgn}(\sin\psi_0) \int_{(-1)^{\ell_0+1}}^{-\cos\psi_0} g\big(\mathrm{Arccos}_3(t)\big)\left[1 + r\log\big|\mathrm{Arccos}_3(t)-\psi_0\big|\right]\frac{1}{\sqrt{1-t^2}}\,e^{ikRt}\,\mathrm{d}t, \tag{B.3.16}$$

It is easily seen that the integrands of the three integrals on the right-hand side of (B.3.16) are only weakly singular, since $\mathrm{Arccos}_j(t)$ is a continuous and g a bounded function, while, by using L'Hôpital's rule, it is not hard to show that $\log|\mathrm{Arccos}_{j_0}(t)-\psi_0| \sim \log|t-t_0|$ for a fixed $j_0 = 1, 2, 3$ and $t_0 \in [-1, 1]$ such that $\mathrm{Arccos}_{j_0}(t_0) = \psi_0$. It follows that the term $[1+r\log|\mathrm{Arccos}_j(t)-\psi_0|]/\sqrt{1-t^2}$ is only weakly singular, even for $|t_0| = 1$. The Riemann-Lebesgue lemma thus proves the statement. ■

To apply Lemma B.3 to integral (B.3.15) it has to be shown that its integrand is at most logarithmically singular. Recall that $f_{\ell,j}\big(n_0'(\psi+\phi_1), 0\big)$ is bounded for all $\psi \in [\psi_0-\pi, \psi_0+\pi]$ (cf. Lemma B.2). Moreover, it is easily shown that the term (cf. (B.3.4))

$$\frac{1}{|n_0'(\psi+\phi_1)-\nu'|} - \frac{1}{|\psi-\psi_0|} = \frac{(\psi-\psi_0)^2 - |n_0'(\psi+\phi_1)-\nu'|^2}{|\psi-\psi_0|\,|n_0'(\psi+\phi_1)-\nu'|\left[|\psi-\psi_0| + |n_0'(\psi+\phi_1)-\nu'|\right]}$$
$$= -\frac{\mathcal{O}\left((\psi-\psi_0)^4\right)}{|\psi-\psi_0|\,|n_0'(\psi+\phi_1)-\nu'|\left[|\psi-\psi_0| + |n_0'(\psi+\phi_1)-\nu'|\right]} \tag{B.3.17}$$

is bounded for all $\psi \in [\psi_0-\pi, \psi_0+\pi]$. Lemma B.3 thus proves that

$$\frac{1}{kRm_z}\int_{\phi_0-\pi}^{\phi_0+\pi} f_{\ell,j}(n_0', 0)\left(\frac{1}{|n_0'-\nu'|} - \frac{1}{|\phi-\phi_0|}\right) e^{ikRn_0'\cdot m'}\,\mathrm{d}\phi = o\left(\frac{1}{R}\right). \tag{B.3.18}$$

The next step is to examine the remaining integral on the right-hand side of (B.3.14) by examining the occurring derivative

$$\partial_\rho\left[f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2})\left(\frac{1}{|\rho n_0'-\nu'|} - \frac{1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\right)\right]$$
$$= \left(n_0', \frac{-\rho}{\sqrt{1-\rho^2}}\right)^\top \cdot \nabla_{\vec{n}}\, f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2})\left(\frac{1}{|\rho n_0'-\nu'|} - \frac{1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\right)$$
$$- f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2})\left(\frac{n_0'\cdot(\rho n_0'-\nu')}{|\rho n_0'-\nu'|^3} - \frac{\rho-1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}^{\,3}}\right). \tag{B.3.19}$$

Since $\nabla_{\vec{n}} f_{\ell,j}(n', n_z)$ has at most a logarithmic singularity (cf. Lemma B.2) and using (B.3.11), it is easily seen that the first summand on the right-hand side is only weakly singular at $\rho = 1$ and $\phi = \phi_0$. To show this for the second summand, it has to be proven that the difference of the two quotients is at most weakly singular. Consider

$$\begin{aligned}
\frac{n_0' \cdot (\rho n_0' - \nu')}{|\rho n_0' - \nu'|^3} &- \frac{\rho - 1}{\sqrt{(\rho-1)^2 + (\phi - \phi_0)^2}^3} \\
&= \frac{n_0' \cdot (\rho n_0' - n_0') + n_0' \cdot (n_0' - \nu')}{|\rho n_0' - \nu'|^3} - \frac{\rho - 1}{\sqrt{(\rho-1)^2 + (\phi - \phi_0)^2}^3} \\
&= (\rho - 1)\left(\frac{1}{|\rho n_0' - \nu'|^3} - \frac{1}{\sqrt{(\rho-1)^2 + (\phi - \phi_0)^2}^3}\right) + \frac{n_0' \cdot (n_0' - \nu')}{|\rho n_0' - \nu'|^3}. \qquad \text{(B.3.20)}
\end{aligned}$$

First, the last term on the right-hand side is examined, (cf. (B.3.2), (B.3.3) and (B.3.4))

$$\begin{aligned}
\frac{n_0' \cdot (n_0' - \nu')}{|\rho n_0' - \nu'|^3} = \frac{n_0' \cdot (n_0' - \nu')}{|\rho n_0' - \nu'|^2} \frac{1}{|\rho n_0' - \nu'|} &= \frac{2 \sin^2\left(\frac{\phi - \phi_0}{2}\right)}{(\rho-1)^2 + 4\rho \sin^2\left(\frac{\phi - \phi_0}{2}\right)} \frac{1}{|\rho n_0' - \nu'|} \\
&\leq \frac{c}{\sqrt{(\rho-1)^2 + (\phi - \phi_0)^2}}. \qquad \text{(B.3.21)}
\end{aligned}$$

Obviously, this is only weakly singular and thus absolutely integrable. On the other hand, examining the first term on the right-hand side of (B.3.20), (cf. (B.3.4))

$$\begin{aligned}
&(\rho - 1)\left(\frac{1}{|\rho n_0' - \nu'|^3} - \frac{1}{\sqrt{(\rho-1)^2 + (\phi - \phi_0)^2}^3}\right) \\
&= (\rho - 1)\frac{\left[(\rho-1)^2 + (\phi-\phi_0)^2\right]^3 - |\rho n_0' - \nu'|^6}{|\rho n_0' - \nu'|^3 \sqrt{(\rho-1)^2 + (\phi - \phi_0)^2}^3 \left[|\rho n_0' - \nu'|^3 + \sqrt{(\rho-1)^2 + (\phi - \phi_0)^2}^3\right]} \\
&= (\rho - 1)\frac{\left[(\rho-1)^2 + (\phi-\phi_0)^2\right]^3 - \left[(\rho-1)^2 + (\phi-\phi_0)^2 + (\rho-1)(\phi-\phi_0)^2 + \rho\,\mathcal{O}\left((\phi-\phi_0)^4\right)\right]^3}{|\rho n_0' - \nu'|^3 \sqrt{(\rho-1)^2 + (\phi - \phi_0)^2}^3 \left[|\rho n_0' - \nu'|^3 + \sqrt{(\rho-1)^2 + (\phi - \phi_0)^2}^3\right]} \\
&= -(\rho - 1)\frac{3\left[(\rho-1)^2 + (\phi-\phi_0)^2\right]^2 \left[(\rho-1)(\phi-\phi_0)^2 + \rho\,\mathcal{O}\left((\phi-\phi_0)^4\right)\right]}{|\rho n_0' - \nu'|^3 \sqrt{(\rho-1)^2 + (\phi - \phi_0)^2}^3 \left[|\rho n_0' - \nu'|^3 + \sqrt{(\rho-1)^2 + (\phi - \phi_0)^2}^3\right]} \\
&\quad - (\rho - 1)\frac{3\left[(\rho-1)^2 + (\phi-\phi_0)^2\right] \left[(\rho-1)(\phi-\phi_0)^2 + \rho\,\mathcal{O}\left((\phi-\phi_0)^4\right)\right]^2}{|\rho n_0' - \nu'|^3 \sqrt{(\rho-1)^2 + (\phi - \phi_0)^2}^3 \left[|\rho n_0' - \nu'|^3 + \sqrt{(\rho-1)^2 + (\phi - \phi_0)^2}^3\right]} \\
&\quad - (\rho - 1)\frac{\left[(\rho-1)(\phi-\phi_0)^2 + \rho\,\mathcal{O}\left((\phi-\phi_0)^4\right)\right]^3}{|\rho n_0' - \nu'|^3 \sqrt{(\rho-1)^2 + (\phi - \phi_0)^2}^3 \left[|\rho n_0' - \nu'|^3 + \sqrt{(\rho-1)^2 + (\phi - \phi_0)^2}^3\right]}
\end{aligned}$$

Using the same approach of substitution as for (B.3.11) it is not hard to show that this term is bounded by $1/\sqrt{(\rho-1)^2 + (\phi-\phi_0)^2}$ at the potential singularity point $(\rho, \phi)^\top = (1, \phi_0)^\top$. Thus, (cf. (B.3.19), (B.3.20), (B.3.11) and (B.3.21))

$$\begin{aligned}
&\left|\partial_\rho \left[f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2}) \left(\frac{1}{|\rho n_0' - \nu'|} - \frac{1}{\sqrt{(\rho-1)^2 + (\phi - \phi_0)^2}}\right)\right]\right| \\
&\qquad \leq c\,\frac{\rho}{\sqrt{\rho^2 - 1}} \left|\log\left((\rho-1)^2 + (\phi-\phi_0)^2\right)\right| + \frac{c}{\sqrt{(\rho-1)^2 + (\phi - \phi_0)^2}} \qquad \text{(B.3.22)}
\end{aligned}$$

for $(\rho, \phi)^\top \to (1, \phi_0)^\top$. It follows that the absolute value of the second integral w.r.t. ρ on the right-hand side of (B.3.14) can be estimated as

$$\begin{aligned}
&\left|\int_1^\infty \partial_\rho \left[f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2}) \left(\frac{1}{|\rho n_0' - \nu'|} - \frac{1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\right)\right] e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho\right| \\
&\quad\le c\int_1^\infty \left\{\frac{\rho}{\sqrt{\rho^2-1}}\left|\log\bigl((\rho-1)^2+(\phi-\phi_0)^2\bigr)\right| + \frac{1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\right\} e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho \\
&\quad= c\int_1^\infty \frac{\rho}{\sqrt{\rho^2-1}}\left|\log\bigl((\rho-1)^2+(\phi-\phi_0)^2\bigr)\right| e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho \\
&\qquad + c\int_1^2 \frac{1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho + c\int_2^\infty \frac{1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho \\
&\quad\le -c\frac{2\log|\phi-\phi_0|}{kRm_z}\int_1^\infty \partial_\rho\Bigl[e^{-\frac{k}{2}Rm_z\sqrt{\rho^2-1}}\Bigr]\,\mathrm{d}\rho \\
&\qquad + c\int_1^2 \frac{1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\,\mathrm{d}\rho + c\int_2^\infty \frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho,
\end{aligned}$$

where

$$\int_1^2 \frac{1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\,\mathrm{d}\rho = \Bigl[\log\bigl((\rho-1)+\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}\Bigr]_{\rho=1}^2$$

such that for $\phi \in [\phi_0-\pi, \phi_0+\pi]$ (cf. (B.3.14))

$$\begin{aligned}
&\left|\int_1^\infty \partial_\rho \left[f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2}) \left(\frac{1}{|\rho n_0' - \nu'|} - \frac{1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\right)\right] e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho\right| \\
&\quad= c\,\frac{2\log|\phi-\phi_0|}{kRm_z} + c\,\log\bigl(1+\sqrt{1+(\phi-\phi_0)^2}\bigr) - c\,\log|\phi-\phi_0| - \frac{c}{kRm_z}\int_2^\infty \partial_\rho\Bigl[e^{-\frac{k}{2}Rm_z\sqrt{\rho^2-1}}\Bigr]\,\mathrm{d}\rho \\
&\quad\le c\,\frac{2\log|\phi-\phi_0|}{kRm_z} + c\,\log\bigl(1+\sqrt{1+\pi^2}\bigr) - c\,\log|\phi-\phi_0| + c\,\frac{e^{-\frac{k}{2}Rm_z\sqrt{3}}}{kRm_z}.
\end{aligned}$$

With this it is easily seen that functions $g_1, g_2, g_3 \in L^\infty$ exist such that

$$\begin{aligned}
&\int_1^\infty \partial_\rho \left[f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2}) \left(\frac{1}{|\rho n_0' - \nu'|} - \frac{1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\right)\right] e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho \\
&\quad= g_1(\phi)\,\frac{\log|\phi-\phi_0|}{R} + g_2(\phi)\,\frac{e^{-cR}}{R} + g_3(\phi)\,[1+\log|\phi-\phi_0|]
\end{aligned}$$

and, substituting $\phi-\phi_1$ by ψ, defining $\psi_0 := \phi_0-\phi_1$ and using Lemma B.3, (cf. (B.3.14) and (B.3.15))

$$\begin{aligned}
&\frac{1}{R}\int_{\phi_0-\pi}^{\phi_0+\pi}\int_1^\infty \partial_\rho\left[f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2}) \left(\frac{1}{|\rho n_0' - \nu'|} - \frac{1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\right)\right] e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho\, e^{ikRn_0'\cdot m'}\,\mathrm{d}\phi \\
&\quad= \frac{1}{R^2}\int_{\phi_0-\pi}^{\phi_0+\pi} \Bigl\{g_1(\phi)\,\log|\phi-\phi_0| + g_2(\phi)\,e^{-cR}\Bigr\} e^{ikRn_0'\cdot m'}\,\mathrm{d}\phi \\
&\qquad + \frac{1}{R}\int_{\phi_0-\pi}^{\phi_0+\pi} g_3(\phi)\bigl[1+\log|\phi-\phi_0|\bigr] e^{ik|m'|R\cos(\phi-\phi_1)}\,\mathrm{d}\phi
\end{aligned}$$

$$= \frac{1}{R} \int\limits_{\psi_0-\pi}^{\psi_0+\pi} g_3(\psi+\phi_1)\big[1+\log|\psi-\psi_0|\big] e^{ik|m'|R\cos\psi}\,\mathrm{d}\psi + o\left(\frac{1}{R}\right)$$
$$= o\left(\frac{1}{R}\right).$$

Consequently, (cf. (B.3.14) and (B.3.18))

$$J_{1.1} = o\left(\frac{1}{R}\right). \tag{B.3.23}$$

B.3.1.1.2 $J_{1.2}$

To obtain the asymptotic behaviour of $J_{1.2}$ (cf. (B.3.13)) define

$$\epsilon_R := C\left(\frac{\log R}{R}\right)^2, \tag{B.3.24}$$

with $C \geq 1/(2k^2 m_z^2)$ and consider (cf. (B.3.11) and Lemma B.2)

$$\begin{aligned}
|J_{1.2}| &\leq c \int\limits_{\phi_0-\pi}^{\phi_0+\pi}\int\limits_{1}^{\infty} \left|e^{ik(\rho-1)Rn_0'\cdot m'}-1\right| \frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho\,\mathrm{d}\phi \\
&\leq c \int\limits_{\phi_0-\pi}^{\phi_0+\pi}\int\limits_{1}^{1+\epsilon_R} \left|e^{ik(\rho-1)Rn_0'\cdot m'}-1\right| \frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho\,\mathrm{d}\phi \\
&\quad - \frac{2c}{kRm_z}\int\limits_{\phi_0-\pi}^{\phi_0+\pi}\int\limits_{1+\epsilon_R}^{\infty} \partial_\rho\left[e^{-kRm_z\sqrt{\rho^2-1}}\right]\mathrm{d}\rho\,\mathrm{d}\phi \\
&= c \int\limits_{\phi_0-\pi}^{\phi_0+\pi}\int\limits_{1}^{1+\epsilon_R} \left|e^{ik(\rho-1)Rn_0'\cdot m'}-1\right| \frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho\,\mathrm{d}\phi + \frac{4c\pi}{kRm_z}\, e^{-kRm_z\sqrt{(1+\epsilon_R)^2-1}}.
\end{aligned} \tag{B.3.25}$$

Since

$$\sqrt{(1+\epsilon_R)^2-1} = \sqrt{2\epsilon_R+{\epsilon_R}^2} \sim \sqrt{2\epsilon_R} \tag{B.3.26}$$

for $R\to\infty$ and $\sqrt{2C}km_z \geq 1$ it follows that (cf. (B.3.24))

$$e^{-kRm_z\sqrt{(1+\epsilon_R)^2-1}} \sim e^{-kRm_z\sqrt{2\epsilon_R}} = e^{-km_z\sqrt{2C}\log R} = R^{-\sqrt{2C}km_z} = \mathcal{O}\left(\frac{1}{R}\right) \tag{B.3.27}$$

for $R\to\infty$. Hence,

$$\frac{4c\pi}{kRm_z}\, e^{-kRm_z\sqrt{(1+\epsilon_R)^2-1}} = o\left(\frac{1}{R}\right). \tag{B.3.28}$$

On the other hand, with $\rho - 1 \leq \epsilon_R = C\left(\frac{\log R}{R}\right)^2$

$$\begin{aligned}
\left|e^{ik(\rho-1)Rn_0'\cdot m'}-1\right| &= \sqrt{\Big[\cos\big(k(\rho-1)Rn_0'\cdot m'\big)-1\Big]^2 + \sin^2\big(k(\rho-1)Rn_0'\cdot m'\big)} \\
&= \sqrt{2-2\cos\Big(\frac{k}{2}(\rho-1)Rn_0'\cdot m'\Big)} = \sqrt{4\sin^2\Big(\frac{k}{4}(\rho-1)Rn_0'\cdot m'\Big)}
\end{aligned}$$

$$\begin{aligned}
&= 2\,\sin\left(\frac{k}{4}(\rho-1)Rn_0'\cdot m'\right)\\
&\sim C\,|n_0'\cdot m'|\,\frac{k}{2}\,\frac{(\log R)^2}{R},
\end{aligned} \tag{B.3.29}$$

for $R\to\infty$. The remaining integral on the right-hand side of (B.3.25) is examined by using this estimate leading to (cf. (B.3.27))

$$\begin{aligned}
c\int\limits_1^{1+\epsilon_R}\int\limits_{\phi_0-\pi}^{\phi_0+\pi}&\left|e^{ik(\rho-1)Rn_0'\cdot m'}-1\right|\,\mathrm{d}\phi\,\frac{\rho}{\sqrt{\rho^2-1}}\,e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho\\
&\sim c\,C\frac{k}{2}\,\frac{(\log R)^2}{R}\int\limits_{\phi_0-\pi}^{\phi_0+\pi}|n_0'\cdot m'|\,\mathrm{d}\phi\int\limits_1^{1+\epsilon_R}\frac{\rho}{\sqrt{\rho^2-1}}\,e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho\\
&= -c\,C\frac{|m'|}{2}\,\frac{(\log R)^2}{R^2m_z}\int\limits_{\phi_0-\pi}^{\phi_0+\pi}|\cos(\phi-\phi_1)|\,\mathrm{d}\phi\int\limits_1^{1+\epsilon_R}\partial_\rho\left[e^{-kRm_z\sqrt{\rho^2-1}}\right]\,\mathrm{d}\rho\\
&= -2c\,C\frac{|m'|}{2}\,\frac{(\log R)^2}{R^2m_z}\left[e^{-kRm_z\sqrt{(1+\epsilon_R)^2-1}}-1\right]\\
&= o\left(\frac{1}{R}\right)
\end{aligned}$$

for $R\to\infty$. Overall, (cf. (B.3.25) and (B.3.28)) $J_{1.2}=o(1/R)$ and (cf. (B.3.12) and (B.3.23))

$$J_1 = o\left(\frac{1}{R}\right). \tag{B.3.30}$$

B.3.1.2 J_2

The first step to show the asymptotic behaviour of (cf. (B.3.7))

$$J_2=\int\limits_{\phi_0-\pi}^{\phi_0+\pi}\int\limits_1^{\infty}\frac{f_{\ell,j}(\rho n_0',\sqrt{1-\rho^2})-f_{\ell,j}(\nu',0)}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\,e^{ikRn_0'\cdot m'}\left[e^{ik(\rho-1)Rn_0'\cdot m'}-1\right]\frac{\rho}{\sqrt{\rho^2-1}}\,e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho\,\mathrm{d}\phi$$

is to change the order of integration. This is valid according to Fubini's theorem, since the integral exists absolutely (cf. Lemma 3.11). Now it can be shown that the quotient

$$\frac{f_{\ell,j}(\rho n_0',\sqrt{1-\rho^2})-f_{\ell,j}(\nu',0)}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}$$

is absolutely integrable w.r.t. $\phi\in[\phi_0-\pi,\phi_0+\pi]$ for any fixed $\rho\geq 1$. Indeed, since $f_{\ell,j}(\rho n_0',\sqrt{1-\rho^2})$ is finite for any ρ and ϕ, the quotient can at most have a singularity at $(\rho,\phi)=(1,\phi_0)$. On the other hand, for $\rho=1$ fixed, this quotient is at most logarithmically singular. This is easily seen by evaluating the limit $\phi\to\phi_0$ of the quotient at $\rho=1$ multiplied with $1/\log|n_0'-\nu'|$. Applying L'Hôpital's rule, (cf. (B.3.1) and $n_0'=(\cos\phi,\sin\phi)^\top$)

$$\begin{aligned}
\lim_{\phi\to\phi_0}\frac{f_{\ell,j}(n_0',0)-f_{\ell,j}(\nu',0)}{|\phi-\phi_0|\,\log|n_0'-\nu'|}&=\lim_{\phi\to\phi_0}\,\mathrm{sgn}(\phi-\phi_0)\frac{\begin{pmatrix}-\sin\phi\\ \cos\phi\end{pmatrix}\cdot\nabla_{n_0'}f_{\ell,j}(n_0',0)}{\log|n_0'-\nu'|-\cos((\phi-\phi_0)/2)\,\frac{\phi-\phi_0}{2\sin((\phi-\phi_0)/2)}}\\
&=\lim_{\phi\to\phi_0}\,\mathrm{sgn}(\phi-\phi_0)\frac{\begin{pmatrix}-\sin\phi\\ \cos\phi\end{pmatrix}\cdot\nabla_{n_0'}f_{\ell,j}(n_0',0)\,\frac{1}{\log|n_0'-\nu'|}}{1-\cos((\phi-\phi_0)/2)\,\frac{\phi-\phi_0}{2\sin((\phi-\phi_0)/2)}\,\frac{1}{\log|n_0'-\nu'|}},
\end{aligned}$$

which is finite, since the occurring limits $\lim_{\phi\to\phi_0} \nabla_{n_0'} f_{\ell,j}(n_0',0)/\log|n_0'-\nu'|$ (cf. Lemma B.2) and $\lim_{\phi\to\phi_0}(\phi-\phi_0)/\sin((\phi-\phi_0)/2)$ are finite. It follows that (cf.(B.3.4))

$$\left|\frac{f_{\ell,j}(\rho n_0',\sqrt{1-\rho^2})-f_{\ell,j}(\nu',0)}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\right| \le c\,|\log|\rho n_0'-\nu'|| \le c\left|\log\big((\rho-1)^2+(\phi-\phi_0)^2\big)\right|$$

in a neighbourhood of $(\rho,\phi)=(1,\phi_0)$. With this it is easily shown that

$$\left|\frac{f_{\ell,j}(\rho n_0',\sqrt{1-\rho^2})-f_{\ell,j}(\nu',0)}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\right| e^{-\frac{k}{2}Rm_z\sqrt{\rho^2-1}} \le c\left|\log\big((\rho-1)^2+(\phi-\phi_0)^2\big)\right| \tag{B.3.31}$$

for any fixed $\rho\in[1,\infty)$, since $f_{\ell,j}(\rho n_0',\sqrt{1-\rho^2})$ grows at most with a finite polynomial degree (cf. (B.2.1)), while $e^{ikRm_z\sqrt{\rho^2-1}}$ decays exponentially for $\rho\to\infty$. Integral J_2 can now be treated similarly to $J_{1.2}$ (cf. (B.3.25)). Consider (cf. (B.3.7) and (B.3.28))

$$\begin{aligned}
|J_2| &\le c\int_1^{1+\epsilon_R}\int_{\phi_0-\pi}^{\phi_0+\pi}\left|e^{ik(\rho-1)Rn_0'\cdot m'}-1\right|\left|\log\big((\rho-1)^2+(\phi-\phi_0)^2\big)\right|\frac{\rho}{\sqrt{\rho^2-1}}\,e^{-\frac{k}{2}Rm_z\sqrt{\rho^2-1}}\,\mathrm{d}\phi\,\mathrm{d}\rho\\
&\quad-\frac{4c}{kRm_z}\int_{1+\epsilon_R}^{\infty}\int_{\phi_0-\pi}^{\phi_0+\pi}\partial_\rho\left[e^{-\frac{k}{2}Rm_z\sqrt{\rho^2-1}}\right]\mathrm{d}\phi\,\mathrm{d}\rho\\
&=c\int_1^{1+\epsilon_R}\int_{\phi_0-\pi}^{\phi_0+\pi}\left|e^{ik(\rho-1)Rn_0'\cdot m'}-1\right|\left|\log\big((\rho-1)^2+(\phi-\phi_0)^2\big)\right|\frac{\rho}{\sqrt{\rho^2-1}}\,e^{-\frac{k}{2}Rm_z\sqrt{\rho^2-1}}\,\mathrm{d}\phi\,\mathrm{d}\rho+o\left(\frac{1}{R}\right).
\end{aligned}$$

In view of (B.3.29),

$$\begin{aligned}
|J_2| &\le 2c\int_1^{1+\epsilon_R}\int_{\phi_0-\pi}^{\phi_0+\pi}2\sin\Big(\frac{k}{4}(\rho-1)Rn_0'\cdot m'\Big)\,|\log|\phi-\phi_0||\,\frac{\rho}{\sqrt{\rho^2-1}}\,e^{-\frac{k}{2}Rm_z\sqrt{\rho^2-1}}\,\mathrm{d}\phi\,\mathrm{d}\rho+o\left(\frac{1}{R}\right)\\
&\sim c\,\frac{Ck\,(\log R)^2}{2R}\int_{\phi_0-\pi}^{\phi_0+\pi}|\log|\phi-\phi_0|\,n_0'\cdot m'|\,\mathrm{d}\phi\int_1^{1+\epsilon_R}\frac{\rho}{\sqrt{\rho^2-1}}\,e^{-\frac{k}{2}Rm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho+o\left(\frac{1}{R}\right)\\
&=-c\,\frac{2Ck|m'|\,(\log R)^2}{2kR^2m_z}\int_{\phi_0-\pi}^{\phi_0+\pi}|\log|\phi-\phi_0|\,\cos(\phi-\phi_1)|\,\mathrm{d}\phi\int_1^{1+\epsilon_R}\partial_\rho\left[e^{-\frac{k}{2}Rm_z\sqrt{\rho^2-1}}\right]\mathrm{d}\rho+o\left(\frac{1}{R}\right)\\
&=-c\,\frac{Ck|m'|\,(\log R)^2}{2kR^2m_z}\int_{\phi_0-\pi}^{\phi_0+\pi}|\log|\phi-\phi_0|\,\cos(\phi-\phi_1)|\,\mathrm{d}\phi\,\left[e^{-\frac{k}{2}Rm_z\sqrt{(1+\epsilon_R)^2-1}}-1\right]+o\left(\frac{1}{R}\right)\\
&=o\left(\frac{1}{R}\right)
\end{aligned}\tag{B.3.32}$$

for $R\to\infty$.

B.3.1.3 J_3

Recall that (cf. (B.3.8))

$$J_3=\int_{\phi_0-\pi}^{\phi_0+\pi}\int_1^{\infty}\frac{f_{\ell,j}(\rho n_0',\sqrt{1-\rho^2})-f_{\ell,j}(\nu',0)}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\,e^{ikRn_0'\cdot m'}\,\frac{\rho}{\sqrt{\rho^2-1}}\,e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho\,\mathrm{d}\phi.$$

As for J_2 the order of integration can be changed. To get the asymptotic behaviour of J_3, integration by parts w.r.t. ρ is applied , giving

$$\begin{aligned} J_3 = &\frac{1}{kRm_z}\int_{\phi_0-\pi}^{\phi_0+\pi}\frac{f_{\ell,j}(n_0',0)-f_{\ell,j}(\nu',0)}{|\phi-\phi_0|}\,e^{ikRn_0'\cdot m'}\,\mathrm{d}\phi \\ &+\frac{1}{kRm_z}\int_1^\infty\int_{\phi_0-\pi}^{\phi_0+\pi}\partial_\rho\left[\frac{f_{\ell,j}(\rho n_0',\sqrt{1-\rho^2})-f_{\ell,j}(\nu',0)}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\right]e^{ikRn_0'\cdot m'}\,\mathrm{d}\phi\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho, \end{aligned} \quad \text{(B.3.33)}$$

where $(f_{\ell,j}(n_0',0)-f_{\ell,j}(\nu',0))/|\phi-\phi_0|$ is bounded by $c\log|\phi-\phi_0|$ (cf. (B.3.31)). Here, Lemma B.3 proves that

$$\frac{1}{kRm_z}\int_{\phi_0-\pi}^{\phi_0+\pi}\frac{f_{\ell,j}(n_0',0)-f_{\ell,j}(\nu',0)}{|\phi-\phi_0|}\,e^{ikRn_0'\cdot m'}\,\mathrm{d}\phi = o\left(\frac{1}{R}\right). \quad \text{(B.3.34)}$$

For the second integral on the right-hand side of (B.3.33) a closer look at the derivative is necessary. Note that

$$\begin{aligned} \partial_\rho\left[\frac{f_{\ell,j}(\rho n_0',\sqrt{1-\rho^2})-f_{\ell,j}(\nu',0)}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\right] = &\frac{\left(n_0',-\frac{\rho}{\sqrt{1-\rho^2}}\right)^\top\cdot\nabla_{\vec{n}}f_{\ell,j}(\rho n_0',\sqrt{1-\rho^2})}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}} \\ &-\frac{(\rho-1)\left[f_{\ell,j}(\rho n_0',\sqrt{1-\rho^2})-f_{\ell,j}(\nu',0)\right]}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}^{\,3}}, \end{aligned}$$

where $(\rho-1)/\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}$ is finite at the point $(\rho,\phi)^\top=(1,\phi_0)^\top$ and where the quotient $[f_{\ell,j}(\rho n_0',\sqrt{1-\rho^2})-f_{\ell,j}(\nu',0)]/\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}$ (cf. (B.3.31)) is logarithmically singular. Hence, with Lemma B.2,

$$\left|\partial_\rho\left[\frac{f_{\ell,j}(\rho n_0',\sqrt{1-\rho^2})-f_{\ell,j}(\nu',0)}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\right]e^{-\frac{k}{2}Rm_z\sqrt{\rho^2-1}}\right| \le c\,\frac{\rho}{\sqrt{1-\rho^2}}\,\frac{\left|\log\left((\rho-1)^2+(\phi-\phi_0)^2\right)\right|}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}. \quad \text{(B.3.35)}$$

Since

$$\begin{aligned} \int_{\phi_0-\pi}^{\phi_0+\pi}\frac{1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\,\mathrm{d}\phi &= 2\int_{\phi_0}^{\phi_0+\pi}\frac{1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\,\mathrm{d}\phi \\ &= 2\log\left(\pi+\sqrt{(\rho-1)^2+\pi^2}\right)-2\log(\rho-1), \end{aligned} \quad \text{(B.3.36)}$$

it follows that (cf. (B.3.33), (B.3.34) and (B.3.35))

$$\begin{aligned} |J_3| &\le \frac{c}{kRm_z}\int_1^\infty\int_{\phi_0-\pi}^{\phi_0+\pi}\frac{\frac{\rho}{\sqrt{1-\rho^2}}\,\left|\log\left((\rho-1)^2+(\phi-\phi_0)^2\right)\right|}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\,\mathrm{d}\phi\, e^{-\frac{k}{2}Rm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho+o\left(\frac{1}{R}\right) \\ &\le \frac{2c}{kRm_z}\int_1^\infty\frac{\rho\,|\log(\rho-1)|}{\sqrt{1-\rho^2}}\int_{\phi_0}^{\phi_0+\pi}\frac{1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\,\mathrm{d}\phi\, e^{-\frac{k}{2}Rm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho+o\left(\frac{1}{R}\right) \\ &= \frac{2c}{kRm_z}\int_1^\infty\frac{\rho\,|\log(\rho-1)|}{\sqrt{1-\rho^2}}\log\left(\pi+\sqrt{(\rho-1)^2+\pi^2}\right)e^{-\frac{k}{2}Rm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho \\ &\quad -\frac{2c}{kRm_z}\int_1^\infty\frac{\rho}{\sqrt{1-\rho^2}}\left[\log(\rho-1)\right]^2e^{-\frac{k}{2}Rm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho+o\left(\frac{1}{R}\right). \end{aligned}$$

$$\leq \frac{c_2}{kRm_z}\int\limits_1^\infty \frac{\rho}{\sqrt{1-\rho^2}}\big[\log(\rho-1)\big]^2\, e^{-\frac{k}{2}Rm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho + o\left(\frac{1}{R}\right).$$

Substituting $u=\sqrt{\rho^2-1}$ and choosing ϵ_R as in (B.3.24) then leads to

$$\begin{aligned}
|J_3| &\leq \frac{c_2}{kRm_z}\int\limits_0^\infty \left[\log\left(\sqrt{u^2+1}-1\right)\right]^2 e^{-\frac{k}{2}Rm_z u}\,\mathrm{d}u + o\left(\frac{1}{R}\right)\\
&= \frac{c_2}{kRm_z}\int\limits_0^{\sqrt{\epsilon_R}} \left[\log\left(\sqrt{u^2+1}-1\right)\right]^2 e^{-\frac{k}{2}Rm_z u}\,\mathrm{d}u + \frac{c_2}{kRm_z}\int\limits_{\sqrt{\epsilon_R}}^\infty \left[\log\left(\sqrt{u^2+1}-1\right)\right]^2 e^{-\frac{k}{2}Rm_z u}\,\mathrm{d}u\\
&\quad + o\left(\frac{1}{R}\right),
\end{aligned}$$

Note that $c_2\,[\log(\sqrt{u^2+1}-1)]^2 \leq c_3[\log u]^2$ for $u\in[0,\sqrt{\epsilon_R}]$ and $\epsilon_R\leq 1$, and that

$$c_2\,\left[\log(\sqrt{u^2+1}-1)\right]^2 e^{-\frac{k}{4}Rm_z u} \leq c_4\left[\log(\sqrt{\epsilon_R+1}-1)\right]^2 \leq c_5\,[\log R]^2,$$

for $u\in[\sqrt{\epsilon_R},\infty)$. Thus

$$\begin{aligned}
|J_3| &\leq \frac{c_3}{kRm_z}\int\limits_0^{\sqrt{\epsilon_R}} [\log u]^2\,\mathrm{d}u + c_3\frac{[\log R]^2}{kRm_z}\int\limits_{\sqrt{\epsilon_R}}^\infty e^{-\frac{k}{4}Rm_z u}\,\mathrm{d}u\\
&= \frac{c_3}{kRm_z}\sqrt{\epsilon_R}\big(2-2\,|\log\sqrt{\epsilon_R}|+[\log\sqrt{\epsilon_R}]^2\big) + c_3\frac{4[\log R]^2}{(kRm_z)^2}\\
&= o\left(\frac{1}{R}\right).
\end{aligned} \tag{B.3.37}$$

B.3.1.4 J_4

Recall that (cf. (B.3.9))

$$J_4 = f_{\ell,j}(\nu',0)\int\limits_{\phi_0-\pi}^{\phi_0+\pi}\int\limits_1^\infty \frac{\left[e^{ik(\rho-1)Rn_0'\cdot m'}-1\right]}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\, e^{ikRn_0'\cdot m'}\frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho\,\mathrm{d}\phi.$$

As for J_2 the first step to finding the asymptotic behaviour is to switch the order of integration. Thus, after splitting the domains of integration w.r.t. ρ, (cf. (B.3.29) and choose ϵ_R according to (B.3.24))

$$\begin{aligned}
|J_4| &\leq |f_{\ell,j}(\nu',0)|\int\limits_1^{1+\epsilon_R}\int\limits_{\phi_0-\pi}^{\phi_0+\pi}\frac{\left|e^{ik(\rho-1)Rn_0'\cdot m'}-1\right|}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\,\mathrm{d}\phi\,\frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho\\
&\quad + 2\,|f_{\ell,j}(\nu',0)|\int\limits_{1+\epsilon_R}^\infty\int\limits_{\phi_0-\pi}^{\phi_0+\pi}\frac{1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\,\mathrm{d}\phi\,\frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho\\
&\leq |f_{\ell,j}(\nu',0)|\,\frac{C|m'|k}{2}\frac{(\log R)^2}{R}\int\limits_1^{1+\epsilon_R}\int\limits_{\phi_0-\pi}^{\phi_0+\pi}\frac{1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\,\mathrm{d}\phi\,\frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho\\
&\quad + 2\,|f_{\ell,j}(\nu',0)|\int\limits_{1+\epsilon_R}^\infty\int\limits_{\phi_0-\pi}^{\phi_0+\pi}\frac{1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\,\mathrm{d}\phi\,\frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho.
\end{aligned} \tag{B.3.38}$$

Consequently, with (B.3.36) and $u := \sqrt{\rho^2 - 1}$,

$$|J_4| \leq c\frac{(\log R)^2}{R^2} \int_1^{1+\epsilon_R} \partial_\rho \left[e^{-kRm_z\sqrt{\rho^2-1}}\right] \mathrm{d}\rho + c\frac{(\log R)^2}{R} \int_0^{\sqrt{(1+\epsilon_R)^2-1}} \left|\log\left(\sqrt{u^2+1}-1\right)\right| e^{-kRm_z u}\,\mathrm{d}u$$
$$+ c\frac{1}{R}\int_{1+\epsilon_R}^{\infty} \partial_\rho \left[e^{-kRm_z\sqrt{\rho^2-1}}\right] \mathrm{d}\rho + c\frac{1}{R}\int_{1+\epsilon_R}^{\infty} |\log(\rho-1)|\, e^{-\frac{k}{2}Rm_z\sqrt{\rho^2-1}}\partial_\rho\left[e^{-\frac{k}{2}Rm_z\sqrt{\rho^2-1}}\right] \mathrm{d}\rho,$$

where $|\log(\rho-1)|\, e^{-\frac{k}{2}Rm_z\sqrt{\rho^2-1}} \leq c\log(\epsilon_R) \sim \log R$ for $\rho \in [1+\epsilon_R, \infty)$ and $R \to \infty$. Hence (cf. (B.3.26) and (B.3.27))

$$\begin{aligned}|J_4| &\leq c\frac{(\log R)^2}{R} \int_0^{\sqrt{2\epsilon_R}} |\log u|\, e^{-kRm_z u}\,\mathrm{d}u + o\left(\frac{1}{R}\right)\\ &\leq -c\frac{(\log R)^2}{R} \int_0^{\sqrt{2\epsilon_R}} \log u\, e^{-kRm_z u}\,\mathrm{d}u + o\left(\frac{1}{R}\right)\\ &\leq -c\frac{(\log R)^2}{R}\sqrt{2\epsilon_R}\left[\log\left(\sqrt{2\epsilon_R}\right) - 1\right] + o\left(\frac{1}{R}\right),\end{aligned}$$

since $|\log u| = -\log u$ for $u \in [0, \sqrt{2\epsilon_R}]$, and where $2\epsilon_R < 1$ for a sufficiently large R. Therefore,

$$J_4 = o\left(\frac{1}{R}\right). \tag{B.3.39}$$

B.3.1.5 J_5

Recall that (cf. (B.3.10))

$$J_5 = f_{\ell,j}(\nu', 0) \int_{\phi_0-\pi}^{\phi_0+\pi}\int_1^{\infty} \frac{1}{\sqrt{(\rho-1)^2 + (\phi-\phi_0)^2}}\, e^{ikRn_0'\cdot m'} \frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho\,\mathrm{d}\phi.$$

To find the behaviour of J_5, the integral is split into integrals where the asymptotic behaviour can be estimated and one integral which can be evaluated explicitly. This split is realised by replacing the exponent $ikRn_0' \cdot m' = ikr|m'|\cos(\phi - \phi_1)$ by its Taylor expansion w.r.t. ϕ at $\phi = \phi_0$. Here, two cases have to be distinguished. The constant $\sin(\phi_0 - \phi_1)$ could either be zero or non-zero. In both cases the integral will be split in correspondence to the Taylor expansion, i.e. for $\sin(\phi_0 - \phi_1) \neq 0$,

$$J_5 = f_{\ell,j}(\nu', 0)\, J^1_{5.1} + f_{\ell,j}(\nu', 0)\, J^1_{5.2}, \tag{B.3.40}$$

where

$$\begin{aligned}J^1_{5.1} &:= \int_{\phi_0-\pi}^{\phi_0+\pi}\int_1^{\infty} \frac{e^{ikRn_0'\cdot m'} - e^{ikR|m'|\cos(\phi_0-\phi_1)}e^{-ikR|m'|\sin(\phi_0-\phi_1)(\phi-\phi_0)}}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}} \frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho\,\mathrm{d}\phi,\\ J^1_{5.2} &:= \int_{\phi_0-\pi}^{\phi_0+\pi}\int_1^{\infty} \frac{e^{-ikR|m'|\sin(\phi_0-\phi_1)(\phi-\phi_0)}}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\, e^{ikR|m'|\cos(\phi_0-\phi_1)} \frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho\,\mathrm{d}\phi.\end{aligned} \tag{B.3.41}$$

Similarly, for $\sin(\phi_0 - \phi_1) = 0$,

$$J_5 = f_{\ell,j}(\nu', 0)\, J^2_{5.1} + f_{\ell,j}(\nu', 0)\, J^2_{5.2}, \tag{B.3.42}$$

where

$$J^2_{5.1} := \int\limits_{\phi_0-\pi}^{\phi_0+\pi}\int\limits_{1}^{\infty} \frac{e^{ikRn_0'\cdot m'} - e^{ikR|m'|\cos(\phi_0-\phi_1)}e^{-ikR\frac{|m'|}{2}\cos(\phi_0-\phi_1)(\phi-\phi_0)^2}}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\,\frac{\rho}{\sqrt{\rho^2-1}}\,e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho\,\mathrm{d}\phi, \tag{B.3.43}$$

$$J^2_{5.2} := \int\limits_{\phi_0-\pi}^{\phi_0+\pi}\int\limits_{1}^{\infty} \frac{e^{-ikR\frac{|m'|}{2}\cos(\phi_0-\phi_1)(\phi-\phi_0)^2}}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\,e^{ikR|m'|\cos(\phi_0-\phi_1)}\,\frac{\rho}{\sqrt{\rho^2-1}}\,e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho\,\mathrm{d}\phi. \tag{B.3.44}$$

B.3.1.5.1 $J^1_{5.1}$

First note that for $\sin(\phi_0-\phi_1)\neq 0$ the Taylor expansion

$$\begin{aligned} n_0'\cdot m' &= |m'|\cos(\phi-\phi_1) \qquad\qquad (\text{B.3.45})\\ &= |m'|\cos(\phi_0-\phi_1) - |m'|\sin(\phi_0-\phi_1)(\phi-\phi_0) - |m'|\sin(\phi_0-\phi_1)\,\mathcal{R}(\phi-\phi_0)\,(\phi-\phi_0)^2 \end{aligned}$$

is obtained, where

$$\mathcal{R}(\phi-\phi_0) := -\frac{1}{\sin(\phi_0-\phi_1)}\sum_{o=0}^{\infty}\frac{a_o\,(\phi-\phi_0)^o}{(o+2)!}, \qquad a_o := \begin{cases} -\cos(\phi_0-\phi_1) & \text{, if } o\equiv 0 \mod 4\\ \sin(\phi_0-\phi_1) & \text{, if } o\equiv 1 \mod 4\\ \cos(\phi_0-\phi_1) & \text{, if } o\equiv 2 \mod 4\\ -\sin(\phi_0-\phi_1) & \text{, if } o\equiv 3 \mod 4 \end{cases}.$$

It is easily shown that $\mathcal{R}(\psi)$ is a continuously differentiable function for $\psi\in[-\pi,\pi]$. By defining

$$a := -k|m'|\sin(\phi_0-\phi_1), \qquad\qquad b := k|m'|\cos(\phi_0-\phi_1), \tag{B.3.46}$$

this gives

$$e^{ikRn_0'\cdot m'} - e^{ikR|m'|\cos(\phi_0-\phi_1)}e^{-ikR|m'|\sin(\phi_0-\phi_1)(\phi-\phi_0)} = \left[e^{iaR\,\mathcal{R}(\phi-\phi_0)\,(\phi-\phi_0)^2}-1\right]e^{ibR}e^{iaR(\phi-\phi_0)}.$$

Moreover, after substituting $\phi-\phi_0$ by ψ and changing the order of integration

$$J^1_{5.1} = \int\limits_{1}^{\infty}\int\limits_{-\pi}^{\pi}\frac{e^{iaR\,\mathcal{R}(\psi)\,\psi^2}-1}{\sqrt{(\rho-1)^2+\psi^2}}\,e^{iaR\psi}\,\mathrm{d}\psi\,\frac{\rho}{\sqrt{\rho^2-1}}\,e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho\,e^{ibR}.$$

This integral is split further by separating the domain of integration w.r.t. ρ into $[1,1+\epsilon_R]$ and $[1+\epsilon_R,\infty)$. The absolute value of the integral over the second domain of integration gives

$$\begin{aligned} &\left|\int\limits_{1+\epsilon_R}^{\infty}\int\limits_{-\pi}^{\pi}\frac{e^{iaR\,\mathcal{R}(\psi)\,\psi^2}-1}{\sqrt{(\rho-1)^2+\psi^2}}\,e^{iaR\psi}\,\mathrm{d}\psi\,\frac{\rho}{\sqrt{\rho^2-1}}\,e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho\right|\\ &\qquad\le \int\limits_{1+\epsilon_R}^{\infty}\int\limits_{-\pi}^{\pi}\frac{2}{\sqrt{(\rho-1)^2+\psi^2}}\,\mathrm{d}\psi\,\frac{\rho}{\sqrt{\rho^2-1}}\,e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho. \end{aligned}$$

On the other hand, it has already been shown that this upper bound decays faster than $1/R$ as R tends to infinity, when this asymptotic behaviour was proven for J_4. Indeed, for $\psi=\phi-\phi_0$, this bound corresponds to the second term on the right-hand side of (B.3.38), which in turn is a bound for $|J_4|$. Thus,

$$J^1_{5.1} = -\frac{1}{kRm_z}\int\limits_{1}^{1+\epsilon_R}\int\limits_{-\pi}^{\pi}\frac{e^{iaR\,\mathcal{R}(\psi)\,\psi^2}-1}{\sqrt{(\rho-1)^2+\psi^2}}\,e^{iaR\psi}\,\mathrm{d}\psi\,\partial_\rho\left[e^{-kRm_z\sqrt{\rho^2-1}}\right]\,\mathrm{d}\rho\,e^{ibR} + o\left(\frac{1}{R}\right).$$

Next, the integral w.r.t. ρ is integrated by parts, leading to

$$J_{5.1}^{1} = J_{5.1}^{1.1}\, e^{ibR} + J_{5.1}^{1.2}\, e^{ibR} + J_{5.1}^{1.3}\, e^{ibR}, \tag{B.3.47}$$

where

$$\begin{aligned}
J_{5.1}^{1.1} &:= -\frac{1}{kRm_z}\int_{-\pi}^{\pi} \frac{e^{iaR\,\mathcal{R}(\psi)\,\psi^2}-1}{\sqrt{{\epsilon_R}^2+\psi^2}}\, e^{iaR\psi}\,\mathrm{d}\psi\, e^{-kRm_z\sqrt{(1+\epsilon_R)^2-1}} \\
J_{5.1}^{1.2} &:= \frac{1}{kRm_z}\int_{-\pi}^{\pi} \frac{e^{iaR\,\mathcal{R}(\psi)\,\psi^2}-1}{|\psi|}\, e^{iaR\psi}\,\mathrm{d}\psi \\
J_{5.1}^{1.3} &:= \frac{1}{kRm_z}\int_{1}^{1+\epsilon_R}\int_{-\pi}^{\pi} (\rho-1)\frac{e^{iaR\,\mathcal{R}(\psi)\,\psi^2}-1}{\sqrt{(\rho-1)^2+\psi^2}^3}\, e^{iaR\psi}\,\mathrm{d}\psi\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho.
\end{aligned} \tag{B.3.48}$$

Consider (cf. (B.3.27) and (B.3.36))

$$\begin{aligned}
\left|J_{5.1}^{1.1}\right| &\le \frac{2}{kRm_z}\int_{-\pi}^{\pi} \frac{1}{\sqrt{{\epsilon_R}^2+\psi^2}}\,\mathrm{d}\psi\, e^{-kRm_z\sqrt{(1+\epsilon_R)^2-1}} \\
&= \frac{4}{kRm_z}\left[\log\!\left(\pi+\sqrt{{\epsilon_R}^2+\pi^2}\right)-\log\epsilon_R\right] e^{-kRm_z\sqrt{(1+\epsilon_R)^2-1}} \\
&\le \frac{4}{kRm_z}\left[\log\!\left(\pi+\sqrt{{\epsilon_R}^2+\pi^2}\right)+c\,|\log R|\right] R^{-\sqrt{2C}km_z},
\end{aligned} \tag{B.3.49}$$

leading to

$$J_{5.1}^{1.1} = o\left(\frac{1}{R}\right). \tag{B.3.50}$$

For $J_{5.1}^{1.2}$, the first step is to apply integration by parts w.r.t. ψ, which results in

$$\begin{aligned}
J_{5.1}^{1.2} &= \frac{-i}{akR^2m_z}\left[\frac{e^{iaR\,\mathcal{R}(\pi)\,\pi^2}-1}{\pi}\, e^{iaR\pi} - \frac{e^{iaR\,\mathcal{R}(-\pi)\,\pi^2}-1}{\pi}\, e^{-iaR\pi}\right] \\
&\quad + \frac{i}{akR^2m_z}\int_{-\pi}^{\pi}\left\{ia\frac{R\,\mathcal{R}'(\psi)\,\psi^2+2R\,\mathcal{R}(\psi)\,\psi}{|\psi|}\, e^{iaR\,\mathcal{R}(\psi)\,\psi^2} - \operatorname{sgn}\psi\frac{e^{iaR\,\mathcal{R}(\psi)\,\psi^2}-1}{\psi^2}\right\} e^{iaR\psi}\,\mathrm{d}\psi \\
&= -I_1 - I_2 + o\left(\frac{1}{R}\right),
\end{aligned}$$

where

$$\begin{aligned}
I_1 &:= \frac{1}{kRm_z}\int_{-\pi}^{\pi} \operatorname{sgn}\psi\,[\mathcal{R}'(\psi)\,\psi+2\mathcal{R}(\psi)]\; e^{iaR\,\mathcal{R}(\psi)\,\psi^2} e^{iaR\psi}\,\mathrm{d}\psi \\
I_2 &:= \frac{i}{akR^2m_z}\int_{-\pi}^{\pi} \operatorname{sgn}\psi\frac{e^{iaR\,\mathcal{R}(\psi)\,\psi^2}-1}{\psi^2}\, e^{iaR\psi}\,\mathrm{d}\psi.
\end{aligned}$$

Recall that $a\mathcal{R}(\psi)\,\psi^2 + aR\psi = |m'|\cos(\phi-\phi_1) - b$ (cf. (B.3.45)) such that (cf. Lemma B.3)

$$I_1 = \frac{1}{kRm_z}\int_{-\pi}^{\pi} \operatorname{sgn}\psi\,[\mathcal{R}'(\psi)\,\psi+2\mathcal{R}(\psi)]\; e^{ikR|m'|\cos(\psi-\psi_0)}\,\mathrm{d}\psi\, e^{-ibR} = o\left(\frac{1}{R}\right),$$

where $\psi_0 = \phi_0 - \phi_1$. The absolute value of I_2 can be estimated as

$$\begin{aligned}
|I_2| &\leq \frac{1}{|a|kR^2 m_z} \int_{-\pi}^{\pi} \frac{\left|e^{iaR\,\mathcal{R}(\psi)\,\psi^2} - 1\right|}{\psi^2}\,\mathrm{d}\psi \\
&= \frac{1}{|a|kR^{\frac{3}{2}} m_z} \Bigg(\int_{-\pi}^{-R^{-\frac{1}{4}}} + \int_{R^{-\frac{1}{4}}}^{\pi} \Bigg) \frac{\left|e^{iaR\,\mathcal{R}(\psi)\,\psi^2} - 1\right|}{\sqrt{R}\,\psi^2}\,\mathrm{d}\psi + \frac{1}{|a|kRm_z} \int_{-R^{-\frac{1}{4}}}^{R^{-\frac{1}{4}}} \frac{\left|e^{iaR\,\mathcal{R}(\psi)\,\psi^2} - 1\right|}{R\,\psi^2}\,\mathrm{d}\psi \\
&\leq \frac{2}{|a|kR^{\frac{3}{2}} m_z} \Bigg(\int_{-\pi}^{-R^{-\frac{1}{4}}} + \int_{R^{-\frac{1}{4}}}^{\pi} \Bigg) 1\,\mathrm{d}\psi + \frac{c}{|a|kRm_z} \int_{-R^{-\frac{1}{4}}}^{R^{-\frac{1}{4}}} 1\,\mathrm{d}\psi \\
&= \mathcal{O}\left(\frac{1}{R^{\frac{3}{2}}}\right) + \mathcal{O}\left(\frac{1}{R^{\frac{5}{4}}}\right),
\end{aligned}$$

since $1/(\sqrt{R}\psi^2) \leq 1$ for $|\psi| \geq R^{-1/4}$, and since $|e^{iaR\,\mathcal{R}(\psi)\,\psi^2} - 1|/(R\,\psi^2)$ is uniformly bounded by a constant $c < \infty$ for all $\psi \in [-R^{-\frac{1}{4}}, R^{-\frac{1}{4}}]$ and $R > 1$. Indeed, the latter can be shown by evaluating the limit $\psi \to 0$ of the quotient, using L'Hôpital's rule, i.e.

$$\lim_{\psi\to 0} \frac{e^{iaR\,\mathcal{R}(\psi)\,\psi^2} - 1}{R\,\psi^2} = \lim_{\psi\to 0} \frac{ia}{2}\left[\mathcal{R}'(\psi)\,\psi + 2\mathcal{R}(\psi)\right] e^{iaR\,\mathcal{R}(\psi)\,\psi^2} = -\frac{ik|m'|}{2}\cos(\phi_0 - \phi_1) \tag{B.3.51}$$

for any fixed $1 < R < \infty$. Thus, since the continuous continuation of $|e^{iaR\,\mathcal{R}(\psi)\,\psi^2} - 1|/(R\,\psi^2)$ to $\psi = 0$, i.e. the right hand side of (B.3.51), is constant, the function $|e^{iaR\,\mathcal{R}(\psi)\,\psi^2} - 1|/(R\,\psi^2)$ is continuous w.r.t. $\psi \in [-1, 1]$ and $1 \leq R < \infty$. Therefore, there exists a finite $R_0 \geq 1$ such that the function $|e^{iaR\,\mathcal{R}(\psi)\,\psi^2} - 1|/(R\,\psi^2)$ is uniformly bounded by a constant c_{R_0} for all $\psi \in [-1, 1]$ and $R \in [1, R_0]$, while, at the same time, $|e^{iaR\,\mathcal{R}(\psi)\,\psi^2} - 1|/(R\,\psi^2) \leq c_{R_0}$ for all $\psi \in [-1, 1]$ and $R > R_0$. The latter follows, since, for any fixed and positive $|\psi|$ with $|\psi| \leq 1$, the limit of $|e^{iaR\,\mathcal{R}(\psi)\,\psi^2} - 1|/(R\,\psi^2)$ for $R \to \infty$ is zero, the continuous continuation to $\psi = 0$ on right-hand side of (B.3.51) is uniformly bounded w.r.t. $R > 1$ and since $|e^{iaR\,\mathcal{R}(\psi)\,\psi^2} - 1|/(R\,\psi^2)$ is continuous w.r.t. $\psi \in [-1, 1]$ for all $R < \infty$. Hence, $|e^{iaR\,\mathcal{R}(\psi)\,\psi^2} - 1|/(R\,\psi^2)$ is uniformly bounded w.r.t. $\psi \in [-1, 1]$ and $R > 1$. Thus

$$J_{5.1}^{1.2} = o\left(\frac{1}{R}\right). \tag{B.3.52}$$

Similar to $J_{5.1}^{1.2}$, the integral w.r.t. ψ in $J_{5.1}^{1.3}$ is integrated by parts w.r.t. ψ, leading to

$$\begin{aligned}
J_{5.1}^{1.3} = {} & \frac{1}{iakR^2 m_z} \int_{1}^{1+\epsilon_R} \left[(\rho - 1) \frac{e^{iaR\,\mathcal{R}(\psi)\,\psi^2} - 1}{\sqrt{(\rho-1)^2 + \psi^2}^3}\, e^{iaR\psi} \right]_{\psi=-\pi}^{\pi} e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho \\
& - \frac{1}{kR^2 m_z} \int_{1}^{1+\epsilon_R} \int_{-\pi}^{\pi} (\rho - 1) \frac{R\,\mathcal{R}'(\psi)\,\psi^2 + 2R\,\mathcal{R}(\psi)\,\psi}{\sqrt{(\rho-1)^2 + \psi^2}^3} e^{iaR\,\mathcal{R}(\psi)\,\psi^2} e^{iaR\psi}\,\mathrm{d}\psi\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho \\
& + \frac{3}{iakR^2 m_z} \int_{1}^{1+\epsilon_R} \int_{-\pi}^{\pi} (\rho - 1) \frac{\left[e^{iaR\,\mathcal{R}(\psi)\,\psi^2} - 1\right]\psi}{\sqrt{(\rho-1)^2 + \psi^2}^5}\, e^{iaR\psi}\,\mathrm{d}\psi\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho.
\end{aligned}$$

The first integral can easily be estimated as

$$\left| \frac{1}{akR^2 m_z} \int_{1}^{1+\epsilon_R} \left[(\rho - 1) \frac{e^{iaR\,\mathcal{R}(\psi)\,\psi^2} - 1}{\sqrt{(\rho-1)^2 + \psi^2}^3}\, e^{iaR\psi} \right]_{\psi=-\pi}^{\pi} e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho \right| \leq \frac{c}{R^2} \int_{1}^{1+\epsilon_R} 1\,\mathrm{d}\rho = o\left(\frac{1}{R}\right).$$

For the second and third integral it is not hard to prove that (cf. the arguments following (B.3.51))

$$\left| -(\rho-1)\frac{\mathcal{R}'(\psi)\,\psi^2 + 2\,\mathcal{R}(\psi)\,\psi}{\sqrt{(\rho-1)^2+\psi^2}^{3}} + (\rho-1)\frac{\left[e^{iaR\,\mathcal{R}(\psi)\,\psi^2}-1\right]\psi}{R\sqrt{(\rho-1)^2+\psi^2}^{5}} \right| \le \frac{c}{\sqrt{(\rho-1)^2+\psi^2}}.$$

Thus, (cf. (B.3.36))

$$\begin{aligned}
\left|J_{5.1}^{1.3}\right| &\le \frac{c}{R}\int_1^{1+\epsilon_R}\int_{-\pi}^{\pi} \frac{1}{\sqrt{(\rho-1)^2+\psi^2}}\,\mathrm{d}\psi\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho + o\left(\frac{1}{R}\right)\\
&= \frac{2c}{R}\int_1^{1+\epsilon_R}\int_{0}^{\pi} \frac{1}{\sqrt{(\rho-1)^2+\psi^2}}\,\mathrm{d}\psi\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho + o\left(\frac{1}{R}\right)\\
&= \frac{2c}{R}\int_1^{1+\epsilon_R} \left[\log\left(\pi+\sqrt{(\rho-1)^2+\pi^2}\right) - \log(\rho-1)\right]\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho + o\left(\frac{1}{R}\right)\\
&\le \frac{c_2}{R}\int_1^{1+\epsilon_R} 1\,\mathrm{d}\rho + \frac{c_2}{R}\int_1^{1+\epsilon_R} \left|\log(\rho-1)\right|\,\mathrm{d}\rho + o\left(\frac{1}{R}\right)\\
&= \frac{c_2}{R}\,\epsilon_R - \frac{c_2}{R}\int_1^{1+\epsilon_R} \log(\rho-1)\,\mathrm{d}\rho + o\left(\frac{1}{R}\right),
\end{aligned} \tag{B.3.53}$$

since $|\log(\rho-1)| = -\log(\rho-1)$ for all $\rho \in [1, 1+\epsilon_R]$ and R sufficiently large, such that $\epsilon_R = C(\log R/R)^2 < 1$. Hence, substituting $u = \rho - 1$,

$$\begin{aligned}
\left|J_{5.1}^{1.3}\right| &\le -\frac{c_2}{R}\int_0^{\epsilon_R} \log u\,\mathrm{d}u + o\left(\frac{1}{R}\right)\\
&= -c_2\frac{\epsilon_R}{R}\left(\log\epsilon_R - 1\right) + o\left(\frac{1}{R}\right).
\end{aligned} \tag{B.3.54}$$

Consequently, $J_{5.1}^{1.3} = o(1/R)$ and (cf. (B.3.47), (B.3.50) and (B.3.52))

$$J_{5.1}^{1} = o\left(\frac{1}{R}\right). \tag{B.3.55}$$

B.3.1.5.2 $J_{5.1}^{2}$

Similar to $J_{5.1}^{1}$, a Taylor expansion of $n_0' \cdot m'$ is found in the case of $\sin(\phi_0 - \phi_1) = 0$. To be exact,

$$\begin{aligned}
n_0' \cdot m' &= |m'|\cos(\phi - \phi_1)\\
&= |m'|\cos(\phi_0-\phi_1) - \frac{|m'|}{2}\cos(\phi_0-\phi_1)(\phi-\phi_0)^2 + |m'|\cos(\phi_0-\phi_1)\,\mathcal{R}_2\big((\phi-\phi_0)^2\big)\,(\phi-\phi_0)^4,
\end{aligned}$$

where

$$\mathcal{R}_2\big((\phi-\phi_0)^2\big) := \sum_{o=0}^{\infty} \frac{(-1)^o\,(\phi-\phi_0)^{2o}}{(2o+4)!}.$$

As for $\mathcal{R}$ the function $\mathcal{R}_2$ and its derivative are continuous. Using this, substituting $\psi = (\phi - \phi_0)$ and changing the order of integration then gives (cf. (B.3.43) and (B.3.46))

$$J_{5.1}^{2} = \int_1^{\infty}\int_{-\pi}^{\pi} \frac{e^{ibR\,\mathcal{R}_2(\psi^2)\,\psi^4}-1}{\sqrt{(\rho-1)^2+\psi^2}}\, e^{-i\frac{b}{2}R\psi^2}\,\mathrm{d}\psi\, \frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho\, e^{ibR}.$$

As for $J_{5.1}^1$ the domain of integration w.r.t. ρ can be split into $[1, 1+\epsilon_R]$ and $[1+\epsilon_R, \infty)$, where ϵ_R is chosen as in (B.3.24) and where it was already shown that the asymptotic behaviour of (cf. the estimate for the second integral in (B.3.38))

$$\left| \int_{1+\epsilon_R}^{\infty} \int_{-\pi}^{\pi} \frac{e^{ibR\,\mathcal{R}_2(\psi^2)\,\psi^4} - 1}{\sqrt{(\rho-1)^2+\psi^2}}\, e^{-i\frac{b}{2}R\psi^2}\, \mathrm{d}\psi \, \frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}}\, \mathrm{d}\rho \right| \\ \leq \int_{1+\epsilon_R}^{\infty} \int_{-\pi}^{\pi} \frac{2}{\sqrt{(\rho-1)^2+\psi^2}}\, \mathrm{d}\psi \, \frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}}\, \mathrm{d}\rho$$

is $o(1/R)$ (cf. (B.3.38)). The remaining integral in

$$J_{5.1}^2 = -\frac{1}{kRm_z} \int_{1}^{1+\epsilon_R} \int_{-\pi}^{\pi} \frac{e^{ibR\,\mathcal{R}_2(\psi^2)\,\psi^4} - 1}{\sqrt{(\rho-1)^2+\psi^2}}\, e^{-i\frac{b}{2}R\psi^2}\, \mathrm{d}\psi \, \partial_\rho \left[e^{-kRm_z\sqrt{\rho^2-1}} \right] \mathrm{d}\rho \, e^{ibR} + o\left(\frac{1}{R}\right)$$

is once again split into three separate integrals by using integration by parts w.r.t. ρ. Hence,

$$J_{5.1}^2 = J_{5.1}^{2.1}\, e^{ibR} + J_{5.1}^{2.2}\, e^{ibR} + J_{5.1}^{2.3}\, e^{ibR}, \tag{B.3.56}$$

where

$$\begin{aligned} J_{5.1}^{2.1} &:= -\frac{1}{kRm_z} \int_{-\pi}^{\pi} \frac{e^{ibR\,\mathcal{R}_2(\psi^2)\,\psi^4} - 1}{\sqrt{\epsilon_R{}^2+\psi^2}}\, e^{-i\frac{b}{2}R\psi^2}\, \mathrm{d}\psi \, e^{-kRm_z\sqrt{(1+\epsilon_R)^2-1}}, \\ J_{5.1}^{2.2} &:= \frac{1}{kRm_z} \int_{-\pi}^{\pi} \frac{e^{ibR\,\mathcal{R}_2(\psi^2)\,\psi^4} - 1}{|\psi|}\, e^{-i\frac{b}{2}R\psi^2}\, \mathrm{d}\psi, \\ J_{5.1}^{2.3} &:= -\frac{1}{kRm_z} \int_{1}^{1+\epsilon_R} \int_{-\pi}^{\pi} (\rho-1) \frac{e^{ibR\,\mathcal{R}_2(\psi^2)\,\psi^4} - 1}{\sqrt{(\rho-1)^2+\psi^2}^3}\, e^{-i\frac{b}{2}R\psi^2}\, \mathrm{d}\psi \, e^{-kRm_z\sqrt{\rho^2-1}}\, \mathrm{d}\rho. \end{aligned} \tag{B.3.57}$$

It is easily seen that (cf. (B.3.49) and (B.3.50))

$$\left| J_{5.1}^{2.1} \right| \leq \frac{2}{kRm_z} \int_{-\pi}^{\pi} \frac{1}{\sqrt{\epsilon_R{}^2+\psi^2}}\, \mathrm{d}\psi \, e^{-kRm_z\sqrt{(1+\epsilon_R)^2-1}} = o\left(\frac{1}{R}\right). \tag{B.3.58}$$

The approach to show the asymptotic behaviour of the integral $J_{5.1}^{2.2}$ is very similar to that of $J_{5.1}^{1.2}$ (cf. Sect. B.3.1.5.1). The only significant difference is that ψ^2 is substituted by ϕ, such that

$$J_{5.1}^{2.2} = \frac{2}{kRm_z} \int_{0}^{\pi} \frac{e^{ibR\,\mathcal{R}_2(\psi^2)\,\psi^4} - 1}{\psi}\, e^{-i\frac{b}{2}R\psi^2}\, \mathrm{d}\psi = \frac{1}{kRm_z} \int_{0}^{\pi^2} \frac{e^{ibR\,\mathcal{R}_2(\phi)\,\phi^2} - 1}{\phi}\, e^{-i\frac{b}{2}R\phi}\, \mathrm{d}\phi.$$

Since L'Hôpital's rule shows that

$$\lim_{\phi\to 0} \frac{e^{ibR\,\mathcal{R}_2(\phi)\,\phi^2} - 1}{R\phi^2} = ib \lim_{\phi\to 0} \left[\mathcal{R}_2'(\phi)\,\phi + 2\mathcal{R}_2(\phi) \right] e^{ibR\,\mathcal{R}_2(\phi)\,\phi^2} = \frac{ik|m'|}{12} \cos(\phi_0 - \phi_1), \tag{B.3.59}$$

the same arguments as for $J_{5.1}^{1.2}$ can be used to prove that

$$J_{5.1}^{2.2} = o\left(\frac{1}{R}\right). \tag{B.3.60}$$

To show the order of decay for $J_{5.1}^{2.3}$, arguments similar to those used in Section B.3.1.5.1 for $J_{5.1}^{1.3}$ can be used as well. As for $J_{5.1}^{2.2}$, ψ^2 is substituted by ϕ, which leads to

$$\begin{aligned} J_{5.1}^{2.3} &= -\frac{2}{kRm_z} \int_1^{1+\epsilon_R} \int_0^{\pi} (\rho-1) \frac{e^{ibR\,\mathcal{R}_2(\psi^2)\,\psi^4}-1}{\sqrt{(\rho-1)^2+\psi^2}^3}\, e^{-i\frac{b}{2}R\psi^2}\,\mathrm{d}\psi\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho \\ &= -\frac{1}{kRm_z} \int_1^{1+\epsilon_R} \int_0^{\pi^2} (\rho-1) \frac{e^{ibR\,\mathcal{R}_2(\phi)\,\phi^2}-1}{\sqrt{\phi}\sqrt{(\rho-1)^2+\phi}^3}\, e^{-i\frac{b}{2}R\phi}\,\mathrm{d}\phi\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho. \end{aligned}$$

Note that (cf. (B.3.59))

$$\lim_{\phi\to 0}\left|(\rho-1)\frac{e^{ibR\,\mathcal{R}_2(\phi)\,\phi^2}-1}{\sqrt{\phi}\sqrt{(\rho-1)^2+\phi}^3}\right| \le \lim_{\phi\to 0}\frac{\rho-1}{\rho-1}\left|\frac{e^{ibR\,\mathcal{R}_2(\phi)\,\phi^2}-1}{\sqrt{\phi}^3}\right| = 0$$

for any fixed $\rho \in [1, 1+\epsilon_R]$. This can then be used to apply integration by parts w.r.t. ϕ, and the formula

$$\begin{aligned} J_{5.1}^{2.3} = &\frac{2}{ibkR^2m_z} \int_1^{1+\epsilon_R} (\rho-1) \frac{e^{ibR\,\mathcal{R}_2(\pi^2)\,\pi^4}-1}{\pi\sqrt{(\rho-1)^2+\pi^2}^3}\, e^{-i\frac{b}{2}R\pi^2} e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho \\ &- \frac{2}{kRm_z} \int_1^{1+\epsilon_R} \int_0^{\pi^2} (\rho-1) \frac{\mathcal{R}_2'(\phi)\,\phi^2 + 2\mathcal{R}_2(\phi)\,\phi}{\sqrt{\phi}\sqrt{(\rho-1)^2+\phi}^3}\, e^{ibR\,\mathcal{R}_2(\phi)\,\phi^2} e^{-i\frac{b}{2}R\phi}\,\mathrm{d}\phi\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho \\ &+ \frac{1}{ibkR^2m_z} \int_1^{1+\epsilon_R} \int_0^{\pi^2} (\rho-1) \frac{\left[e^{ibR\,\mathcal{R}_2(\phi)\,\phi^2}-1\right]\left[(\rho-1)^2+4\phi\right]}{\sqrt{\phi}^3\sqrt{(\rho-1)^2+\phi}^5}\, e^{-i\frac{b}{2}R\phi}\,\mathrm{d}\phi\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho \end{aligned}$$

is obtained. Furthermore, it is easily shown that

$$\left|(\rho-1)\frac{e^{ibR\,\mathcal{R}_2(\pi^2)\,\pi^4}-1}{\pi\sqrt{(\rho-1)^2+\pi^2}^3}\, e^{-ibR\pi^2} e^{-kRm_z\sqrt{\rho^2-1}}\right| \le c$$

and that

$$\left|(\rho-1)\frac{\mathcal{R}_2'(\phi)\,\phi^2+2\mathcal{R}_2(\phi)\,\phi}{(\rho-1)^2+\phi}\right| \le c, \qquad \left|(\rho-1)\frac{\left[e^{ibR\,\mathcal{R}_2(\phi)\,\phi^2}-1\right]\left[(\rho-1)^2+4\phi\right]}{R\phi\left[(\rho-1)^2+\phi\right]^2}\right| \le c.$$

It follows that, by undoing the substitution $\phi = \psi^2$,

$$\begin{aligned} \left|J_{5.1}^{2.3}\right| &\le \frac{2c}{|b|kR^2m_z} \int_1^{1+\epsilon_R} 1\,\mathrm{d}\rho + \frac{2c}{kRm_z}\left(1+\frac{1}{2|b|}\right) \int_1^{1+\epsilon_R}\int_0^{\pi^2} \frac{1}{\sqrt{\phi}\sqrt{(\rho-1)^2+\phi}}\,\mathrm{d}\phi\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho \\ &= \frac{2c}{kRm_z}\left(1+\frac{1}{2|b|}\right) \int_1^{1+\epsilon_R}\int_0^{\pi} \frac{1}{\sqrt{(\rho-1)^2+\psi^2}}\,\mathrm{d}\psi\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho + o\left(\frac{1}{R}\right). \end{aligned}$$

The previous estimates (B.3.53) and (B.3.54) now show that $J_{5.1}^{2.3} = o(1/R)$ and thus that (cf. (B.3.56), (B.3.58) and (B.3.60))

$$J_{5.1}^{2} = o\left(\frac{1}{R}\right). \tag{B.3.61}$$

B.3.1.5.3 $J^1_{5.2}$

As before, the order of integration can be changed, such that (cf. (B.3.41) and (B.3.46))

$$J^1_{5.2} = \int_1^\infty \int_{\phi_0-\pi}^{\phi_0+\pi} \frac{1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\, e^{iaR(\phi-\phi_0)}\,\mathrm{d}\phi\, \frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho\, e^{ibR}.$$

To determine the asymptotic behaviour it is the goal to obtain an integral in the form of a Fourier transform, such that known formulas can be applied to evaluate that integral explicitly. To this end, the integral is split into

$$J^1_{5.2} = J^{1.1}_{5.2}\, e^{ibR} - J^{1.2}_{5.2}\, e^{ibR} + 2\, J^{1.3}_{5.2}\, e^{ibR}, \tag{B.3.62}$$

where (cf. (B.3.24))

$$J^{1.1}_{5.2} := \int_{1+\epsilon_R}^\infty \int_{\phi_0-\pi}^{\phi_0+\pi} \frac{1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\, e^{iaR(\phi-\phi_0)}\,\mathrm{d}\phi\, \frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho,$$

$$J^{1.2}_{5.2} := \int_1^{1+\epsilon_R} \left(\int_{-\infty}^{\phi_0-\pi} + \int_{\phi_0+\pi}^{\infty} \right) \frac{1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\, e^{iaR(\phi-\phi_0)}\,\mathrm{d}\phi\, \frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho, \tag{B.3.63}$$

$$J^{1.3}_{5.2} := \frac{1}{2} \int_1^{1+\epsilon_R} \int_{\mathbb{R}} \frac{1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\, e^{iaR(\phi-\phi_0)}\,\mathrm{d}\phi\, \frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho. \tag{B.3.64}$$

Applying integration by parts w.r.t. ρ to $J^{1.1}_{5.2}$ leads to

$$\begin{aligned} J^{1.1}_{5.2} &= \frac{1}{kRm_z} \int_{\phi_0-\pi}^{\phi_0+\pi} \frac{1}{\sqrt{{\epsilon_R}^2+(\phi-\phi_0)^2}}\, e^{iaR(\phi-\phi_0)}\,\mathrm{d}\phi\, e^{-kRm_z\sqrt{(1+\epsilon_R)^2-1}} \\ &\quad - \frac{1}{kRm_z} \int_{1+\epsilon_R}^\infty \int_{\phi_0-\pi}^{\phi_0+\pi} \frac{\rho-1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}^3}\, e^{iaR(\phi-\phi_0)}\,\mathrm{d}\phi\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho, \end{aligned} \tag{B.3.65}$$

where (cf. (B.3.27))

$$\begin{aligned} &\frac{1}{kRm_z} \left| \int_{\phi_0-\pi}^{\phi_0+\pi} \frac{1}{\sqrt{{\epsilon_R}^2+(\phi-\phi_0)^2}}\, e^{iaR(\phi-\phi_0)}\,\mathrm{d}\phi\, e^{-kRm_z\sqrt{(1+\epsilon_R)^2-1}} \right| \\ &\quad \le \frac{1}{kRm_z} \int_{\phi_0-\pi}^{\phi_0+\pi} \frac{1}{\sqrt{{\epsilon_R}^2+(\phi-\phi_0)^2}}\,\mathrm{d}\phi\, e^{-kRm_z\sqrt{(1+\epsilon_R)^2-1}} \\ &\quad = \frac{2}{kRm_z} \left[\log\left(\pi + \sqrt{{\epsilon_R}^2+\pi^2}\right) - \log \epsilon_R \right] e^{-kRm_z\sqrt{(1+\epsilon_R)^2-1}} \\ &\quad = o\left(\frac{1}{R}\right). \end{aligned} \tag{B.3.66}$$

On the other hand, (cf. [3, Equ. (58), p. 621])

$$\begin{aligned} &\frac{1}{kRm_z} \left| \int_{1+\epsilon_R}^\infty \int_{\phi_0-\pi}^{\phi_0+\pi} \frac{\rho-1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}^3}\, e^{iaR(\phi-\phi_0)}\,\mathrm{d}\phi\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho \right| \\ &\quad \le \frac{c}{kRm_z} \int_{1+\epsilon_R}^\infty \int_{\phi_0-\pi}^{\phi_0+\pi} \frac{1}{(\rho-1)^2+(\phi-\phi_0)^2}\,\mathrm{d}\phi\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho \end{aligned}$$

$$= \frac{2c}{kRm_z} \int_{1+\epsilon_R}^{\infty} \frac{\arctan\left(\frac{\pi}{\rho-1}\right)}{\rho - 1} e^{-kRm_z\sqrt{\rho^2-1}} \,\mathrm{d}\rho$$
$$\leq \frac{c\,\pi}{kR\epsilon_R m_z} \int_{1+\epsilon_R}^{\infty} e^{-kRm_z\sqrt{\rho^2-1}} \,\mathrm{d}\rho,$$

such that by substituting $u = \sqrt{\rho^2 - 1}$

$$\frac{1}{kRm_z} \left| \int_{1+\epsilon_R}^{\infty} \int_{\phi_0-\pi}^{\phi_0+\pi} \frac{\rho - 1}{\sqrt{(\rho-1)^2 + (\phi-\phi_0)^2}^3} e^{iaR(\phi-\phi_0)} \,\mathrm{d}\phi \, e^{-kRm_z\sqrt{\rho^2-1}} \,\mathrm{d}\rho \right|$$
$$\leq \frac{c\,\pi}{kR\epsilon_R m_z} \int_{\sqrt{(1+\epsilon_R)^2-1}}^{\infty} \frac{u}{\sqrt{u^2+1}} e^{-kRm_z u} \,\mathrm{d}u$$
$$\leq \frac{c_2\,\pi}{kR\epsilon_R m_z} \int_{\sqrt{(1+\epsilon_R)^2-1}}^{\infty} e^{-kRm_z u} \,\mathrm{d}u$$
$$= \frac{c_2\,\pi}{k^2R^2\epsilon_R m_z^2} e^{-kRm_z\sqrt{(1+\epsilon_R)^2-1}}$$
$$= \frac{c_2\,\pi}{k^2C(\log R)^2 m_z^2} e^{-kRm_z\sqrt{(1+\epsilon_R)^2-1}}.$$

Thus (cf. (B.3.27), (B.3.65) and (B.3.66))

$$J_{5.2}^{1.1} = o\left(\frac{1}{R}\right). \tag{B.3.67}$$

For $J_{5.2}^{1.2}$ (cf. (B.3.63)), substituting $\psi = \phi - \phi_0$ and integrating by parts w.r.t. ρ, gives

$$J_{5.2}^{1.2} = -\frac{1}{kRm_z}\left(\int_{-\infty}^{-\pi} + \int_{\pi}^{\infty}\right) \frac{1}{\sqrt{\epsilon_R{}^2 + \psi^2}} e^{iaR\psi} \,\mathrm{d}\psi \, e^{-kRm_z\sqrt{(1+\epsilon_R)^2-1}} + \frac{1}{kRm_z}\left(\int_{-\infty}^{-\pi} + \int_{\pi}^{\infty}\right) \frac{1}{|\psi|} e^{iaR\psi} \,\mathrm{d}\psi$$
$$- \frac{1}{kRm_z} \int_{1}^{1+\epsilon_R} \left(\int_{-\infty}^{-\pi} + \int_{\pi}^{\infty}\right) \frac{\rho-1}{\sqrt{(\rho-1)^2+\psi^2}^3} e^{iaR\psi} \,\mathrm{d}\psi \, e^{-kRm_z\sqrt{\rho^2-1}} \,\mathrm{d}\rho, \tag{B.3.68}$$

where, using integration by parts w.r.t. ψ for any fixed $\epsilon \geq 0$, it can be shown that

$$\frac{1}{R}\left(\int_{-\infty}^{-\pi} + \int_{\pi}^{\infty}\right) \frac{1}{\sqrt{\epsilon^2+\psi^2}} e^{iaR\psi} \,\mathrm{d}\psi = \frac{1}{iaR^2}\left[\frac{1}{\sqrt{\epsilon^2+\pi^2}} e^{-iaR\pi} - \frac{1}{\sqrt{\epsilon^2+\pi^2}} e^{iaR\pi}\right]$$
$$+ \frac{1}{iaR^2}\left(\int_{-\infty}^{-\pi} + \int_{\pi}^{\infty}\right) \frac{\psi}{\sqrt{\epsilon^2+\psi^2}^3} e^{iaR\psi} \,\mathrm{d}\psi$$
$$= o\left(\frac{1}{R}\right). \tag{B.3.69}$$

Furthermore,

$$\frac{1}{kRm_z} \left| \int_{1}^{1+\epsilon_R} \left(\int_{-\infty}^{-\pi} + \int_{\pi}^{\infty}\right) \frac{\rho-1}{\sqrt{(\rho-1)^2+\psi^2}^3} e^{iaR\psi} \,\mathrm{d}\psi \, e^{-kRm_z\sqrt{\rho^2-1}} \,\mathrm{d}\rho \right|$$

$$\begin{aligned}
&\leq \frac{c}{kRm_z} \int_1^{1+\epsilon_R} \left(\int_{-\infty}^{-\pi} + \int_{\pi}^{\infty} \right) \frac{1}{|\psi|^2} \, \mathrm{d}\psi \, \mathrm{d}\rho \\
&\leq \frac{c_2}{kRm_z} \epsilon_R.
\end{aligned}$$

Consequently, (B.3.24), (B.3.68) and (B.3.69) with $\epsilon = 0$ and $\epsilon = \epsilon_R$ imply

$$J_{5.2}^{1.2} = o\left(\frac{1}{R}\right). \tag{B.3.70}$$

Finally, recall that (cf. (B.3.64))

$$J_{5.2}^{1.3} = \frac{1}{2} \int_1^{1+\epsilon_R} \int_{\mathbb{R}} \frac{1}{\sqrt{(\rho-1)^2 + (\phi-\phi_0)^2}} \, e^{iaR(\phi-\phi_0)} \, \mathrm{d}\phi \, \frac{\rho}{\sqrt{\rho^2-1}} \, e^{-kRm_z\sqrt{\rho^2-1}} \, \mathrm{d}\rho.$$

Note that the integral w.r.t. ϕ is very similar to the definition of a Fourier transform (cf. (2.3.7)). To utilise this fact, $\phi - \phi_0$ is substituted by $(\rho-1)\,t$ leading to

$$\int_{\mathbb{R}} \frac{1}{\sqrt{(\rho-1)^2 + (\phi-\phi_0)^2}} \, e^{iaR(\phi-\phi_0)} \, \mathrm{d}\phi = \int_{\mathbb{R}} \frac{1}{\sqrt{1+t^2}} \, e^{iaR(\rho-1)t} \, \mathrm{d}t = 2\, K_0(|a|R(\rho-1)). \tag{B.3.71}$$

Indeed, [32, Eqn. 42, p. 21 for $\nu = 1$] gives that

$$\int_{\mathbb{R}} \frac{1}{\sqrt{1+t^2}^3} \, e^{iyt} \, \mathrm{d}t = 2\, y\, K_1(y), \quad y \geq 0, \qquad \int_{\mathbb{R}} \frac{1}{\sqrt{1+t^2}^3} \, e^{iyt} \, \mathrm{d}t = 2\,(-y)\, K_1(-y), \quad y < 0.$$

On the other hand, using integration by parts, (cf. [1, Eqn. 9.6.28, p. 120])

$$\begin{aligned}
\int_{\mathbb{R}} \frac{1}{\sqrt{1+t^2}} \, e^{iyt} \, \mathrm{d}t &= -\frac{1}{iy} \int_{\mathbb{R}} \partial_t \left[\frac{1}{\sqrt{1+t^2}} \right] e^{iyt} \, \mathrm{d}t = \frac{1}{iy} \int_{\mathbb{R}} \frac{t}{\sqrt{1+t^2}^3} \, e^{iyt} \, \mathrm{d}t \\
&= -\frac{1}{y} \int_{\mathbb{R}} \frac{it}{\sqrt{1+t^2}^3} \, e^{iyt} \, \mathrm{d}t = -\frac{1}{y} \partial_y \left[\int_{\mathbb{R}} \frac{1}{\sqrt{1+t^2}^3} \, e^{iyt} \, \mathrm{d}t \right] \\
&= -\frac{2}{y} \partial_y \left[|y|\, K_1(|y|) \right] = \operatorname{sgn} y \, \frac{2}{y} \partial_{|y|} \left[|y|\, K_1(|y|) \right] = \frac{2}{|y|} \partial_{|y|} \left[|y|\, e^{i\pi}\, K_1(|y|) \right] \\
&= 2\, K_0(|y|).
\end{aligned}$$

Thus

$$J_{5.2}^{1.3} = \int_1^{1+\epsilon_R} K_0(|a|R(\rho-1)) \, \frac{\rho}{\sqrt{\rho^2-1}} \, e^{-kRm_z\sqrt{\rho^2-1}} \, \mathrm{d}\rho.$$

First of all, note that this integral is well defined since $K_0(\rho-1)$ has only a logarithmic singularity at $\rho = 1$ (cf. [1, Eqn. 9.6.53, p. 121]). To separate the singularity from the integrand, the integral is split once more such that

$$\begin{aligned}
J_{5.2}^{1.3} = &-\frac{1}{kRm_z} \int_1^{1+\epsilon_R} \left[K_0(|a|R(\rho-1)) + \log\left(\frac{|a|}{2} R(\rho-1)\right) + \tilde{\gamma} \right] \partial_\rho \left[e^{-kRm_z\sqrt{\rho^2-1}} \right] \mathrm{d}\rho \\
&- \int_1^{1+\epsilon_R} \left[\log\left(\frac{|a|}{2} R(\rho-1)\right) + \tilde{\gamma} \right] \frac{\rho}{\sqrt{\rho^2-1}} \, e^{-kRm_z\sqrt{\rho^2-1}} \, \mathrm{d}\rho.
\end{aligned} \tag{B.3.72}$$

Applying integration by parts to the first integral on the right-hand side, (cf. [1, Eqn. 9.6.27, p. 120])

$$
\begin{aligned}
-\frac{1}{kRm_z}\int_1^{1+\epsilon_R}&\left[K_0(|a|R(\rho-1))+\log\left(\frac{|a|}{2}R(\rho-1)\right)+\tilde{\gamma}\right]\partial_\rho\left[e^{-kRm_z\sqrt{\rho^2-1}}\right]\mathrm{d}\rho\\
&=-\frac{1}{kRm_z}\left[K_0(|a|R\epsilon_R)+\log\left(\frac{|a|}{2}R\epsilon_R\right)+\tilde{\gamma}\right]e^{-kRm_z\sqrt{\epsilon_R{}^2+2\epsilon_R}}\\
&\quad+\frac{1}{kRm_z}\lim_{\rho\searrow 1}\left[K_0(|a|R(\rho-1))+\log\left(\frac{|a|}{2}R(\rho-1)\right)+\tilde{\gamma}\right]\\
&\quad+\frac{|a|}{km_z}\int_1^{1+\epsilon_R}\left[-K_1(|a|R(\rho-1))+\frac{1}{|a|R(\rho-1)}\right]e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho,
\end{aligned}
$$

where (cf. [1, Eqns. 9.6.12 and 9.6.13, p. 119])

$$
\begin{aligned}
K_0(|a|R\epsilon_R)+\log\left(\frac{|a|}{2}R\epsilon_R\right)+\tilde{\gamma}&=\mathcal{O}\left(\log(R\epsilon_R)\,(R\epsilon_R)^2\right)=\mathcal{O}\left(\frac{(\log R)^5}{R^2}\right),\\
\lim_{\rho\searrow 1}\left[K_0(|a|R(\rho-1))+\log\left(\frac{|a|}{2}R(\rho-1)\right)+\tilde{\gamma}\right]&=0.
\end{aligned}
\tag{B.3.73}
$$

Moreover, since $|-K_1(|a|R(\rho-1))+1/(|a|R(\rho-1))|\leq c<\infty$ (cf. [1, Eqns. 9.6.10 and 9.6.11, p. 119]) for $\rho\in[1,1+\epsilon_R]$,

$$
\frac{|a|}{km_z}\left|\int_1^{1+\epsilon_R}\left[-K_1(|a|R(\rho-1))+\frac{1}{|a|R(\rho-1)}\right]e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho\right|\leq\frac{|a|\,c}{km_z}\int_1^{1+\epsilon_R}1\,\mathrm{d}\rho=\mathcal{O}\left(\epsilon_R\right)=o\left(\frac{1}{R}\right)
$$

and (cf. (B.3.72) and (B.3.27))

$$
\begin{aligned}
J_{5.2}^{1.3}&=-\int_1^{1+\epsilon_R}\left[\log\left(\frac{|a|}{2}R(\rho-1)\right)+\tilde{\gamma}\right]\frac{\rho}{\sqrt{\rho^2-1}}\,e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho+o\left(\frac{1}{R}\right)\\
&=\frac{\log\left(\frac{|a|}{2}R\right)+\tilde{\gamma}}{kRm_z}\int_1^{1+\epsilon_R}\partial_\rho\left[e^{-kRm_z\sqrt{\rho^2-1}}\right]\mathrm{d}\rho-\int_1^{1+\epsilon_R}\log(\rho-1)\,\frac{\rho}{\sqrt{\rho^2-1}}\,e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho+o\left(\frac{1}{R}\right)\\
&=-\frac{\log\left(\frac{|a|}{2}R\right)+\tilde{\gamma}}{kRm_z}-\int_1^{1+\epsilon_R}\log(\rho-1)\,\frac{\rho}{\sqrt{\rho^2-1}}\,e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho+o\left(\frac{1}{R}\right).
\end{aligned}
\tag{B.3.74}
$$

Substituting $u=\sqrt{\rho^2-1}$ in the remaining integral on the right-hand side of (B.3.74) and defining $d_R:=\sqrt{\epsilon_R{}^2+2\epsilon_R}$ then gives

$$
\begin{aligned}
\int_1^{1+\epsilon_R}&\log(\rho-1)\,\frac{\rho}{\sqrt{\rho^2-1}}\,e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho\\
&=\int_0^{d_R}\log\left(\sqrt{1+u^2}-1\right)e^{-kRm_zu}\,\mathrm{d}u\\
&=\int_0^{d_R}\left[\log\left(\sqrt{1+u^2}-1\right)-2\log u\right]e^{-kRm_zu}\,\mathrm{d}u+2\int_0^{d_R}\log u\,e^{-kRm_zu}\,\mathrm{d}u \qquad \text{(B.3.75)}\\
&=-\int_0^{d_R}\log\left(1+\sqrt{1+u^2}\right)e^{-kRm_zu}\,\mathrm{d}u+\frac{2}{kRm_z}\int_0^{kRm_zd_R}\log u\,e^{-u}\,\mathrm{d}u-2\frac{\log(kRm_z)}{kRm_z}\int_0^{kRm_zd_R}e^{-u}\,\mathrm{d}u,
\end{aligned}
$$

where $[\sqrt{u^2+1}-1]/u^2 = [1+u^2-1]/[u^2(\sqrt{u^2+1}+1)] = 1/[\sqrt{u^2+1}+1]$ is bounded and greater than some positive constant c. The first of the integrals on the right-hand side can be examined using integration by parts, resulting in (cf. (B.3.27))

$$
\begin{aligned}
&-\int_0^{d_R} \log\left(1+\sqrt{1+u^2}\right) e^{-kRm_z u}\, \mathrm{d}u \\
&\qquad = \frac{\log(2+\epsilon_R)}{kRm_z} e^{-kRm_z d_R} - \frac{\log 2}{kRm_z} - \frac{1}{kRm_z}\int_0^{d_R} \frac{1}{\sqrt{1+u^2}} \frac{u}{1+\sqrt{1+u^2}}\, e^{-kRm_z u}\, \mathrm{d}u \\
&\qquad = -\frac{\log 2}{kRm_z} + o\left(\frac{1}{R}\right).
\end{aligned}
$$

Thus (cf. (B.3.75) and (B.3.27))

$$
\int_1^{1+\epsilon_R} \log(\rho-1)\, \frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}}\, \mathrm{d}\rho = -\frac{\log 2}{kRm_z} - 2\frac{\log(kRm_z)}{kRm_z} + \frac{2}{kRm_z}\int_0^{kRm_z d_R} \log u\, e^{-u}\, \mathrm{d}u + o\left(\frac{1}{R}\right), \tag{B.3.76}
$$

where

$$
\begin{aligned}
\int_0^{kRm_z d_R} \log u\, e^{-u}\, \mathrm{d}u &= \lim_{\epsilon\to 0} \int_\epsilon^{kRm_z d_R} \log u\, e^{-u}\, \mathrm{d}u \\
&= -\log(kRm_z d_R)\, e^{-kRm_z d_R} + \lim_{\epsilon\to 0}\left[\log\epsilon\, e^{-\epsilon} + \int_\epsilon^{kRm_z d_R} \frac{1}{u}\, e^{-u}\, \mathrm{d}u\right] \\
&= -\log(kRm_z d_R)\, e^{-kRm_z d_R} - \int_{kRm_z d_R}^{\infty} \frac{1}{u}\, e^{-u}\, \mathrm{d}u + \lim_{\epsilon\to 0}\left[\log\epsilon\, e^{-\epsilon} + \int_\epsilon^{\infty} \frac{1}{u}\, e^{-u}\, \mathrm{d}u\right] \\
&= -\log(kRm_z d_R)\, e^{-kRm_z d_R} - E_1(kRm_z d_R) + \lim_{\epsilon\to 0}\left[\log\epsilon\, e^{-\epsilon} + E_1(\epsilon)\right]
\end{aligned} \tag{B.3.77}
$$

and E_1 the exponential integral (cf. [1, Eqn. 5.1.1, p. 56]). In view of [1, Eqn. 5.1.11, p. 57] it is easily seen that

$$
\lim_{\epsilon\to 0}\left[\log\epsilon\, e^{-\epsilon} + E_1(\epsilon)\right] = \lim_{\epsilon\to 0}\left[\log\epsilon\, e^{-\epsilon} - \tilde{\gamma} - \log\epsilon\right] = -\tilde{\gamma}.
$$

On the other hand, since $Rd_R = R\sqrt{\epsilon_R}\sqrt{\epsilon_R+2} = \mathcal{O}(\log R)$ as R tends to infinity, (cf. [1, Eqn. 5.1.51, p. 59])

$$
E_1(kRm_z d_R) = E_1\left(kRm_z\sqrt{\epsilon_R{}^2+2\epsilon_R}\right) = \frac{1}{kRm_z\sqrt{\epsilon_R{}^2+2\epsilon_R}}\, e^{-kRm_z\sqrt{\epsilon_R{}^2+2\epsilon_R}}\left[1+\mathcal{O}\left(\frac{1}{R}\right)\right].
$$

Thus (cf. (B.3.27))

$$
\begin{aligned}
&\log(kRm_z d_R)\, e^{-kRm_z d_R} + E_1(kRm_z d_R) \\
&\qquad = \left[\log\left(kRm_z\sqrt{\epsilon_R{}^2+2\epsilon_R}\right) + \frac{1}{kRm_z\sqrt{\epsilon_R{}^2+2\epsilon_R}}\right] e^{-kRm_z\sqrt{\epsilon_R{}^2+2\epsilon_R}} + o\left(\frac{1}{R}\right) \\
&\qquad = \mathcal{O}\left(\frac{\log R}{R}\right)
\end{aligned}
$$

and (cf. (B.3.76) and (B.3.77))

$$
\int_1^{1+\epsilon_R} \log(\rho-1)\, \frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}}\, \mathrm{d}\rho = -\frac{\log 2}{kRm_z} - 2\frac{\log(kRm_z)}{kRm_z} - 2\frac{\tilde{\gamma}}{kRm_z} + o\left(\frac{1}{R}\right). \tag{B.3.78}
$$

At last, (cf. (B.3.74))

$$J_{5.2}^{1.3} = -\frac{\log|a| - 2\log 2 - \log R - 2\log(km_z) - \tilde{\gamma}}{kRm_z} + o\left(\frac{1}{R}\right).$$

and (cf. (B.3.62), (B.3.67) and (B.3.70))

$$J_{5.2}^{1} = -2\frac{\log|a| - 2\log 2 - \log R - 2\log(km_z) - \tilde{\gamma}}{kRm_z}\, e^{ibR} + o\left(\frac{1}{R}\right).$$

Altogether, (cf. (B.3.5), (B.3.30), (B.3.32), (B.3.37), (B.3.39), (B.3.40) and (B.3.55))

$$\mathcal{J}_2 = -2f_{\ell,j}(\nu',0)\,\frac{\log|a| - 2\log 2 - \log R - 2\log(km_z) - \tilde{\gamma}}{ikRm_z}\, e^{ibR} + o\left(\frac{1}{R}\right) \tag{B.3.79}$$

for $\sin(\phi_0 - \phi_1) \neq 0$.

B.3.1.5.4 $J_{5.2}^{2}$

As for $J_{5.2}^{1}$, the order of integration in $J_{5.2}^{2}$ (cf. (B.3.44) with (B.3.46)) is interchanged and $\phi - \phi_0$ is substituted by ψ.

$$J_{5.2}^{2} = \int_1^\infty \int_{-\pi}^{\pi} \frac{1}{\sqrt{(\rho-1)^2 + \psi^2}}\, e^{-i\frac{b}{2}R\psi^2}\,\mathrm{d}\psi\, \frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho\, e^{ibR}.$$

Again, it is the goal to obtain an integral that can be evaluated explicitly. For this purpose, the domains of integration are split, such that

$$J_{5.2}^{2} = J_{5.2}^{2.1}\, e^{ibR} + J_{5.2}^{2.2}\, e^{ibR} + J_{5.2}^{2.3}\, e^{ibR}, \tag{B.3.80}$$

where

$$\begin{aligned}
J_{5.2}^{2.1} &:= \int_{1+\epsilon_R}^{\infty} \int_{-\pi}^{\pi} \frac{1}{\sqrt{(\rho-1)^2 + \psi^2}}\, e^{-i\frac{b}{2}R\psi^2}\,\mathrm{d}\psi\, \frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho,\\
J_{5.2}^{2.2} &:= -\int_{1}^{1+\epsilon_R} \left(\int_{-\infty}^{-\pi} + \int_{\pi}^{\infty}\right) \frac{1}{\sqrt{(\rho-1)^2 + \psi^2}}\, e^{-i\frac{b}{2}R\psi^2}\,\mathrm{d}\psi\, \frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho,\\
J_{5.2}^{2.3} &:= \int_{1}^{1+\epsilon_R} \int_{\mathbb{R}} \frac{1}{\sqrt{(\rho-1)^2 + \psi^2}}\, e^{-i\frac{b}{2}R\psi^2}\,\mathrm{d}\psi\, \frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho.
\end{aligned} \tag{B.3.81}$$

It is easily seen that the same approach that was used to show that $J_{5.2}^{1.1} = o(1/R)$ (cf. Sect. B.3.1.5.3) can be applied here to prove that

$$J_{5.2}^{2.1} = o\left(\frac{1}{R}\right). \tag{B.3.82}$$

Integrating $J_{5.2}^{2.2}$ by parts w.r.t. ρ gives

$$\begin{aligned}
J_{5.2}^{2.2} &= \frac{2}{kRm_z} \int_{1}^{1+\epsilon_R} \int_{\pi}^{\infty} \frac{1}{\sqrt{(\rho-1)^2 + \psi^2}}\, e^{-i\frac{b}{2}R\psi^2}\,\mathrm{d}\psi\, \partial_\rho \left[e^{-kRm_z\sqrt{\rho^2-1}}\right] \mathrm{d}\rho\\
&= \frac{2}{kRm_z} \int_{\pi}^{\infty} \frac{1}{\sqrt{{\epsilon_R}^2 + \psi^2}}\, e^{-i\frac{b}{2}R\psi^2}\,\mathrm{d}\psi\, e^{-kRm_z\sqrt{(1+\epsilon_R)^2-1}} - \frac{2}{kRm_z} \int_{\pi}^{\infty} \frac{1}{|\psi|}\, e^{-i\frac{b}{2}R\psi^2}\,\mathrm{d}\psi\\
&\quad + \frac{2}{kRm_z} \int_{1}^{1+\epsilon_R} \int_{\pi}^{\infty} \frac{\rho-1}{\sqrt{(\rho-1)^2 + \psi^2}^{3}}\, e^{-i\frac{b}{2}R\psi^2}\,\mathrm{d}\psi\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho.
\end{aligned} \tag{B.3.83}$$

Note that by substituting $\phi = \psi^2$ and then integrating by parts w.r.t. ϕ, for any $\epsilon \geq 0$

$$\begin{aligned}
\frac{1}{R}\int_{\pi}^{\infty} \frac{1}{\sqrt{\epsilon^2+\psi^2}}\, e^{-i\frac{b}{2}R\psi^2}\,\mathrm{d}\psi &= \frac{1}{R}\int_{\pi^2}^{\infty} \frac{1}{2\sqrt{\phi}\sqrt{\epsilon^2+\phi}}\, e^{-i\frac{b}{2}R\phi}\,\mathrm{d}\phi \\
&= \frac{1}{ibR^2}\frac{1}{\pi\sqrt{\epsilon^2+\pi^2}}\, e^{-i\frac{b}{2}R\pi^2} - \frac{1}{ibR^2}\int_{\pi^2}^{\infty} \frac{\epsilon^2+2\phi}{2\sqrt{\phi\,(\epsilon^2+\phi)}^{\,3}}\, e^{-i\frac{b}{2}R\phi}\,\mathrm{d}\phi \\
&= o\Big(\frac{1}{R}\Big). \qquad \text{(B.3.84)}
\end{aligned}$$

This can be applied to the first two integrals on the right-hand side of (B.3.83) such that, with $\rho{-}1 \leq \epsilon_R$,

$$\big|J_{5.2}^{2.2}\big| \leq \frac{2}{kRm_z}\epsilon_R \int_1^{1+\epsilon_R}\int_{\pi}^{\infty} \frac{1}{\psi^3}\,\mathrm{d}\psi\,\mathrm{d}\rho + o\Big(\frac{1}{R}\Big) = o\Big(\frac{1}{R}\Big). \qquad \text{(B.3.85)}$$

Recall that (cf. (B.3.81))

$$J_{5.2}^{2.3} = \int_1^{1+\epsilon_R}\int_{\mathbb{R}} \frac{1}{\sqrt{(\rho-1)^2+\psi^2}}\, e^{-i\frac{b}{2}R\psi^2}\,\mathrm{d}\psi\, \frac{\rho}{\sqrt{\rho^2{-}1}}\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho.$$

First, a closer look at the integral w.r.t. ψ is necessary. The aim is to evaluate this integral explicitly using known integral representations of Bessel functions. To do so, ψ^2 is substituted by $(\rho{-}1)^2(\phi{-}1)/2$ for any $\rho \in [1, 1{+}\epsilon_R]$. To be precise, the integral w.r.t. ρ has to be evaluated as an improper integral at the lower bound $\rho = 1$. In this sense, the mentioned substitution results in (cf. [1, Eqn. 9.1.24, p. 104 with Eqn. 6.1.8, p. 76])

$$\begin{aligned}
&\int_{\mathbb{R}} \frac{1}{\sqrt{(\rho-1)^2+\psi^2}}\, e^{-i\frac{b}{2}R\psi^2}\,\mathrm{d}\psi \\
&= 2\int_0^{\infty} \frac{1}{\sqrt{(\rho-1)^2+\psi^2}}\, e^{-i\frac{b}{2}R\psi^2}\,\mathrm{d}\psi \\
&= \int_1^{\infty} \frac{1}{\sqrt{\phi^2-1}}\, e^{-i\frac{b}{4}R(\rho-1)^2\phi}\,\mathrm{d}\phi\, e^{i\frac{b}{4}R(\rho-1)^2} \\
&= \Bigg\{\int_1^{\infty} \frac{\cos\!\big({-\frac{b}{4}}R(\rho{-}1)^2\,\phi\big)}{\sqrt{\phi^2-1}}\,\mathrm{d}\phi + i\int_1^{\infty} \frac{\sin\!\big({-\frac{b}{4}}R(\rho{-}1)^2\,\phi\big)}{\sqrt{\phi^2-1}}\,\mathrm{d}\phi\Bigg\}\, e^{i\frac{b}{4}R(\rho-1)^2} \\
&= \Bigg\{\int_1^{\infty} \frac{\cos\!\Big(\frac{|b|}{4}R(\rho{-}1)^2\,\phi\Big)}{\sqrt{\phi^2-1}}\,\mathrm{d}\phi - i\,\mathrm{sgn}(b)\int_1^{\infty} \frac{\sin\!\Big(\frac{|b|}{4}R(\rho{-}1)^2\,\phi\Big)}{\sqrt{\phi^2-1}}\,\mathrm{d}\phi\Bigg\}\, e^{i\frac{b}{4}R(\rho-1)^2} \\
&= -\Bigg\{\frac{\pi}{2}\,Y_0\Big(\frac{|b|}{4}R(\rho-1)^2\Big) + i\frac{\pi}{2}\,\mathrm{sgn}(b)\,J_0\Big(\frac{|b|}{4}R(\rho-1)^2\Big)\Bigg\}\, e^{i\frac{b}{4}R(\rho-1)^2} \qquad \text{(B.3.86)}
\end{aligned}$$

such that

$$J_{5.2}^{2.3} = -\int_1^{1+\epsilon_R}\Bigg\{\frac{\pi}{2}\,Y_0\Big(\frac{|b|}{4}R(\rho{-}1)^2\Big) + i\frac{\pi}{2}\,\mathrm{sgn}(b)\,J_0\Big(\frac{|b|}{4}R(\rho{-}1)^2\Big)\Bigg\}\, e^{i\frac{b}{4}R(\rho-1)^2}\, \frac{\rho}{\sqrt{\rho^2{-}1}}\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho$$

where J_0 and Y_0 are the zero order Bessel functions of the first and second kind. This integral is once more split by separating the singularity from the integrand. As a result,

$$J_{5.2}^{2.3} = I_3 + I_4, \qquad \text{(B.3.87)}$$

where

$$I_3 := -\int_1^{1+\epsilon_R} \Bigg[\left\{ \frac{\pi}{2} Y_0\Big(\frac{|b|}{4} R(\rho-1)^2\Big) - \log\Big(\frac{|b|}{8} R(\rho-1)^2\Big) + i\frac{\pi}{2}\,\mathrm{sgn}(b)\, J_0\Big(\frac{|b|}{4} R(\rho-1)^2\Big) \right\} e^{i\frac{b}{4}R(\rho-1)^2} \frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}} \Bigg] \,\mathrm{d}\rho,$$

$$I_4 := -\int_1^{1+\epsilon_R} \log\Big(\frac{|b|}{8} R(\rho-1)^2\Big)\, e^{i\frac{b}{4}R(\rho-1)^2} \frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}} \,\mathrm{d}\rho,$$

To derive the asymptotic behaviour of I_3, note that (cf. [1, Eqns. 9.1.12 and 9.1.13, p. 104])

$$\frac{\pi}{2} Y_0(\upsilon) - \log\Big(\frac{\upsilon}{2}\Big) = \tilde{\gamma} + \mathcal{O}(\upsilon), \qquad J_0(\upsilon) = 1 + \mathcal{O}\left(\upsilon^2\right), \qquad \upsilon \in \mathbb{R}_+ \tag{B.3.88}$$

for $\upsilon \to 0$. With this and by integrating I_3 by parts, it can be shown that (cf. [1, Eqn. 9.1.28, p. 105])

$$\begin{aligned} I_3 = &\frac{1}{kRm_z} \left\{ \frac{\pi}{2} Y_0\Big(\frac{|b|}{4} R{\epsilon_R}^2\Big) - \log\Big(\frac{|b|}{8} R{\epsilon_R}^2\Big) + i\frac{\pi}{2}\,\mathrm{sgn}(b)\, J_0\Big(\frac{|b|}{4} R{\epsilon_R}^2\Big) \right\} e^{i\frac{b}{4}R{\epsilon_R}^2} e^{-kRm_z\sqrt{(1+\epsilon_R)^2-1}} \\ &- \frac{\tilde{\gamma} + i\frac{\pi}{2}\,\mathrm{sgn}(b)}{kRm_z} \\ &- \frac{|b|}{4km_z} \int_1^{1+\epsilon_R} \Bigg[(\rho-1) \left\{ -\pi Y_1\Big(\frac{|b|}{4} R(\rho-1)^2\Big) - \frac{1}{\frac{|b|}{8} R(\rho-1)^2} - i\pi\,\mathrm{sgn}(b)\, J_1\Big(\frac{|b|}{4} R(\rho-1)^2\Big) \right\} \\ &\qquad e^{i\frac{b}{4}R(\rho-1)^2} e^{-kRm_z\sqrt{\rho^2-1}} \Bigg] \,\mathrm{d}\rho \\ &- \frac{ib}{2km_z} \int_1^{1+\epsilon_R} \Bigg[(\rho-1) \left\{ \frac{\pi}{2} Y_0\Big(\frac{|b|}{4} R(\rho-1)^2\Big) - \log\Big(\frac{|b|}{8} R(\rho-1)^2\Big) + i\frac{\pi}{2}\,\mathrm{sgn}(b)\, J_0\Big(\frac{|b|}{4} R(\rho-1)^2\Big) \right\} \\ &\qquad e^{i\frac{b}{4}R(\rho-1)^2} e^{-kRm_z\sqrt{\rho^2-1}} \Bigg] \,\mathrm{d}\rho, \end{aligned} \tag{B.3.89}$$

where J_1 and Y_1 are the first order Bessel functions of the first and second kind and (cf. (B.3.27) and (B.3.88))

$$\begin{aligned} &\frac{1}{kRm_z} \left\{ \frac{\pi}{2} Y_0\Big(\frac{|b|}{4} R{\epsilon_R}^2\Big) - \log\Big(\frac{|b|}{8} R{\epsilon_R}^2\Big) + i\frac{\pi}{2}\,\mathrm{sgn}(b)\, J_0\Big(\frac{|b|}{4} R{\epsilon_R}^2\Big) \right\} e^{i\frac{b}{4}R{\epsilon_R}^2} e^{-kRm_z\sqrt{(1+\epsilon_R)^2-1}} \\ &\qquad = \mathcal{O}\Big(\frac{1}{R}\Big) \left[\tilde{\gamma} + \mathcal{O}\left(R{\epsilon_R}^2\right) + 1 + \mathcal{O}\left(R^2{\epsilon_R}^4\right)\right] \mathcal{O}\Big(\frac{1}{R}\Big) = o\Big(\frac{1}{R}\Big), \end{aligned}$$

since $R{\epsilon_R}^2 \to 0$ as $R \to \infty$. Furthermore, [1, Eqns. 9.1.10 and 9.1.11, p. 104 with Eqn. 6.3.2, p. 79] shows that both integrands of the remaining two integrals in (B.3.89) are uniformly bounded by a constant $c > 0$ for $\rho \in [1, 1+\epsilon_R]$, such that (cf. (B.3.24))

$$\left| I_3 + \frac{\tilde{\gamma} + i\frac{\pi}{2}\,\mathrm{sgn}(b)}{kRm_z} \right| \le \frac{3\,|b|\,c}{2km_z} \int_1^{1+\epsilon_R} 1 \,\mathrm{d}\rho = \frac{3\,|b|\,c}{2km_z}\epsilon_R = \frac{3\,|b|\,c}{2km_z} C \frac{(\log R)^2}{R^2} = o\Big(\frac{1}{R}\Big). \tag{B.3.90}$$

At last, it only remains to derive the asymptotic behaviour of I_4. Consider

$$I_4 = -\int_1^{1+\epsilon_R} \log\Big(\frac{|b|}{8} R(\rho-1)^2\Big)\, e^{i\frac{b}{4}R(\rho-1)^2} \frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}} \,\mathrm{d}\rho$$

$$
\begin{aligned}
&= \frac{\log\left(\frac{|b|}{8}R\right)}{kRm_z} \int\limits_1^{1+\epsilon_R} e^{i\frac{b}{4}R(\rho-1)^2} \partial_\rho \left[e^{-kRm_z\sqrt{\rho^2-1}}\right] \mathrm{d}\rho \\
&\quad + \frac{2}{kRm_z} \int\limits_1^{1+\epsilon_R} \log(\rho-1)\, e^{i\frac{b}{4}R(\rho-1)^2} \partial_\rho \left[e^{-kRm_z\sqrt{\rho^2-1}}\right] \mathrm{d}\rho \\
&= \frac{\log\left(\frac{|b|}{8}R\right)}{kRm_z} \int\limits_1^{1+\epsilon_R} e^{i\frac{b}{4}R(\rho-1)^2} \partial_\rho \left[e^{-kRm_z\sqrt{\rho^2-1}}\right] \mathrm{d}\rho \\
&\quad + \frac{2}{kRm_z} \int\limits_1^{1+\epsilon_R} \log(\rho-1) \left[e^{i\frac{b}{4}R(\rho-1)^2} - 1\right] \partial_\rho \left[e^{-kRm_z\sqrt{\rho^2-1}}\right] \mathrm{d}\rho \\
&\quad - 2 \int\limits_1^{1+\epsilon_R} \log(\rho-1) \frac{\rho}{\sqrt{\rho^2-1}}\, e^{-kRm_z\sqrt{\rho^2-1}} \mathrm{d}\rho,
\end{aligned} \tag{B.3.91}
$$

where, by integrating by parts, (cf. (B.3.27))

$$
\begin{aligned}
\frac{1}{R} \int\limits_1^{1+\epsilon_R} e^{i\frac{b}{4}R(\rho-1)^2} \partial_\rho \left[e^{-kRm_z\sqrt{\rho^2-1}}\right] \mathrm{d}\rho &= \frac{1}{R} e^{i\frac{b}{4}R{\epsilon_R}^2} e^{-kRm_z\sqrt{(1+\epsilon_R)^2-1}} - \frac{1}{R} \\
&\quad - i\frac{b}{2} \int\limits_1^{1+\epsilon_R} (\rho-1) e^{i\frac{b}{4}R(\rho-1)^2} e^{-kRm_z\sqrt{\rho^2-1}} \mathrm{d}\rho \\
&= -\frac{1}{R} + \mathcal{O}(\epsilon_R) + o\left(\frac{1}{R}\right) = -\frac{1}{R} + o\left(\frac{1}{R}\right).
\end{aligned}
$$

With this and (B.3.78) the right-hand side of (B.3.91) reduces to

$$
\begin{aligned}
I_4 &= -\frac{\log\left(\frac{|b|}{8}R\right)}{kRm_z} + 2\frac{\log 2}{kRm_z} + 4\frac{\log(kRm_z)}{kRm_z} + 4\frac{\tilde{\gamma}}{kRm_z} \\
&\quad + \frac{2}{kRm_z} \int\limits_1^{1+\epsilon_R} \log(\rho-1) \left[e^{i\frac{b}{4}R(\rho-1)^2} - 1\right] \partial_\rho \left[e^{-kRm_z\sqrt{\rho^2-1}}\right] \mathrm{d}\rho + o\left(\frac{1}{R}\right).
\end{aligned} \tag{B.3.92}
$$

The remaining integral is also examined using integration by parts. Hence,

$$
\begin{aligned}
&\frac{2}{kRm_z} \int\limits_1^{1+\epsilon_R} \log(\rho-1) \left[e^{i\frac{b}{4}R(\rho-1)^2} - 1\right] \partial_\rho \left[e^{-kRm_z\sqrt{\rho^2-1}}\right] \mathrm{d}\rho \\
&\quad = \frac{2}{kRm_z} \log(\epsilon_R) \left[e^{i\frac{b}{4}R{\epsilon_R}^2} - 1\right] e^{-kRm_z\sqrt{(1+\epsilon_R)^2-1}} - \lim_{\rho\searrow 1} \frac{2}{kRm_z} \frac{e^{i\frac{b}{4}R(\rho-1)^2} - 1}{\frac{1}{\log(\rho-1)}} \\
&\quad\quad - \frac{2}{km_z} \int\limits_1^{1+\epsilon_R} \frac{e^{i\frac{b}{4}R(\rho-1)^2} - 1}{R(\rho-1)} e^{-kRm_z\sqrt{\rho^2-1}} \mathrm{d}\rho \\
&\quad\quad - \frac{ib}{km_z} \int\limits_1^{1+\epsilon_R} \log(\rho-1)\,(\rho-1)\, e^{i\frac{b}{4}R(\rho-1)^2} e^{-kRm_z\sqrt{\rho^2-1}} \mathrm{d}\rho,
\end{aligned}
$$

where, using L'Hôpital's rule,

$$
\lim_{\rho\searrow 1} \frac{2}{kRm_z} \frac{e^{i\frac{b}{4}R(\rho-1)^2} - 1}{\frac{1}{\log(\rho-1)}} = \lim_{\rho\searrow 1} \frac{ib}{km_z} (\rho-1)^2 \left(\log(\rho-1)\right)^2 e^{i\frac{b}{4}R(\rho-1)^2} = 0, \tag{B.3.93}
$$

and where it is easily shown that a constant c with $0 < c < \infty$ independent of R and $\rho \in [1, 1+\epsilon_R]$ exists such that

$$\left| \frac{e^{i\frac{b}{4}R(\rho-1)^2} - 1}{R(\rho-1)} \right| < c, \qquad |\log(\rho-1)|\,(\rho-1) \le c \log R\, \epsilon_R. \tag{B.3.94}$$

Together with (B.3.27)

$$\frac{2}{kRm_z} \int\limits_1^{1+\epsilon_R} \log(\rho-1) \left[e^{i\frac{b}{4}R(\rho-1)^2} - 1 \right] \partial_\rho \left[e^{-kRm_z\sqrt{\rho^2-1}} \right] \mathrm{d}\rho$$
$$= \frac{\log R}{R}\,\mathcal{O}\left(\frac{1}{R}\right) + \mathcal{O}\left(\epsilon_R\right) + \log R\,\mathcal{O}\left({\epsilon_R}^2\right) = o\left(\frac{1}{R}\right)$$

and thus, with (B.3.92), it follows that

$$I_4 = -\frac{\log|b| - 5\log 2 - 3\log R - 4\log(km_z) - 4\tilde{\gamma}}{kRm_z} + o\left(\frac{1}{R}\right).$$

Finally, (cf. (B.3.87) and (B.3.90))

$$J_{5.2}^{2.3} = -\frac{\log|b| - 5\log 2 - 3\log R - 4\log(km_z) - 3\tilde{\gamma} + i\frac{\pi}{2}\operatorname{sgn}(b)}{kRm_z} + o\left(\frac{1}{R}\right)$$

and (cf. (B.3.80), (B.3.82) and (B.3.85))

$$\begin{aligned} J_{5.2}^{2} &= -\frac{\log|b| - 5\log 2 - 3\log R - 4\log(km_z) - 3\tilde{\gamma} + i\frac{\pi}{2}\operatorname{sgn} b}{kRm_z}\, e^{ibR} + o\left(\frac{1}{R}\right) \\ &= -\frac{\log|m'| - 5\log 2 - 4\log m_z - 3\big(\tilde{\gamma} + \log(kR)\big) + i\frac{\pi}{2}\cos(\phi_0-\phi_1)}{kRm_z}\, e^{ikR|m'|\cos(\phi_0-\phi_1)} + o\left(\frac{1}{R}\right), \end{aligned}$$

since $b = k|m'|\cos(\phi_0-\phi_1)$, $\operatorname{sgn} b = \operatorname{sgn}(\cos(\phi_0-\phi_1))$ and (cf. beginning of Subsect. B.3.1.5.2)

$$\cos(\phi_0-\phi_1) = \begin{cases} 1 & \text{if } m'/|m'| = \nu' \\ -1 & \text{if } m'/|m'| = -\nu' \end{cases},$$

which gives $\operatorname{sgn} b = \cos(\phi_0-\phi_1)$. Consequently (cf. (B.3.5), (B.3.30), (B.3.32), (B.3.37), (B.3.39), (B.3.42) and (B.3.61))

$$\begin{aligned} \mathcal{J}_2 = -f_{\ell,j}(\nu',0)\, &\frac{\log|m'| - 5\log 2 - 4\log m_z - 3\big[\tilde{\gamma} + \log(kR)\big] + i\frac{\pi}{2}\cos(\phi_0-\phi_1)}{ikRm_z}\, e^{ikR|m'|\cos(\phi_0-\phi_1)} \\ &+ o\left(\frac{1}{R}\right) \end{aligned} \tag{B.3.95}$$

B.3.2 Normal reflection

As mentioned before, the integrals J_2 and J_4 (cf. (B.3.7) and (B.3.9)) reduce to zero if the reflection direction is orthogonal to the x-y-plane, i.e. $m' = (0,0)^\top$, such that $\mathcal{J}_2 = -i(J_1 + J_3 + J_5)$ (cf. (B.3.5)). First consider J_1 (cf. (B.3.6) for $m' = (0,0)^\top$ and thus $m_z = 1$) by applying integration by parts w.r.t. ρ.

$$\begin{aligned} J_1 = &\frac{1}{kR} \int\limits_{\phi_0-\pi}^{\phi_0+\pi} f_{\ell,j}(n_0',0) \left(\frac{1}{|n_0'-\nu'|} - \frac{1}{|\phi-\phi_0|} \right) \mathrm{d}\phi \\ &+ \frac{1}{kR} \int\limits_{\phi_0-\pi}^{\phi_0+\pi} \int\limits_1^{\infty} \partial_\rho \left[f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2}) \left(\frac{1}{|\rho n_0'-\nu'|} - \frac{1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}} \right) \right] e^{-kR\sqrt{\rho^2-1}}\, \mathrm{d}\rho\, \mathrm{d}\phi. \end{aligned} \tag{B.3.96}$$

The existence of these two integrals has already been shown in Subsection B.3.1.1.1 (cf. (B.3.17) and (B.3.22)). Obviously, the first term on the right-hand side does not decay faster than $1/R$. On the other hand, the term will also occur with the opposite sign when examining the asymptotics of the inner integral $\mathcal{J}_1$ for $m' = (0,0)^\top$ (cf. the subsequent (B.4.106)). Thus, the two will cancel when added to get the asymptotic behaviour of $\mathcal{J}$ (cf. (B.2.4)). It remains to examine the asymptotic behaviour of the last term on the right-hand side of (B.3.96). It has already be shown that the occurring derivative can be bounded by the weakly singular term (B.3.22). Thus, since $|\log((\rho-1)^2+(\phi-\phi_0)^2)|\, e^{-k/4R\sqrt{\rho^2-1}} \leq c\,|\log((\phi-\phi_0)^2)|$ for $\rho \geq 1$ and $\phi_0 - \pi \leq \phi \leq \phi_0 + \pi$,

$$
\begin{aligned}
&\frac{1}{kR}\left|\int_{\phi_0-\pi}^{\phi_0+\pi}\int_1^\infty \partial_\rho\left[f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2})\left(\frac{1}{|\rho n_0' - \nu'|} - \frac{1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\right)\right] e^{-kR\sqrt{\rho^2-1}}\,\mathrm{d}\rho\,\mathrm{d}\phi\right| \\
&\leq \frac{c}{kR}\int_{\phi_0-\pi}^{\phi_0+\pi}\int_1^\infty \left\{\frac{\left|\log\big((\rho-1)^2+(\phi-\phi_0)^2\big)\right|\,\rho}{\sqrt{\rho^2-1}} + \frac{1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\right\} e^{-\frac{k}{2}R\sqrt{\rho^2-1}}\,\mathrm{d}\rho\,\mathrm{d}\phi \\
&\leq 2\frac{c}{kR}\int_1^\infty\int_{\phi_0}^{\phi_0+\pi}\left\{\frac{2\,|\log(\phi-\phi_0)|\,\rho}{\sqrt{\rho^2-1}} + \frac{1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\,\mathrm{d}\phi\right\} e^{-\frac{k}{4}R\sqrt{\rho^2-1}}\,\mathrm{d}\rho.
\end{aligned}
$$

Moreover, with (B.3.36) and since $\log(\pi + \sqrt{(\rho-1)^2+\pi^2})\, e^{-k/8R\sqrt{\rho^2-1}} \leq c$,

$$
\begin{aligned}
&\frac{1}{kR}\left|\int_{\phi_0-\pi}^{\phi_0+\pi}\int_1^\infty \partial_\rho\left[f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2})\left(\frac{1}{|\rho n_0' - \nu'|} - \frac{1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\right)\right] e^{-kR\sqrt{\rho^2-1}}\,\mathrm{d}\rho\,\mathrm{d}\phi\right| \\
&\leq 4c\,\frac{2-\pi+\pi\,\log\pi}{kR}\int_1^\infty \frac{\rho}{\sqrt{\rho^2-1}}\, e^{-\frac{k}{4}R\sqrt{\rho^2-1}}\,\mathrm{d}\rho + 2\frac{c}{kR}\int_1^\infty \log\Big(\pi+\sqrt{(\rho-1)^2+\pi^2}\Big)\, e^{-\frac{k}{4}R\sqrt{\rho^2-1}}\,\mathrm{d}\rho \\
&\quad - 2\frac{c}{kR}\int_1^\infty \log(\rho-1)\, e^{-\frac{k}{4}R\sqrt{\rho^2-1}}\,\mathrm{d}\rho \\
&\leq -16c\,\frac{2-\pi+\pi\,\log\pi}{(kR)^2}\int_1^\infty \partial_\rho\left[e^{-\frac{k}{4}R\sqrt{\rho^2-1}}\right]\mathrm{d}\rho + 2\frac{c}{kR}\int_1^\infty e^{-\frac{k}{8}R\sqrt{\rho^2-1}}\,\mathrm{d}\rho \\
&\quad - 2\frac{c}{kR}\int_1^\infty \log(\rho-1)\, e^{-\frac{k}{4}R\sqrt{\rho^2-1}}\,\mathrm{d}\rho \\
&= 2\frac{c}{kR}\int_1^\infty e^{-\frac{k}{8}R\sqrt{\rho^2-1}}\,\mathrm{d}\rho - 2\frac{c}{kR}\int_1^\infty \log(\rho-1)\, e^{-\frac{k}{4}R\sqrt{\rho^2-1}}\,\mathrm{d}\rho + o\left(\frac{1}{R}\right).
\end{aligned}
$$

Substituting $u = \sqrt{\rho^2-1}$ then leads to

$$
\begin{aligned}
&\frac{1}{kR}\left|\int_{\phi_0-\pi}^{\phi_0+\pi}\int_1^\infty \partial_\rho\left[f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2})\left(\frac{1}{|\rho n_0' - \nu'|} - \frac{1}{\sqrt{(\rho-1)^2+(\phi-\phi_0)^2}}\right)\right] e^{-kR\sqrt{\rho^2-1}}\,\mathrm{d}\rho\,\mathrm{d}\phi\right| \\
&\leq 2\frac{c}{kR}\int_0^\infty \frac{u}{\sqrt{u^2+1}}\, e^{-\frac{k}{8}Ru}\,\mathrm{d}u - 2\frac{c}{kR}\int_0^\infty \frac{u\,\log\big(\sqrt{u^2+1}-1\big)}{\sqrt{u^2+1}}\, e^{-\frac{k}{4}Ru}\,\mathrm{d}u \\
&\leq 2\frac{c}{kR}\int_0^\infty e^{-\frac{k}{8}Ru}\,\mathrm{d}u
\end{aligned}
$$

$$= o\left(\frac{1}{R}\right).$$

Consequently, (cf. (B.3.96))

$$J_1 = \frac{1}{kR} \int\limits_{\phi_0-\pi}^{\phi_0+\pi} f_{\ell,j}(n_0', 0) \left(\frac{1}{|n_0' - \nu'|} - \frac{1}{|\phi - \phi_0|} \right) \mathrm{d}\phi + o\left(\frac{1}{R}\right) \tag{B.3.97}$$

for $m' = (0,0)^\top$.

Next, consider J_3. Recall that for $m' = (0,0)^\top$, (cf. (B.3.8))

$$J_3 = \int\limits_1^\infty \int\limits_{-\pi}^{\pi} \frac{f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2}) - f_{\ell,j}(\nu', 0)}{\sqrt{(\rho-1)^2 + \psi^2}} \, \mathrm{d}\psi \, \frac{\rho}{\sqrt{\rho^2-1}} \, e^{-kR\sqrt{\rho^2-1}} \, \mathrm{d}\rho,$$

where $n_0' := n_0'(\psi) := (\cos(\psi + \phi_0), \sin(\psi + \phi_0))^\top$ and $\nu' = \vec{n}_0'(0)$. To obtain the asymptotic behaviour of J_3, integration by parts w.r.t. ρ is applied, such that

$$\begin{aligned} J_3 = {} & \frac{1}{kR} \int\limits_{-\pi}^{\pi} \frac{f_{\ell,j}(n_0', 0) - f_{\ell,j}(\nu', 0)}{|\psi|} \, \mathrm{d}\psi \\ & + \frac{1}{kR} \int\limits_1^\infty \int\limits_{-\pi}^{\pi} \partial_\rho \left[\frac{f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2}) - f_{\ell,j}(\nu', 0)}{\sqrt{(\rho-1)^2 + \psi^2}} \right] \mathrm{d}\psi \, e^{-kR\sqrt{\rho^2-1}} \, \mathrm{d}\rho, \end{aligned} \tag{B.3.98}$$

where (cf. (B.3.31))

$$\left| \frac{f_{\ell,j}(n_0', 0) - f_{\ell,j}(\nu', 0)}{|\psi|} \right| \le c \log |\psi|.$$

This shows that the first integral on the right-hand side of (B.3.98) is well defined. Note that the second integral on the right-hand side is the same as the second integral on the right-hand side of (B.3.33), except that now $m' = (0,0)^\top$ and $\phi - \phi_0$ was substituted by ψ. Nonetheless, the same estimates can be applied to show that the integral decays faster than $1/R$ as R tends to infinity. Altogether, undoing the substitution $\psi = \phi - \phi_0$, (cf. (B.3.98))

$$J_3 = \frac{1}{kR} \int\limits_{\phi_0-\pi}^{\phi_0+\pi} \frac{f_{\ell,j}(n_0', 0) - f_{\ell,j}(\nu', 0)}{|\phi - \phi_0|} \, \mathrm{d}\phi + o\left(\frac{1}{R}\right). \tag{B.3.99}$$

Finally, it remains to examine J_5 (cf. (B.3.10)). To obtain the asymptotic behaviour of (cf. (B.3.10))

$$J_5 = 2 f_{\ell,j}(\nu', 0) \int\limits_1^\infty \int\limits_0^\pi \frac{1}{\sqrt{(\rho-1)^2 + \psi^2}} \, \mathrm{d}\psi \, \frac{\rho}{\sqrt{\rho^2-1}} \, e^{-kR\sqrt{\rho^2-1}} \, \mathrm{d}\rho,$$

the integral w.r.t. ψ is evaluated explicitly (cf. (B.3.36)), giving

$$\begin{aligned} J_5 &= 2 f_{\ell,j}(\nu', 0) \int\limits_1^\infty \int\limits_0^\pi \frac{1}{\sqrt{(\rho-1)^2 + \psi^2}} \, \mathrm{d}\psi \, \frac{\rho}{\sqrt{\rho^2-1}} \, e^{-kR\sqrt{\rho^2-1}} \, \mathrm{d}\rho \\ &= 2 f_{\ell,j}(\nu', 0) \int\limits_1^\infty \log\Big(\pi + \sqrt{(\rho-1)^2 + \pi^2}\Big) \, \frac{\rho}{\sqrt{\rho^2-1}} \, e^{-kR\sqrt{\rho^2-1}} \, \mathrm{d}\rho \\ &\quad - 2 f_{\ell,j}(\nu', 0) \int\limits_1^\infty \log(\rho - 1) \, \frac{\rho}{\sqrt{\rho^2-1}} \, e^{-kR\sqrt{\rho^2-1}} \, \mathrm{d}\rho. \end{aligned} \tag{B.3.100}$$

The first of the two integrals on the right-hand side of (B.3.100) can be examined, by applying integration by parts, which leads to

$$
\begin{aligned}
&\int_1^\infty \log\Big(\pi+\sqrt{(\rho-1)^2+\pi^2}\Big)\,\frac{\rho}{\sqrt{\rho^2-1}}\,e^{-kR\sqrt{\rho^2-1}}\,\mathrm{d}\rho\\
&\qquad= -\frac{1}{kR}\int_1^\infty \log\Big(\pi+\sqrt{(\rho-1)^2+\pi^2}\Big)\,\partial_\rho\left[e^{-kR\sqrt{\rho^2-1}}\right]\,\mathrm{d}\rho\\
&\qquad= \frac{\log(2\pi)}{kR}+\frac{1}{kR}\int_1^\infty \frac{\frac{\rho-1}{\sqrt{(\rho-1)^2+\pi^2}}}{\pi+\sqrt{(\rho-1)^2+\pi^2}}\,e^{-kR\sqrt{\rho^2-1}}\,\mathrm{d}\rho,
\end{aligned}
\tag{B.3.101}
$$

where, substituting $u=\sqrt{\rho^2-1}$,

$$
\begin{aligned}
\frac{1}{R}\left|\int_1^\infty \frac{\frac{\rho-1}{\sqrt{(\rho-1)^2+\pi^2}}}{\pi+\sqrt{(\rho-1)^2+\pi^2}}\,e^{-kR\sqrt{\rho^2-1}}\,\mathrm{d}\rho\right| &\le \frac{c}{R}\int_1^\infty e^{-\frac{k}{2}R\sqrt{\rho^2-1}}\,\mathrm{d}\rho\\
&= \frac{c}{R}\int_0^\infty \frac{u}{\sqrt{u^2+1}}\,e^{-\frac{k}{2}Ru}\,\mathrm{d}u\\
&\le \frac{c_2}{R}\int_0^\infty e^{-\frac{k}{2}Ru}\,\mathrm{d}u\\
&= \frac{2c}{kR^2}.
\end{aligned}
$$

Hence, (cf. (B.3.100) and (B.3.101))

$$
J_5 = 2f_{\ell,j}(\nu',0)\,\frac{\log(2\pi)}{kR} - 2f_{\ell,j}(\nu',0)\int_1^\infty \log(\rho-1)\,\frac{\rho}{\sqrt{\rho^2-1}}\,e^{-kR\sqrt{\rho^2-1}}\,\mathrm{d}\rho + o\left(\frac{1}{R}\right).
$$

Using (B.3.24) and (B.3.78), this can further be transformed to

$$
\begin{aligned}
J_5 &= 2f_{\ell,j}(\nu',0)\,\frac{\log(2\pi)}{kR} - 2f_{\ell,j}(\nu',0)\int_1^{1+\epsilon_R} \log(\rho-1)\,\frac{\rho}{\sqrt{\rho^2-1}}\,e^{-kR\sqrt{\rho^2-1}}\,\mathrm{d}\rho \qquad \text{(B.3.102)}\\
&\quad - 2f_{\ell,j}(\nu',0)\int_{1+\epsilon_R}^\infty \frac{\log(\rho-1)\,\rho}{\sqrt{\rho^2-1}}\,e^{-kR\sqrt{\rho^2-1}}\,\mathrm{d}\rho + o\left(\frac{1}{R}\right)\\
&= 2f_{\ell,j}(\nu',0)\left\{\frac{\log(2\pi)}{kR}+\frac{\log 2}{kR}+2\frac{\log(kR)}{kR}+2\frac{\tilde\gamma}{kR}\right\}\\
&\quad - 2f_{\ell,j}(\nu',0)\int_{1+\epsilon_R}^\infty \log(\rho-1)\,\frac{\rho}{\sqrt{\rho^2-1}}\,e^{-kR\sqrt{\rho^2-1}}\,\mathrm{d}\rho + o\left(\frac{1}{R}\right). \qquad \text{(B.3.103)}
\end{aligned}
$$

The remaining integral can be estimated as (cf. (B.3.27))

$$
\begin{aligned}
\left|\int_{1+\epsilon_R}^\infty \log(\rho-1)\,\frac{\rho}{\sqrt{\rho^2-1}}\,e^{-kR\sqrt{\rho^2-1}}\,\mathrm{d}\rho\right| &\le c\log\epsilon_R\int_{1+\epsilon_R}^\infty \frac{\rho}{\sqrt{\rho^2-1}}\,e^{-\frac{k}{2}R\sqrt{\rho^2-1}}\,\mathrm{d}\rho\\
&= \frac{c\log\epsilon_R}{kR}e^{-\frac{k}{2}R\sqrt{(1+\epsilon_R)^2-1}} = o\left(\frac{1}{R}\right),
\end{aligned}
$$

since, for $R \geq 1$, $|\log(\rho-1)|\, e^{-k/2R\sqrt{\rho^2-1}} \leq c \log \epsilon_R$ for all ρ in the interval $[1+\epsilon_R, \infty)$. At last, (cf. (B.3.103))

$$J_5 = 2 f_{\ell,j}(\nu', 0) \left\{ \frac{\log(2\pi)}{kR} + \frac{\log 2 + 2\log(kR)}{kR} + 2\frac{\tilde{\gamma}}{kR} \right\} + o\left(\frac{1}{R}\right)$$

and for $m' = (0,0)^\top$ (cf. (B.3.5), (B.3.97) and (B.3.99))

$$\begin{aligned} \mathcal{J}_2 = {} & 2 f_{\ell,j}(\nu', 0) \frac{\log(2\pi) + \log 2 + 2\log(kR) + 2\tilde{\gamma}}{ikR} \\ & + \frac{1}{ikR} \int_{\phi_0-\pi}^{\phi_0+\pi} f_{\ell,j}(n_0', 0) \left(\frac{1}{|n_0' - \nu'|} + \frac{1}{|\phi - \phi_0|} \right) \mathrm{d}\phi + \frac{1}{ikR} \int_{\phi_0-\pi}^{\phi_0+\pi} \frac{f_{\ell,j}(n_0', 0) - f_{\ell,j}(\nu', 0)}{|\phi - \phi_0|} \mathrm{d}\phi + o\left(\frac{1}{R}\right). \end{aligned} \tag{B.3.104}$$

B.4 Integrating over plane-wave modes

Similar to $\mathcal{J}_2$ it is the goal to split the integral $\mathcal{J}_1$ into separate parts for which the asymptotic behaviour can be estimated. At the end many integrals will be of order $o(1/R)$, and one integral will remain that can be evaluated explicitly, such that known asymptotic expansions can be used to prove the asymptotic behaviour proposed in Theorem B.1. Again, it is also necessary to distinguish between the cases that the reflection direction is orthogonal (normal) or oblique to the x-y-plane. As before, the orthogonal case is considered last (cf. Sect. B.4.4).

B.4.1 Oblique reflection

Recall that (cf. (B.2.5))

$$\mathcal{J}_1 = \int_{\phi_0-\pi}^{\phi_0+\pi} \int_0^1 \frac{f_{\ell,j}(\rho n_0'(\phi), \sqrt{1-\rho^2})}{|\rho n_0'(\phi) - \nu'|} e^{ik\rho R n_0'(\phi)\cdot m'} \frac{\rho}{\sqrt{1-\rho^2}} e^{ikRm_z\sqrt{1-\rho^2}} \mathrm{d}\rho\, \mathrm{d}\phi, \tag{B.4.1}$$

where $\nu' = n_0'(\phi_0)$ and $|\nu'| = 1$. Since the singularity lies at the boundary of the domain of integration, the latter can be split into an inner part, where the integrand is non-singular and a narrow outer annulus that includes the singularity. The width of the outer part is to be defined in such a way that it excludes m'. The splitting of the domain is accomplished by introducing a monotonic cut-off function $\chi(n') \in C^\infty(B_2(1))$, defined such that $m' \notin \operatorname{supp}\chi$ with $\chi(n') \equiv 1$ for all n' close to and on the unit circle. Since $m_z > 0$ and $\|\vec{m}\| = 1$ it can always be assured that the support of χ is non-empty. Later on, as the need arises, the cut-off function will be specified further. With this,

$$\mathcal{J}_1 = \tilde{J}_1 + \tilde{J}_2, \tag{B.4.2}$$

where

$$\begin{aligned} \tilde{J}_1 &:= \int_{\phi_0-\pi}^{\phi_0+\pi} \int_0^1 \bar{\chi}\big(\rho n_0'(\phi)\big) \frac{f_{\ell,j}(\rho n_0'(\phi), \sqrt{1-\rho^2})}{|\rho n_0'(\phi) - \nu'|} e^{ik\rho R n_0'(\phi)\cdot m'} \frac{\rho}{\sqrt{1-\rho^2}} e^{ikRm_z\sqrt{1-\rho^2}} \mathrm{d}\rho\, \mathrm{d}\phi, \\ \tilde{J}_2 &:= \int_{\phi_0-\pi}^{\phi_0+\pi} \int_0^1 \chi\big(\rho n_0'(\phi)\big) \frac{f_{\ell,j}(\rho n_0'(\phi), \sqrt{1-\rho^2})}{|\rho n_0'(\phi) - \nu'|} e^{ik\rho R n_0'(\phi)\cdot m'} \frac{\rho}{\sqrt{1-\rho^2}} e^{ikRm_z\sqrt{1-\rho^2}} \mathrm{d}\rho\, \mathrm{d}\phi, \end{aligned} \tag{B.4.3}$$

where $\bar{\chi}(\rho n_0'(\phi)) := 1 - \chi(\rho n_0'(\phi))$.

To obtain the asymptotic behaviour of $\tilde{J}_1$, the same substitution into spherical coordinates $(\psi, \phi)^\top$ w.r.t. $\vec{m}$, that was introduced at the beginning of Section 4.2.3 (cf. (4.2.22)), is used. Following these transformations after undoing the transformation to polar coordinates,

$$\tilde{J}_1 := \int_{\phi_0-\pi}^{\phi_0+\pi} \int_{\cos\theta(\phi)}^1 \bar{\chi}\big(n'(\psi,\phi)\big) \frac{f_{\ell,j}\Big(n'(\psi,\phi), \sqrt{1 - \left|n'(\psi,\phi)\right|^2}\Big)}{|n'(\psi,\phi) - \nu'|} e^{ikR\psi} \mathrm{d}\psi\, \mathrm{d}\phi, \tag{B.4.4}$$

where $\theta(\phi)$ is defined as the polar angle at which $|n'(\cos\theta(\phi),\phi)| = 1$. Note that $\bar{\chi}(m') = 1-\chi(m') = 1$. The integral can now be integrated by parts w.r.t. ψ, leading to

$$\begin{aligned}\tilde{J}_1 = &\frac{1}{ikR}\int\limits_{\phi_0-\pi}^{\phi_0+\pi} \bar{\chi}\big(n'(1,\phi)\big)\frac{f_{\ell,j}\Big(n'(1,\phi),\sqrt{1-n'(1,\phi)^2}\Big)}{|n'(1,\phi)-\nu'|}\,e^{ikR}\,\mathrm{d}\phi\\
&-\frac{1}{ikR}\int\limits_{\phi_0-\pi}^{\phi_0+\pi} \bar{\chi}\big(n'(\cos\theta(\phi),\phi)\big)\frac{f_{\ell,j}\Big(n'(\cos\theta(\phi),\phi),0\Big)}{|n'(\cos\theta(\phi),\phi)-\nu'|}\,e^{ikR\cos\theta(\phi)}\,\mathrm{d}\phi\\
&-\frac{1}{ikR}\int\limits_{\phi_0-\pi}^{\phi_0+\pi}\int\limits_{\cos\theta(\phi)}^{1} \partial_\psi\left[\bar{\chi}\big(n'(\psi,\phi)\big)\frac{f_{\ell,j}\Big(n'(\psi,\phi),\sqrt{1-n'(\psi,\phi)^2}\Big)}{|n'(\psi,\phi)-\nu'|}\right]e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi.\end{aligned}$$

Since $n'(1,\phi) = m'$ (cf.(4.2.22)) is independent of ϕ, the first integral on the right-hand side can be evaluated explicitly. Moreover, with $\bar{\chi}(n'(\cos\theta(\phi),\phi)) \equiv 0$, the second integral is equal to zero. For the last integral on the right-hand side, the Riemann-Lebesgue lemma can be used to show that the integral tends to zero as R tends to infinity. Indeed, the cut-off function $\bar{\chi}$ and its derivative ensure that all possible singularities at $n' = \nu'$ are removed and only weak singularities $1/\sqrt{1-\psi^2}$ remain, which shows that the integral exists absolutely. Altogether,

$$\tilde{J}_1 = \frac{2\pi}{ikR}\frac{f_{\ell,j}(m',m_z)}{|m'-\nu'|}\,e^{ikR} + o\left(\frac{1}{R}\right), \tag{B.4.5}$$

where $m' \neq \nu'$, since $|\nu'| = 1$ and $|m'| < 1$.

B.4.2 Singular integral part for oblique reflection with singularity in same direction

In this section the asymptotic behaviour of $\tilde{J}_2$ (cf. (B.4.3)) in the cases that $m'/|m'| = \nu'$, which is equivalent to $\phi_0 = 0$, will be determined. This is necessary, since the nature of the substitution to the spherical coordinate system w.r.t. $\vec{m}$ from the previous subsection, changes the behaviour of the singularity in the specific case that the two vectors m' and ν' have the same direction. All the other cases will be considered in the following Subsection B.4.3.

Transforming $\tilde{J}_2$ to the spherical coordinate system $(\psi,\phi)^\top$ w.r.t. $\vec{m}$, that was introduced at the beginning of Section 4.2.3 (cf. (4.2.22) and (4.2.23)),

$$\tilde{J}_2 = \int\limits_{0}^{2\pi}\int\limits_{\cos\theta(\phi)}^{1} \chi(n'(\psi,\phi))\frac{f_{\ell,j}\big(n'(\psi,\phi),n_z^r(\psi,\phi)\big)}{|n'(\psi,\phi)-\nu'|}\,e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi. \tag{B.4.6}$$

For this section only, it will be assumed that the cut-off function is dependent only on ψ such that $\chi(n'(\psi,\phi)) = \chi(\psi) \in C_0^\infty(\mathbb{R})$ with $\chi(1) = 0$, $\operatorname{supp}\chi \subset [-\sin\alpha, 1)$ and $\chi(\psi) \equiv 1$ for all $\psi \in [-\sin\alpha,\sin\alpha]$. These restrictions ensure that the assumptions made on $\chi(n')$ at the beginning of Section B.4.1 are satisfied, since it can be shown that $[-\sin\alpha,\sin\alpha]$ is the range of $\cos\theta(\phi)$, while $n'(1,\phi) = m'$.

First note, that for $\nu' = n'(\psi_0,\phi_0)$ it is easily seen that $\psi_0 := \cos\theta(\phi_0) = \sin\alpha$ for $\phi_0 = 0$ (cf. (4.2.28)). To show the asymptotic order of $\tilde{J}_2$, it is necessary to change the order of integration to apply the Riemann-Lebesgue lemma to the integral w.r.t. ψ. Special care has to be given to the lower bound of the integral w.r.t. ψ, which is depending on ϕ. Recall that (cf. (4.2.28) and Figure B.2)

$$\psi(\phi) := \cos\theta(\phi) = \frac{\tan\alpha\cos\phi}{\sqrt{1+\tan^2\alpha\cos^2\phi}},$$

which is finite for any $\phi \in [0,2\pi]$, as well as continuous and strictly monotonically decreasing for all $\phi \in [0,\pi]$ and $\alpha > 0$ ($m' \neq (0,0)^\top$). Consequently, $\psi(\phi)$ is a bijective mapping for all $\phi \in [0,\pi]$ and

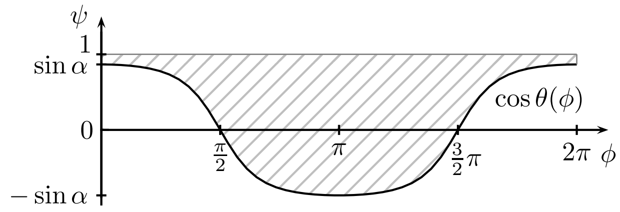


Figure B.2: Integration boundary $\cos\theta(\phi)$ for $\alpha = \frac{\pi}{3}$ and the corresponding area of integration of $\tilde{J}_2$

ψ in the range of $\psi(\phi)$, which can be shown is $[-\sin\alpha, \sin\alpha]$. Thus, a corresponding inverse function $\phi(\psi)$ can be found. Indeed,

$$\phi(\psi) = \arccos\left(\frac{\cot\alpha}{\tan(\arccos\psi)}\right) = \arccos\left(\cot\alpha\,\frac{\psi}{\sqrt{1-\psi^2}}\right). \tag{B.4.7}$$

Using the implicit definition of $\psi(\phi)$ (cf. (4.2.26)), it is not hard to show that $\psi(2\pi-\phi) = \psi(\phi)$, which mirrors the properties of $\psi(\phi)$ onto all $\phi \in [\pi, 2\pi]$. It follows that changing the order of integration leads to

$$\begin{aligned}\tilde{J}_2 = &\int_{-\sin\alpha}^{\sin\alpha} \chi(\psi) \int_{\phi(\psi)}^{2\pi-\phi(\psi)} \frac{f_{\ell,j}\big(n'(\psi,\phi), n_z^r(\psi,\phi)\big)}{|n'(\psi,\phi)-\nu'|}\,\mathrm{d}\phi\, e^{ikR\psi}\,\mathrm{d}\psi \\ &+ \int_{\sin\alpha}^{1} \chi(\psi) \int_{0}^{2\pi} \frac{f_{\ell,j}\big(n'(\psi,\phi), n_z^r(\psi,\phi)\big)}{|n'(\psi,\phi)-\nu'|}\,\mathrm{d}\phi\, e^{ikR\psi}\,\mathrm{d}\psi.\end{aligned} \tag{B.4.8}$$

Moreover, it is easily seen that $n'(\psi,\phi)$ and $n_z^r(\psi,\phi)$ (cf. (4.2.22) and (4.2.23)) are 2π-periodic w.r.t. ϕ and that $n_z^r(\psi,-\phi) = n_z^r(\psi,\phi)$ and $|n'(\psi,-\phi)-\nu'| = |n'(\psi,\phi)-\nu'|$. Indeed, the last statement follows for $\phi_0 = 0$, since (cf. (4.2.22))

$$\begin{aligned}|n'(\psi,\phi)-\nu'|^2 &= |n'(\psi,\phi) - n'(\psi_0,\phi_0)|^2 \\ &= \Big[\sin\alpha\,(\psi-\psi_0) + \cos\alpha\,(\cos\phi\sqrt{1-\psi^2} - \cos\alpha)\Big]^2 + \sin^2\phi\,(1-\psi^2).\end{aligned} \tag{B.4.9}$$

Integral $\tilde{J}_2$ now simplifies to

$$\begin{aligned}\tilde{J}_2 = &\int_{-\sin\alpha}^{\sin\alpha} \chi(\psi) \int_{\phi(\psi)}^{\pi} \frac{f_{\ell,j}^2\big(n'(\psi,\phi), n_z^r(\psi,\phi)\big)}{|n'(\psi,\phi)-\nu'|}\,\mathrm{d}\phi\, e^{ikR\psi}\,\mathrm{d}\psi \\ &+ \int_{\sin\alpha}^{1} \chi(\psi) \int_{0}^{\pi} \frac{f_{\ell,j}^2\big(n'(\psi,\phi), n_z^r(\psi,\phi)\big)}{|n'(\psi,\phi)-\nu'|}\,\mathrm{d}\phi\, e^{ikR\psi}\,\mathrm{d}\psi,\end{aligned} \tag{B.4.10}$$

where

$$f_{\ell,j}^2\big(n'(\psi,\phi), n_z^r(\psi,\phi)\big) := f_{\ell,j}\big(n'(\psi,\phi), n_z^r(\psi,\phi)\big) + f_{\ell,j}\big(n'(\psi,-\phi), n_z^r(\psi,-\phi)\big). \tag{B.4.11}$$

Once again, the integrals are split to separate the singularity. To be precise, taking into account that (cf. (B.3.36))

$$\int_{-\sin\alpha}^{\sin\alpha} \chi(\psi) \int_{\phi(\psi)}^{\pi} \frac{1}{\sqrt{\bar{b}\,\phi^2 + \bar{d}\,(\psi-\psi_0)^4}}\,\mathrm{d}\phi\, e^{ikR\psi}\,\mathrm{d}\psi + \int_{\sin\alpha}^{1} \chi(\psi) \int_{0}^{\pi} \frac{1}{\sqrt{\bar{b}\,\phi^2 + \bar{d}\,(\psi-\psi_0)^4}}\,\mathrm{d}\phi\, e^{ikR\psi}\,\mathrm{d}\psi$$

$$
\begin{aligned}
&= \int_{-\sin\alpha}^{\sin\alpha} \frac{\chi(\psi)}{\sqrt{\bar b}} \log\Big(\bar b\,\pi + \sqrt{\bar b}\sqrt{\bar b\,\pi^2 + \bar d\,(\psi-\psi_0)^4}\Big)\, e^{ikR\psi}\,\mathrm{d}\psi \\
&\quad - \int_{-\sin\alpha}^{\sin\alpha} \frac{\chi(\psi)}{\sqrt{\bar b}} \log\Big(\bar b\,\phi(\psi) + \sqrt{\bar b}\sqrt{\bar b\,\phi(\psi)^2 + \bar d\,(\psi-\psi_0)^4}\Big)\, e^{ikR\psi}\,\mathrm{d}\psi \\
&\quad + \int_{\sin\alpha}^{1} \frac{\chi(\psi)}{\sqrt{\bar b}} \log\Big(\bar b\,\pi + \sqrt{\bar b}\sqrt{\bar b\,\pi^2 + \bar d\,(\psi-\psi_0)^4}\Big)\, e^{ikR\psi}\,\mathrm{d}\psi - \int_{\sin\alpha}^{1} \frac{\chi(\psi)}{\sqrt{\bar b}} \log\Big(\sqrt{\bar b\bar d}\,(\psi-\psi_0)^2\Big)\, e^{ikR\psi}\,\mathrm{d}\psi \\
&= \int_{-\sin\alpha}^{1} \frac{\chi(\psi)}{\sqrt{\bar b}} \log\Big(\bar b\,\pi + \sqrt{\bar b}\sqrt{\bar b\,\pi^2 + \bar d\,(\psi-\psi_0)^4}\Big)\, e^{ikR\psi}\,\mathrm{d}\psi \\
&\quad - \int_{-\sin\alpha}^{\sin\alpha} \frac{\chi(\psi)}{\sqrt{\bar b}} \log\Big(\bar b\,\phi(\psi) + \sqrt{\bar b}\sqrt{\bar b\,\phi(\psi)^2 + \bar d\,(\psi-\psi_0)^4}\Big)\, e^{ikR\psi}\,\mathrm{d}\psi \\
&\quad - \int_{\sin\alpha}^{1} \frac{\chi(\psi)}{\sqrt{\bar b}} \log\Big(\sqrt{\bar b\bar d}\,(\psi-\psi_0)^2\Big)\, e^{ikR\psi}\,\mathrm{d}\psi,
\end{aligned}
$$

the integrals in $\tilde J_2$ (cf. (B.4.10)) are split into

$$
\tilde J_2 = \tilde J_3 + f_{\ell,j}(\nu',0)\,\tilde J_4 + f_{\ell,j}(\nu',0)\,\tilde J_5 + f_{\ell,j}(\nu',0)\,\tilde J_6, \tag{B.4.12}
$$

where

$$
\begin{aligned}
\tilde J_3 :=& \int_{-\sin\alpha}^{\sin\alpha} \chi(\psi) \int_{\phi(\psi)}^{\pi} \frac{f_{\ell,j}^2\big(n'(\psi,\phi), n_z^r(\psi,\phi)\big) - 2 f_{\ell,j}(\nu',0)}{|n'(\psi,\phi)-\nu'|}\,\mathrm{d}\phi\, e^{ikR\psi}\,\mathrm{d}\psi \\
&+ \int_{\sin\alpha}^{1} \chi(\psi) \int_{0}^{\pi} \frac{f_{\ell,j}^2\big(n'(\psi,\phi), n_z^r(\psi,\phi)\big) - 2 f_{\ell,j}(\nu',0)}{|n'(\psi,\phi)-\nu'|}\,\mathrm{d}\phi\, e^{ikR\psi}\,\mathrm{d}\psi,
\end{aligned} \tag{B.4.13}
$$

$$
\begin{aligned}
\tilde J_4 :=& \,2 \int_{-\sin\alpha}^{\sin\alpha} \chi(\psi) \int_{\phi(\psi)}^{\pi} \frac{1}{|n'(\psi,\phi)-\nu'|} - \frac{1}{\sqrt{\bar b\,\phi^2 + \bar d\,(\psi-\psi_0)^4}}\,\mathrm{d}\phi\, e^{ikR\psi}\,\mathrm{d}\psi \\
&+ 2 \int_{\sin\alpha}^{1} \chi(\psi) \int_{0}^{\pi} \frac{1}{|n'(\psi,\phi)-\nu'|} - \frac{1}{\sqrt{\bar b\,\phi^2 + \bar d\,(\psi-\psi_0)^4}}\,\mathrm{d}\phi\, e^{ikR\psi}\,\mathrm{d}\psi,
\end{aligned} \tag{B.4.14}
$$

$$
\tilde J_5 := \frac{2}{\sqrt{\bar b}} \int_{-\sin\alpha}^{1} \chi(\psi)\, \log\Big(\bar b\,\pi + \sqrt{\bar b}\sqrt{\bar b\,\pi^2 + \bar d\,(\psi-\psi_0)^4}\Big)\, e^{ikR\psi}\,\mathrm{d}\psi, \tag{B.4.15}
$$

$$
\begin{aligned}
\tilde J_6 :=& -\frac{2}{\sqrt{\bar b}} \int_{-\sin\alpha}^{\sin\alpha} \chi(\psi)\, \log\Big(\bar b\,\phi(\psi) + \sqrt{\bar b}\sqrt{\bar b\,\phi(\psi)^2 + \bar d\,(\psi-\psi_0)^4}\Big)\, e^{ikR\psi}\,\mathrm{d}\psi \\
&- \frac{2}{\sqrt{\bar b}} \int_{\sin\alpha}^{1} \chi(\psi)\, \log\Big(\sqrt{\bar b\bar d}\,(\psi-\psi_0)^2\Big)\, e^{ikR\psi}\,\mathrm{d}\psi.
\end{aligned} \tag{B.4.16}
$$

The constants

$$
\bar b := \cos^2\alpha = m_z^2, \qquad \bar d := \frac{1}{4\cos^4\alpha} \tag{B.4.17}
$$

are obtained by calculating the Taylor expansion of $|n'(\psi,\phi)-\nu'|^2$ w.r.t. ψ and ϕ at $\phi_0 = 0$ and $\psi_0 = \sin\alpha$ up to the fourth order. To be exact,

$$\begin{aligned}|n'(\psi,\phi)-\nu'|^2 &= \cos^2\alpha\,\phi^2 - 2\sin\alpha\,\phi^2\,(\psi-\psi_0) + \frac{1}{4\cos^4\alpha}\,(\psi-\psi_0)^4 - \frac{1}{2}\,\phi^2\,(\psi-\psi_0)^2 \\ &\quad + \left[\frac{\cos^4\alpha}{4} - \frac{\cos^2\alpha}{3}\right]\phi^4 + \mathcal{O}\big((\phi+|\psi-\psi_0|)^5\big). \end{aligned} \tag{B.4.18}$$

Indeed, defining $T(\psi,\phi) := \sin\alpha\,(\psi-\psi_0)+\cos\alpha\,(\cos\phi\,\sqrt{1-\psi^2}-\cos\alpha)$ and $\mathcal{T}(\psi,\phi) := |n'(\psi,\phi)-\nu'|^2 = [T(\psi,\phi)]^2 + \sin^2\phi\,(1-\psi^2)$ (cf. (B.4.9)), all necessary derivatives of T at $\phi = 0$ and $\psi = \psi_0 = \sin\alpha$ can be calculated. For simplicity in these calculations, the symbols $T_{\psi_0^n,\phi_0^m} := [\partial_\psi^n\partial_\phi^m T(\psi,\phi)]_{(\psi,\phi)=(\psi_0,\phi_0)}$ and $\mathcal{T}_{\psi_0^n,\phi_0^m} := [\partial_\psi^n\partial_\phi^m \mathcal{T}(\psi,\phi)]_{(\psi,\phi)=(\psi_0,\phi_0)}$ for $(\psi_0,\phi_0) = (\sin\alpha, 0)$ will be used. Thus,

$$\begin{aligned}
T_{\psi_0} &= \sin\alpha - \cos\alpha\cos\phi_0\,\frac{\psi_0}{\sqrt{1-\psi_0^2}} = 0, & T_{\phi_0} &= -\cos\alpha\sin\phi_0\,\sqrt{1-\psi_0^2} = 0,\\
T_{\psi_0^2} &= -\cos\alpha\cos\phi_0\,\frac{1}{\sqrt{1-\psi_0^2}^3} = -\frac{1}{\cos^2\alpha}, & T_{\phi_0^2} &= -\cos\alpha\cos\phi_0\,\sqrt{1-\psi_0^2} = -\cos^2\alpha,\\
T_{\psi_0,\phi_0} &= \cos\alpha\sin\phi_0\,\frac{\psi_0}{\sqrt{1-\psi_0^2}} = 0, & T_{\psi_0^3} &= -3\cos\alpha\cos\phi_0\,\frac{\psi_0}{\sqrt{1-\psi_0^2}^5} = -3\frac{\sin\alpha}{\cos^4\alpha},
\end{aligned}$$

such that

$$\begin{aligned}
\mathcal{T}_{\psi_0} &= 2T_{\psi_0}\,T - 2\sin^2\phi_0\,\psi_0 && = 0,\\
\mathcal{T}_{\phi_0} &= 2T_{\phi_0}\,T + 2\sin\phi_0\cos\phi_0\,(1-\psi_0^2) && = 0,\\
\mathcal{T}_{\psi_0^2} &= 2T_{\psi_0^2}\,T + 2\,[T_{\psi_0}]^2 - 2\sin^2\phi_0 && = 0\\
\mathcal{T}_{\psi_0,\phi_0} &= 2T_{\psi_0,\phi_0}\,T + 2T_{\psi_0}\,T_{\phi_0} - 4\sin\phi_0\cos\phi_0\,\psi_0 && = 0,\\
\mathcal{T}_{\phi_0^2} &= 2T_{\phi_0^2}\,T + 2\,[T_{\phi_0}]^2 + 2(1-\psi_0^2)\,\left[\cos^2\phi_0 - \sin^2\phi_0\right] && = 2\cos^2\alpha,\\
\mathcal{T}_{\psi_0^3} &= 2T_{\psi_0^3}\,T + 6T_{\psi_0^2}\,T_{\psi_0} && = 0\\
\mathcal{T}_{\psi_0^2,\phi_0} &= 2T_{\psi_0^2,\phi_0}\,T + 2T_{\psi_0^2}\,T_{\phi_0} + 4T_{\psi_0,\phi_0}\,T_{\psi_0} - 4\sin\phi_0\cos\phi_0 && = 0,\\
\mathcal{T}_{\psi_0,\phi_0^2} &= 2T_{\psi_0,\phi_0^2}\,T + 2T_{\phi_0^2}\,T_{\psi_0} + 4T_{\psi_0,\phi_0}\,T_{\phi_0} - 4\,\psi_0\,\left[\cos^2\phi_0 - \sin^2\phi_0\right] && = -4\sin\alpha,\\
\mathcal{T}_{\phi_0^3} &= 2T_{\phi_0^3}\,T + 6T_{\phi_0^2}\,T_{\phi_0} - 8\sin\phi_0\cos\phi_0\,(1-\psi_0^2) && = 0,\\
\mathcal{T}_{\psi_0^4} &= 2T_{\psi_0^4}\,T + 8T_{\psi_0^3}\,T_{\psi_0} + 6\big[T_{\psi_0^2}\big]^2 && = \frac{6}{\cos^4\alpha},\\
\mathcal{T}_{\psi_0^3,\phi_0} &= 2T_{\psi_0^3,\phi_0}\,T + 6T_{\psi_0^2,\phi_0}\,T_{\psi_0} + 2T_{\psi_0^3}\,T_{\phi_0} + 6T_{\psi_0^2}\,T_{\psi_0,\phi_0} && = 0,\\
\mathcal{T}_{\psi_0^2,\phi_0^2} &= 2T_{\psi_0^2,\phi_0^2}\,T + 4T_{\psi_0,\phi_0^2}\,T_{\psi_0} + 2T_{\psi_0^2}\,T_{\phi_0^2} + 4T_{\psi_0^2,\phi_0}\,T_{\phi_0} + 4\,[T_{\psi_0,\phi_0}]^2 && \\
&\quad - 4\,\left[\cos^2\phi_0 - \sin^2\phi_0\right] && = -2,\\
\mathcal{T}_{\psi_0,\phi_0^3} &= 2T_{\psi_0,\phi_0^3}\,T + 2T_{\phi_0^3}\,T_{\psi_0} + 6T_{\psi_0,\phi_0^2}\,T_{\phi_0} + 6T_{\phi_0^2}\,T_{\psi_0,\phi_0} + 16\psi_0\sin\phi_0\cos\phi_0 && = 0,\\
\mathcal{T}_{\phi_0^4} &= 2T_{\phi_0^4}\,T + 8T_{\phi_0^3}\,T_{\phi_0} + 6\big[T_{\phi_0^2}\big]^2 - 8\,(1-\psi_0^2)\,\left[\cos^2\phi_0 - \sin^2\phi_0\right] && = 6\cos^4\alpha - 8\cos^2\alpha
\end{aligned}$$

leading to (B.4.18). Later on, it will also be used that

$$\mathcal{T}_{\psi_0^5} = 2T_{\psi_0^5}\,T + 10T_{\psi_0^4}\,T_{\psi_0} + 20T_{\psi_0^3}\,T_{\psi_0^2} = 60\,\frac{\sin\alpha}{\cos^6\alpha}. \tag{B.4.19}$$

B.4.2.1 $\tilde{J}_3$

First note that the integrands w.r.t. ϕ of $\tilde{J}_3$ (cf. (B.4.13)) are absolutely integrable for any fixed ψ. Indeed, this follows since, with L'Hôpital's rule, it is easily shown that

$$\frac{f_{\ell,j}^2(n'(\psi,\phi), n_z(\psi,\phi)) - 2f_{\ell,j}(\nu',0)}{|n'(\psi,\phi)-\nu'|}$$

is bounded for $\psi \neq \psi_0$ and has a logarithmic singularity at $\phi = \phi_0$ for $\psi = \psi_0$ (cf. Lemma B.2), while $\partial_\phi \vec{n}^r(\psi,\phi)$ (cf. (4.2.22) and (4.2.23)) is bounded. Keeping in mind that $\psi_0 = \sin\alpha$, $\chi(1) = 0$, $\chi(\sin\alpha) = \chi(-\sin\alpha) = 1$ and $\phi(\sin\alpha) = \phi_0 = 0$, integration by parts w.r.t. ψ is applied to $\tilde{J}_3$, giving

$$\begin{aligned}
\tilde{J}_3 = {} & \frac{1}{ikR} \int\limits_0^\pi \frac{f_{\ell,j}^2\big(n'(\psi_0,\phi), n_z^r(\psi_0,\phi)\big) - 2 f_{\ell,j}(\nu',0)}{|n'(\psi_0,\phi) - \nu'|} \,\mathrm{d}\phi\, e^{ikR\psi_0} \\
& - \frac{1}{ikR} \int\limits_\pi^\pi \frac{f_{\ell,j}^2\big(n'(-\psi_0,\phi), n_z^r(-\psi_0,\phi)\big) - 2 f_{\ell,j}(\nu',0)}{|n'(-\psi_0,\phi) - \nu'|} \,\mathrm{d}\phi\, e^{-ikR\psi_0} \\
& - \frac{1}{ikR} \int\limits_{-\sin\alpha}^{\sin\alpha} \chi'(\psi) \int\limits_{\phi(\psi)}^{\pi} \frac{f_{\ell,j}^2\big(n'(\psi,\phi), n_z^r(\psi,\phi)\big) - 2 f_{\ell,j}(\nu',0)}{|n'(\psi,\phi) - \nu'|} \,\mathrm{d}\phi\, e^{ikR\psi} \,\mathrm{d}\psi \\
& + \frac{1}{ikR} \int\limits_{-\sin\alpha}^{\sin\alpha} \chi(\psi) \frac{f_{\ell,j}^2\big(n'(\psi,\phi(\psi)), n_z^r(\psi,\phi(\psi))\big) - 2 f_{\ell,j}(\nu',0)}{|n'(\psi,\phi(\psi)) - \nu'|} \,\phi'(\psi)\, e^{ikR\psi} \,\mathrm{d}\psi \\
& - \frac{1}{ikR} \int\limits_{-\sin\alpha}^{\sin\alpha} \chi(\psi) \int\limits_{\phi(\psi)}^{\pi} \partial_\psi \left[\frac{f_{\ell,j}^2\big(n'(\psi,\phi), n_z^r(\psi,\phi)\big) - 2 f_{\ell,j}(\nu',0)}{|n'(\psi,\phi) - \nu'|} \right] \mathrm{d}\phi\, e^{ikR\psi} \,\mathrm{d}\psi \\
& - \frac{1}{ikR} \int\limits_0^\pi \frac{f_{\ell,j}^2\big(n'(\psi_0,\phi), n_z^r(\psi_0,\phi)\big) - 2 f_{\ell,j}(\nu',0)}{|n'(\psi_0,\phi) - \nu'|} \,\mathrm{d}\phi\, e^{ikR\psi_0} \\
& - \frac{1}{ikR} \int\limits_{\sin\alpha}^{1} \chi'(\psi) \int\limits_0^{2\pi} \frac{f_{\ell,j}\big(n'(\psi,\phi), n_z^r(\psi,\phi)\big) - f_{\ell,j}(\nu',0)}{|n'(\psi,\phi) - \nu'|} \,\mathrm{d}\phi\, e^{ikR\psi} \,\mathrm{d}\psi \\
& - \frac{1}{ikR} \int\limits_{\sin\alpha}^{1} \chi(\psi) \int\limits_0^{\pi} \partial_\psi \left[\frac{f_{\ell,j}^2\big(n'(\psi,\phi), n_z^r(\psi,\phi)\big) - 2 f_{\ell,j}(\nu',0)}{|n'(\psi,\phi) - \nu'|} \right] \mathrm{d}\phi\, e^{ikR\psi} \,\mathrm{d}\psi,
\end{aligned} \tag{B.4.20}$$

where (cf. (B.4.7))

$$\phi'(\psi) = \partial_\psi \left[\arccos\left(\cot\alpha \, \frac{\psi}{\sqrt{1-\psi^2}} \right) \right] = - \frac{\cos\alpha}{1-\psi^2} \, \frac{1}{\sqrt{\sin^2\alpha - \psi^2}}. \tag{B.4.21}$$

It is easily seen that the integrand of the second integral on the right-hand side is non-singular, which shows that the integral is zero, since the upper and lower integration bounds are identical. On the other hand, the first and the sixth line on the right-hand side of (B.4.20) cancel each other, since they are identical except for the sign. Moreover, the derivative of the cut-off function $\chi(\psi)$ is bounded for all ψ such that the integrands w.r.t. ψ of the integrals on the third and seventh line on the right-hand side of (B.4.20) are absolutely integrable, since the integral w.r.t. ϕ is finite for any fixed ψ from the compact set $[-\sin\alpha, 1]$. The Riemann-Lebesgue lemma then proves that these two integrals tend to zero as R tends to infinity. To show this for the remaining integrals on the fourth, fifth and eighth line as well, a closer look at their integrands is necessary. Starting with that of the integral on the fourth line, it will be shown that this integrand is absolutely integrable.

Since $\phi'(\psi)$ (cf. (B.4.21)) is weakly singular at $\psi = \psi_0 = \sin\alpha$, it is sufficient to show that

$$\left| \frac{f_{\ell,j}^2\big(n'(\psi,\phi(\psi)), n_z^r(\psi,\phi(\psi))\big) - 2 f_{\ell,j}(\nu',0)}{|n'(\psi,\phi(\psi)) - \nu'|} \right| \leq c \left| \log|\psi - \psi_0| \right|, \tag{B.4.22}$$

to deduce that the integrand of the integral on the fourth line of (B.4.20) is absolutely integrable. Indeed, this holds since (cf. (B.4.11) and Lemma B.2)

$$\left| \frac{f_{\ell,j}^2\big(n'(\psi,\phi(\psi)), n_z^r(\psi,\phi(\psi))\big) - 2 f_{\ell,j}(\nu',0)}{|n'(\psi,\phi(\psi)) - \nu'|} \right| \leq c \left| \log|n'(\psi,\phi(\psi)) - \nu'| \right| \tag{B.4.23}$$

and, recalling that $\psi_0 = \sin\alpha$, (cf. (B.4.7) and (B.4.9))

$$\begin{aligned}|n'(\psi,\phi(\psi)) - \nu'|^2 &= \Big[\sin\alpha\,(\psi-\psi_0) + \cos\alpha\Big(\frac{\cos\alpha}{\sin\alpha}\,\psi - \cos\alpha\Big)\Big]^2 + \Big[1 - \frac{\cos^2\alpha}{\sin^2\alpha}\frac{\psi^2}{1-\psi^2}\Big](1-\psi^2)\\ &= \Big[\sin\alpha\,(\psi-\psi_0) + \frac{\cos^2\alpha}{\sin\alpha}\,(\psi-\psi_0)\Big]^2 - \frac{1}{\sin^2\alpha}\,(\psi^2-\psi_0^2)\\ &= \frac{1}{\sin^2\alpha}\big[(\psi-\psi_0)^2 - (\psi+\psi_0)\,(\psi-\psi_0)\big] = -\frac{2}{\sin\alpha}\,(\psi-\psi_0). \end{aligned}\tag{B.4.24}$$

Consequently, the integral on the fourth line of (B.4.20) exists absolutely and the Riemann-Lebesgue lemma once more proves that it tends to zero as R tends to infinity.

Next, to obtain the asymptotic behaviour of the integrals on the fifth and eighth line of (B.4.20), consider the derivative

$$\begin{aligned}&\partial_\psi\left[\frac{f_{\ell,j}^2\big(n'(\psi,\phi),n_z^r(\psi,\phi)\big) - 2f_{\ell,j}(\nu',0)}{|n'(\psi,\phi)-\nu'|}\right]\\ &\quad= \frac{\partial_\psi n'(\psi,\phi)\cdot\nabla_{n'}f_{\ell,j}^2\big(n'(\psi,\phi),n_z^r(\psi,\phi)\big) + \partial_\psi n_z^r(\psi,\phi)\cdot\nabla_{n_z^r}f_{\ell,j}^2\big(n'(\psi,\phi),n_z^r(\psi,\phi)\big)}{|n'(\psi,\phi)-\nu'|}\\ &\quad\quad - \frac{\partial_\psi n'(\psi,\phi)\cdot\big(n'(\psi,\phi)-\nu'\big)\Big[f_{\ell,j}^2\big(n'(\psi,\phi),n_z^r(\psi,\phi)\big) - 2f_{\ell,j}(\nu',0)\Big]}{|n'(\psi,\phi)-\nu'|^3},\end{aligned}$$

where $[n'(\psi,\phi)-\nu']/|n'(\psi,\phi)-\nu'|$ is bounded w.r.t. ϕ for any fixed $\psi\in[-\sin\alpha,1]$. Furthermore, it was already seen that the partial derivatives of $n'(\psi,\phi)$ and $n_z^r(\psi,\phi)$ are finite at $(\psi,\phi)^\top = (\psi_0,\phi_0)^\top$, with $\psi_0 \neq 1$. On the other hand,

$$\frac{f_{\ell,j}^2\big(n'(\psi,\phi),n_z^r(\psi,\phi)\big) - 2f_{\ell,j}(\nu',0)}{|n'(\psi,\phi)-\nu'|},$$

$\nabla_{\vec{n}^r}f_{\ell,j}(n',n_z^r)$ and thus of $\nabla_{\vec{n}^r}f_{\ell,j}^2(n',n_z^r)$ (cf. (B.4.11)) are absolutely bounded by $c|\log|n'(\psi,\phi)-\nu'||$ (cf. Lemma B.2). Hence

$$\left|\partial_\psi\left[\frac{f_{\ell,j}^2\big(n'(\psi,\phi),n_z^r(\psi,\phi)\big) - 2f_{\ell,j}(\nu',0)}{|n'(\psi,\phi)-\nu'|}\right]\right| \le c\frac{\big|\log|n'(\psi,\phi)-\nu'|\big|}{|n'(\psi,\phi)-\nu'|}.$$

It follows that, if the integrands on the right-hand sides of

$$\left|\chi(\psi)\int_{\phi(\psi)}^{\pi}\partial_\psi\left[\frac{f_{\ell,j}^2\big(n'(\psi,\phi),n_z^r(\psi,\phi)\big) - 2f_{\ell,j}(\nu',0)}{|n'(\psi,\phi)-\nu'|}\right]\mathrm{d}\phi\right| \le c\,\chi(\psi)\int_{\phi(\psi)}^{\pi}\frac{\big|\log|n'(\psi,\phi)-\nu'|\big|}{|n'(\psi,\phi)-\nu'|}\,\mathrm{d}\phi,$$

$$\left|\chi(\psi)\int_{0}^{\pi}\partial_\psi\left[\frac{f_{\ell,j}^2\big(n'(\psi,\phi),n_z^r(\psi,\phi)\big) - 2f_{\ell,j}(\nu',0)}{|n'(\psi,\phi)-\nu'|}\right]\mathrm{d}\phi\right| \le c\,\chi(\psi)\int_{0}^{\pi}\frac{\big|\log|n'(\psi,\phi)-\nu'|\big|}{|n'(\psi,\phi)-\nu'|}\,\mathrm{d}\phi$$

are integrable w.r.t. ψ, the Riemann-Lebesgue lemma shows that the fifth and eighth line of (B.4.20) decay with the order $o(1/R)$ as R tends to infinity. On the other hand, the integrability is easily shown by undoing the substitution (4.2.22) to spherical coordinates (ψ,ϕ) and returning to the Cartesian coordinate system n' (compare with the difference between (4.2.16) and the first line of (4.2.21)). First, however, the order of integration is switched back (compare with switch from (B.4.6) to (B.4.8)).

Thus, recalling that $\chi(\psi)$ was defined as $\chi(n'(\psi,\phi))$ for this section,

$$\begin{aligned}
&\int_{-\sin\alpha}^{\sin\alpha} \chi(\psi) \int_{\phi(\psi)}^{\pi} \frac{\left|\log|n'(\psi,\phi)-\nu'|\right|}{|n'(\psi,\phi)-\nu'|}\,\mathrm{d}\phi\,\mathrm{d}\psi + \int_{\sin\alpha}^{1} \chi(\psi) \int_{0}^{\pi} \frac{\left|\log|n'(\psi,\phi)-\nu'|\right|}{|n'(\psi,\phi)-\nu'|}\,\mathrm{d}\phi\,\mathrm{d}\psi \\
&\qquad = \int_0^{2\pi} \int_{\cos\theta(\phi)}^{1} \chi(\psi)\, \frac{\left|\log|n'(\psi,\phi)-\nu'|\right|}{|n'(\psi,\phi)-\nu'|}\,\mathrm{d}\psi\,\mathrm{d}\phi \\
&\qquad = \int_{B_2(1)} \chi(n')\, \frac{\left|\log|n'-\nu'|\right|}{|n'-\nu'|}\, \frac{1}{\sqrt{1-|n'|^2}}\,\mathrm{d}n',
\end{aligned}$$

which is finite according to Lemma 3.11. Thus the integrands w.r.t. ψ in the fifth and eighth line of (B.4.20) are absolutely integrable, such that the Riemann-Lebesgue lemma reveals that both lines decay as proposed. Finally, it was proven for all terms on the right-hand side of (B.4.20) that they decay faster than $1/R$, and thus that

$$\tilde{J}_3 = o\left(\frac{1}{R}\right) \tag{B.4.25}$$

for $m'/|m'| = \nu'$.

B.4.2.2 $\tilde{J}_4$

For the integrand w.r.t. ϕ of $\tilde{J}_4$ (cf. (B.4.14)) it can also be shown that it is bounded for any fixed $\psi \in [-\sin\alpha, 1]$. Indeed, (cf. (B.4.18))

$$\begin{aligned}
&\frac{1}{|n'(\psi,\phi)-\nu'|} - \frac{1}{\sqrt{\bar{b}\,\phi^2 + \bar{d}\,(\psi-\psi_0)^4}} \\
&\quad = \frac{-|n'(\psi,\phi)-\nu'|^2 + \bar{b}\,\phi^2 + \bar{d}\,(\psi-\psi_0)^4}{|n'(\psi,\phi)-\nu'|\sqrt{\bar{b}\,\phi^2 + \bar{d}\,(\psi-\psi_0)^4}\left[|n'(\psi,\phi)-\nu'| + \sqrt{\bar{b}\,\phi^2 + \bar{d}\,(\psi-\psi_0)^4}\right]} \\
&\quad = \frac{2\sin\alpha\,\phi^2\,(\psi-\psi_0) + \frac{1}{2}\,\phi^2\,(\psi-\psi_0)^2 - \left[\frac{\cos^4\alpha}{4} - \frac{\cos^2\alpha}{3}\right]\phi^4 + \mathcal{O}\left((\phi+|\psi-\psi_0|)^5\right)}{|n'(\psi,\phi)-\nu'|\sqrt{\bar{b}\,\phi^2 + \bar{d}\,(\psi-\psi_0)^4}\left[|n'(\psi,\phi)-\nu'| + \sqrt{\bar{b}\,\phi^2 + \bar{d}\,(\psi-\psi_0)^4}\right]}.
\end{aligned}$$

Using the expansion (B.4.18), the statement is easily proven, which shows that the integrals w.r.t. ϕ are finite for any fixed ψ. As for $\tilde{J}_3$ the integrals w.r.t. ψ are integrated by parts, leading to

$$\begin{aligned}
\tilde{J}_4 = &\ \frac{2}{ikR}\int_0^{\pi} \frac{1}{|n'(\psi_0,\phi)-\nu'|} - \frac{1}{\sqrt{\bar{b}}\,\phi}\,\mathrm{d}\phi\, e^{ikR\psi_0} \\
&- \frac{2}{ikR}\int_{\pi}^{\pi} \frac{1}{|n'(-\psi_0,\phi)-\nu'|} - \frac{1}{\sqrt{\bar{b}\,\phi^2 + 16\bar{d}\,\psi_0^4}}\,\mathrm{d}\phi\, e^{-ikR\psi_0} \\
&- \frac{2}{ikR}\int_{-\sin\alpha}^{\sin\alpha} \chi'(\psi) \int_{\phi(\psi)}^{\pi} \frac{1}{|n'(\psi,\phi)-\nu'|} - \frac{1}{\sqrt{\bar{b}\,\phi^2 + \bar{d}\,(\psi-\psi_0)^4}}\,\mathrm{d}\phi\, e^{ikR\psi}\,\mathrm{d}\psi \\
&+ \frac{2}{ikR}\int_{-\sin\alpha}^{\sin\alpha} \chi(\psi) \left[\frac{1}{|n'(\psi,\phi(\psi))-\nu'|} - \frac{1}{\sqrt{\bar{b}\,\phi(\psi)^2 + \bar{d}\,(\psi-\psi_0)^4}}\right] \phi'(\psi)\, e^{ikR\psi}\,\mathrm{d}\psi \\
&- \frac{2}{ikR}\int_{-\sin\alpha}^{\sin\alpha} \chi(\psi) \int_{\phi(\psi)}^{\pi} \partial_\psi \left[\frac{1}{|n'(\psi,\phi)-\nu'|} - \frac{1}{\sqrt{\bar{b}\,\phi^2 + \bar{d}\,(\psi-\psi_0)^4}}\right] \mathrm{d}\phi\, e^{ikR\psi}\,\mathrm{d}\psi
\end{aligned}$$

$$
\begin{aligned}
&- \frac{2}{ikR} \int\limits_0^\pi \frac{1}{|n'(\psi_0, \phi) - \nu'|} - \frac{1}{\sqrt{\bar b}\,\phi} \,\mathrm{d}\phi\, e^{ikR\psi_0} \\
&- \frac{2}{ikR} \int\limits_{\sin\alpha}^1 \chi'(\psi) \int\limits_0^\pi \frac{1}{|n'(\psi, \phi) - \nu'|} - \frac{1}{\sqrt{\bar b\,\phi^2 + \bar d\,(\psi - \psi_0)^4}} \,\mathrm{d}\phi\, e^{ikR\psi} \,\mathrm{d}\psi \\
&- \frac{2}{ikR} \int\limits_{\sin\alpha}^1 \chi(\psi) \int\limits_0^\pi \partial_\psi \left[\frac{1}{|n'(\psi, \phi) - \nu'|} - \frac{1}{\sqrt{\bar b\,\phi^2 + \bar d\,(\psi - \psi_0)^4}} \right] \mathrm{d}\phi\, e^{ikR\psi} \,\mathrm{d}\psi. \qquad \text{(B.4.26)}
\end{aligned}
$$

The integrals on the first and sixth line cancel each other once more, while the integrand on the second line is again zero, since the integrand is bounded and the area of integration a zero set. Moreover, since the derivative of the cut-off function is bounded and zero in a neighbourhood of $(\psi, \phi)^\top = (\psi_0, \phi_0)^\top$, the integrals w.r.t. ψ on the third and seventh line exist absolutely and the Riemann-Lebesgue lemma states that they tend to zero as R tends to infinity. To show the same for the fourth line, it is used that $\phi(\psi) \sim \sqrt{\psi_0 - \psi}$ for $\psi \to \psi_0 = \sin\alpha$. Indeed, by using L'Hôpital's rule it is easily shown that (cf. (B.4.21))

$$
\begin{aligned}
\lim_{\psi\to\psi_0} \frac{\phi(\psi)}{\sqrt{\psi_0 - \psi}} &= \lim_{\psi\to\psi_0} -2\,\phi'(\psi)\sqrt{\psi_0 - \psi} = 2 \lim_{\psi\to\psi_0} \frac{\cos\alpha}{1 - \psi^2} \frac{1}{\sqrt{\sin\alpha + \psi}} \frac{\sqrt{\psi_0 - \psi}}{\sqrt{\sin\alpha - \psi}} \\
&= \frac{\sqrt{2}}{\cos\alpha\sqrt{\sin\alpha}} < \infty
\end{aligned}
$$

for $\alpha \in (0, \pi/2)$, such that

$$
\phi(\psi) \sim \frac{\sqrt{2}}{\cos\alpha\sqrt{\sin\alpha}} \sqrt{\psi_0 - \psi} \qquad \text{(B.4.27)}
$$

for $\psi \to \psi_0$. With this, $\bar b = \cos^2\alpha$ and $|n'(\psi, \phi(\psi)) - \nu'|^2 = 2/\sin\alpha\, |\psi - \psi_0|$ (cf. (B.4.24) for $\psi \le \psi_0 = \sin\alpha$) it is easily shown that the term

$$
\begin{aligned}
&\frac{1}{|n'(\psi, \phi(\psi)) - \nu'|} - \frac{1}{\sqrt{\bar b\,\phi(\psi)^2 + \bar d\,(\psi - \psi_0)^4}} \\
&\qquad \sim \frac{1}{\sqrt{\frac{2}{\sin\alpha}}\,\sqrt{|\psi - \psi_0|}} - \frac{1}{\sqrt{\frac{2}{\sin\alpha}\,|\psi - \psi_0| + \bar d\,(\psi - \psi_0)^4}} \\
&\qquad = \frac{\bar d\,(\psi - \psi_0)^4}{\sqrt{|\psi - \psi_0|}^3 \sqrt{\frac{4}{\sin^2\alpha} + \frac{2\,\bar d}{\sin\alpha}\,|\psi - \psi_0|^3} \left[\sqrt{\frac{2}{\sin\alpha}} + \sqrt{\frac{2}{\sin\alpha} + \bar d\,|\psi - \psi_0|^3} \right]}
\end{aligned}
$$

is bounded for all $\psi \in [-\sin\alpha, \sin\alpha]$. It follows that the integrand of the integral on the fourth line on the right-hand side of (B.4.26) is only weakly singular (cf. (B.4.21)) and thus absolutely integrable. Consequently, (cf. the Riemann-Lebesgue lemma) this integral tends to zero as R tends to infinity. To determine the asymptotic behaviour of the remaining two integrals, it is necessary to examine the occurring derivative w.r.t. ψ at the possible singularity point $(\psi_0, \phi_0)^\top$. Consider

$$
\begin{aligned}
&\partial_\psi \left[\frac{1}{|n'(\psi, \phi) - \nu'|} - \frac{1}{\sqrt{\bar b\,\phi^2 + \bar d\,(\psi - \psi_0)^4}} \right] \\
&\quad = -\frac{1}{2} \frac{\partial_\psi \left[|n'(\psi, \phi) - \nu'|^2 \right]}{|n'(\psi, \phi) - \nu'|^3} + 2 \frac{\bar d\,(\psi - \psi_0)^3}{\sqrt{\bar b\,\phi^2 + \bar d\,(\psi - \psi_0)^4}^3} \\
&\quad = \frac{1}{|n'(\psi, \phi) - \nu'|} \frac{-\frac{1}{2}\partial_\psi \left[|n'(\psi, \phi) - \nu'|^2 \right] + 2\bar d\,(\psi - \psi_0)^3 \sqrt{\frac{|n'(\psi,\phi) - \nu'|^2}{\bar b\,\phi^2 + \bar d\,(\psi - \psi_0)^4}}^3}{|n'(\psi, \phi) - \nu'|^2}, \qquad \text{(B.4.28)}
\end{aligned}
$$

where the Taylor expansions

$$\partial_\psi\left[|n'(\psi,\phi)-\nu'|^2\right] = -2\sin\alpha\,\phi^2 + 4\bar{d}\,(\psi-\psi_0)^3 + \ldots$$

and $\sqrt{1+x}^{\,3} = 1+\mathcal{O}(x)$ are easily derived. It can further be shown that with $\bar{d}_0 := -2\sin\alpha$, $\bar{d}_1 := -1/2$, $\bar{d}_2 := \cos^4\alpha/4 - \cos^2\alpha/3$ and $\bar{d}_3 := 1/2\,\sin\alpha/\cos^6\alpha$, (cf. (B.4.18) and (B.4.19))

$$\begin{aligned}
&\frac{|n'(\psi,\phi)-\nu'|^2}{\bar{b}\,\phi^2+\bar{d}\,(\psi-\psi_0)^4} \\
&\quad = 1 + \frac{\bar{d}_0\,\phi^2\,(\psi-\psi_0)+\bar{d}_1\,\phi^2\,(\psi-\psi_0)^2+\bar{d}_2\,\phi^4+\bar{d}_3\,(\psi-\psi_0)^5+\mathcal{O}\left(\phi\,(\phi+|\psi-\psi_0|)^4+|\psi-\psi_0|^6\right)}{\bar{b}\,\phi^2+\bar{d}\,(\psi-\psi_0)^4} \\
&\quad = 1+\mathcal{O}\left(\phi+|\psi-\psi_0|\right)
\end{aligned}$$

for $(\psi,\phi)^\top \to (\psi_0,\phi_0)^\top$. Thus (cf. (B.4.28))

$$\begin{aligned}
&\frac{-\frac{1}{2}\partial_\psi\left[|n'(\psi,\phi)-\nu'|^2\right]+2\bar{d}\,(\psi-\psi_0)^3\sqrt{\frac{|n'(\psi,\phi)-\nu'|^2}{\bar{b}\,\phi^2+\bar{d}\,(\psi-\psi_0)^4}}^{\,3}}{|n'(\psi,\phi)-\nu'|^2} \\
&\qquad \le c\frac{-\frac{1}{2}\bar{d}_0\,\phi^2-2\bar{d}\,(\psi-\psi_0)^3+2\bar{d}\,(\psi-\psi_0)^3\left[1+\mathcal{O}\left(\phi+|\psi-\psi_0|\right)\right]}{\bar{b}\,\phi^2+\bar{d}_0\,\phi^2\,(\psi-\psi_0)+\bar{d}\,(\psi-\psi_0)^4} \\
&\qquad = c\frac{-\frac{1}{2}\bar{d}_0\,\phi^2+2\bar{d}\,(\psi-\psi_0)^3\,\mathcal{O}\left(\phi+|\psi-\psi_0|\right)}{\bar{b}\,\phi^2+\bar{d}_0\,\phi^2\,(\psi-\psi_0)+\bar{d}\,(\psi-\psi_0)^4}
\end{aligned}$$

is bounded for $(\psi,\phi)^\top \to (\psi_0,\phi_0)^\top$ and (B.4.28) is absolutely integrable w.r.t. ϕ and then ψ, similar to $\tilde{J}_3$. Altogether, the Riemann-Lebesgue lemma gives that

$$\tilde{J}_4 = o\left(\frac{1}{R}\right) \tag{B.4.29}$$

for $m'/|m'| = \nu'$.

B.4.2.3 $\tilde{J}_5$

Recall that (cf. (B.4.15))

$$\tilde{J}_5 := \frac{2}{\sqrt{\bar{b}}}\int\limits_{-\sin\alpha}^{1}\chi(\psi)\,\log\left(\bar{b}\,\pi+\sqrt{\bar{b}}\sqrt{\bar{b}\,\pi^2+\bar{d}\,(\psi-\psi_0)^4}\right)\,e^{ikR\psi}\,\mathrm{d}\psi.$$

It is easily seen that the integrand of $\tilde{J}_5$ is uniformly bounded for all $\psi \in [-\sin\alpha, 1]$. Since $\chi(1) = 0$ and $\chi(-\sin\alpha) = 1$, applying integration by parts to $\tilde{J}_5$ gives

$$\begin{aligned}
\tilde{J}_5 = &-\frac{2}{\sqrt{\bar{b}}ikR}\log\left(\bar{b}\,\pi+\sqrt{\bar{b}}\sqrt{\bar{b}\,\pi^2+16\bar{d}\,\psi_0^4}\right)\,e^{-ikR\psi_0} \\
&-\frac{2}{\sqrt{\bar{b}}ikR}\int\limits_{-\sin\alpha}^{1}\chi'(\psi)\log\left(\bar{b}\,\pi+\sqrt{\bar{b}}\sqrt{\bar{b}\,\pi^2+\bar{d}\,(\psi-\psi_0)^4}\right)\,e^{ikR\psi}\,\mathrm{d}\psi \\
&-\frac{2}{\sqrt{\bar{b}}ikR}\int\limits_{-\sin\alpha}^{1}\chi(\psi)\,\partial_\psi\left[\log\left(\bar{b}\,\pi+\sqrt{\bar{b}}\sqrt{\bar{b}\,\pi^2+\bar{d}\,(\psi-\psi_0)^4}\right)\right]\,e^{ikR\psi}\,\mathrm{d}\psi.
\end{aligned}$$

Obviously, the remaining integrals are absolutely integrable. By applying the Riemann-Lebesgue lemma this, in turn, shows that they tend to zero as R tends to infinity. Indeed, both integrands are bounded since $\chi'(\psi)$, the logarithm and its derivative are bounded for $-\sin\alpha \le \psi \le 1$. Hence

$$\tilde{J}_5 = -\frac{2}{\sqrt{\bar{b}}ikR}\log\left(\bar{b}\,\pi+\sqrt{\bar{b}}\sqrt{\bar{b}\,\pi^2+16\bar{d}\,\psi_0^4}\right)\,e^{-ikR\psi_0}+o\left(\frac{1}{R}\right) \tag{B.4.30}$$

for $m'/|m'| = \nu'$.

B.4.2.4 $\tilde{J}_6$

The remaining integral $\tilde{J}_6$ (cf. (B.4.16)) can be rewritten as

$$
\begin{aligned}
\tilde{J}_6 = &-\frac{2}{\sqrt{\bar{b}}} \int\limits_{-\sin\alpha}^{\sin\alpha} \chi(\psi)\, \log\Big(\bar{b}\,\phi(\psi) + \sqrt{\bar{b}}\sqrt{\bar{b}\,\phi(\psi)^2 + \bar{d}\,(\psi-\psi_0)^4}\Big)\; e^{ikR\psi}\,\mathrm{d}\psi \\
&- \frac{2}{\sqrt{\bar{b}}} \int\limits_{\sin\alpha}^{1} \chi(\psi)\, \log\Big(\sqrt{\bar{b}\bar{d}}\,(\psi-\psi_0)^2\Big)\; e^{ikR\psi}\,\mathrm{d}\psi \\
= &-\frac{2}{\sqrt{\bar{b}}} \int\limits_{-\sin\alpha}^{\sin\alpha} \chi(\psi)\, \Big[\log\Big(\bar{b}\,\phi(\psi) + \sqrt{\bar{b}}\sqrt{\bar{b}\,\phi(\psi)^2 + \bar{d}\,(\psi-\psi_0)^4}\Big) - \frac{1}{2}\log(\psi_0-\psi)\Big]\, e^{ikR\psi}\,\mathrm{d}\psi \\
&- \frac{1}{\sqrt{\bar{b}}} \int\limits_{-\sin\alpha}^{\sin\alpha} \chi(\psi)\log(\psi_0-\psi)\, e^{ikR\psi}\,\mathrm{d}\psi \\
&- \frac{\log(\bar{b}\bar{d})}{\sqrt{\bar{b}}} \int\limits_{\sin\alpha}^{1} \chi(\psi)\, e^{ikR\psi}\,\mathrm{d}\psi - \frac{4}{\sqrt{\bar{b}}} \int\limits_{\sin\alpha}^{1} \chi(\psi)\, \log(\psi-\psi_0)\, e^{ikR\psi}\,\mathrm{d}\psi \\
= &-I_1 - I_2 - I_3,
\end{aligned}
\tag{B.4.31}
$$

where

$$
\begin{aligned}
I_1 &:= \frac{1}{\sqrt{\bar{b}}} \int\limits_{-\sin\alpha}^{\sin\alpha} \big[\chi(\psi)-1\big]\log(\psi_0-\psi)\, e^{ikR\psi}\,\mathrm{d}\psi + \frac{4}{\sqrt{\bar{b}}} \int\limits_{\sin\alpha}^{1} \big[\chi(\psi)-1\big]\log(\psi-\psi_0)\, e^{ikR\psi}\,\mathrm{d}\psi \\
&\quad + \frac{\log(\bar{b}\bar{d})}{\sqrt{\bar{b}}} \int\limits_{\sin\alpha}^{1} \chi(\psi)\, e^{ikR\psi}\,\mathrm{d}\psi, \\
I_2 &:= \frac{2}{\sqrt{\bar{b}}} \int\limits_{-\sin\alpha}^{\sin\alpha} \chi(\psi)\, \Big[\log\Big(\bar{b}\,\phi(\psi) + \sqrt{\bar{b}}\sqrt{\bar{b}\,\phi(\psi)^2 + \bar{d}\,(\psi-\psi_0)^4}\Big) - \frac{1}{2}\log(\psi_0-\psi)\Big]\, e^{ikR\psi}\,\mathrm{d}\psi, \\
I_3 &:= \frac{1}{\sqrt{\bar{b}}} \int\limits_{-\sin\alpha}^{\sin\alpha} \log(\psi_0-\psi)\, e^{ikR\psi}\,\mathrm{d}\psi + \frac{4}{\sqrt{\bar{b}}} \int\limits_{\sin\alpha}^{1} \log(\psi-\psi_0)\, e^{ikR\psi}\,\mathrm{d}\psi
\end{aligned}
\tag{B.4.32}
$$

and $\bar{b}\bar{d} = 1/(4\cos^2\alpha) \neq 0$ (cf. (B.4.17)).

Since $\chi(1) = 0$ and $\chi(\sin\alpha) = \chi(-\sin\alpha) = 1$, integrating I_1 by parts results in

$$
\begin{aligned}
I_1 = &-\frac{1}{\sqrt{\bar{b}}\,ikR} \int\limits_{-\sin\alpha}^{\sin\alpha} \Big[\chi'(\psi)\, \log(\psi_0-\psi) - \frac{\chi(\psi)-1}{\psi_0-\psi}\Big]\, e^{ikR\psi}\,\mathrm{d}\psi \\
&- \frac{4}{\sqrt{\bar{b}}\,ikR}\log(1-\psi_0)\, e^{ikR} - \frac{4}{\sqrt{\bar{b}}\,ikR} \int\limits_{\sin\alpha}^{1} \Big[\chi'(\psi)\, \log(\psi-\psi_0) + \frac{\chi(\psi)-1}{\psi-\psi_0}\Big]\, e^{ikR\psi}\,\mathrm{d}\psi \\
&- \frac{\log(\bar{b}\bar{d})}{\sqrt{\bar{b}}\,ikR}\, e^{ikR\psi_0} - \frac{\log(\bar{b}\bar{d})}{\sqrt{\bar{b}}\,ikR} \int\limits_{\sin\alpha}^{1} \chi'(\psi)\, e^{ikR\psi}\,\mathrm{d}\psi.
\end{aligned}
$$

It is easily seen that the remaining integrals exist absolutely since $\chi'(\psi)$ is bounded and $\chi(\psi)$ is identically one in a small neighbourhood of $\psi = \psi_0 = \sin\alpha$. The Riemann-Lebesgue lemma then proves that

$$I_1 = -4\frac{\log(1-\psi_0)}{\sqrt{\bar{b}}\,ikR}\,e^{ikR} - \frac{\log(\bar{b}\bar{d})}{\sqrt{\bar{b}}\,ikR}\,e^{ikR\psi_0} + o\left(\frac{1}{R}\right) \tag{B.4.33}$$

for $m'/|m'| = \nu'$.

Integral I_2 is treated similarly by applying integration by parts. To do so, it has to be shown that the limit $\psi \nearrow \psi_0$ of the integrand is bounded. Consider, with $\phi(\psi_0) = 0$, (cf. (B.4.27) and (B.4.17))

$$\begin{aligned}
&\lim_{\psi\nearrow\psi_0}\left[\log\left(\bar{b}\,\phi(\psi) + \sqrt{\bar{b}}\sqrt{\bar{b}\,\phi(\psi)^2 + \bar{d}\,(\psi-\psi_0)^4}\right) - \frac{1}{2}\log(\psi_0-\psi)\right]\\
&\quad= \lim_{\psi\nearrow\psi_0}\log\left(\bar{b}\frac{\phi(\psi)}{\sqrt{\psi_0-\psi}} + \sqrt{\bar{b}}\sqrt{\bar{b}\left[\frac{\phi(\psi)}{\sqrt{\psi_0-\psi}}\right]^2 + \bar{d}\,(\psi-\psi_0)^3}\right)\\
&\quad= \log\left(2\sqrt{2}\frac{\cos\alpha}{\sqrt{\sin\alpha}}\right),
\end{aligned}$$

which is finite for $\alpha > 0$. With this and $\phi(-\sin\alpha) = \pi$, integration by parts in I_2 leads to

$$\begin{aligned}
I_2 &= \frac{2}{\sqrt{\bar{b}}\,ikR}\log\left(2\sqrt{2}\frac{\cos\alpha}{\sqrt{\sin\alpha}}\right)e^{ikR\psi_0}\\
&\quad - \frac{2}{\sqrt{\bar{b}}\,ikR}\left\{\log\left(\bar{b}\,\pi + \sqrt{\bar{b}}\sqrt{\bar{b}\,\pi^2 + 16\bar{d}\,\psi_0^4}\right) - \frac{1}{2}\log(2\psi_0)\right\}e^{-ikR\psi_0}\\
&\quad - \frac{2}{\sqrt{\bar{b}}\,ikR}\int_{-\sin\alpha}^{\sin\alpha}\chi'(\psi)\left[\log\left(\bar{b}\,\phi(\psi) + \sqrt{\bar{b}}\sqrt{\bar{b}\,\phi(\psi)^2 + \bar{d}\,(\psi-\psi_0)^4}\right) - \frac{1}{2}\log(\psi_0-\psi)\right]e^{ikR\psi}\,\mathrm{d}\psi\\
&\quad - \frac{2}{\sqrt{\bar{b}}\,ikR}\int_{-\sin\alpha}^{\sin\alpha}\chi(\psi)\,\partial_\psi\left[\log\left(\bar{b}\,\phi(\psi) + \sqrt{\bar{b}}\sqrt{\bar{b}\,\phi(\psi)^2 + \bar{d}\,(\psi-\psi_0)^4}\right) - \frac{1}{2}\log(\psi_0-\psi)\right]e^{ikR\psi}\,\mathrm{d}\psi.
\end{aligned} \tag{B.4.34}$$

Since $\chi'(\psi)$ is bounded for all $\psi \in [-\sin\alpha, \sin\alpha]$, the integral on the third line exists absolutely and the Riemann-Lebesgue lemma can be applied. For the remaining integral it has to be shown that the occurring derivative is absolutely integrable to apply the Riemann-Lebesgue lemma. It is easily calculated that

$$\begin{aligned}
&\partial_\psi\left[\log\left(\bar{b}\,\phi(\psi) + \sqrt{\bar{b}}\sqrt{\bar{b}\,\phi(\psi)^2 + \bar{d}\,(\psi-\psi_0)^4}\right) - \frac{1}{2}\log(\psi_0-\psi)\right]\\
&\quad= \frac{\bar{b}\,\phi'(\psi) + \sqrt{\bar{b}}\frac{\bar{b}\,\phi'(\psi)\,\phi(\psi) + 2\bar{d}\,(\psi-\psi_0)^3}{\sqrt{\bar{b}\,\phi(\psi)^2 + \bar{d}\,(\psi-\psi_0)^4}}}{\bar{b}\,\phi(\psi) + \sqrt{\bar{b}}\sqrt{\bar{b}\,\phi(\psi)^2 + \bar{d}\,(\psi-\psi_0)^4}} + \frac{1}{2}\frac{1}{\psi_0-\psi}\\
&\quad= \frac{\sqrt{\bar{b}}\,\phi'(\psi)}{\sqrt{\bar{b}\,\phi(\psi)^2 + \bar{d}\,(\psi-\psi_0)^4}} + 2\sqrt{\bar{b}}\bar{d}\frac{(\psi-\psi_0)^3}{\sqrt{\bar{b}\,\phi(\psi)^2 + \bar{d}\,(\psi-\psi_0)^4}\left[\bar{b}\,\phi(\psi) + \sqrt{\bar{b}}\sqrt{\bar{b}\,\phi(\psi)^2 + \bar{d}\,(\psi-\psi_0)^4}\right]}\\
&\qquad + \frac{1}{2}\frac{1}{\psi_0-\psi},
\end{aligned} \tag{B.4.35}$$

where (cf. (B.4.27))

$$\begin{aligned}
&\lim_{\psi\nearrow\psi_0}\frac{(\psi-\psi_0)^3}{\sqrt{\bar{b}\,\phi(\psi)^2 + \bar{d}\,(\psi-\psi_0)^4}\left[\bar{b}\,\phi(\psi) + \sqrt{\bar{b}}\sqrt{\bar{b}\,\phi(\psi)^2 + \bar{d}\,(\psi-\psi_0)^4}\right]}\\
&\quad= \lim_{\psi\nearrow\psi_0}\frac{-(\psi-\psi_0)^2}{\sqrt{\bar{b}\left[\frac{\phi(\psi)}{\sqrt{\psi_0-\psi}}\right]^2 + \bar{d}\,(\psi_0-\psi)^3}\left[\bar{b}\,\frac{\phi(\psi)}{\sqrt{\psi_0-\psi}} + \sqrt{\bar{b}}\sqrt{\bar{b}\left[\frac{\phi(\psi)}{\sqrt{\psi_0-\psi}}\right]^2 + \bar{d}\,(\psi_0-\psi)^3}\right]} = -\lim_{\psi\nearrow\psi_0}\frac{(\psi-\psi_0)^2}{4\frac{\cos^2\alpha}{\sin\alpha}} = 0.
\end{aligned}$$

Furthermore, it can be shown that the sum of the remaining two terms on the right-hand side of (B.4.35) is finite at $\psi = \psi_0$. To be precise, it can be shown that

$$\lim_{\psi\nearrow\psi_0}\left[\frac{\sqrt{\bar b}\,\phi'(\psi)}{\sqrt{\bar b\,\phi(\psi)^2+\bar d\,(\psi-\psi_0)^4}}+\frac{1}{2}\frac{1}{\psi_0-\psi}\right]=\lim_{\psi\nearrow\psi_0}\frac{\frac{\sqrt{\bar b}\,\phi'(\psi)\,\sqrt{\psi_0-\psi}}{\sqrt{\bar b\left[\frac{\phi(\psi)}{\sqrt{\psi_0-\psi}}\right]^2+\bar d\,(\psi_0-\psi)^3}}+\frac{1}{2}}{\psi_0-\psi}.$$

is finite using L'Hôpital's rule. Indeed, since $\lim_{\psi\nearrow\psi_0}\phi(\psi)/\sqrt{\psi_0-\psi}$ is non-zero and finite (cf. (B.4.27)), and since $\lim_{\psi\nearrow\psi_0}\phi'(\psi)\,\sqrt{\psi_0-\psi}$ is finite (cf. (B.4.27)) it is not hard to show that the numerator of the quotient on the right-hand side tends to zero as ψ tends to ψ_0. Thus, L'Hôpital's rule can be applied to get

$$\begin{aligned}
&\lim_{\psi\nearrow\psi_0}\left[\frac{\sqrt{\bar b}\,\phi'(\psi)}{\sqrt{\bar b\,\phi(\psi)^2+\bar d\,(\psi-\psi_0)^4}}+\frac{1}{2}\frac{1}{\psi_0-\psi}\right]\\
&=-\lim_{\psi\nearrow\psi_0}\left\{\frac{\sqrt{\bar b}\left[\phi''(\psi)\,\sqrt{\psi_0-\psi}-\frac{1}{2}\frac{\phi'(\psi)}{\sqrt{\psi_0-\psi}}\right]}{\sqrt{\bar b\left[\frac{\phi(\psi)}{\sqrt{\psi_0-\psi}}\right]^2+\bar d\,(\psi_0-\psi)^3}}\right. \qquad\qquad (B.4.36)\\
&\qquad\left.-\frac{\sqrt{\bar b}}{2}\,\phi'(\psi)\,\sqrt{\psi_0-\psi}\,\frac{2\bar b\left[\frac{\phi'(\psi)}{\sqrt{\psi_0-\psi}}+\frac{1}{2}\frac{\phi(\psi)}{\sqrt{\psi_0-\psi}^3}\right]\left[\frac{\phi(\psi)}{\sqrt{\psi_0-\psi}}\right]-3\bar d\,(\psi_0-\psi)^3}{\sqrt{\bar b\left[\frac{\phi(\psi)}{\sqrt{\psi_0-\psi}}\right]^2+\bar d\,(\psi_0-\psi)^3}^{\,3}}\right\},
\end{aligned}$$

where (cf. (B.4.21))

$$\phi''(\psi)=-\frac{\cos\alpha}{1-\psi^2}\frac{\psi}{\sqrt{\sin^2\alpha-\psi^2}}\left[\frac{2}{1-\psi^2}+\frac{1}{\sin^2\alpha-\psi^2}\right].$$

Using the same arguments for $\phi(\psi)/\sqrt{\psi_0-\psi}$ and $\phi'(\psi)\,\sqrt{\psi_0-\psi}$ as before and since, applying L'Hôpital's rule, (cf. (B.4.21))

$$\begin{aligned}
\lim_{\psi\nearrow\psi_0}\left[\frac{\phi'(\psi)}{\sqrt{\psi_0-\psi}}+\frac{1}{2}\frac{\phi(\psi)}{\sqrt{\psi_0-\psi}^3}\right]&=\lim_{\psi\nearrow\psi_0}\frac{\phi'(\psi)\,(\psi_0-\psi)+\frac{1}{2}\,\phi(\psi)}{\sqrt{\psi_0-\psi}^3}\\
&=-\frac{2}{3}\lim_{\psi\nearrow\psi_0}\left[\phi''(\psi)\,\sqrt{\psi_0-\psi}-\frac{1}{2}\frac{\phi'(\psi)}{\sqrt{\psi_0-\psi}}\right]\\
&=\frac{2}{3}\lim_{\psi\nearrow\psi_0}\left[\frac{\cos\alpha}{(1-\psi^2)^2}\frac{2\psi}{\sqrt{\psi_0+\psi}}+\frac{\cos\alpha}{1-\psi^2}\frac{\psi}{\sqrt{\psi_0+\psi}^3}\frac{1}{\psi_0-\psi}-\frac{1}{2}\frac{\cos\alpha}{1-\psi^2}\frac{1}{\sqrt{\psi_0+\psi}}\frac{1}{\psi_0-\psi}\right]\\
&=\frac{2}{3}\lim_{\psi\nearrow\psi_0}\left[\frac{\cos\alpha}{(1-\psi^2)^2}\frac{2\psi}{\sqrt{\psi_0+\psi}}-\frac{1}{2}\frac{\cos\alpha}{1-\psi^2}\frac{1}{\sqrt{\psi_0+\psi}^3}\right]=\frac{2}{3}\frac{\sqrt{2\sin\alpha}}{\cos\alpha}\left[\frac{1}{\cos^2\alpha}-\frac{1}{8\sin^2\alpha}\right]
\end{aligned}$$

is finite, it can be proven that (B.4.36) is also finite. It follows that the last integral on the right-hand side of (B.4.34) exists absolutely and the Riemann-Lebesgue lemma gives

$$\begin{aligned}
I_2&=\frac{2}{\sqrt{\bar b}\,ikR}\log\!\left(2\sqrt{2}\frac{\cos\alpha}{\sqrt{\sin\alpha}}\right)e^{ikR\psi_0}\\
&\quad-\frac{2}{\sqrt{\bar b}\,ikR}\left\{\log\!\left(\bar b\,\pi+\sqrt{\bar b}\sqrt{\bar b\,\pi^2+16\bar d\,\psi_0^4}\right)-\frac{1}{2}\,\log(2\psi_0)\right\}e^{-ikR\psi_0}+o\left(\frac{1}{R}\right) \qquad (B.4.37)
\end{aligned}$$

for $m'/|m'|=\nu'$.

Now only the evaluation of the integrals in I_3 (cf. (B.4.32)) remains. The first step is to substitute $(\psi_0-\psi)/(2\sin\alpha)$ by u in the first integral and $(\psi-\psi_0)/(1-\sin\alpha)$ by u in the second integral, such that

$$I_3=2\frac{\sin\alpha}{\sqrt{\bar b}}\int_0^1\log(2\sin\alpha\,u)\,e^{-ikR2\sin\alpha u}\,\mathrm{d}u\,e^{ikR\psi_0}+4\frac{1-\sin\alpha}{\sqrt{\bar b}}\int_0^1\log\big((1-\sin\alpha)\,u\big)\,e^{ikR(1-\sin\alpha)u}\,\mathrm{d}u\,e^{ikR\psi_0}$$

$$= 2\frac{\sin\alpha\,\log(2\sin\alpha)}{\sqrt{b}}\int_0^1 e^{-ikR2\sin\alpha u}\,\mathrm{d}u\,e^{ikR\psi_0} + 4\frac{(1-\sin\alpha)\,\log(1-\sin\alpha)}{\sqrt{b}}\int_0^1 e^{ikR(1-\sin\alpha)u}\,\mathrm{d}u\,e^{ikR\psi_0}$$
$$+ 2\frac{\sin\alpha}{\sqrt{b}}\int_0^1 \log u\, e^{-ikR2\sin\alpha u}\,\mathrm{d}u\,e^{ikR\psi_0} + 4\frac{1-\sin\alpha}{\sqrt{b}}\int_0^1 \log u\, e^{ikR(1-\sin\alpha)u}\,\mathrm{d}u\,e^{ikR\psi_0}$$
$$= -\frac{\log(2\sin\alpha)}{ikR\sqrt{b}}\left[e^{-ikR2\sin\alpha}-1\right]e^{ikR\psi_0} + 4\frac{\log(\sin\alpha-1)}{ikR\sqrt{b}}\left[e^{ikR(1-\sin\alpha)}-1\right]e^{ikR\psi_0}$$
$$+ 2\frac{\sin\alpha}{\sqrt{b}}\int_0^1 \log u\, e^{-ikR2\sin\alpha u}\,\mathrm{d}u\,e^{ikR\psi_0} - 4\frac{\sin\alpha-1}{\sqrt{b}}\int_0^1 \log u\, e^{ikR(1-\sin\alpha)u}\,\mathrm{d}u\,e^{ikR\psi_0},$$

where, defining $s := -2\sin\alpha < 0$ or $s := 1-\sin\alpha > 0$, (cf. [32, Eqn. 106, pp. 27 and 82] and [1, Eqns. 5.2.8, 5.2.9, 5.2.34 and 5.2.35, pp. 60 and 61])

$$\int_0^1 \log u\, e^{iksR\,u}\,\mathrm{d}u = \frac{\tilde{\gamma}+\log(ksR)-\mathrm{Ci}(ksR)-i\,\mathrm{Si}(ksR)}{iksR} = \frac{\tilde{\gamma}+\log(ksR)-i\frac{\pi}{2}}{iksR} + o\left(\frac{1}{R}\right),$$

for $ksR > 0$. Note that the definitions of Ci and Si (cf. [1, Eqns. 5.2.1 and 5.2.2, p. 59]) yield that $\mathrm{Ci}(-kR2\sin\alpha) = \mathrm{Ci}(kR2\sin\alpha) + \log(-1)$ and $\mathrm{Si}(-kR2\sin\alpha) = -\,\mathrm{Si}(kR2\sin\alpha)$, where $kR2\sin\alpha > 0$. With this, I_3 reduces to

$$I_3 = -\frac{\log(2\sin\alpha)}{ikR\sqrt{b}}\left[e^{-ikR2\sin\alpha}-1\right]e^{ikR\psi_0} + 4\frac{\log(1-\sin\alpha)}{ikR\sqrt{b}}\left[e^{ikR(1-\sin\alpha)}-1\right]e^{ikR\psi_0}$$
$$- \frac{\tilde{\gamma}+\log(-kR)-\log(-1)+i\frac{\pi}{2}}{ikR\sqrt{b}}\,e^{ikR\psi_0} - \frac{\log(2\sin\alpha)}{ikR\sqrt{b}}\,e^{ikR\psi_0} + 4\frac{\tilde{\gamma}+\log(kR)-i\frac{\pi}{2}}{ikR\sqrt{b}}\,e^{ikR\psi_0}$$
$$+ 4\frac{\log(1-\sin\alpha)}{ikR\sqrt{b}}\,e^{ikR\psi_0} + o\left(\frac{1}{R}\right)$$
$$= -\frac{\log(2\sin\alpha)}{ikR\sqrt{b}}\,e^{-ikR2\sin\alpha}e^{ikR\psi_0} + 4\frac{\log(1-\sin\alpha)}{ikR\sqrt{b}}\,e^{ikR(1-\sin\alpha)}e^{ikR\psi_0}$$
$$+ \frac{3\tilde{\gamma}+3\log(kR)-5\,i\frac{\pi}{2}}{ikR\sqrt{b}}\,e^{ikR\psi_0} + o\left(\frac{1}{R}\right),$$

since $\log(-1) = i\pi$. Consequently, (cf. (B.4.12), (B.4.25), (B.4.29), (B.4.30), (B.4.31), (B.4.33) and (B.4.37))

$$\tilde{J}_2 = f_{\ell,j}(\nu',0)\left\{\frac{\log(\bar{b}\bar{d})}{\sqrt{b}\,ikR}\,e^{ikR\psi_0} - \frac{2}{\sqrt{b}\,ikR}\log\left(2\sqrt{2}\frac{\cos\alpha}{\sqrt{\sin\alpha}}\right)e^{ikR\psi_0} - \frac{3\tilde{\gamma}+3\log(kR)-5\,i\frac{\pi}{2}}{ikR\sqrt{b}}\,e^{ikR\psi_0}\right\}$$
$$+ o\left(\frac{1}{R}\right)$$
$$= f_{\ell,j}(\nu',0)\,\frac{-2\log m_z-2\log 2-2\log 2-\log 2-2\log m_z+\log|m'|-3\left(\tilde{\gamma}+\log(kR)\right)+5\,i\frac{\pi}{2}}{ikRm_z}\,e^{ikR\,|m'|}$$
$$+ o\left(\frac{1}{R}\right)$$
$$= f_{\ell,j}(\nu',0)\,\frac{\log|m'|-5\log 2-4\log m_z-3\left(\tilde{\gamma}+\log(kR)\right)+5\,i\frac{\pi}{2}}{ikRm_z}\,e^{ikR\,|m'|} + o\left(\frac{1}{R}\right),$$

since $\bar{b}\bar{d} = 1/(4\cos^2\alpha)$ (cf. (B.4.17)), $m_z = \cos\alpha$ and $|m'| = \sin\alpha = \psi_0$. At last, for $m'/|m'| = \nu'$ (cf. (B.4.2) and (B.4.5))

$$\mathcal{J}_1 = \frac{2\pi}{ikR}\frac{f_{\ell,j}(m',m_z)}{|m'-\nu'|}\,e^{ikR} + f_{\ell,j}(\nu',0)\,\frac{\log|m'|-5\log 2-4\log m_z-3\left(\tilde{\gamma}+\log(kR)\right)+5\,i\frac{\pi}{2}}{ikRm_z}\,e^{ikR\,|m'|}$$
$$+ o\left(\frac{1}{R}\right).$$

Adding this to $\mathcal{J}_2$ (cf. (B.2.4) and (B.3.95)) for the case of $m'/|m'| = \nu'$ gives the final formula

$$\mathcal{J} = \frac{2\pi}{ikR}\frac{f_{\ell,j}(m',m_z)}{|m'-\nu'|}\, e^{ikR} + f_{\ell,j}(\nu',0)\frac{2\pi}{kRm_z}\, e^{ikR\,|m'|} + o\left(\frac{1}{R}\right). \tag{B.4.38}$$

B.4.3 Singular integral part for oblique reflection with singularity in different direction

To show the asymptotic behaviour of $\tilde{J}_2$ (cf. (B.4.3)) in the case that $m'/|m'| \neq \nu'$, the order of integration is changed and the integral is split into five different parts. For each of these parts, the order of decay as R tends to infinity will be shown separately in the following subsections. To do so, the cut-off function $\chi(n')$ is specified as a cut off function $\chi(|n'|)$, only depending on the distance from the origin. Furthermore, the variable $\tilde{\epsilon}_R$ is defined as

$$\tilde{\epsilon}_R := \frac{1}{R^3} \tag{B.4.39}$$

for all $R > 1$ such that $\chi(1-\tilde{\epsilon}_R) = 1$. Thus

$$\tilde{J}_2 = \tilde{J}_3 + \tilde{J}_4 + \tilde{J}_5 + \tilde{J}_6 + \tilde{J}_7, \tag{B.4.40}$$

where

$$\begin{aligned}
\tilde{J}_3 &:= \int\limits_{\phi_0-\pi}^{\phi_0+\pi}\int\limits_{|m'|}^{1-\tilde{\epsilon}_R} \chi(\rho)\frac{f_{\ell,j}(\rho n_0'(\phi),\sqrt{1-\rho^2})}{|\rho n_0'(\phi)-\nu'|}\, e^{ik\rho R n_0'(\phi)\cdot m'}\,\frac{\rho}{\sqrt{1-\rho^2}}\, e^{ikRm_z\sqrt{1-\rho^2}}\,\mathrm{d}\rho\,\mathrm{d}\phi,\\
\tilde{J}_4 &:= \int\limits_{1-\tilde{\epsilon}_R}^{1}\left\{\int\limits_{\phi_0-\pi}^{\phi_0+\pi} f_{\ell,j}(\rho n_0'(\phi),\sqrt{1-\rho^2})\left[\frac{\chi(\rho)}{|\rho n_0'(\phi)-\nu'|} - \frac{1}{\sqrt{(1-\rho)^2+(\phi-\phi_0)^2}}\right] e^{ik\rho R n_0'(\phi)\cdot m'}\,\mathrm{d}\phi\right.\\
&\qquad\left.\frac{\rho}{\sqrt{1-\rho^2}}\, e^{ikRm_z\sqrt{1-\rho^2}}\right\}\mathrm{d}\rho,
\end{aligned} \tag{B.4.41}$$

$$\tilde{J}_5 := \int\limits_{1-\tilde{\epsilon}_R}^{1}\int\limits_{\phi_0-\pi}^{\phi_0+\pi}\frac{f_{\ell,j}(\rho n_0'(\phi),\sqrt{1-\rho^2}) - f_{\ell,j}(\nu',0)}{\sqrt{(1-\rho)^2+(\phi-\phi_0)^2}}\, e^{ik\rho R n_0'(\phi)\cdot m'}\,\mathrm{d}\phi\,\frac{\rho}{\sqrt{1-\rho^2}}\, e^{ikRm_z\sqrt{1-\rho^2}}\,\mathrm{d}\rho, \tag{B.4.42}$$

$$\tilde{J}_6 := f_{\ell,j}(\nu',0)\int\limits_{1-\tilde{\epsilon}_R}^{1}\int\limits_{\phi_0-\pi}^{\phi_0+\pi}\frac{e^{ik(\rho-1)Rn_0'(\phi)\cdot m'}-1}{\sqrt{(1-\rho)^2+(\phi-\phi_0)^2}}\, e^{ikRn_0'(\phi)\cdot m'}\,\mathrm{d}\phi\,\frac{\rho}{\sqrt{1-\rho^2}}\, e^{ikRm_z\sqrt{1-\rho^2}}\,\mathrm{d}\rho, \tag{B.4.43}$$

$$\tilde{J}_7 := f_{\ell,j}(\nu',0)\int\limits_{1-\tilde{\epsilon}_R}^{1}\int\limits_{\phi_0-\pi}^{\phi_0+\pi}\frac{1}{\sqrt{(1-\rho)^2+(\phi-\phi_0)^2}}\, e^{ikRn_0'(\phi)\cdot m'}\,\mathrm{d}\phi\,\frac{\rho}{\sqrt{1-\rho^2}}\, e^{ikRm_z\sqrt{1-\rho^2}}\,\mathrm{d}\rho. \tag{B.4.44}$$

For convenience the term $n_0'(\phi)$ will be shortly denoted by n_0' for the remainder of this section.

B.4.3.1 $\tilde{J}_3$

To show the asymptotic behaviour of $\tilde{J}_3$, the term is integrated by parts w.r.t. ρ, such that with $\chi(1-\tilde{\epsilon}_R) = 1$ and $\chi(|m'|) = 0$,

$$\begin{aligned}
\tilde{J}_3 &= -\frac{1}{ikRm_z}\int\limits_{\phi_0-\pi}^{\phi_0+\pi}\int\limits_{|m'|}^{1-\tilde{\epsilon}_R}\chi(\rho)\frac{f_{\ell,j}(\rho n_0',\sqrt{1-\rho^2})}{|\rho n_0'-\nu'|}\, e^{ik\rho Rn_0'\cdot m'}\,\partial_\rho\Big[e^{ikRm_z\sqrt{1-\rho^2}}\Big]\,\mathrm{d}\rho\,\mathrm{d}\phi\\
&= -\frac{1}{ikRm_z}\int\limits_{\phi_0-\pi}^{\phi_0+\pi}\frac{f_{\ell,j}((1-\tilde{\epsilon}_R)n_0',\sqrt{2\tilde{\epsilon}_R-\tilde{\epsilon}_R^2})}{|(1-\tilde{\epsilon}_R)n_0'-\nu'|}\, e^{ik(1-\tilde{\epsilon}_R)Rn_0'\cdot m'}\, e^{ikRm_z\sqrt{2\tilde{\epsilon}_R-\tilde{\epsilon}_R^2}}\,\mathrm{d}\phi\\
&\quad + \tilde{J}_{3.1} + \tilde{J}_{3.2} + \tilde{J}_{3.3} + \tilde{J}_{3.4},
\end{aligned} \tag{B.4.45}$$

where

$$\tilde{J}_{3.1} := \frac{1}{ikRm_z} \int_{\phi_0-\pi}^{\phi_0+\pi} \int_{|m'|}^{1-\tilde{\epsilon}_R} \chi'(\rho) \frac{f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2})}{|\rho n_0' - \nu'|} \, e^{ik\rho R n_0' \cdot m'} \, e^{ikRm_z\sqrt{1-\rho^2}} \, \mathrm{d}\rho \, \mathrm{d}\phi,$$

$$\tilde{J}_{3.2} := \frac{1}{ikRm_z} \int_{\phi_0-\pi}^{\phi_0+\pi} \int_{|m'|}^{1-\tilde{\epsilon}_R} \chi(\rho) \frac{\left(n_0', -\frac{\rho}{\sqrt{1-\rho^2}}\right)^\top \cdot \nabla_{\vec{n}} f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2})}{|\rho n_0' - \nu'|} \, e^{ik\rho R n_0' \cdot m'} \, e^{ikRm_z\sqrt{1-\rho^2}} \, \mathrm{d}\rho \, \mathrm{d}\phi,$$

$$\tilde{J}_{3.3} := -\frac{1}{ikRm_z} \int_{\phi_0-\pi}^{\phi_0+\pi} \int_{|m'|}^{1-\tilde{\epsilon}_R} \chi(\rho) \frac{f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2}) \, n_0' \cdot (\rho n_0' - \nu')}{|\rho n_0' - \nu'|^3} \, e^{ik\rho R n_0' \cdot m'} \, e^{ikRm_z\sqrt{1-\rho^2}} \, \mathrm{d}\rho \, \mathrm{d}\phi,$$

$$\tilde{J}_{3.4} := \frac{1}{m_z} \int_{\phi_0-\pi}^{\phi_0+\pi} \int_{|m'|}^{1-\tilde{\epsilon}_R} \chi(\rho) \frac{f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2}) \, n_0' \cdot m'}{|\rho n_0' - \nu'|} \, e^{ik\rho R n_0' \cdot m'} \, e^{ikRm_z\sqrt{1-\rho^2}} \, \mathrm{d}\rho \, \mathrm{d}\phi.$$

First consider $\tilde{J}_{3.1}$. Note, that the derivative $\chi'(\rho)$ in $\tilde{J}_{3.1}$ removes the singularity at $(\rho, \phi)^\top = (1, \phi_0)^\top$, since $\operatorname{supp}\chi' \subseteq [|m'|, (1+|m'|)/2]$, with $|m'| < 1$ (cf. beginnings of Sections B.4.1 and B.4.3). Thus, after switching the order of integration of $\tilde{J}_{3.1}$, it is easily seen that, for any fixed $\rho \in [|m'|, (|m'|+1)/2]$, the integrand of the integral w.r.t. ϕ in

$$\left|\tilde{J}_{3.1}\right| \leq \frac{1}{kRm_z} \int_{|m'|}^{1-\tilde{\epsilon}_R} \left| \int_{\phi_0-\pi}^{\phi_0+\pi} \chi'(\rho) \, \frac{f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2})}{|\rho n_0' - \nu'|} \, e^{ik\rho R n_0' \cdot m'} \, \mathrm{d}\phi \right| \mathrm{d}\rho$$

is bounded for any fixed ρ in the bounded set $[|m'|, (|m'|+1)/2]$. Since $n_0' \cdot m' = |m'| \cos(\psi_0 - \phi_1)$, where $n_0'(\phi_0) = \nu'$ and $|m'| \, n_0'(\phi_1) = m'$, Lemma B.3 with the occurring r set to zero and Lebesgue's theorem now show that

$$\tilde{J}_{3.1} = o\left(\frac{1}{R}\right). \tag{B.4.46}$$

To determine the asymptotic behaviour of $\tilde{J}_{3.2}$ to $\tilde{J}_{3.4}$ the coordinate system is changed to the modified spherical system used for $\tilde{J}_1$ in Section B.4.1. To be precise, the currently used system of polar coordinates $(\rho, \phi)^\top$ is returned to the Cartesian system n' and afterwards the transformation, introduced in Section 4.2.3 (cf. (4.2.22) and (4.2.23)), leading to (B.4.4) in Section B.4.1 is applied. Taking into account that $n' = \rho n_0'$, $\rho = |n'|$, $\sqrt{1-\rho^2} = n_z^r$ and $\mathrm{d}\phi \, \mathrm{d}\rho = n_z^r(\psi, \phi)/|n'(\psi, \phi)| \, \mathrm{d}\psi \, \mathrm{d}\phi$, this transformation gives

$$\tilde{J}_{3.2} := \frac{1}{ikRm_z} \int_0^{2\pi} \int_{\psi_R(\phi)}^1 \chi(|n'(\psi, \phi)|) \frac{\left(\frac{n'(\psi,\phi)}{|n'(\psi,\phi)|^2} \, n_z^r(\psi, \phi), -1\right)^\top \cdot \nabla_{\vec{n}} f_{\ell,j}\Big(n'(\psi, \phi), n_z^r(\psi, \phi)\Big)}{\big|n'(\psi, \phi) - \nu'\big|} \, e^{ikR\psi} \, \mathrm{d}\psi \, \mathrm{d}\phi, \tag{B.4.47}$$

$$\tilde{J}_{3.3} := -\frac{1}{ikRm_z} \int_0^{2\pi} \int_{\psi_R(\phi)}^1 \Bigg\{ \chi(|n'(\psi, \phi)|) \, \frac{f_{\ell,j}\Big(n'(\psi, \phi), n_z^r(\psi, \phi)\Big)}{\big|n'(\psi, \phi)\big|^2} \frac{n'(\psi, \phi) \cdot \big[n'(\psi, \phi) - \nu'\big] \, n_z^r(\psi, \phi)}{\big|n'(\psi, \phi) - \nu'\big|^3} \, e^{ikR\psi} \Bigg\} \mathrm{d}\psi \, \mathrm{d}\phi, \tag{B.4.48}$$

$$\tilde{J}_{3.4} := \frac{1}{m_z} \int_0^{2\pi} \int_{\psi_R(\phi)}^1 \chi(|n'(\psi, \phi)|) \frac{f_{\ell,j}\Big(n'(\psi, \phi), n_z^r(\psi, \phi)\Big) \, n'(\psi, \phi) \cdot m' \, n_z^r(\psi, \phi)}{\big|n'(\psi, \phi) - \nu'\big| \, \big|n'(\psi, \phi)\big|^2} \, e^{ikR\psi} \, \mathrm{d}\psi \, \mathrm{d}\phi, \tag{B.4.49}$$

where $\psi_R(\phi) := \cos\theta_R(\phi)$ and $\theta_R(\phi)$ the polar angle at which

$$\left|n'(\psi_R(\phi),\phi)\right| = 1 - \tilde{\epsilon}_R \tag{B.4.50}$$

for all $\phi \in [0,2\pi]$. Note that $0 \notin \operatorname{supp}\chi$, such that the term $\chi(|n'(\psi,\phi)|)/|n'(\psi,\phi)|^2$ in (B.4.47) to (B.4.49) does not introduce a singularity into the integrands. The term $n_z^r(\psi,\phi)$ on the other hand is zero at $\psi = \psi(\phi) := \lim_{R\to\infty}\psi_R(\phi)$.

To obtain the asymptotic behaviour of $\tilde{J}_{3.2}$ to $\tilde{J}_{3.4}$, consider the following lemma.

Lemma B.4. *Assuming any locally integrable function* $(\psi,\phi) \mapsto F(n'(\psi,\phi))\, e^{ikR\psi}$ *for* $\psi \in [\psi(\phi),1]$ *and* $\phi \in [0,2\pi]$, *where*

$$\left|F\big(n'(\psi,\phi)\big)\right| \le c\frac{\log\left|n'(\psi,\phi)-\nu'\right|}{\left|n'(\psi,\phi)-\nu'\right|}$$

at $(\psi,\phi) = (\psi(\phi_0),\phi_0)$ *and* ϕ_0 *is defined such that* $n'(\psi(\phi_0),\phi_0) = \nu'$. *Then, with* $\psi_R(\phi)$ *defined as above,*

$$\lim_{R\to\infty}\int_0^{2\pi}\int_{\psi_R(\phi)}^{1} F(n'(\psi,\phi))\, e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi = 0.$$

Proof. The first step is to split the integral into two parts, i.e.

$$\int_0^{2\pi}\int_{\psi_R(\phi)}^{1} F\big(n'(\psi,\phi)\big)\, e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi = \int_0^{2\pi}\int_{\psi(\phi)}^{1} F\big(n'(\psi,\phi)\big)\, e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi - \int_0^{2\pi}\int_{\psi(\phi)}^{\psi_R(\phi)} F\big(n'(\psi,\phi)\big)\, e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi. \tag{B.4.51}$$

To show that the first integral on the right-hand side tends to zero, the Riemann-Lebesgue lemma and Lebesgue's theorem have to be applied. To do so, it has to be shown that

$$\int_0^{2\pi}\left|\int_{\psi(\phi)}^{1} F\big(n'(\psi,\phi)\big)\, e^{ikR\psi}\,\mathrm{d}\psi\right|\mathrm{d}\phi \le \int_0^{2\pi}\int_{\psi(\phi)}^{1}\left|F\big(n'(\psi,\phi)\big)\right|\mathrm{d}\psi\,\mathrm{d}\phi \le c\int_0^{2\pi}\int_{\psi(\phi)}^{1}\frac{\left|\log|n'(\psi,\phi)-\nu'|\right|}{\left|n'(\psi,\phi)-\nu'\right|}\,\mathrm{d}\psi\,\mathrm{d}\phi$$

is finite. On the other hand, undoing the substitution (4.2.22) and returning to Cartesian coordinates n' leads to

$$\int_0^{2\pi}\int_{\psi(\phi)}^{1}\frac{\left|\log|n'(\psi,\phi)-\nu'|\right|}{\left|n'(\psi,\phi)-\nu'\right|}\,\mathrm{d}\psi\,\mathrm{d}\phi = \int_{B_2(1)}\frac{\left|\log|n'-\nu'|\right|}{\left|n'-\nu'\right|}\,\frac{1}{\sqrt{1-|n'|^2}}\,\mathrm{d}n',$$

which is finite according to Lemma 3.11. Thus, the Riemann-Lebesgue lemma implies

$$\lim_{R\to\infty}\int_0^{2\pi}\int_{\psi(\phi)}^{1} F\big(n'(\psi,\phi)\big)\, e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi = 0.$$

It is more involved to prove the same for the second integral on the right-hand side of (B.4.51). Similarly to the first integral, the integral is bounded from above and the substitution (4.2.22) is undone, i.e.

$$\begin{aligned}\left|\int_0^{2\pi}\int_{\psi(\phi)}^{\psi_R(\phi)} F\big(n'(\psi,\phi)\big)\, e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi\right| &\le \int_0^{2\pi}\int_{\psi(\phi)}^{\psi_R(\phi)}\left|F\big(n'(\psi,\phi)\big)\right|\mathrm{d}\psi\,\mathrm{d}\phi\\ &\le c\int_0^{2\pi}\int_{\psi(\phi)}^{\psi_R(\phi)}\frac{\left|\log|n'(\psi,\phi)-\nu'|\right|}{\left|n'(\psi,\phi)-\nu'\right|}\,\mathrm{d}\psi\,\mathrm{d}\phi\\ &= c\int_{D_R}\frac{\left|\log|n'-\nu'|\right|}{\left|n'-\nu'\right|}\,\frac{1}{\sqrt{1-|n'|^2}}\,\mathrm{d}n',\end{aligned} \tag{B.4.52}$$

where $\nu' \in D_R \subset B_2(1)$. Note that $D_R := \{n' = n'(\psi,\phi) \in \mathbb{R}^2 | \, \phi \in [0,2\pi] \text{ and } \psi \in [\psi(\phi), \psi_R(\phi)]\}$ is the annulus $\{n' \in \mathbb{R}^2 | 1-\tilde{\epsilon}_R \le |n'| \le 1\}$, since $\psi_R(\phi)$ is defined such that $|n'(\psi_R(\phi),\phi)| = 1-\tilde{\epsilon}_R$ (cf. (B.4.50)) and $\psi(\phi)$ such that $|n'(\psi(\phi),\phi)| = 1$. Naturally, D_R tends to the zero set of the unit circle as R tends to infinity (cf. (B.4.39)) and $\nu' = n'(\psi(\phi_0),\phi_0) \in D_R$ for any fixed $R > 1$, since $|\nu'| = 1$. Next, it will be shown that the integral over D_R tends to zero as R tends to infinity. For this, the same approach as for the proof of Lemma 3.11 is used. First, however, the domain of integration D_R is split into a small neighbourhood around the singularity $n' = \nu'$ and the rest. To be precise, as in the proof of Lemma 3.11, it is assumed w.l.o.g. that $\nu' = (0,1)^\top$ such that the small neighbourhood around the singularity $n' = \nu'$ can be defined as all $n' \in D_R$ with $n_x \in [-\epsilon,\epsilon]$ and $n_y > 0$ for a small and fixed $\epsilon > 0$. Now, it is not hard to show that the complement of this neighbourhood w.r.t. D_R is contained in the section of the annulus

$$\left\{ n' = \rho \begin{pmatrix} \cos\gamma \\ \sin\gamma \end{pmatrix} \in \mathbb{R}^2 \,\middle|\, \rho \in [1-\tilde{\epsilon}_R, 1] \text{ and } \gamma \in \left[\frac{\pi}{2}-\gamma_\epsilon, \frac{\pi}{2}+\gamma_\epsilon\right] \text{ with } \sin\gamma_\epsilon = \epsilon \text{ s.t. } n_x\Big(1, \frac{\pi}{2}\pm\gamma_\epsilon\Big) = \mp\epsilon \right\}.$$

Thus, representing the integral over this annulus section in the polar coordinate system (ρ,γ) and defining $n_0' := n_0'(\gamma) := (\cos\gamma, \sin\gamma)$ gives (cf. (B.4.52))

$$\begin{aligned} \left| \int_0^{2\pi} \int_{\psi(\phi)}^{\psi_R(\phi)} F\big(n'(\psi,\phi)\big)\, e^{ikR\psi}\, \mathrm{d}\psi\, \mathrm{d}\phi \right| &\le c \int_{D_R} \frac{\big|\log|n'-\nu'|\big|}{|n'-\nu'|} \frac{1}{\sqrt{1-|n'|^2}}\, \mathrm{d}n' \\ &\le c \int_{-\epsilon}^{\epsilon} \int_{\sqrt{(1-\tilde{\epsilon}_R)^2-n_x^2}}^{\sqrt{1-n_x^2}} \frac{\big|\log|n'-\nu'|\big|}{|n'-\nu'|} \frac{1}{\sqrt{1-|n'|^2}}\, \mathrm{d}n' \\ &\quad + c \left(\int_0^{\frac{\pi}{2}-\gamma_\epsilon} + \int_{\frac{\pi}{2}+\gamma_\epsilon}^{2\pi} \right) \int_{1-\tilde{\epsilon}_R}^{1} \frac{\big|\log|\rho n_0'-\nu'|\big|}{|\rho n_0'-\nu'|} \frac{\rho}{\sqrt{1-\rho^2}}\, \mathrm{d}\rho\, \mathrm{d}\gamma. \end{aligned}$$

Since $|\gamma - \pi/2| \ge \gamma_\epsilon > 0$ and $\nu' = n_0'(\pi/2)$, it is easily seen that $|\log|\rho n_0' - \nu'||/|\rho n_0' - \nu'| \le c_\epsilon$ in the second integral on the right-hand side. Therefore,

$$\left(\int_0^{\frac{\pi}{2}-\gamma_\epsilon} + \int_{\frac{\pi}{2}+\gamma_\epsilon}^{2\pi} \right) \int_{1-\tilde{\epsilon}_R}^{1} \frac{\big|\log|\rho n_0'-\nu'|\big|}{|\rho n_0'-\nu'|} \frac{\rho}{\sqrt{1-\rho^2}}\, \mathrm{d}\rho\, \mathrm{d}\gamma \le 2\pi c_\epsilon \int_{1-\tilde{\epsilon}_R}^{1} \frac{\rho}{\sqrt{1-\rho^2}}\, \mathrm{d}\rho = \mathcal{O}\left(\frac{1}{R^{\frac{3}{2}}}\right)$$

such that

$$\begin{aligned} \left| \int_0^{2\pi} \int_{\psi(\phi)}^{\psi_R(\phi)} F\big(n'(\psi,\phi)\big)\, e^{ikR\psi}\, \mathrm{d}\psi\, \mathrm{d}\phi \right| &\le c \int_{-\epsilon}^{\epsilon} \int_{\sqrt{(1-\tilde{\epsilon}_R)^2-n_x^2}}^{\sqrt{1-n_x^2}} \frac{\big|\log|n'-\nu'|\big|}{|n'-\nu'|} \frac{1}{\sqrt{1-|n'|^2}}\, \mathrm{d}n' + \mathcal{O}\left(\frac{1}{R^{\frac{3}{2}}}\right) \\ &\le c \int_{-\epsilon}^{\epsilon} \int_{\sqrt{1-\tilde{\epsilon}_R^2-n_x^2}}^{\sqrt{1+\tilde{\epsilon}_R^2-n_x^2}} \frac{\big|\log|n'-\nu'|\big|}{|n'-\nu'|} \frac{1}{\sqrt{1-|n'|^2}}\, \mathrm{d}n' + \mathcal{O}\left(\frac{1}{R^{\frac{3}{2}}}\right). \end{aligned}$$

Using (3.3.36), (3.3.37) and (3.3.38) from the proof of Lemma 3.11 with $\epsilon_x = \epsilon$ and $\epsilon_y = \tilde{\epsilon}_R$, it is easily shown that

$$\left| \int_0^{2\pi} \int_{\psi(\phi)}^{\psi_R(\phi)} F\big(n'(\psi,\phi)\big)\, e^{ikR\psi}\, \mathrm{d}\psi\, \mathrm{d}\phi \right| \le c \int_{-\epsilon}^{\epsilon} \int_{\sqrt{1-1/R^3-n_x^2}}^{\sqrt{1+1/R^3-n_x^2}} \frac{\big|\log|n'-\nu'|\big|}{|n'-\nu'|} \frac{1}{\sqrt{|1-|n'|^2|}}\, \mathrm{d}n_y\, \mathrm{d}n_x + \mathcal{O}\left(\frac{1}{R^{\frac{3}{2}}}\right)$$

$$
\begin{aligned}
&\leq c \int_0^{1/R^3} \frac{(\log t_y)^2}{\sqrt{t_y}}\, \mathrm{d}t_y + c \int_0^{1/R^3} \frac{1}{\sqrt{t_y}}\, \mathrm{d}t_y + \frac{c}{\epsilon^{\frac{1}{3}}} \int_0^{1/R^3} \frac{1}{t_y^{\frac{5}{6}}}\, \mathrm{d}t_y + \mathcal{O}\left(\frac{1}{R^{\frac{3}{2}}}\right) \\
&\leq c \int_0^{1/R^3} \frac{1}{t_y^{\frac{2}{3}}}\, \mathrm{d}t_y + 2c\frac{1}{R^{3/2}} + 6\,\frac{c}{\epsilon^{\frac{1}{3}}}\,\frac{1}{R^{1/2}} + \mathcal{O}\left(\frac{1}{R^{\frac{3}{2}}}\right) \\
&= \mathcal{O}\left(\frac{1}{\sqrt{R}}\right),
\end{aligned}
$$

proving the lemma. ■

For the integrand of $\tilde{J}_{3.2}$ (cf. (B.4.47)) it is easily seen that the assumptions of Lemma B.4 are satisfied, since $\nabla_{\vec{n}} f_{\ell,j}(n', n_z)$ has at most a logarithmic singularity, while the cut-off function χ ensures that $1/|n'| \geq 1/|m'| < \infty$, such that the integrand can be bounded by $c|\log|n'(\psi,\phi)-\nu'||/|n'(\psi,\phi)-\nu'|$ at $n' = \nu'$. The lemma thus shows that

$$
\tilde{J}_{3.2} = o\left(\frac{1}{R}\right). \tag{B.4.53}
$$

In the following, the integrals $\tilde{J}_{3.3}$ and $\tilde{J}_{3.4}$ will be examined similarly to $\tilde{J}_{3.2}$. For $\tilde{J}_{3.3}$ (cf. B.4.48) it will be shown that the integrand satisfies the assumptions of Lemma B.4. Indeed, since $f_{\ell,j}$ is a bounded function and the cut-off function χ removes the singularity at $|n'(\psi,\phi)| = 0$, it follows that $\chi(|n'(\psi,\phi)|)\, f_{\ell,j}(n'(\psi,\phi), n_z^r(\psi,\phi))/|n'(\psi,\phi)|^2$ is bounded. Moreover, since $|\nu'| = 1$, $|n'(\psi,\phi)| \leq 1$ and $n_z^r(\psi,\phi) = -\sqrt{1-|n'(\psi,\phi)|^2}$,

$$
\begin{aligned}
\left|\frac{n'(\psi,\phi)\cdot\left[n'(\psi,\phi)-\nu'\right] n_z^r(\psi,\phi)}{\left|n'(\psi,\phi)-\nu'\right|^2}\right|^2 &\leq c\frac{\left|n'(\psi,\phi)-\nu'\right|^2 \left|n_z^r(\psi,\phi)\right|^2}{\left|n'(\psi,\phi)-\nu'\right|^4} = c\frac{1-\left|n'(\psi,\phi)\right|^2}{\left|n'(\psi,\phi)-\nu'\right|^2} \\
&\leq c\frac{|\nu'|^2-\left|n'(\psi,\phi)\right|^2}{|\nu'|^2-\left|n'(\psi,\phi)\right|^2} = c < \infty.
\end{aligned} \tag{B.4.54}
$$

Hence the integrand of $\tilde{J}_{3.3}$ is absolutely bounded from above by

$$
\frac{c}{\left|n'(\psi,\phi)-\nu'\right|} \leq c\frac{\left|\log|n'(\psi,\phi)-\nu'|\right|}{\left|n'(\psi,\phi)-\nu'\right|},
$$

for $\psi \in [\psi(\phi), 1]$ and $\phi \in [0, 2\pi]$, such that Lemma B.4 can be applied, giving

$$
\tilde{J}_{3.3} = o\left(\frac{1}{R}\right). \tag{B.4.55}
$$

To consider the asymptotic behaviour of $\tilde{J}_{3.4}$ (cf. (B.4.49)), the integral is split into

$$
\begin{aligned}
\tilde{J}_{3.4} = \frac{1}{m_z}\int_0^{2\pi}\int_{\psi(\phi)}^{1} &\chi(|n'(\psi,\phi)|)\frac{f_{\ell,j}\Big(n'(\psi,\phi), n_z^r(\psi,\phi)\Big)\, n'(\psi,\phi)\cdot m'\, n_z^r(\psi,\phi)}{\left|n'(\psi,\phi)-\nu'\right|\left|n'(\psi,\phi)\right|^2}\, e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi \\
-\frac{1}{m_z}\int_0^{2\pi}\int_{\psi(\phi)}^{\psi_R(\phi)} &\chi(|n'(\psi,\phi)|)\frac{f_{\ell,j}\Big(n'(\psi,\phi), n_z^r(\psi,\phi)\Big)\, n'(\psi,\phi)\cdot m'\, n_z^r(\psi,\phi)}{\left|n'(\psi,\phi)-\nu'\right|\left|n'(\psi,\phi)\right|^2}\, e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi.
\end{aligned} \tag{B.4.56}
$$

The asymptotic behaviour of the second integral on the right-hand side is easily proven, since the estimates done for $\tilde{J}_{3.3}$ (e.g. (B.4.54)) show that the integrand is uniformly bounded for all $\psi \in [\psi(\phi), 1]$ and $\phi \in [0, 2\pi]$. Moreover, by undoing the substitution (4.2.22) for this bound and introducing polar coordinates to the new domain of integration D_R, which is the annulus with the radii $1-\tilde{\epsilon}_R$ and 1, it follows that

$$\left|\int_0^{2\pi}\int_{\psi(\phi)}^{\psi_R(\phi)} \chi(|n'(\psi,\phi)|)\frac{f_{\ell,j}\Big(n'(\psi,\phi),n_z^r(\psi,\phi)\Big)\,n'(\psi,\phi)\cdot m'\,n_z^r(\psi,\phi)}{\big|n'(\psi,\phi)-\nu'\big|\,\big|n'(\psi,\phi)\big|^2}\,e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi\right|$$
$$\le \int_0^{2\pi}\int_{\psi(\phi)}^{\psi_R(\phi)} c\,\mathrm{d}\psi\,\mathrm{d}\phi = c\int_{D_R}\frac{1}{n_z^r}\,\mathrm{d}n' = 2\pi c\int_{1-\tilde{\epsilon}_R}^{1}\frac{\rho}{\sqrt{1-\rho^2}}\,\mathrm{d}\rho = \mathcal{O}\left(\frac{1}{R^{\frac{3}{2}}}\right).$$

Hence, (cf. (B.4.56))

$$\tilde{J}_{3.4} = \frac{1}{m_z}\int_0^{2\pi}\int_{\psi(\phi)}^{1} \chi(|n'(\psi,\phi)|)\frac{f_{\ell,j}\Big(n'(\psi,\phi),n_z^r(\psi,\phi)\Big)\,n'(\psi,\phi)\cdot m'\,n_z^r(\psi,\phi)}{\big|n'(\psi,\phi)-\nu'\big|\,\big|n'(\psi,\phi)\big|^2}\,e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi + o\left(\frac{1}{R}\right).$$

Next, the remaining integral is integrated by parts w.r.t. ψ, leading to (cf. $\chi(|n'(1,\phi)|) = 0$ and $|n'(\psi(\phi),\phi)| = 1$)

$$\begin{aligned}\tilde{J}_{3.4} = &-\frac{1}{ikRm_z}\int_0^{2\pi}\frac{f_{\ell,j}\Big(n'(\psi(\phi),\phi),n_z^r(\psi(\phi),\phi)\Big)\,n'(\psi(\phi),\phi)\cdot m'\,n_z^r(\psi(\phi),\phi)}{\big|n'(\psi(\phi),\phi)-\nu'\big|}\,e^{ikR\psi(\phi)}\,\mathrm{d}\phi\\ &-\frac{1}{ikRm_z}\int_0^{2\pi}\int_{\psi(\phi)}^{1}\partial_\psi\left[\chi(|n'(\psi,\phi)|)\frac{f_{\ell,j}\Big(n'(\psi,\phi),n_z^r(\psi,\phi)\Big)\,n'(\psi,\phi)\cdot m'\,n_z^r(\psi,\phi)}{\big|n'(\psi,\phi)-\nu'\big|\,\big|n'(\psi,\phi)\big|^2}\right]e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi.\\ &+o\left(\frac{1}{R}\right).\end{aligned}\tag{B.4.57}$$

To get the asymptotic behaviour of the second integral on the right-hand side, it is necessary to analyse the singular behaviour of the derivative, i.e. of

$$\begin{aligned}&\partial_\psi\left[\chi(|n'(\psi,\phi)|)\frac{f_{\ell,j}\Big(n'(\psi,\phi),n_z^r(\psi,\phi)\Big)\,n'(\psi,\phi)\cdot m'\,n_z^r(\psi,\phi)}{\big|n'(\psi,\phi)-\nu'\big|\,\big|n'(\psi,\phi)\big|^2}\right]\\
&\quad=\frac{1}{2}\frac{\partial_\psi\,n'(\psi,\phi)\cdot n'(\psi,\phi)}{|n'(\psi,\phi)|}\chi'(|n'(\psi,\phi)|)\frac{f_{\ell,j}\Big(n'(\psi,\phi),n_z^r(\psi,\phi)\Big)\,n'(\psi,\phi)\cdot m'\,n_z^r(\psi,\phi)}{\big|n'(\psi,\phi)-\nu'\big|\,\big|n'(\psi,\phi)\big|^2}\\
&\qquad+\chi(|n'(\psi,\phi)|)\frac{\partial_\psi\vec{n}^r(\psi,\phi)\cdot\nabla_{\vec{n}}f_{\ell,j}\Big(n'(\psi,\phi),n_z^r(\psi,\phi)\Big)\,n'(\psi,\phi)\cdot m'\,n_z^r(\psi,\phi)}{\big|n'(\psi,\phi)-\nu'\big|\,\big|n'(\psi,\phi)\big|^2}\\
&\qquad+\chi(|n'(\psi,\phi)|)\frac{f_{\ell,j}\Big(n'(\psi,\phi),n_z^r(\psi,\phi)\Big)\,\partial_\psi\left[n'(\psi,\phi)\right]\cdot m'\,n_z^r(\psi,\phi)}{\big|n'(\psi,\phi)-\nu'\big|\,\big|n'(\psi,\phi)\big|^2}\\
&\qquad+\chi(|n'(\psi,\phi)|)\frac{f_{\ell,j}\Big(n'(\psi,\phi),n_z^r(\psi,\phi)\Big)\,n'(\psi,\phi)\cdot m'\,\partial_\psi\left[n_z^r(\psi,\phi)\right]}{\big|n'(\psi,\phi)-\nu'\big|\,\big|n'(\psi,\phi)\big|^2}\\
&\qquad-\chi(|n'(\psi,\phi)|)\frac{f_{\ell,j}\Big(n'(\psi,\phi),n_z^r(\psi,\phi)\Big)\,n'(\psi,\phi)\cdot m'\,n_z^r(\psi,\phi)}{\big|n'(\psi,\phi)-\nu'\big|^2\,\big|n'(\psi,\phi)\big|^2}\,\frac{\partial_\psi\,n'(\psi,\phi)\cdot\big(n'(\psi,\phi)-\nu'\big)}{\big|n'(\psi,\phi)-\nu'\big|}\\
&\qquad-2\chi(|n'(\psi,\phi)|)\frac{f_{\ell,j}\Big(n'(\psi,\phi),n_z^r(\psi,\phi)\Big)\,n'(\psi,\phi)\cdot m'\,n_z^r(\psi,\phi)}{\big|n'(\psi,\phi)-\nu'\big|}\,\frac{\partial_\psi\,n'(\psi,\phi)\cdot n'(\psi,\phi)}{\big|n'(\psi,\phi)\big|^4}.\end{aligned}$$

Here $\chi(|n'(\psi,\phi)|)$ and $\chi'(|n'(\psi,\phi)|)$ cut off the singularity of $1/|n'(\psi,\phi)|$ at $n'(\psi,\phi)=(0,0)^\top$ and of

$$\partial_\psi \vec{n}^r(\psi,\phi) = \begin{pmatrix} \partial_\psi n'(\psi,\phi) \\ \partial_\psi n_z^r(\psi,\phi) \end{pmatrix} = \begin{pmatrix} \sin\alpha\cos\beta - (\cos\alpha\cos\beta\cos\phi - \sin\beta\sin\phi)\frac{\psi}{\sqrt{1-\psi^2}} \\ \sin\alpha\sin\beta - (\cos\alpha\sin\beta\cos\phi + \cos\beta\sin\phi)\frac{\psi}{\sqrt{1-\psi^2}} \\ \cos\alpha + \sin\alpha\cos\phi\frac{\psi}{\sqrt{1-\psi^2}} \end{pmatrix}$$

at $\psi=1$. As stated before, the gradient of $f_{\ell,j}$ has at most a logarithmic singularity (cf. Lemma B.2). With this, it is not hard to show that

$$\left|\partial_\psi\left[\chi(|n'(\psi,\phi)|)\frac{f_{\ell,j}\Big(n'(\psi,\phi),n_z^r(\psi,\phi)\Big)\,n'(\psi,\phi)\cdot m'\,n_z^r(\psi,\phi)}{\big|n'(\psi,\phi)-\nu'\big|\,\big|n'(\psi,\phi)\big|^2}\right]\right| \le c\frac{\big|\log|n'(\psi,\phi)-\nu'|\big|}{\big|n'(\psi,\phi)-\nu'\big|}$$

for all $\psi\in[\psi(\phi),1]$ and $\phi\in[0,2\pi]$. Thus, by undoing the coordinate transformation (ψ,ϕ), it can be shown, very similar to the beginning of the proof of Lemma B.4, that the Riemann-Lebesgue lemma can be applied to the second term on the right-hand side of (B.4.57). Hence, it is shown that the term decays faster than $1/R$ as R tends to infinity. It remains to examine

$$\tilde{J}_{3.4} = -\frac{1}{ikRm_z}\int_0^{2\pi}\frac{f_{\ell,j}\Big(n'(\psi(\phi),\phi),n_z^r(\psi(\phi),\phi)\Big)\,n'(\psi(\phi),\phi)\cdot m'\,n_z^r(\psi(\phi),\phi)}{\big|n'(\psi(\phi),\phi)-\nu'\big|}\,e^{ikR\psi(\phi)}\,\mathrm{d}\phi + o\left(\frac{1}{R}\right).$$

To determine the asymptotic behaviour of the remaining integral, the goal is to apply the Riemann-Lebesgue lemma once again. To realise this, the continuous function $\psi(\phi)$ (cf. (4.2.28) and Figure B.2) has to be substituted. Recall that $\psi(\phi)$ is strictly monotonic for $\phi\in[0,\pi]$ and $\phi\in[\pi,2\pi]$ with the range $[-\sin\alpha,\sin\alpha]$. Thus (cf. (B.4.7))

$$\begin{aligned}\tilde{J}_{3.4} = &-\frac{1}{ikRm_z}\int_{-\sin\alpha}^{\sin\alpha}\frac{f_{\ell,j}\Big(n'(\psi,\phi(\psi)),n_z^r(\psi,\phi(\psi))\Big)\,n'(\psi,\phi(\psi))\cdot m'\,n_z^r(\psi,\phi(\psi))}{\big|n'(\psi,\phi(\psi))-\nu'\big|}\phi'(\psi)\,e^{ikR\psi}\,\mathrm{d}\psi \\ &+\frac{1}{ikRm_z}\int_{-\sin\alpha}^{\sin\alpha}\Bigg\{f_{\ell,j}\Big(n'(\psi,2\pi-\phi(\psi)),n_z^r(\psi,2\pi-\phi(\psi))\Big)\,n'(\psi,2\pi-\phi(\psi))\cdot m' \\ &\qquad\frac{n_z^r(\psi,2\pi-\phi(\psi))}{\big|n'(\psi,2\pi-\phi(\psi))-\nu'\big|}\phi'(\psi)\,e^{ikR\psi}\Bigg\}\,\mathrm{d}\psi + o\left(\frac{1}{R}\right),\end{aligned}$$

since $\psi(\phi)=\psi(2\pi-\phi)$ for $\phi\in[\pi,2\pi]$ and where $\phi'(\psi)$ (cf. (B.4.21)) is weakly singular for $\phi=\pi$ and thus $\psi=-\sin\alpha$. Since $f_{\ell,j}$ and $n_z^r(\psi,\phi(\psi))/|n'(\psi,\phi(\psi))-\nu'|$ (cf. (B.4.54)) are bounded, the Riemann-Lebesgue lemma directly gives that

$$\tilde{J}_{3.4} = o\left(\frac{1}{R}\right)$$

for $R\to\infty$. In total (cf. (B.4.45), (B.4.46), (B.4.53) and (B.4.55))

$$\tilde{J}_3 = -\frac{1}{ikRm_z}\int_{\phi_0-\pi}^{\phi_0+\pi}\frac{f_{\ell,j}((1-\tilde{\epsilon}_R)n_0',\sqrt{2\tilde{\epsilon}_R-\tilde{\epsilon}_R^2})}{|(1-\tilde{\epsilon}_R)n_0'-\nu'|}\,e^{ik(1-\tilde{\epsilon}_R)Rn_0'\cdot m'}\,e^{ikRm_z\sqrt{2\tilde{\epsilon}_R-\tilde{\epsilon}_R^2}}\,\mathrm{d}\phi + o\left(\frac{1}{R}\right) \tag{B.4.58}$$

for $m'/|m'|\neq\nu'$

B.4.3.2 $\tilde{J}_4$

The asymptotic behaviour of $\tilde{J}_4$ (cf. (B.4.41)) is determined next. Note that using the fact that $\chi(\rho)$ is identically equal to one in a neighbourhood of $\rho n_0'=\nu'$, it was already shown in Subsection B.3.1.1

that (cf. (B.3.11))

$$f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2}) \left\{ \frac{\chi(\rho)}{|\rho n_0' - \nu'|} - \frac{1}{\sqrt{(1-\rho)^2 + (\phi-\phi_0)^2}} \right\}$$

is finite at $\rho n_0' = \nu'$. Thus the integrand of $\tilde{J}_4$ (cf. (B.4.41)) is uniformly bounded by a constant c for all $\rho \in [1-\tilde{\epsilon}_R, 1]$ and $\phi \in [\phi_0 - \pi, \phi_0 + \pi]$. Furthermore, it was shown that locally (cf. (B.3.22))

$$\begin{aligned} &\left| \partial_\rho \left[f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2}) \left[\frac{\chi(\rho)}{|\rho n_0' - \nu'|} - \frac{1}{\sqrt{(1-\rho)^2 + (\phi-\phi_0)^2}} \right] \right] \right| \\ &\qquad \le \frac{\rho}{\sqrt{1-\rho^2}} \left| \log\big(\sqrt{(1-\rho)^2 + (\phi-\phi_0)^2}\big) \right| + \frac{c}{\sqrt{(1-\rho)^2 + (\phi-\phi_0)^2}}. \end{aligned}$$

After applying integration by parts w.r.t. ρ, this will be used to show that all occurring terms decay faster than $1/R$. Consider, (cf. (B.4.41) and $\chi(1-\tilde{\epsilon}_R) = 1$)

$$\begin{aligned} \tilde{J}_4 = &-\frac{1}{ikRm_z} \int_{1-\tilde{\epsilon}_R}^{1} \left\{ \int_{\phi_0-\pi}^{\phi_0+\pi} f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2}) \left[\frac{\chi(\rho)}{|\rho n_0' - \nu'|} - \frac{1}{\sqrt{(1-\rho)^2 + (\phi-\phi_0)^2}} \right] e^{ik\rho R n_0' \cdot m'} \, \mathrm{d}\phi \right. \\ &\qquad \left. \partial_\rho \left[e^{ikRm_z\sqrt{1-\rho^2}} \right] \right\} \mathrm{d}\rho \\ = &-\frac{1}{ikRm_z} \int_{\phi_0-\pi}^{\phi_0+\pi} f_{\ell,j}(n_0', 0) \left[\frac{1}{|n_0' - \nu'|} - \frac{1}{|\phi - \phi_0|} \right] e^{ikRn_0' \cdot m'} \, \mathrm{d}\phi \\ &+ \frac{1}{ikRm_z} \int_{\phi_0-\pi}^{\phi_0+\pi} \left\{ f_{\ell,j}((1-\tilde{\epsilon}_R) n_0', \sqrt{2\tilde{\epsilon}_R - \tilde{\epsilon}_R^2}) \left[\frac{1}{|(1-\tilde{\epsilon}_R) n_0' - \nu'|} - \frac{1}{\sqrt{\tilde{\epsilon}_R^2 + (\phi-\phi_0)^2}} \right] \right. \\ &\qquad \left. e^{ik(1-\tilde{\epsilon}_R) R n_0' \cdot m'} \right\} \mathrm{d}\phi \; e^{ikRm_z\sqrt{2\tilde{\epsilon}_R - \tilde{\epsilon}_R^2}} \\ &+ \frac{1}{ikRm_z} \int_{1-\tilde{\epsilon}_R}^{1} \left\{ \int_{\phi_0-\pi}^{\phi_0+\pi} \partial_\rho \left[f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2}) \left[\frac{\chi(\rho)}{|\rho n_0' - \nu'|} - \frac{1}{\sqrt{(1-\rho)^2 + (\phi-\phi_0)^2}} \right] \right] e^{ik\rho R n_0' \cdot m'} \, \mathrm{d}\phi \right. \\ &\qquad \left. e^{ikRm_z\sqrt{1-\rho^2}} \right\} \mathrm{d}\rho \\ &+ \frac{1}{m_z} \int_{1-\tilde{\epsilon}_R}^{1} \left\{ \int_{\phi_0-\pi}^{\phi_0+\pi} f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2}) \left[\frac{\chi(\rho)\, n_0' \cdot m'}{|\rho n_0' - \nu'|} - \frac{n_0' \cdot m'}{\sqrt{(1-\rho)^2 + (\phi-\phi_0)^2}} \right] e^{ik\rho R n_0' \cdot m'} \, \mathrm{d}\phi \right. \\ &\qquad \left. e^{ikRm_z\sqrt{1-\rho^2}} \right\} \mathrm{d}\rho. \end{aligned}$$

In view of (B.3.18) and $\tilde{\epsilon}_R = 1/R^3 = o(1/R)$, and since $\int_{\phi_0-\pi}^{\phi_0+\pi} |\log((1-\rho)^2 + (\phi-\phi_0)^2)| \, \mathrm{d}\phi$ is bounded by $2\int_{\phi_0-\pi}^{\phi_0+\pi} |\log|\phi - \phi_0|| \, \mathrm{d}\phi$ for $\rho \in [1-\tilde{\epsilon}_R, 1]$, it is easily seen that the sum of the absolute values of all integrals on the right-hand side, except the second, are bounded by (cf. (B.3.36) and (B.4.39))

$$\begin{aligned} &\frac{c}{kRm_z} \int_{1-\tilde{\epsilon}_R}^{1} \int_{\phi_0-\pi}^{\phi_0+\pi} \frac{1}{\sqrt{(1-\rho)^2 + (\phi-\phi_0)^2}} \, \mathrm{d}\phi \, \mathrm{d}\rho + \frac{c}{kRm_z} \int_{1-\tilde{\epsilon}_R}^{1} \int_{\phi_0-\pi}^{\phi_0+\pi} \left| \log\big((1-\rho)^2 + (\phi-\phi_0)^2\big) \right| \mathrm{d}\phi \, \frac{\rho}{\sqrt{1-\rho^2}} \, \mathrm{d}\rho \\ &\qquad + c \, \frac{2\pi\, |m'|}{m_z} \int_{1-\tilde{\epsilon}_R}^{1} 1 \, \mathrm{d}\rho + o\left(\frac{1}{R} \right) \end{aligned}$$

$$
\begin{aligned}
&\le \frac{2c}{kRm_z} \int\limits_{1-\tilde\epsilon_R}^{1} \int\limits_{\phi_0}^{\phi_0+\pi} \frac{1}{\sqrt{(1-\rho)^2+(\phi-\phi_0)^2}}\,\mathrm{d}\phi\,\mathrm{d}\rho + \frac{2c}{kRm_z} \int\limits_{1-\tilde\epsilon_R}^{1} \frac{\rho}{\sqrt{1-\rho^2}}\,\mathrm{d}\rho \int\limits_{\phi_0-\pi}^{\phi_0+\pi} |\log|\phi-\phi_0||\,\mathrm{d}\phi \\
&\quad + o\left(\frac{1}{R}\right) \\
&= \frac{2c}{kRm_z} \int\limits_{1-\tilde\epsilon_R}^{1} \left|\log\left(\pi+\sqrt{(1-\rho)^2+\pi^2}\right) - \log(1-\rho)\right|\mathrm{d}\rho + \frac{c_3}{R}\sqrt{2\tilde\epsilon_R+\tilde\epsilon_R^2} + o\left(\frac{1}{R}\right) \\
&\le \frac{c_2}{R} \int\limits_{1-\tilde\epsilon_R}^{1} 1\,\mathrm{d}\rho + \frac{2c}{kRm_z} \int\limits_{1-\tilde\epsilon_R}^{1} |\log(1-\rho)|\,\mathrm{d}\rho + o\left(\frac{1}{R}\right) \\
&\le \frac{2c}{kRm_z}\left|-\tilde\epsilon_R + \log\tilde\epsilon_R\,\tilde\epsilon_R\right| + o\left(\frac{1}{R}\right) \\
&= o\left(\frac{1}{R}\right).
\end{aligned}
$$

In total,

$$
\begin{aligned}
\tilde J_4 = \frac{1}{ikRm_z} \int\limits_{\phi_0-\pi}^{\phi_0+\pi} \Bigg\{ & f_{\ell,j}((1-\tilde\epsilon_R)n_0', \sqrt{2\tilde\epsilon_R-\tilde\epsilon_R^2}) \left[\frac{1}{|(1-\tilde\epsilon_R)n_0'-\nu'|} - \frac{1}{\sqrt{\tilde\epsilon_R^2+(\phi-\phi_0)^2}}\right] \\
& e^{ik(1-\tilde\epsilon_R)Rn_0'\cdot m'}\Bigg\}\,\mathrm{d}\phi\; e^{ikRm_z\sqrt{2\tilde\epsilon_R-\tilde\epsilon_R^2}} + o\left(\frac{1}{R}\right).
\end{aligned}
\tag{B.4.59}
$$

B.4.3.3 $\tilde J_5$

To obtain the asymptotic behaviour of $\tilde J_5$, recall that (cf. (B.4.42))

$$
\tilde J_5 = -\frac{1}{ikRm_z} \int\limits_{1-\tilde\epsilon_R}^{1} \int\limits_{\phi_0-\pi}^{\phi_0+\pi} \frac{f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2}) - f_{\ell,j}(\nu',0)}{\sqrt{(1-\rho)^2+(\phi-\phi_0)^2}}\, e^{ik\rho Rn_0'\cdot m'}\,\mathrm{d}\phi\,\partial_\rho\left[e^{ikRm_z\sqrt{1-\rho^2}}\right]\mathrm{d}\rho.
$$

As for $\tilde J_4$ the singular behaviour of the integrand was already examined in a previous section. It was shown in Subsection B.3.1.2 that (cf. (B.3.31))

$$
\left|\frac{f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2}) - f_{\ell,j}(\nu',0)}{\sqrt{(1-\rho)^2+(\phi-\phi_0)^2}}\right| \le \left|\log\left((1-\rho)^2+(\phi-\phi_0)^2\right)\right| \tag{B.4.60}
$$

for any fixed $\rho \in [1-\tilde\epsilon_R, 1]$ and thus that the integrand of $\tilde J_5$ is absolutely integrable. Moreover, the derivative w.r.t. ρ of the quotient is bounded by $c|\log((1-\rho)^2+(\phi-\phi_0)^2)|\rho/[\sqrt{1-\rho^2}\sqrt{(1-\rho)^2+(\phi-\phi_0)^2}]$ (cf. (B.3.35)). Integration by parts w.r.t. ρ is used once more, and

$$
\begin{aligned}
\tilde J_5 = &-\frac{1}{ikRm_z} \int\limits_{\phi_0-\pi}^{\phi_0+\pi} \frac{f_{\ell,j}(n_0',0) - f_{\ell,j}(\nu',0)}{|\phi-\phi_0|} e^{ikRn_0'\cdot m'}\,\mathrm{d}\phi \\
&+ \frac{1}{ikRm_z} \int\limits_{\phi_0-\pi}^{\phi_0+\pi} \frac{f_{\ell,j}((1-\tilde\epsilon_R)n_0', \sqrt{2\tilde\epsilon_R-\tilde\epsilon_R^2}) - f_{\ell,j}(\nu',0)}{\sqrt{\tilde\epsilon_R^2+(\phi-\phi_0)^2}}\, e^{ik(1-\tilde\epsilon_R)Rn_0'\cdot m'}\,\mathrm{d}\phi\, e^{ikRm_z\sqrt{2\tilde\epsilon_R-\tilde\epsilon_R^2}} \\
&+ \frac{1}{ikRm_z} \int\limits_{1-\tilde\epsilon_R}^{1} \int\limits_{\phi_0-\pi}^{\phi_0+\pi} \partial_\rho\left[\frac{f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2}) - f_{\ell,j}(\nu',0)}{\sqrt{(1-\rho)^2+(\phi-\phi_0)^2}}\right] e^{ik\rho Rn_0'\cdot m'}\,\mathrm{d}\phi\, e^{ikRm_z\sqrt{1-\rho^2}}\,\mathrm{d}\rho \\
&+ \frac{1}{m_z} \int\limits_{1-\tilde\epsilon_R}^{1} \int\limits_{\phi_0-\pi}^{\phi_0+\pi} (n_0'\cdot m') \frac{f_{\ell,j}(\rho n_0', \sqrt{1-\rho^2}) - f_{\ell,j}(\nu',0)}{\sqrt{(1-\rho)^2+(\phi-\phi_0)^2}}\, e^{ik\rho Rn_0'\cdot m'}\,\mathrm{d}\phi\, e^{ikRm_z\sqrt{1-\rho^2}}\,\mathrm{d}\rho.
\end{aligned}
$$

With the bounds of (B.4.60), the absolute value of $\tilde{J}_5$ minus the second integral on the right-hand side can then be estimated as (cf. (B.3.34), (B.3.35) and (B.3.36))

$$\begin{aligned}
&\frac{c}{kRm_z}\int_{1-\tilde{\epsilon}_R}^{1}\int_{\phi_0-\pi}^{\phi_0+\pi}\frac{\left|\log\left((1-\rho)^2+(\phi-\phi_0)^2\right)\right|}{\sqrt{(1-\rho)^2+(\phi-\phi_0)^2}}\,\mathrm{d}\phi\,\frac{\rho}{\sqrt{1-\rho^2}}\,\mathrm{d}\rho \\
&\qquad+\frac{c}{m_z}\int_{1-\tilde{\epsilon}_R}^{1}\int_{\phi_0-\pi}^{\phi_0+\pi}\left|\log\left((1-\rho)^2+(\phi-\phi_0)^2\right)\right|\,\mathrm{d}\phi\,\mathrm{d}\rho+o\left(\frac{1}{R}\right) \\
&\qquad\le\frac{c}{kRm_z}\int_{1-\tilde{\epsilon}_R}^{1}\int_{\phi_0-\pi}^{\phi_0+\pi}\frac{1}{\sqrt{(1-\rho)^2+(\phi-\phi_0)^2}}\,\mathrm{d}\phi\,\left|\log(1-\rho)\right|\frac{\rho}{\sqrt{1-\rho^2}}\,\mathrm{d}\rho \\
&\qquad+\frac{c}{m_z}\int_{1-\tilde{\epsilon}_R}^{1}\int_{\phi_0-\pi}^{\phi_0+\pi}1\,\mathrm{d}\phi\,\left|\log(1-\rho)\right|\,\mathrm{d}\rho+o\left(\frac{1}{R}\right) \\
&\qquad=\frac{c}{kRm_z}\int_{1-\tilde{\epsilon}_R}^{1}\int_{\phi_0-\pi}^{\phi_0+\pi}\left\{\log\left(\pi+\sqrt{(1-\rho)^2+\pi^2}\right)+\log(1-\rho)\right\}\left|\log(1-\rho)\right|\frac{\rho}{\sqrt{1-\rho^2}}\,\mathrm{d}\rho \\
&\qquad+\frac{2\pi\,c}{m_z}\,\tilde{\epsilon}_R\left[1-\log\tilde{\epsilon}_R\right]+o\left(\frac{1}{R}\right) \\
&\qquad=\frac{2c}{kRm_z}\int_{1-\tilde{\epsilon}_R}^{1}\left[\log(1-\rho)\right]^2\frac{\rho}{\sqrt{1-\rho^2}}\,\mathrm{d}\rho+o\left(\frac{1}{R}\right),
\end{aligned}$$

since $|\log(1-\rho)|=-\log(1-\rho)$ for $\rho\in[1-\tilde{\epsilon}_R,1]$ and R sufficiently large. Furthermore, substituting $u=\sqrt{1-\rho^2}$,

$$\begin{aligned}
\frac{1}{R}\int_{1-\tilde{\epsilon}_R}^{1}\left[\log(1-\rho)\right]^2\frac{\rho}{\sqrt{1-\rho^2}}\,\mathrm{d}\rho&=\frac{1}{R}\int_{0}^{\sqrt{2\tilde{\epsilon}_R-\tilde{\epsilon}_R^2}}\left[\log\left(1-\sqrt{1-u^2}\right)\right]^2\mathrm{d}u \\
&\le\frac{c_2}{R}\int_{0}^{\sqrt{2\tilde{\epsilon}_R-\tilde{\epsilon}_R^2}}\left[\log u\right]^2\mathrm{d}u \\
&\le\frac{c_2}{R}\sqrt{2\tilde{\epsilon}_R-\tilde{\epsilon}_R^2}\left|2-2\log\sqrt{2\tilde{\epsilon}_R-\tilde{\epsilon}_R^2}+\left[\log\sqrt{2\tilde{\epsilon}_R-\tilde{\epsilon}_R^2}\right]^2\right| \\
&=o\left(\frac{1}{R}\right)
\end{aligned}$$

such that

$$\tilde{J}_5=\frac{1}{ikRm_z}\int_{\phi_0-\pi}^{\phi_0+\pi}\frac{f_{\ell,j}((1-\tilde{\epsilon}_R)n_0',\sqrt{2\tilde{\epsilon}_R-\tilde{\epsilon}_R^2})-f_{\ell,j}(\nu',0)}{\sqrt{\tilde{\epsilon}_R^2+(\phi-\phi_0)^2}}\,e^{ik(1-\tilde{\epsilon}_R)Rn_0'\cdot m'}\,\mathrm{d}\phi\,e^{ikRm_z\sqrt{2\tilde{\epsilon}_R-\tilde{\epsilon}_R^2}}+o\left(\frac{1}{R}\right). \tag{B.4.61}$$

B.4.3.4 $\tilde{J}_6$

Next, the asymptotic behaviour of $\tilde{J}_6$ is derived. Recall that (cf. (B.4.43))

$$\tilde{J}_6=-\frac{f_{\ell,j}(\nu',0)}{ikRm_z}\int_{1-\tilde{\epsilon}_R}^{1}\int_{\phi_0-\pi}^{\phi_0+\pi}\frac{e^{ik(\rho-1)Rn_0'\cdot m'}-1}{\sqrt{(1-\rho)^2+(\phi-\phi_0)^2}}\,e^{ikRn_0'\cdot m'}\,\mathrm{d}\phi\,\partial_\rho\left[e^{ikRm_z\sqrt{1-\rho^2}}\right]\mathrm{d}\rho.$$

As in the previous subsections, $\tilde{J}_6$ is integrated by parts w.r.t. ρ, resulting in

$$\begin{aligned}\tilde{J}_6 = \frac{f_{\ell,j}(\nu',0)}{ikRm_z}\int\limits_{\phi_0-\pi}^{\phi_0+\pi}\frac{e^{-ik\tilde{\epsilon}_R Rn_0'\cdot m'}-1}{\sqrt{\tilde{\epsilon}_R^2+(\phi-\phi_0)^2}}\,e^{ikRn_0'\cdot m'}\,\mathrm{d}\phi\, e^{ikRm_z\sqrt{2\tilde{\epsilon}_R-\tilde{\epsilon}_R^2}}\\ + \frac{f_{\ell,j}(\nu',0)}{ikm_z}\int\limits_{1-\tilde{\epsilon}_R}^{1}\int\limits_{\phi_0-\pi}^{\phi_0+\pi}\Bigg\{ikn_0'\cdot m'\frac{e^{ik(\rho-1)Rn_0'\cdot m'}}{\sqrt{(1-\rho)^2+(\phi-\phi_0)^2}}\\ - \frac{(\rho-1)\left[e^{ik(\rho-1)Rn_0'\cdot m'}-1\right]}{R\sqrt{(1-\rho)^2+(\phi-\phi_0)^2}^3}\Bigg\}\,e^{ikRn_0'\cdot m'}\,\mathrm{d}\phi\, e^{ikRm_z\sqrt{1-\rho^2}}\,\mathrm{d}\rho,\end{aligned} \tag{B.4.62}$$

where it is easily shown that

$$\left|\frac{e^{ik(1-\rho)Rn_0'\cdot m'}-1}{R\sqrt{(1-\rho)^2+(\phi-\phi_0)^2}}\right|$$

is bounded uniformly for all ρ, ϕ and R, such that

$$\left|ikn_0'\cdot m'\frac{e^{ik(\rho-1)Rn_0'\cdot m'}}{\sqrt{(1-\rho)^2+(\phi-\phi_0)^2}} - \frac{(\rho-1)\left[e^{ik(1-\rho)Rn_0'\cdot m'}-1\right]}{R\sqrt{(1-\rho)^2+(\phi-\phi_0)^2}^3}\right| \le \frac{c}{\sqrt{(1-\rho)^2+(\phi-\phi_0)^2}}.$$

With this and keeping in mind that $|\log(1-\rho)| = -\log(1-\rho)$ for all $\rho\in[1-\tilde{\epsilon}_R,1]$ and R sufficiently large, the absolute value of the second integral on the right-hand side of (B.4.62) is bounded by (cf. (B.4.39))

$$\begin{aligned}&c\frac{|f_{\ell,j}(\nu',0)|}{km_z}\int\limits_{1-\tilde{\epsilon}_R}^{1}\int\limits_{\phi_0-\pi}^{\phi_0+\pi}\frac{1}{\sqrt{(1-\rho)^2+(\phi-\phi_0)^2}}\,\mathrm{d}\phi\,\mathrm{d}\rho\\ &= 2c\frac{|f_{\ell,j}(\nu',0)|}{km_z}\int\limits_{1-\tilde{\epsilon}_R}^{1}\int\limits_{\phi_0}^{\phi_0+\pi}\frac{1}{\sqrt{(1-\rho)^2+(\phi-\phi_0)^2}}\,\mathrm{d}\phi\,\mathrm{d}\rho\\ &= 2c\frac{|f_{\ell,j}(\nu',0)|}{km_z}\int\limits_{1-\tilde{\epsilon}_R}^{1}\log\Big(\pi+\sqrt{(1-\rho)^2+\pi^2}\Big)-\log(1-\rho)\,\mathrm{d}\rho\\ &\le 2c\frac{|f_{\ell,j}(\nu',0)|}{km_z}\log(2\pi)\tilde{\epsilon}_R - 2c\frac{|f_{\ell,j}(\nu',0)|}{km_z}\int\limits_{1-\tilde{\epsilon}_R}^{1}\log(1-\rho)\,\mathrm{d}\rho\\ &= o\left(\frac{1}{R}\right) + 2c\frac{|f_{\ell,j}(\nu',0)|}{km_z}\Big[1-\tilde{\epsilon}_R\,\log(\tilde{\epsilon}_R)-1+\tilde{\epsilon}_R\Big]\\ &= o\left(\frac{1}{R}\right).\end{aligned}$$

Therefore,

$$\tilde{J}_6 = \frac{f_{\ell,j}(\nu',0)}{ikRm_z}\int\limits_{\phi_0-\pi}^{\phi_0+\pi}\frac{e^{-ik\tilde{\epsilon}_R Rn_0'\cdot m'}-1}{\sqrt{\tilde{\epsilon}_R^2+(\phi-\phi_0)^2}}\,e^{ikRn_0'\cdot m'}\,\mathrm{d}\phi\, e^{ikRm_z\sqrt{2\tilde{\epsilon}_R-\tilde{\epsilon}_R^2}} + o\left(\frac{1}{R}\right). \tag{B.4.63}$$

B.4.3.5 $\tilde{J}_7$

To obtain the asymptotic behaviour of $\tilde{J}_7$, the integral has to be split. Recall that (cf. (B.4.44))

$$\tilde{J}_7 = f_{\ell,j}(\nu',0) \int\limits_{1-\tilde{\epsilon}_R}^{1} \int\limits_{\phi_0-\pi}^{\phi_0+\pi} \frac{1}{\sqrt{(1-\rho)^2+(\phi-\phi_0)^2}}\, e^{ikRn_0'\cdot m'}\, \mathrm{d}\phi\, \frac{\rho}{\sqrt{1-\rho^2}}\, e^{ikRm_z\sqrt{1-\rho^2}}\, \mathrm{d}\rho.$$

The goal is to get an integral w.r.t. ϕ that can be evaluated explicitly. For this, the exponent $n_0'\cdot m' = |m'|\cos(\phi-\phi_1)$ has to be transformed to a linear function of ϕ and the domain of integration has to be extended to $\mathbb{R}$. To linearise the exponent, the Taylor expansion of $\cos(\phi-\phi_1)$ at $\phi=\phi_0$ is used.

For $\sin(\phi_0-\phi_1)\neq 0$,

$$n_0'\cdot m' = |m'|\cos(\phi_0-\phi_1) - |m'|\sin(\phi_0-\phi_1)\,(\phi-\phi_0) - |m'|\sin(\phi_0-\phi_1)\,\mathcal{R}_1(\phi-\phi_0)\,(\phi-\phi_0)^2,$$

where

$$\mathcal{R}_1(\psi) := -\frac{1}{\sin(\phi_0-\phi_1)} \sum_{o=0}^{\infty} \frac{a_o\,\psi^o}{(o+2)!}$$

and $a_o := (-1)^{o/2+1}\cos(\phi_0-\phi_1)$ if o is even and $a_o := (-1)^{(o-1)/2}\sin(\phi_0-\phi_1)$ otherwise, such that $|a_o|\leq 1$. Similarly, for $\sin(\phi_0-\phi_1)=0$,

$$n_0'\cdot m' = |m'|\cos(\phi_0-\phi_1) - \frac{|m'|}{2}\cos(\phi_0-\phi_1)\,(\phi-\phi_0)^2 + |m'|\cos(\phi_0-\phi_1)\,\mathcal{R}_2\big((\phi-\phi_0)^2\big)\,(\phi-\phi_0)^4,$$

where

$$\mathcal{R}_2(\psi) := \sum_{o=0}^{\infty} (-1)^o \frac{\psi^o}{(2o+4)!}.$$

Note that the case $\sin(\phi_0-\phi_1)=0$ corresponds to either $m'/|m'| = -\nu'$ or $m'/|m'| = \nu'$, where the latter was already examined in Section B.4.2, such that only the case of $m'/|m'| = -\nu'$ remains to be analysed. It is easily seen, that $\mathcal{R}_1$, $\mathcal{R}_2$ and their derivatives are continuous functions. Defining the constants $a := -k|m'|\sin(\phi_0-\phi_1)$ and $b := k|m'|\cos(\phi_0-\phi_1)$, and substituting $\psi = \phi-\phi_0$ such that

$$kn_0'\cdot m' = \begin{cases} b + a\,\psi + a\,\mathcal{R}_1(\psi)\,\psi^2, & \text{if } \sin(\phi_0-\phi_1)\neq 0, \\ b - \frac{b}{2}\,\psi^2 + b\,\mathcal{R}_2(\psi^2)\,\psi^4, & \text{if } \sin(\phi_0-\phi_1)=0 \end{cases}, \tag{B.4.64}$$

the integral $\tilde{J}_7$ can be split as

$$\tilde{J}_7 = f_{\ell,j}(\nu',0)\,\left(\tilde{J}^1_{7.1} - \tilde{J}^1_{7.2} + \tilde{J}^1_{7.3}\right) e^{ibR} \tag{B.4.65}$$

for $\sin(\phi_0-\phi_1)\neq 0$. Here,

$$\tilde{J}^1_{7.1} := \int\limits_{1-\tilde{\epsilon}_R}^{1} \int\limits_{-\pi}^{\pi} \frac{e^{iaR\,\mathcal{R}_1(\psi)\,\psi^2}-1}{\sqrt{(1-\rho)^2+\psi^2}}\, e^{iaR\,\psi}\, \mathrm{d}\psi\, \frac{\rho}{\sqrt{1-\rho^2}}\, e^{ikRm_z\sqrt{1-\rho^2}}\, \mathrm{d}\rho, \tag{B.4.66}$$

$$\tilde{J}^1_{7.2} := \int\limits_{1-\tilde{\epsilon}_R}^{1} \left(\int\limits_{-\infty}^{-\pi} + \int\limits_{\pi}^{\infty} \right) \frac{1}{\sqrt{(1-\rho)^2+\psi^2}}\, e^{iaR\,\psi}\, \mathrm{d}\psi\, \frac{\rho}{\sqrt{1-\rho^2}}\, e^{ikRm_z\sqrt{1-\rho^2}}\, \mathrm{d}\rho, \tag{B.4.67}$$

$$\tilde{J}^1_{7.3} := \int\limits_{1-\tilde{\epsilon}_R}^{1} \int\limits_{\mathbb{R}} \frac{1}{\sqrt{(1-\rho)^2+\psi^2}}\, e^{iaR\,\psi}\, \mathrm{d}\psi\, \frac{\rho}{\sqrt{1-\rho^2}}\, e^{ikRm_z\sqrt{1-\rho^2}}\, \mathrm{d}\rho. \tag{B.4.68}$$

In the same way, for $m'/|m'| = -\nu'$,

$$\tilde{J}_7 = f_{\ell,j}(\nu',0)\,\left(\tilde{J}^2_{7.1} - \tilde{J}^2_{7.2} + \tilde{J}^2_{7.3}\right) e^{ibR}, \tag{B.4.69}$$

where

$$\tilde{J}^2_{7.1} := \int\limits_{1-\tilde{\epsilon}_R}^{1} \int\limits_{-\pi}^{\pi} \frac{e^{ibR\,\mathcal{R}_2(\psi^2)\,\psi^4} - 1}{\sqrt{(1-\rho)^2+\psi^2}}\, e^{-i\frac{b}{2}R\,\psi^2}\, \mathrm{d}\psi\, \frac{\rho}{\sqrt{1-\rho^2}}\, e^{ikRm_z\sqrt{1-\rho^2}}\, \mathrm{d}\rho, \tag{B.4.70}$$

$$\tilde{J}^2_{7.2} := \int\limits_{1-\tilde{\epsilon}_R}^{1} \left(\int\limits_{-\infty}^{-\pi} + \int\limits_{\pi}^{\infty} \right) \frac{1}{\sqrt{(1-\rho)^2+\psi^2}}\, e^{-i\frac{b}{2}R\,\psi^2}\, \mathrm{d}\psi\, \frac{\rho}{\sqrt{1-\rho^2}}\, e^{ikRm_z\sqrt{1-\rho^2}}\, \mathrm{d}\rho, \tag{B.4.71}$$

$$\tilde{J}^2_{7.3} := \int\limits_{1-\tilde{\epsilon}_R}^{1} \int\limits_{\mathbb{R}} \frac{1}{\sqrt{(1-\rho)^2+\psi^2}}\, e^{-i\frac{b}{2}R\,\psi^2}\, \mathrm{d}\psi\, \frac{\rho}{\sqrt{1-\rho^2}}\, e^{ikRm_z\sqrt{1-\rho^2}}\, \mathrm{d}\rho. \tag{B.4.72}$$

Obviously, in this case, the exponent of $e^{-i\frac{b}{2}R\,\psi^2}$ is not linear. This will be resolved in the corresponding subsections by introducing an additional substitution of variable.

B.4.3.5.1 $\tilde{J}^1_{7.1}$

Again, to examine the asymptotic behaviour of $\tilde{J}^1_{7.1}$ (cf. (B.4.66)), integration by parts w.r.t. ρ is used. For this, note that a $c > 0$ exists such that

$$(1-\rho)\left| \frac{e^{iaR\,\mathcal{R}_1(\psi)\,\psi^2} - 1}{R\sqrt{(1-\rho)^2+\psi^2}^3} \right| \le \frac{1-\rho}{1-\rho}\, \frac{\left| e^{iaR\,\mathcal{R}_1(\psi)\,\psi^2} - 1 \right|}{R\,\psi^2} \le c < \infty$$

uniformly for all $\rho \in [1-\tilde{\epsilon}_R, 1]$, $\psi \in [-\pi, \pi]$ and $R \ge 1$. Hence, the absolute value of $\tilde{J}^1_{7.1}$ minus the boundary term at the lower bound from integrating by parts w.r.t. ρ is bounded by (cf. (B.3.48) and (B.3.52))

$$\begin{aligned}
&\frac{1}{kRm_z} \left| \int\limits_{-\pi}^{\pi} \frac{e^{iaR\,\mathcal{R}_1(\psi)\,\psi^2} - 1}{|\psi|}\, e^{iaR\,\psi}\, \mathrm{d}\psi \right| \\
&\qquad + \frac{1}{km_z} \left| \int\limits_{1-\tilde{\epsilon}_R}^{1} \int\limits_{-\pi}^{\pi} (1-\rho)\, \frac{e^{iaR\,\mathcal{R}_1(\psi)\,\psi^2} - 1}{R\sqrt{(1-\rho)^2+\psi^2}^3}\, e^{iaR\,\psi}\, \mathrm{d}\psi\, e^{ikRm_z\sqrt{1-\rho^2}}\, \mathrm{d}\rho \right| \\
&\le \frac{2\pi\, c}{km_z} \int\limits_{1-\tilde{\epsilon}_R}^{1} 1\, \mathrm{d}\rho + o\left(\frac{1}{R}\right) = o\left(\frac{1}{R}\right),
\end{aligned}$$

such that, undoing the substitution $\psi = \phi - \phi_0$,

$$\tilde{J}^1_{7.1} = \frac{1}{ikRm_z} \int\limits_{\phi_0-\pi}^{\phi_0+\pi} \frac{e^{iaR\,\mathcal{R}_1(\phi-\phi_0)\,(\phi-\phi_0)^2} - 1}{\sqrt{\tilde{\epsilon}_R^2 + (\phi-\phi_0)^2}}\, e^{iaR\,(\phi-\phi_0)}\, \mathrm{d}\phi\, e^{ikRm_z\sqrt{2\tilde{\epsilon}_R - \tilde{\epsilon}_R^2}} + o\left(\frac{1}{R}\right). \tag{B.4.73}$$

B.4.3.5.2 $\tilde{J}^2_{7.1}$

Considering integral $\tilde{J}^2_{7.1}$ (cf. (B.4.70)), similar to $\tilde{J}^1_{7.1}$ it is not hard to shown that a constant $0 < c < \infty$ exists such that

$$(1-\rho)\, \frac{e^{ibR\,\mathcal{R}_2(\psi^2)\,\psi^4} - 1}{R\sqrt{(1-\rho)^2+\psi^2}^3} \le \frac{1-\rho}{1-\rho}\, \frac{e^{ibR\,\mathcal{R}_2(\psi^2)\,\psi^4} - 1}{R\,\psi^2} \le c,$$

for $\rho \in [1-\tilde{\epsilon}_R, 1]$ and $\psi \in [-\pi, \pi]$. With this, the asymptotic behaviour of $\tilde{J}^2_{7.1}$ is easily estimated by integrating by parts w.r.t. ρ, such that the absolute value of $\tilde{J}^2_{7.1}$ minus the boundary term at the lower bound from integrating by parts w.r.t. ρ is bounded by (cf. (B.3.57) and (B.3.60))

$$\begin{aligned}
&\frac{1}{kRm_z}\left|\int_{-\pi}^{\pi}\frac{e^{ibR\,\mathcal{R}_2(\psi^2)\,\psi^4}-1}{|\psi|}\,e^{-i\frac{b}{2}R\,\psi^2}\,\mathrm{d}\psi\right| \\
&\qquad+\frac{1}{km_z}\left|\int_{1-\tilde{\epsilon}_R}^{1}\int_{-\pi}^{\pi}(1-\rho)\,\frac{e^{ibR\,\mathcal{R}_2(\psi^2)\,\psi^4}-1}{R\sqrt{(1-\rho)^2+\psi^2}^3}\,e^{-i\frac{b}{2}R\,\psi^2}\,\mathrm{d}\psi\,e^{ikRm_z\sqrt{1-\rho^2}}\,\mathrm{d}\rho\right| \\
&\qquad\le\frac{2\pi\,c}{km_z}\int_{1-\tilde{\epsilon}_R}^{1}1\,\mathrm{d}\rho+o\left(\frac{1}{R}\right)=o\left(\frac{1}{R}\right),
\end{aligned}$$

which, undoing the substitution $\psi=\phi-\phi_0$, leads to

$$\tilde{J}^2_{7.1}=\frac{1}{ikRm_z}\int_{\phi_0-\pi}^{\phi_0+\pi}\frac{e^{ibR\,\mathcal{R}_2((\phi-\phi_0)^2)\,(\phi-\phi_0)^4}-1}{\sqrt{\tilde{\epsilon}_R^2+(\phi-\phi_0)^2}}\,e^{-i\frac{b}{2}R\,(\phi-\phi_0)^2}\,\mathrm{d}\phi\,e^{ikRm_z\sqrt{2\tilde{\epsilon}_R-\tilde{\epsilon}_R^2}}+o\left(\frac{1}{R}\right). \tag{B.4.74}$$

B.4.3.5.3 $\tilde{J}^1_{7.2}$

Next, integral $\tilde{J}^1_{7.2}$ (cf. (B.4.67)) is examined. Recall that

$$\tilde{J}^1_{7.2}=-\frac{1}{ikRm_z}\int_{1-\tilde{\epsilon}_R}^{1}\left(\int_{-\infty}^{-\pi}+\int_{\pi}^{\infty}\right)\frac{1}{\sqrt{(1-\rho)^2+\psi^2}}\,e^{iaR\,\psi}\,\mathrm{d}\psi\;\partial_\rho\Big[e^{ikRm_z\sqrt{1-\rho^2}}\Big]\,\mathrm{d}\rho.$$

First, the integral w.r.t. ρ is integrated by parts, giving

$$\begin{aligned}
\tilde{J}^1_{7.2}=&-\frac{1}{ikRm_z}\left(\int_{-\infty}^{-\pi}+\int_{\pi}^{\infty}\right)\frac{1}{|\psi|}\,e^{iaR\,\psi}\,\mathrm{d}\psi \\
&+\frac{1}{ikRm_z}\left(\int_{-\infty}^{-\pi}+\int_{\pi}^{\infty}\right)\frac{1}{\sqrt{\tilde{\epsilon}_R^2+\psi^2}}\,e^{iaR\,\psi}\,\mathrm{d}\psi\,e^{ikRm_z\sqrt{2\tilde{\epsilon}_R-\tilde{\epsilon}_R^2}} \\
&+\frac{1}{ikRm_z}\int_{1-\tilde{\epsilon}_R}^{1}\left(\int_{-\infty}^{-\pi}+\int_{\pi}^{\infty}\right)\frac{1-\rho}{\sqrt{(1-\rho)^2+\psi^2}^3}\,e^{iaR\,\psi}\,\mathrm{d}\psi\,e^{ikRm_z\sqrt{1-\rho^2}}\,\mathrm{d}\rho,
\end{aligned}$$

where, since $1-\rho\le\tilde{\epsilon}_R$

$$\begin{aligned}
\frac{1}{R}\left|\int_{1-\tilde{\epsilon}_R}^{1}\left(\int_{-\infty}^{-\pi}+\int_{\pi}^{\infty}\right)\frac{1-\rho}{\sqrt{(1-\rho)^2+\psi^2}^3}\,e^{iaR\,\psi}\,\mathrm{d}\psi\,e^{ikRm_z\sqrt{1-\rho^2}}\,\mathrm{d}\rho\right|&\le\frac{\tilde{\epsilon}_R}{R}\int_{1-\tilde{\epsilon}_R}^{1}\left(\int_{-\infty}^{-\pi}+\int_{\pi}^{\infty}\right)\frac{1}{|\psi|^3}\,\mathrm{d}\psi\,\mathrm{d}\rho \\
&=\frac{\tilde{\epsilon}_R^2}{\pi^2\,R}=\mathcal{O}\left(\frac{1}{R^5}\right)=o\left(\frac{1}{R}\right).
\end{aligned} \tag{B.4.75}$$

Hence, in view of (B.3.69) and undoing the substitution $\psi=\phi-\phi_0$,

$$\tilde{J}^1_{7.2}=\frac{1}{ikRm_z}\left(\int_{-\infty}^{\phi_0-\pi}+\int_{\phi_0+\pi}^{\infty}\right)\frac{1}{\sqrt{\tilde{\epsilon}_R^2+(\phi-\phi_0)^2}}\,e^{iaR\,(\phi-\phi_0)}\,\mathrm{d}\phi\,e^{ikRm_z\sqrt{2\tilde{\epsilon}_R-\tilde{\epsilon}_R^2}}+o\left(\frac{1}{R}\right). \tag{B.4.76}$$

B.4.3.5.4 $\tilde{J}^2_{7.2}$

The asymptotic behaviour of $\tilde{J}^2_{7.2}$ (cf. (B.4.71)) is just as easily shown. Integration by parts w.r.t. ρ gives

$$\begin{aligned}
\tilde{J}^2_{7.2} &= -\frac{2}{ikRm_z} \int\limits_{1-\tilde{\epsilon}_R}^{1} \int\limits_{\pi}^{\infty} \frac{1}{\sqrt{(1-\rho)^2+\psi^2}}\, e^{-i\frac{b}{2}R\,\psi^2}\, \mathrm{d}\psi\, \partial_\rho \left[e^{ikRm_z\sqrt{1-\rho^2}}\right] \mathrm{d}\rho \\
&= -\frac{2}{ikRm_z} \int\limits_{\pi}^{\infty} \frac{1}{|\psi|}\, e^{-i\frac{b}{2}R\,\psi^2}\, \mathrm{d}\psi \\
&\quad + \frac{2}{ikRm_z} \int\limits_{\pi}^{\infty} \frac{1}{\sqrt{\tilde{\epsilon}_R^2+\psi^2}}\, e^{-i\frac{b}{2}R\,\psi^2}\, \mathrm{d}\psi\, e^{ikRm_z\sqrt{2\tilde{\epsilon}_R-\tilde{\epsilon}_R^2}} \\
&\quad + \frac{2}{ikRm_z} \int\limits_{1-\tilde{\epsilon}_R}^{1} \int\limits_{\pi}^{\infty} \frac{1-\rho}{\sqrt{(1-\rho)^2+\psi^2}^3}\, e^{-i\frac{b}{2}R\,\psi^2}\, \mathrm{d}\psi\, e^{ikRm_z\sqrt{1-\rho^2}}\, \mathrm{d}\rho,
\end{aligned}$$

where the last integral on the right hand side can be estimated the same as for $\tilde{J}^1_{7.2}$ (cf. (B.4.75)). Furthermore, (B.3.84) can be used to estimate the first integral on the right-hand side such that, undoing the substitution $\psi = \phi - \phi_0$,

$$\tilde{J}^2_{7.2} = \frac{1}{ikRm_z} \left(\int\limits_{-\infty}^{\phi_0-\pi} + \int\limits_{\phi_0+\pi}^{\infty} \right) \frac{1}{\sqrt{\tilde{\epsilon}_R^2+(\phi-\phi_0)^2}}\, e^{-i\frac{b}{2}R\,(\phi-\phi_0)^2}\, \mathrm{d}\phi\, e^{ikRm_z\sqrt{2\tilde{\epsilon}_R-\tilde{\epsilon}_R^2}} + o\left(\frac{1}{R}\right). \tag{B.4.77}$$

B.4.3.5.5 $\tilde{J}^1_{7.3}$

Finally the asymptotic behaviour of $\tilde{J}^1_{7.3}$ (cf. (B.4.68)) is determined. Recall that

$$\tilde{J}^1_{7.3} = \int\limits_{1-\tilde{\epsilon}_R}^{1} \int\limits_{\mathbb{R}} \frac{1}{\sqrt{(1-\rho)^2+\psi^2}}\, e^{iaR\,\psi}\, \mathrm{d}\psi\, \frac{\rho}{\sqrt{1-\rho^2}}\, e^{ikRm_z\sqrt{1-\rho^2}}\, \mathrm{d}\rho.$$

The integral w.r.t. ψ can be evaluated in the sense of a Fourier transform (cf. (B.3.71)). Furthermore, the resulting integral

$$\tilde{J}^1_{7.3} = 2 \int\limits_{1-\tilde{\epsilon}_R}^{1} K_0(|a|R(1-\rho))\, \frac{\rho}{\sqrt{1-\rho^2}}\, e^{ikRm_z\sqrt{1-\rho^2}}\, \mathrm{d}\rho$$

is split into the two integrals

$$\tilde{J}^1_{7.3} = I^1_1 + I^1_2, \tag{B.4.78}$$

where

$$\begin{aligned}
I^1_1 &:= 2 \int\limits_{1-\tilde{\epsilon}_R}^{1} \left[K_0(|a|R(1-\rho)) + \log\left(\frac{|a|}{2}R(1-\rho)\right) + \tilde{\gamma} \right] \frac{\rho}{\sqrt{1-\rho^2}}\, e^{ikRm_z\sqrt{1-\rho^2}}\, \mathrm{d}\rho, \\
I^1_2 &:= -2 \int\limits_{1-\tilde{\epsilon}_R}^{1} \left[\log\left(\frac{|a|}{2}R(1-\rho)\right) + \tilde{\gamma} \right] \frac{\rho}{\sqrt{1-\rho^2}}\, e^{ikRm_z\sqrt{1-\rho^2}}\, \mathrm{d}\rho
\end{aligned}$$

to separate the logarithmic singularity of K_0. The integral I_1^1 is evaluated using integration by parts. Given (B.3.73),

$$\begin{aligned} I_1^1 &= -\frac{2}{ikRm_z} \int\limits_{1-\tilde{\epsilon}_R}^{1} \left[K_0(|a|R(1-\rho)) + \log\left(\frac{|a|}{2}R(1-\rho)\right) + \tilde{\gamma}\right] \partial_\rho \left[e^{ikRm_z\sqrt{1-\rho^2}}\right] \,\mathrm{d}\rho \\ &= \frac{2}{ikRm_z} \left[K_0(|a|R\tilde{\epsilon}_R) + \log\left(\frac{|a|}{2}R\tilde{\epsilon}_R\right) + \tilde{\gamma}\right] e^{ikRm_z\sqrt{2\tilde{\epsilon}_R - \tilde{\epsilon}_R^2}} \\ &\quad - \frac{2|a|}{ikm_z} \int\limits_{1-\tilde{\epsilon}_R}^{1} \left[-K_1(|a|R(1-\rho)) + \frac{1}{|a|R(1-\rho)}\right] e^{ikRm_z\sqrt{1-\rho^2}} \,\mathrm{d}\rho, \end{aligned}$$

where (cf. [1, Eqns. 9.6.10 and 9.6.11, p. 119]) $|K_1(|a|R(1-\rho)) - 1/(|a|R(1-\rho))| < c$ for all $\rho \in [1-\tilde{\epsilon}_R, 1]$ and $R \geq 1$, which leads to

$$I_1^1 = \frac{2}{ikRm_z} \left[K_0(|a|R\tilde{\epsilon}_R) + \log\left(\frac{|a|}{2}R\tilde{\epsilon}_R\right) + \tilde{\gamma}\right] e^{ikRm_z\sqrt{2\tilde{\epsilon}_R - \tilde{\epsilon}_R^2}} + \mathcal{O}\left(\tilde{\epsilon}_R\right). \tag{B.4.79}$$

Consider I_2^1 and substitute $u = \sqrt{1-\rho^2}$

$$\begin{aligned} I_2^1 &= \frac{2}{ikRm_z} \left[\log\left(\frac{|a|}{2}R\right) + \tilde{\gamma}\right] \int\limits_{1-\tilde{\epsilon}_R}^{1} \partial_\rho \left[e^{ikRm_z\sqrt{1-\rho^2}}\right] \,\mathrm{d}\rho - 2 \int\limits_{1-\tilde{\epsilon}_R}^{1} \log(1-\rho) \frac{\rho}{\sqrt{1-\rho^2}} e^{ikRm_z\sqrt{1-\rho^2}} \,\mathrm{d}\rho \\ &= 2\frac{\log\left(\frac{|a|}{2}R\right) + \tilde{\gamma}}{ikRm_z} \left[1 - e^{ikRm_z\sqrt{2\tilde{\epsilon}_R - \tilde{\epsilon}_R^2}}\right] - 2 \int\limits_{0}^{\sqrt{2\tilde{\epsilon}_R - \tilde{\epsilon}_R^2}} \log\left(1 - \sqrt{1-u^2}\right) e^{ikRm_z u} \,\mathrm{d}u. \end{aligned} \tag{B.4.80}$$

To evaluate the remaining integral, first note that employing [32, Eqn. 106, p. 27 and 82] and [1, Eqns. 5.2.8, 5.2.9, 5.2.34 and 5.2.35, p. 60 and 61] gives

$$\begin{aligned} \int\limits_0^1 \log x \, e^{icRx} \,\mathrm{d}x &= \left[\tilde{\gamma} + \log(cR) - \mathrm{Ci}(cR) - i\,\mathrm{Si}(cR)\right] \frac{1}{icR} \\ &= \left[\tilde{\gamma} + \log(cR) - i\frac{\pi}{2}\right] \frac{1}{icR} + o\left(\frac{1}{R}\right). \end{aligned} \tag{B.4.81}$$

Moreover, it is used that

$$\lim_{u\to 0} \left[\log\left(1 - \sqrt{1-u^2}\right) - 2\log u\right] = \lim_{u\to 0} \log\left(\frac{1 - \sqrt{1-u^2}}{u^2}\right) = \lim_{u\to 0} \log\left(\frac{1}{1 + \sqrt{1-u^2}}\right) = -\log 2.$$

With this, (B.4.81), defining $d_R := \sqrt{2\tilde{\epsilon}_R - \tilde{\epsilon}_R^2} = \mathcal{O}(1/R)$ and using integration by parts for the remaining integral on the right-hand side of (B.4.80), it follows that

$$\begin{aligned} &\int\limits_0^{d_R} \log\left(1 - \sqrt{1-u^2}\right) e^{ikRm_z u} \,\mathrm{d}u \\ &= \int\limits_0^{d_R} \left[\log\left(1 - \sqrt{1-u^2}\right) - 2\log u\right] e^{ikRm_z u} \,\mathrm{d}u + 2\int\limits_0^{d_R} \log u \, e^{ikRm_z u} \,\mathrm{d}u \\ &= \frac{\log\tilde{\epsilon}_R - 2\log(d_R)}{ikRm_z} e^{ikRm_z d_R} + \frac{\log 2}{ikRm_z} - \frac{1}{ikRm_z} \int\limits_0^{d_R} \partial_u \left[\log\left(1 - \sqrt{1-u^2}\right) - 2\log u\right] e^{ikRm_z u} \,\mathrm{d}u \\ &\quad + 2\log(d_R)\, d_R \int\limits_0^1 e^{ikRm_z d_R u} \,\mathrm{d}u + 2d_R \int\limits_0^1 \log u \, e^{ikRm_z d_R u} \,\mathrm{d}u \end{aligned}$$

$$
\begin{aligned}
&= \frac{\log\tilde{\epsilon}_R - 2\log(d_R)}{ikRm_z}\, e^{ikRm_z d_R} + \frac{\log 2}{ikRm_z} - \frac{1}{ikRm_z}\int_0^{d_R} \frac{1}{\sqrt{1-u^2}}\frac{u}{1+\sqrt{1-u^2}}\, e^{ikRm_z u}\,\mathrm{d}u \\
&\quad + 2\frac{\log(d_R)\, d_R}{ikRm_z d_R}\left[e^{ikRm_z d_R} - 1\right] + 2\frac{d_R}{ikRm_z d_R}\left[\tilde{\gamma} + \log(kRm_z d_R) - i\frac{\pi}{2}\right] + o\left(\frac{1}{R}\right) \\
&= \frac{\log\tilde{\epsilon}_R}{ikRm_z}\, e^{ikRm_z d_R} + \frac{\log 2}{ikRm_z} + 2\frac{\tilde{\gamma} + \log(kRm_z) - i\frac{\pi}{2}}{ikRm_z} + o\left(\frac{1}{R}\right).
\end{aligned}
\tag{B.4.82}
$$

Hence,

$$
I_2^1 = 2\frac{\log\left(\frac{|a|}{2}R\right) - \tilde{\gamma}}{ikRm_z} - 2\frac{\log\left(\frac{|a|}{2}R\tilde{\epsilon}_R\right) + \tilde{\gamma}}{ikRm_z}\, e^{ikRm_z\sqrt{2\tilde{\epsilon}_R - \tilde{\epsilon}_R^2}} - 2\frac{\log 2}{ikRm_z} - 4\frac{\log(kRm_z) - i\frac{\pi}{2}}{ikRm_z} + o\left(\frac{1}{R}\right),
$$

and (cf. (B.4.78) and (B.4.79))

$$
\tilde{J}_{7.3}^1 = \frac{2}{ikRm_z}\, K_0(|a|R\tilde{\epsilon}_R)\, e^{ikRm_z\sqrt{2\tilde{\epsilon}_R - \tilde{\epsilon}_R^2}} + 2\frac{\log|a| - 2\log 2 - \log R - 2\log(km_z) - \tilde{\gamma} + i\pi}{ikRm_z} + o\left(\frac{1}{R}\right),
$$

where (cf. (B.3.71))

$$
2\, K_0(|a|R\tilde{\epsilon}_R) = \int_{\mathbb{R}} \frac{1}{\sqrt{\tilde{\epsilon}_R^2 + (\phi-\phi_0)^2}}\, e^{iaR\,(\phi-\phi_0)}\,\mathrm{d}\phi.
$$

In total, (cf. (B.4.65), (B.4.64) (B.4.73) and (B.4.76))

$$
\begin{aligned}
\tilde{J}_7 &= \frac{f_{\ell,j}(\nu',0)}{ikRm_z}\Bigg\{\int_{\phi_0-\pi}^{\phi_0+\pi} \frac{e^{iR[b + a\,(\phi-\phi_0) + \mathcal{R}_1(\phi-\phi_0)\,(\phi-\phi_0)^2]} - e^{iR[b + a\,(\phi-\phi_0)]}}{\sqrt{\tilde{\epsilon}_R^2 + (\phi-\phi_0)^2}}\,\mathrm{d}\phi \\
&\qquad - \left(\int_{-\infty}^{\phi_0-\pi} + \int_{\phi_0+\pi}^{\infty}\right)\frac{e^{iR[b + a\,(\phi-\phi_0)]}}{\sqrt{\tilde{\epsilon}_R^2 + (\phi-\phi_0)^2}}\,\mathrm{d}\phi + \int_{\mathbb{R}} \frac{e^{iR[b + a\,(\phi-\phi_0)]}}{\sqrt{\tilde{\epsilon}_R^2 + (\phi-\phi_0)^2}}\,\mathrm{d}\phi\Bigg\}\, e^{ikRm_z\sqrt{2\tilde{\epsilon}_R - \tilde{\epsilon}_R^2}} \\
&\quad + 2f_{\ell,j}(\nu',0)\,\frac{\log|a| - 2\log 2 - \log R - 2\log(km_z) - \tilde{\gamma} + i\pi}{ikRm_z}\, e^{ibR} + o\left(\frac{1}{R}\right) \\
&= \frac{f_{\ell,j}(\nu',0)}{ikRm_z}\int_{\phi_0-\pi}^{\phi_0+\pi} \frac{1}{\sqrt{\tilde{\epsilon}_R^2 + (\phi-\phi_0)^2}}\, e^{ikRn_0'\cdot m'}\,\mathrm{d}\phi\, e^{ikRm_z\sqrt{2\tilde{\epsilon}_R - \tilde{\epsilon}_R^2}} \\
&\quad + 2f_{\ell,j}(\nu',0)\,\frac{\log|a| - 2\log 2 - \log R - 2\log(km_z) - \tilde{\gamma} + i\pi}{ikRm_z}\, e^{ibR} + o\left(\frac{1}{R}\right).
\end{aligned}
$$

Thus (cf. (B.4.2), (B.4.5), (B.4.40), (B.4.58), (B.4.59), (B.4.61), (B.4.63) and $a = k|m'|\sin(\phi_0 - \phi_1)$)

$$
\mathcal{J}_1 = \frac{2\pi}{ikR}\frac{f_{\ell,j}(m', m_z)}{|m' - \nu'|}\, e^{ikR} + 2f_{\ell,j}(\nu',0)\,\frac{\log|a| - 2\log 2 - \log R - 2\log(km_z) - \tilde{\gamma} + i\pi}{ikRm_z}\, e^{ibR} + o\left(\frac{1}{R}\right)
$$

for $\sin(\phi_0 - \phi_1) \neq 0$. Finally, (cf. (B.2.4) and (B.3.79))

$$
\begin{aligned}
\mathcal{J} &= \frac{2\pi}{ikR}\frac{f_{\ell,j}(m', m_z)}{|m' - \nu'|}\, e^{ikR} + 2f_{\ell,j}(\nu',0)\,\frac{\log|a| - 2\log 2 - \log R - 2\log(km_z) - \tilde{\gamma} + i\pi}{ikRm_z}\, e^{ibR} \\
&\quad - 2f_{\ell,j}(\nu',0)\,\frac{\log|a| - 2\log 2 - \log R - 2\log(km_z) - \tilde{\gamma}}{ikRm_z}\, e^{ibR} + o\left(\frac{1}{R}\right) \\
&= \frac{2\pi}{ikR}\frac{f_{\ell,j}(m', m_z)}{|m' - \nu'|}\, e^{ikR} + f_{\ell,j}(\nu',0)\,\frac{2\pi}{kRm_z}\, e^{ikR\,\nu'\cdot m'} + o\left(\frac{1}{R}\right)
\end{aligned}
\tag{B.4.83}
$$

for $m'/|m'| \neq \pm\nu'$, since $b = k|m'|\cos(\phi_0 - \phi_1) = k\,\nu'\cdot m'$.

B.4.3.5.6 $\tilde{J}^2_{7.3}$

Only the asymptotic behaviour of $\tilde{J}^2_{7.3}$ (cf. (B.4.72)) is left to be derived. Recall that

$$\tilde{J}^2_{7.3} = \int\limits_{1-\tilde{\epsilon}_R}^{1} \int\limits_{\mathbb{R}} \frac{1}{\sqrt{(1-\rho)^2+\psi^2}}\, e^{-i\frac{b}{2}R\,\psi^2}\, \mathrm{d}\psi\, \frac{\rho}{\sqrt{1-\rho^2}}\, e^{ikRm_z\sqrt{1-\rho^2}}\, \mathrm{d}\rho,$$

which in view of (B.3.86) transforms to

$$\tilde{J}^2_{7.3} = -\int\limits_{1-\tilde{\epsilon}_R}^{1} \left\{\frac{\pi}{2}\, Y_0\!\left(\frac{|b|}{4}R(\rho-1)^2\right) + i\frac{\pi}{2}\,\mathrm{sgn}(b)\, J_0\!\left(\frac{|b|}{4}R(\rho-1)^2\right)\right\} e^{i\frac{b}{4}R(\rho-1)^2}\, \frac{\rho}{\sqrt{1-\rho^2}}\, e^{ikRm_z\sqrt{1-\rho^2}}\, \mathrm{d}\rho$$

such that

$$\tilde{J}^2_{7.3} = I_1^2 + I_2^2, \tag{B.4.84}$$

with

$$I_1^2 := \frac{1}{ikRm_z}\int\limits_{1-\tilde{\epsilon}_R}^{1} \Bigg[\left\{\frac{\pi}{2}\, Y_0\!\left(\frac{|b|}{4}R(\rho-1)^2\right) - \log\!\left(\frac{|b|}{8}R(\rho-1)^2\right) + i\frac{\pi}{2}\,\mathrm{sgn}(b)\, J_0\!\left(\frac{|b|}{4}R(\rho-1)^2\right)\right\}$$
$$e^{i\frac{b}{4}R(\rho-1)^2}\, \partial_\rho\!\left[e^{ikRm_z\sqrt{1-\rho^2}}\right]\Bigg]\, \mathrm{d}\rho,$$

$$I_2^2 := -\int\limits_{1-\tilde{\epsilon}_R}^{1} \log\!\left(\frac{|b|}{8}R(1-\rho)^2\right) e^{i\frac{b}{4}R(\rho-1)^2}\, \frac{\rho}{\sqrt{1-\rho^2}}\, e^{ikRm_z\sqrt{1-\rho^2}}\, \mathrm{d}\rho.$$

To determine the asymptotic behaviour of I_1^2, the integral w.r.t. ρ is integrated by parts, and (cf. (B.3.88) and [1, Eqn. 9.1.28, p. 105])

$$\begin{aligned}
I_1^2 = {} & \frac{\tilde{\gamma} + i\frac{\pi}{2}\,\mathrm{sgn}(b)}{ikRm_z} \\
& - \frac{1}{ikRm_z}\left\{\frac{\pi}{2}\, Y_0\!\left(\frac{|b|}{4}R\tilde{\epsilon}_R^2\right) - \log\!\left(\frac{|b|}{8}R\tilde{\epsilon}_R^2\right) + i\frac{\pi}{2}\,\mathrm{sgn}(b)\, J_0\!\left(\frac{|b|}{4}R\tilde{\epsilon}_R^2\right)\right\} e^{i\frac{b}{4}R\tilde{\epsilon}_R^2}\, e^{ikRm_z\sqrt{2\tilde{\epsilon}_R-\tilde{\epsilon}_R^2}} \\
& - \frac{|b|}{i2km_z}\int\limits_{1-\tilde{\epsilon}_R}^{1} \Bigg[(\rho-1)\left\{-\frac{\pi}{2}\, Y_1\!\left(\frac{|b|}{4}R(\rho-1)^2\right) - \frac{\frac{1}{2}}{\frac{|b|}{8}R(\rho-1)^2} - i\frac{\pi}{2}\,\mathrm{sgn}(b)\, J_1\!\left(\frac{|b|}{4}R(\rho-1)^2\right)\right\} \\
& \qquad e^{i\frac{b}{4}R(\rho-1)^2}\, e^{ikRm_z\sqrt{1-\rho^2}}\Bigg]\, \mathrm{d}\rho \\
& - \frac{b}{2km_z}\int\limits_{1-\tilde{\epsilon}_R}^{1} \Bigg[(\rho-1)\left\{\frac{\pi}{2}\, Y_0\!\left(\frac{|b|}{4}R(\rho-1)^2\right) - \log\!\left(\frac{|b|}{8}R(\rho-1)^2\right) + i\frac{\pi}{2}\,\mathrm{sgn}(b)\, J_0\!\left(\frac{|b|}{4}R(\rho-1)^2\right)\right\} \\
& \qquad e^{i\frac{b}{4}R(\rho-1)^2}\, \frac{\rho}{\sqrt{1-\rho^2}}\, e^{ikRm_z\sqrt{1-\rho^2}}\Bigg]\, \mathrm{d}\rho.
\end{aligned}$$

In view of [1, Eqns. 9.1.10 and 9.1.11, p. 104 with Eqn. 6.3.2, p. 79] for $R\tilde{\epsilon}_R^2 = 1/R^5 \to 0$ as $R \to \infty$, it is easily seen that the integrands of the remaining two integrals are uniformly bounded w.r.t. $\rho \in [1-\tilde{\epsilon}_R, 1]$ and $R > 1$. These two integrals, thus, decay at least as fast as their area of integration, which decreases with the order $\mathcal{O}(\tilde{\epsilon}_R) = \mathcal{O}(1/R^3) = o(1/R)$. Consequently, (cf. (B.3.88))

$$\begin{aligned}
I_1^2 = {} & -\frac{1}{ikRm_z}\left\{\frac{\pi}{2}\, Y_0\!\left(\frac{|b|}{4}R\tilde{\epsilon}_R^2\right) - \log\!\left(\frac{|b|}{8}R\tilde{\epsilon}_R^2\right) + i\frac{\pi}{2}\,\mathrm{sgn}(b)\, J_0\!\left(\frac{|b|}{4}R\tilde{\epsilon}_R^2\right)\right\} e^{i\frac{b}{4}R\tilde{\epsilon}_R^2}\, e^{ikRm_z\sqrt{2\tilde{\epsilon}_R-\tilde{\epsilon}_R^2}} \\
& + \frac{\tilde{\gamma} + i\frac{\pi}{2}\,\mathrm{sgn}(b)}{ikRm_z} + o\!\left(\frac{1}{R}\right).
\end{aligned} \tag{B.4.85}$$

At last, it only remains to analyse the asymptotic behaviour of I_2^2. The first step is to split the integral further to obtain

$$\begin{aligned} I_2^2 &= \frac{1}{ikRm_z} \int\limits_{1-\tilde{\epsilon}_R}^{1} \log\left(\frac{|b|}{8} R(1-\rho)^2\right) e^{i\frac{b}{4}R(\rho-1)^2}\, \partial_\rho \left[e^{ikRm_z\sqrt{1-\rho^2}}\right] \mathrm{d}\rho \\ &= \frac{\log\left(\frac{|b|}{8}R\right)}{ikRm_z} \int\limits_{1-\tilde{\epsilon}_R}^{1} e^{i\frac{b}{4}R(\rho-1)^2}\, \partial_\rho \left[e^{ikRm_z\sqrt{1-\rho^2}}\right] \mathrm{d}\rho \\ &\quad + \frac{2}{ikRm_z} \int\limits_{1-\tilde{\epsilon}_R}^{1} \log(1-\rho) \left[e^{i\frac{b}{4}R(\rho-1)^2} - 1\right] \partial_\rho \left[e^{ikRm_z\sqrt{1-\rho^2}}\right] \mathrm{d}\rho \\ &\quad - 2 \int\limits_{1-\tilde{\epsilon}_R}^{1} \log(1-\rho)\, \frac{\rho}{\sqrt{1-\rho^2}}\, e^{ikRm_z\sqrt{1-\rho^2}}\, \mathrm{d}\rho, \end{aligned} \tag{B.4.86}$$

where, by integration by parts and since $\mathcal{O}(\tilde{\epsilon}_R) = o(1/R)$,

$$\begin{aligned} \frac{\log\left(\frac{|b|}{8}R\right)}{ikRm_z} \int\limits_{1-\tilde{\epsilon}_R}^{1} e^{i\frac{b}{4}R(\rho-1)^2} \partial_\rho\left[e^{ikRm_z\sqrt{1-\rho^2}}\right] \mathrm{d}\rho &= \frac{\log\left(\frac{|b|}{8}R\right)}{ikRm_z} - \frac{\log\left(\frac{|b|}{8}R\right)}{ikRm_z}\, e^{i\frac{b}{4}R\tilde{\epsilon}_R^2}\, e^{ikRm_z\sqrt{2\tilde{\epsilon}_R-\tilde{\epsilon}_R^2}} \\ &\quad - \frac{b\,\log\left(\frac{|b|}{8}R\right)}{2km_z} \int\limits_{1-\tilde{\epsilon}_R}^{1} (\rho-1)\, e^{i\frac{b}{4}R(\rho-1)^2}\, e^{ikRm_z\sqrt{1-\rho^2}}\, \mathrm{d}\rho \\ &= \frac{\log\left(\frac{|b|}{8}R\right)}{ikRm_z} - \frac{\log\left(\frac{|b|}{8}R\right)}{ikRm_z}\, e^{i\frac{b}{4}R\tilde{\epsilon}_R^2} e^{ikRm_z\sqrt{2\tilde{\epsilon}_R-\tilde{\epsilon}_R^2}} + o\left(\frac{1}{R}\right). \end{aligned}$$

Furthermore, integrating the second integral on the right-hand side of (B.4.86) by parts as well, gives (cf. (B.3.93))

$$\begin{aligned} &\frac{2}{ikRm_z} \int\limits_{1-\tilde{\epsilon}_R}^{1} \log(1-\rho) \left[e^{i\frac{b}{4}R(\rho-1)^2} - 1\right] \partial_\rho \left[e^{ikRm_z\sqrt{1-\rho^2}}\right] \mathrm{d}\rho \\ &\qquad = -2\frac{\log\tilde{\epsilon}_R}{ikRm_z} \left[e^{i\frac{b}{4}R\tilde{\epsilon}_R^2} - 1\right] e^{ikRm_z\sqrt{2\tilde{\epsilon}_R-\tilde{\epsilon}_R^2}} \\ &\qquad\quad + \frac{2}{ikRm_z} \int\limits_{1-\tilde{\epsilon}_R}^{1} \frac{e^{i\frac{b}{4}R(\rho-1)^2} - 1}{1-\rho}\, e^{ikRm_z\sqrt{1-\rho^2}}\, \mathrm{d}\rho \\ &\qquad\quad + \frac{b}{km_z} \int\limits_{1-\tilde{\epsilon}_R}^{1} \log(1-\rho)\,(1-\rho)\, e^{i\frac{b}{4}R(\rho-1)^2}\, e^{ikRm_z\sqrt{1-\rho^2}}\, \mathrm{d}\rho \\ &\qquad = -2\frac{\log\tilde{\epsilon}_R}{ikRm_z} \left[e^{i\frac{b}{4}R\tilde{\epsilon}_R^2} - 1\right] e^{ikRm_z\sqrt{2\tilde{\epsilon}_R-\tilde{\epsilon}_R^2}} + o\left(\frac{1}{R}\right), \end{aligned}$$

since the estimates in (B.3.94) also hold for $\rho \in [1-\tilde{\epsilon}_R, 1]$. Now only the asymptotic behaviour of the third integral on the right-hand side of (B.4.86) remains to be determined. Here, $\sqrt{1-\rho^2}$ is substituted by u, which leads to (cf. (B.4.82))

$$\begin{aligned} -2\int\limits_{1-\tilde{\epsilon}_R}^{1} \frac{\log(1-\rho)\,\rho}{\sqrt{1-\rho^2}}\, e^{ikRm_z\sqrt{1-\rho^2}}\, \mathrm{d}\rho &= -2\int\limits_{0}^{d_R} \log\left(1-\sqrt{1-u^2}\right) e^{ikRm_z u}\, \mathrm{d}u \\ &= -2\frac{\log\tilde{\epsilon}_R}{ikRm_z} e^{ikRm_z d_R} - 2\frac{\log 2}{ikRm_z} - 4\frac{\tilde{\gamma} + \log(kRm_z) - i\frac{\pi}{2}}{ikRm_z} + o\left(\frac{1}{R}\right) \end{aligned}$$

such that

$$I_2^2 = -\frac{\log\left(\frac{|b|}{8} R\tilde{\epsilon}_R^2\right)}{ikRm_z}\, e^{i\frac{b}{4}R\tilde{\epsilon}_R^2} e^{ikRm_z\sqrt{2\tilde{\epsilon}_R-\tilde{\epsilon}_R^2}} + \frac{\log|b| - 5\log 2 - 3\log R - 4\log(km_z) - 4\tilde{\gamma} + i\,2\pi}{ikRm_z} + o\left(\frac{1}{R}\right)$$

and (cf. (B.4.84) and (B.4.85))

$$\begin{aligned}\tilde{J}_{7.3}^2 = &-\frac{1}{ikRm_z}\left\{\frac{\pi}{2}\, Y_0\left(\frac{|b|}{4} R\tilde{\epsilon}_R^2\right) + i\frac{\pi}{2}\,\mathrm{sgn}(b)\, J_0\left(\frac{|b|}{4} R\tilde{\epsilon}_R^2\right)\right\} e^{i\frac{b}{4}R\tilde{\epsilon}_R^2}\, e^{ikRm_z\sqrt{2\tilde{\epsilon}_R-\tilde{\epsilon}_R^2}} \\ &+ \frac{\log|b| - 5\log 2 - 3\log R - 4\log(km_z) - 3\tilde{\gamma} + i\frac{\pi}{2}\,\mathrm{sgn}(b) + i\,2\pi}{ikRm_z} + o\left(\frac{1}{R}\right).\end{aligned}$$

Note that (cf. (B.3.86) and $\psi = \phi - \phi_0$)

$$\begin{aligned}&\int\limits_{\mathbb{R}} \frac{1}{\sqrt{\tilde{\epsilon}_R^2 + (\phi-\phi_0)^2}}\, e^{-i\frac{b}{2}R(\phi-\phi_0)^2}\,\mathrm{d}\phi\, e^{ikRm_z\sqrt{2\tilde{\epsilon}_R-\tilde{\epsilon}_R^2}} \\ &\qquad = -\left\{\frac{\pi}{2}\, Y_0\left(\frac{|b|}{4} R\tilde{\epsilon}_R^2\right) + i\frac{\pi}{2}\,\mathrm{sgn}(b)\, J_0\left(\frac{|b|}{4} R\tilde{\epsilon}_R^2\right)\right\} e^{i\frac{b}{4}R\tilde{\epsilon}_R^2}\, e^{ikRm_z\sqrt{2\tilde{\epsilon}_R-\tilde{\epsilon}_R^2}}.\end{aligned}$$

Using this equality, (cf. (B.4.69), (B.4.64), (B.4.74) and (B.4.77))

$$\begin{aligned}\tilde{J}_7 = &\frac{f_{\ell,j}(\nu',0)}{ikRm_z}\left\{\int\limits_{\phi_0-\pi}^{\phi_0+\pi} \frac{e^{iR\left[b-\frac{b}{2}(\phi-\phi_0)^2 + b\,\mathcal{R}_2((\phi-\phi_0)^2)\,(\phi-\phi_0)^4\right]} - e^{iR\left[b-\frac{b}{2}(\phi-\phi_0)^2\right]}}{\sqrt{\tilde{\epsilon}_R^2 + (\phi-\phi_0)^2}}\,\mathrm{d}\phi\right. \\ &\left. - \left(\int\limits_{-\infty}^{\phi_0-\pi} + \int\limits_{\phi_0+\pi}^{\infty}\right)\frac{e^{iR\left[b-\frac{b}{2}(\phi-\phi_0)^2\right]}}{\sqrt{\tilde{\epsilon}_R^2 + (\phi-\phi_0)^2}}\,\mathrm{d}\phi + \int\limits_{\mathbb{R}}\frac{e^{iR\left[b-\frac{b}{2}(\phi-\phi_0)^2\right]}}{\sqrt{\tilde{\epsilon}_R^2 + (\phi-\phi_0)^2}}\,\mathrm{d}\phi\right\} e^{ikRm_z\sqrt{2\tilde{\epsilon}_R-\tilde{\epsilon}_R^2}} \\ &+ f_{\ell,j}(\nu',0)\,\frac{\log|b| - 5\log 2 - 3\log R - 4\log(km_z) - 3\tilde{\gamma} + i\frac{\pi}{2}\,\mathrm{sgn}(b) + i\,2\pi}{ikRm_z}\, e^{ibR} + o\left(\frac{1}{R}\right) \\ = &\frac{f_{\ell,j}(\nu',0)}{ikRm_z}\int\limits_{\phi_0-\pi}^{\phi_0+\pi}\frac{1}{\sqrt{\tilde{\epsilon}_R^2 + (\phi-\phi_0)^2}}\, e^{ikRn_0'\cdot m'}\,\mathrm{d}\phi\, e^{ikRm_z\sqrt{2\tilde{\epsilon}_R-\tilde{\epsilon}_R^2}} \\ &+ f_{\ell,j}(\nu',0)\,\frac{\log|b| - 5\log 2 - 3\log R - 4\log(km_z) - 3\tilde{\gamma} + i\frac{\pi}{2}\,\mathrm{sgn}(b) + i\,2\pi}{ikRm_z}\, e^{ibR} + o\left(\frac{1}{R}\right).\end{aligned}$$

Therefore, (cf. (B.4.2), (B.4.5), (B.4.40), (B.4.58), (B.4.59), (B.4.61), (B.4.63) and $b = k|m'|\cos(\phi_0-\phi_1)$ and $\log|\cos(\phi_0-\phi_1)| = \log 1 = 0$)

$$\begin{aligned}\mathcal{J}_1 = &\frac{2\pi}{ikR}\,\frac{f_{\ell,j}(m',m_z)}{|m'-\nu'|}\, e^{ikR} \\ &+ f_{\ell,j}(\nu',0)\,\frac{\log|m'| - 5\log 2 - 4\log(m_z) - 3\left[\tilde{\gamma} + \log(kR)\right] + i\frac{\pi}{2}\,\cos(\phi_0-\phi_1) + i\,2\pi}{ikRm_z}\, e^{ikR|m'|\cos(\phi_0-\phi_1)} \\ &+ o\left(\frac{1}{R}\right)\end{aligned}$$

for $m'/|m'| = -\nu'$. Finally, adding $\mathcal{J}_2$ (cf. (B.3.95)) to $\mathcal{J}_1$, (cf. (B.2.4))

$$\mathcal{J} = \frac{2\pi}{ikR}\,\frac{f_{\ell,j}(m',m_z)}{|m'-\nu'|}\, e^{ikR} + f_{\ell,j}(\nu',0)\,\frac{2\pi}{kRm_z}\, e^{ikR\nu'\cdot m'} + o\left(\frac{1}{R}\right) \tag{B.4.87}$$

for $m'/|m'| = -\nu'$, since $|m'|\cos(\phi_0-\phi_1) = \nu'\cdot m'$.

B.4.4 Normal reflection

To show the asymptotic behaviour of $\mathcal{J}_1$ in the case that the far-field is evaluated in 'normal' direction, i.e. orthogonal to the x-y-plane ($m' = (0,0)^\top$), the same substitution into spherical coordinates $(\psi, \phi)^\top$ w.r.t. $\vec{m}$, that was introduced at the beginning of Section 4.2.3 (cf. (4.2.22) and (4.2.23)), is used. For $m' = (0,0)^\top$, or equivalently $\alpha = 0$, it follows that $\psi_0 = 0$ since $\cos\theta(\phi) \equiv 0$ (cf. (4.2.28)). Thus, by applying Fubini's theorem, (cf. (B.4.1))

$$\begin{aligned}\mathcal{J}_1 &= \int_{\phi_0-\pi}^{\phi_0+\pi}\int_0^1 \frac{f_{\ell,j}(n'(\psi,\phi), \sqrt{1-n'(\psi,\phi)^2})}{|n'(\psi,\phi)-\nu'|}\, e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi \\ &= \int_0^1\int_{\phi_0-\pi}^{\phi_0+\pi} \frac{f_{\ell,j}(n'(\psi,\phi), \sqrt{1-n'(\psi,\phi)^2})}{|n'(\psi,\phi)-\nu'|}\,\mathrm{d}\phi\, e^{ikR\psi}\,\mathrm{d}\psi. \qquad \text{(B.4.88)}\end{aligned}$$

Moreover, assuming ϕ_0 is defined such that $n'(0,\phi_0) = \nu'$, it is easily shown that (cf. 4.2.22)

$$\begin{aligned}|n'(\psi,\phi)-\nu'|^2 &= \Big[\big(\cos\beta\cos\phi - \sin\beta\sin\phi\big)\sqrt{1-\psi^2} - \cos\beta\cos\phi_0 + \sin\beta\sin\phi_0\Big]^2 \\ &\quad + \Big[\big(\sin\beta\cos\phi + \cos\beta\sin\phi\big)\sqrt{1-\psi^2} - \sin\beta\cos\phi_0 - \cos\beta\sin\phi_0\Big]^2 \\ &= \Big[\cos\phi\sqrt{1-\psi^2} - \cos\phi_0\Big]^2 + \Big[\sin\phi\sqrt{1-\psi^2} - \sin\phi_0\Big]^2 \\ &= 2 - \psi^2 - 2\sqrt{1-\psi^2}\cos(\phi-\phi_0), \qquad \text{(B.4.89)}\end{aligned}$$

which is an element of C^∞ w.r.t. $\psi \in (-1,1)$ and $\phi \in [\phi_0-\pi, \phi_0+\pi)$. The corresponding Taylor-series expansion is

$$\begin{aligned}G(\psi,\phi) &:= |n'(\psi,\phi)-\nu'|^2 = G_4(\psi,\phi) + \mathcal{O}\left((|\psi|^2 + |\phi-\phi_0|^2)^3\right), \qquad \text{(B.4.90)} \\ G_4(\psi,\phi) &:= (\phi-\phi_0)^2 + \frac{1}{4}\psi^4 - \frac{1}{2}\psi^2(\phi-\phi_0)^2 - \frac{1}{12}(\phi-\phi_0)^4.\end{aligned}$$

The order $\mathcal{O}\left((|\psi|^2 + |\phi-\phi_0|^2)^3\right)$ of the higher order terms is easily seen, since $G(\psi,\phi)$ (cf. (B.4.89)) is an even function w.r.t. $\psi = 0$ and $\phi = \phi_0$, such that only even terms can appear in the Taylor expansion. Motivated by the Taylor expansion of G, integral $\mathcal{J}_1$ is split into

$$\mathcal{J}_1 = \tilde{J}_1^0 + \tilde{J}_2^0 + f_{\ell,j}(\nu',0)\,\tilde{J}_3^0, \qquad \text{(B.4.91)}$$

where (cf. (B.4.88))

$$\begin{aligned}\tilde{J}_1^0 &:= \int_0^1\int_{\phi_0-\pi}^{\phi_0+\pi} f_{\ell,j}(n'(\psi,\phi), \sqrt{1-n'(\psi,\phi)^2})\left[\frac{1}{|n'(\psi,\phi)-\nu'|} - \frac{1}{\sqrt{(\phi-\phi_0)^2+\psi^4/4}}\right]\mathrm{d}\phi\, e^{ikR\psi}\,\mathrm{d}\psi \\ \tilde{J}_2^0 &:= \int_0^1\int_{\phi_0-\pi}^{\phi_0+\pi} \frac{f_{\ell,j}(n'(\psi,\phi), \sqrt{1-n'(\psi,\phi)^2}) - f(\nu',0)}{\sqrt{(\phi-\phi_0)^2+\psi^4/4}}\,\mathrm{d}\phi\, e^{ikR\psi}\,\mathrm{d}\psi \qquad \text{(B.4.92)} \\ \tilde{J}_3^0 &:= \int_0^1\int_{\phi_0-\pi}^{\phi_0+\pi} \frac{1}{\sqrt{(\phi-\phi_0)^2+\psi^4/4}}\,\mathrm{d}\phi\, e^{ikR\psi}\,\mathrm{d}\psi. \qquad \text{(B.4.93)}\end{aligned}$$

Applying integration by parts w.r.t. ψ to the first integral,

$$\begin{aligned}\tilde{J}_1^0 = & \frac{1}{ikR}\int\limits_{\phi_0-\pi}^{\phi_0+\pi} f_{\ell,j}(m',1)\left[\frac{1}{|m'-\nu'|}-\frac{1}{\sqrt{(\phi-\phi_0)^2+1/4}}\right]\mathrm{d}\phi\, e^{ikR}\\ & -\frac{1}{ikR}\int\limits_{\phi_0-\pi}^{\phi_0+\pi} f_{\ell,j}(n'(0,\phi),0)\left[\frac{1}{|n'(0,\phi)-\nu'|}-\frac{1}{|\phi-\phi_0|}\right]\mathrm{d}\phi \\ & -\frac{1}{ikR}\int\limits_0^1\int\limits_{\phi_0-\pi}^{\phi_0+\pi}\partial_\psi\left[f_{\ell,j}(n'(\psi,\phi),\sqrt{1-n'(\psi,\phi)^2})\left[\frac{1}{|n'(\psi,\phi)-\nu'|}-\frac{1}{\sqrt{(\phi-\phi_0)^2+\frac{\psi^4}{4}}}\right]\right]\mathrm{d}\phi\, e^{ikR\psi}\mathrm{d}\psi,\end{aligned} \tag{B.4.94}$$

since $n'(\psi,\phi)$ reduces to the constant m' for $\psi=1$. It is easy to see that the first integral on the right-hand side exists, since the integrand is bounded for every $\phi\in[\phi_0-\pi,\phi_0+\pi]$. For the remaining two integrals, the Riemann-Lebesgue lemma is once again to be applied to show that they tend to zero as R tends to infinity. To apply the Riemann-Lebesgue lemma, it remains to be shown that

$$\frac{1}{|n'(0,\phi)-\nu'|}-\frac{1}{|\phi-\phi_0|} \tag{B.4.95}$$

and

$$\partial_\psi\left[f_{\ell,j}(n'(\psi,\phi),\sqrt{1-n'(\psi,\phi)^2})\left[\frac{1}{|n'(\psi,\phi)-\nu'|}-\frac{1}{\sqrt{(\phi-\phi_0)^2+\psi^4/4}}\right]\right] \tag{B.4.96}$$

are absolutely integrable w.r.t. ϕ. First, consider (B.4.95) by replacing $|n'(\psi,\phi)-\nu'|=\sqrt{G(\psi,\phi)}$ and using the series expansion (B.4.90)

$$\begin{aligned}&\frac{1}{|n'(\psi,\phi)-\nu'|}-\frac{1}{\sqrt{(\phi-\phi_0)^2+\frac{1}{4}\psi^4}}\\ &=\frac{(\phi-\phi_0)^2+\frac14\psi^4-G(\psi,\phi)}{|n'(\psi,\phi)-\nu'|\sqrt{(\phi-\phi_0)^2+\frac14\psi^4}\left[\sqrt{(\phi-\phi_0)^2+\frac14\psi^4}+|n'(\psi,\phi)-\nu'|\right]}\\ &=\frac{\frac12\psi^2(\phi-\phi_0)^2+\frac{1}{12}(\phi-\phi_0)^4+\mathcal{O}\left((|\psi|^2+|\phi-\phi_0|^2)^3\right)}{\sqrt{G_4(\psi,\phi)+\mathcal{O}\left((|\psi|^2+|\phi-\phi_0|^2)^3\right)}\sqrt{(\phi-\phi_0)^2+\frac14\psi^4}}\\ &\qquad\frac{1}{\sqrt{(\phi-\phi_0)^2+\frac14\psi^4}+\sqrt{G_4(\psi,\phi)+\mathcal{O}\left((|\psi|^2+|\phi-\phi_0|^2)^3\right)}}.\end{aligned} \tag{B.4.97}$$

Replacing $(\psi,\phi-\phi_0)^\top$ by $r\,(\cos\gamma,\sin\gamma)$, for $\gamma\neq 0,\pi$, and evaluating the limit $r\to 0$ will then lead to

$$\lim_{r\to 0}\left[\frac{1}{|n'(\psi,\phi)-\nu'|}-\frac{1}{\sqrt{(\phi-\phi_0)^2+\frac14\psi^4}}\right]_{\binom{\psi}{\phi-\phi_0}\to r\binom{\cos\gamma}{\sin\gamma}}=0. \tag{B.4.98}$$

The same can be done for $\gamma=0,\pi$ by extending the Taylor expansion of G to sixth-order polynomials. It can easily be shown that $\partial_\psi^5 G(0,\phi_0)=0$ and

$$\partial_\psi^6 G(0,\phi_0)=90\lim_{\substack{\psi\to 0\\ \phi\to\phi_0}}\left(\frac{21\,\psi^6}{\sqrt{1-\psi^2}^{11}}+\frac{35\,\psi^4}{\sqrt{1-\psi^2}^{9}}+\frac{15\,\psi^2}{\sqrt{1-\psi^2}^{7}}+\frac{1}{\sqrt{1-\psi^2}^{5}}\right)\cos(\phi-\phi_0)=90$$

is finite, which shows that the limit in (B.4.98) is uniformly bounded for $\gamma\in[0,2\pi]$. Consequently, Lemma 4.4 proves that the difference of quotients in (B.4.98) is absolutely bounded in a neighbourhood of $(\psi,\phi)^\top = (0,\phi_0)^\top$ such that (B.4.95) is uniformly bounded for all $\phi \in [0,2\pi]$. Hence, the integrand of the second integral on the right-hand side of (B.4.94) is bounded and thus absolutely integrable for $\phi \in [\phi_0-\pi, \phi_0+\pi]$. Now examine (B.4.96), keeping in mind that $\vec{n}(\psi,\phi) = (n'(\psi,\phi), n_z(\psi,\phi))^\top$,

$$\begin{aligned}
&\partial_\psi\left[f_{\ell,j}(n'(\psi,\phi),n_z(\psi,\phi))\left[\frac{1}{|n'(\psi,\phi)-\nu'|}-\frac{1}{\sqrt{(\phi-\phi_0)^2+\psi^4/4}}\right]\right]\\
&\quad= \partial_\psi\vec{n}(\psi,\phi)\cdot\nabla_{\vec{n}}\, f_{\ell,j}(n'(\psi,\phi),n_z(\psi,\phi))\left[\frac{1}{|n'(\psi,\phi)-\nu'|}-\frac{1}{\sqrt{(\phi-\phi_0)^2+\psi^4/4}}\right]\\
&\quad\quad-\frac{1}{2}\, f_{\ell,j}(n'(\psi,\phi),n_z(\psi,\phi))\left[\frac{\partial_\psi G(\psi,\phi)}{|n'(\psi,\phi)-\nu'|^3}-\frac{\psi^3}{\sqrt{(\phi-\phi_0)^2+\psi^4/4}^3}\right],
\end{aligned} \tag{B.4.99}$$

where (cf. (4.2.22) and (4.2.23) for $\alpha = 0$)

$$\partial_\psi\vec{n}(\psi,\phi) = \begin{pmatrix} -(\cos\beta\cos\phi-\sin\beta\sin\phi)\frac{\psi}{\sqrt{1-\psi^2}}\\ -(\sin\beta\cos\phi+\cos\beta\sin\phi)\frac{\psi}{\sqrt{1-\psi^2}}\\ 1\end{pmatrix}$$

is uniformly bounded w.r.t. ψ in a neighbourhood of $\psi_0 = 0$. Furthermore, the same has already been shown above for $1/|n'(\psi,\phi)-\nu'| - 1/\sqrt{(\phi-\phi_0)^2+\psi^4/4}$, while Lemma B.2 states that $\nabla_{\vec{n}} f_{\ell,j}(n',n_z)$ is at most logarithmically singular. Similar to (B.4.97), it can also be shown that the derivative w.r.t. ψ of (B.4.97) is absolutely integrable w.r.t. ϕ. This is done by using the Taylor expansion of $\partial_\psi G(\psi,\phi)$ (cf. (B.4.90))

$$\partial_\psi G(\psi,\phi) = \psi^3 - \psi\,(\phi-\phi_0)^2 + \mathcal{O}\left(|\psi|\left(|\psi|^2+|\phi-\phi_0|^2\right)^2\right).$$

Thus

$$\begin{aligned}
&-2\partial_\psi\left[\frac{1}{\sqrt{G(\psi,\phi)}}-\frac{1}{\sqrt{(\phi-\phi_0)^2+\psi^4/4}}\right]\sqrt{(\phi-\phi_0)^2+\psi^4/4}\\
&\quad=\left[\frac{\partial_\psi G(\psi,\phi)}{\sqrt{G(\psi,\phi)}^3}-\frac{\psi^3}{\sqrt{(\phi-\phi_0)^2+\psi^4/4}^3}\right]\sqrt{(\phi-\phi_0)^2+\psi^4/4}\\
&\quad=\frac{[\partial_\psi G(\psi,\phi)]^2\left[(\phi-\phi_0)^2+\psi^4/4\right]^3-\psi^6\,[G(\psi,\phi)]^3}{\sqrt{G(\psi,\phi)}^3\left[(\phi-\phi_0)^2+\psi^4/4\right]\left\{\partial_\psi G(\psi,\phi)\sqrt{(\phi-\phi_0)^2+\psi^4/4}^3+\psi^3\sqrt{G(\psi,\phi)}^3\right\}}\\
&\quad=\frac{\left\{\psi^3-\psi\,(\phi-\phi_0)^2+\mathcal{O}\left(|\psi|\left(|\psi|^2+|\phi-\phi_0|^2\right)^2\right)\right\}^2\left[(\phi-\phi_0)^2+\psi^4/4\right]^3}{\sqrt{G(\psi,\phi)}^3\left[(\phi-\phi_0)^2+\psi^4/4\right]\left\{\partial_\psi G(\psi,\phi)\sqrt{(\phi-\phi_0)^2+\psi^4/4}^3+\psi^3\sqrt{G(\psi,\phi)}^3\right\}}\\
&\quad\quad-\frac{\psi^6\left[(\phi-\phi_0)^2+\frac{1}{4}\,\psi^4-\frac{1}{2}\,\psi^2\,(\phi-\phi_0)^2-\frac{1}{12}\,(\phi-\phi_0)^4+\mathcal{O}\left(\left(|\psi|^2+|\phi-\phi_0|^2\right)^3\right)\right]^3}{\sqrt{G(\psi,\phi)}^3\left[(\phi-\phi_0)^2+\psi^4/4\right]\left\{\partial_\psi G(\psi,\phi)\sqrt{(\phi-\phi_0)^2+\psi^4/4}^3+\psi^3\sqrt{G(\psi,\phi)}^3\right\}}\\
&\quad=\frac{2\psi^3\left\{-\psi\,(\phi-\phi_0)^2+\mathcal{O}\left(|\psi|\left(|\psi|^2+|\phi-\phi_0|^2\right)^2\right)\right\}\left[(\phi-\phi_0)^2+\psi^4/4\right]^3}{\sqrt{G(\psi,\phi)}^3\left[(\phi-\phi_0)^2+\psi^4/4\right]\left\{\partial_\psi G(\psi,\phi)\sqrt{(\phi-\phi_0)^2+\psi^4/4}^3+\psi^3\sqrt{G(\psi,\phi)}^3\right\}}\\
&\quad\quad+\frac{\left\{-\psi\,(\phi-\phi_0)^2+\mathcal{O}\left(|\psi|\left(|\psi|^2+|\phi-\phi_0|^2\right)^2\right)\right\}^2\left[(\phi-\phi_0)^2+\psi^4/4\right]^3}{\sqrt{G(\psi,\phi)}^3\left[(\phi-\phi_0)^2+\psi^4/4\right]\left\{\partial_\psi G(\psi,\phi)\sqrt{(\phi-\phi_0)^2+\psi^4/4}^3+\psi^3\sqrt{G(\psi,\phi)}^3\right\}}\\
&\quad\quad-\frac{3\psi^6\left[(\phi-\phi_0)^2+\frac{1}{4}\,\psi^4\right]^2\left[-\frac{1}{2}\,\psi^2\,(\phi-\phi_0)^2-\frac{1}{12}\,(\phi-\phi_0)^4+\mathcal{O}\left(\left(|\psi|^2+|\phi-\phi_0|^2\right)^3\right)\right]}{\sqrt{G(\psi,\phi)}^3\left[(\phi-\phi_0)^2+\psi^4/4\right]\left\{\partial_\psi G(\psi,\phi)\sqrt{(\phi-\phi_0)^2+\psi^4/4}^3+\psi^3\sqrt{G(\psi,\phi)}^3\right\}}
\end{aligned}$$

$$- \frac{3\psi^6 \left[(\phi-\phi_0)^2 + \frac{1}{4}\,\psi^4\right] \left[-\frac{1}{2}\,\psi^2\,(\phi-\phi_0)^2 - \frac{1}{12}\,(\phi-\phi_0)^4 + \mathcal{O}\left(\left(|\psi|^2+|\phi-\phi_0|^2\right)^3\right)\right]^2}{\sqrt{G(\psi,\phi)}^3 \left[(\phi-\phi_0)^2+\psi^4/4\right] \left\{\partial_\psi G(\psi,\phi)\sqrt{(\phi-\phi_0)^2+\psi^4/4}^3 + \psi^3\,\sqrt{G(\psi,\phi)}^3\right\}}$$
$$- \frac{\psi^6 \left[-\frac{1}{2}\,\psi^2\,(\phi-\phi_0)^2 - \frac{1}{12}\,(\phi-\phi_0)^4 + \mathcal{O}\left(\left(|\psi|^2+|\phi-\phi_0|^2\right)^3\right)\right]^3}{\sqrt{G(\psi,\phi)}^3 \left[(\phi-\phi_0)^2+\psi^4/4\right] \left\{\partial_\psi G(\psi,\phi)\sqrt{(\phi-\phi_0)^2+\psi^4/4}^3 + \psi^3\,\sqrt{G(\psi,\phi)}^3\right\}}$$

and, using the substitution $(\psi, \phi-\phi_0)^\top = r\,(\cos\gamma, \sin\gamma)$ as before, it can be shown that, for $\gamma \neq 0, \pi$,

$$\lim_{r\to 0}\left[\frac{\partial_\psi G(\psi,\phi)}{|n'(\psi,\phi)-\nu'|^3} - \frac{\psi^3}{\sqrt{(\phi-\phi_0)^2+\psi^4/4}^3}\right]\sqrt{(\phi-\phi_0)^2+\psi^4/4} = 0.$$

Similarly, it can be shown that, for $\gamma = 0, \pi$,

$$\lim_{r\to 0}\left[\frac{\partial_\psi G(\psi,\phi)}{|n'(\psi,\phi)-\nu'|^3} - \frac{\psi^3}{\sqrt{(\phi-\phi_0)^2+\psi^4/4}^3}\right]\sqrt{(\phi-\phi_0)^2+\psi^4/4} < \infty$$

by once more extending the Taylor expansions of G and $\partial_\psi G$ by one order. Indeed, as mentioned before, $\partial_\psi^5 G(0,\phi_0) = 0$ and $|\partial_\psi^6 G(0,\phi_0)| < \infty$. Lemma 4.4 thus proves that

$$\left[\frac{\partial_\psi G(\psi,\phi)}{|n'(\psi,\phi)-\nu'|^3} - \frac{\psi^3}{\sqrt{(\phi-\phi_0)^2+\psi^4/4}^3}\right]\sqrt{(\phi-\phi_0)^2+\psi^4/4}$$

is uniformly bounded in a neighbourhood of $(\psi,\phi) = (\psi_0,\phi_0)$. It follows that

$$\frac{\partial_\psi G(\psi,\phi)}{|n'(\psi,\phi)-\nu'|^3} - \frac{\psi^3}{\sqrt{(\phi-\phi_0)^2+\psi^4/4}^3} \sim \frac{1}{\sqrt{(\phi-\phi_0)^2+\psi^4/4}}$$

for $(\psi,\phi)^\top \to (0,\phi_0)^\top$, which shows that the third integral on the right-hand side of (B.4.94) is absolutely integrable w.r.t. ψ (cf. (B.4.99)). Knowing this, the Riemann-Lebesgue lemma can be applied, leading to

$$\begin{aligned}\tilde{J}_1^0 &= \frac{1}{ikR}\int\limits_{\phi_0-\pi}^{\phi_0+\pi} f_{\ell,j}(m',1)\left[\frac{1}{|m'-\nu'|} - \frac{1}{\sqrt{(\phi-\phi_0)^2+1/4}}\right]\mathrm{d}\phi\, e^{ikR} \\ &\quad - \frac{1}{ikR}\int\limits_{\phi_0-\pi}^{\phi_0+\pi} f_{\ell,j}(n'(0,\phi),0)\left[\frac{1}{|n'(0,\phi)-\nu'|} - \frac{1}{|\phi-\phi_0|}\right]\mathrm{d}\phi + o\left(\frac{1}{R}\right). \qquad \text{(B.4.100)}\end{aligned}$$

To examine $\tilde{J}_2^0$, recall that (cf. (B.4.92))

$$\tilde{J}_2^0 = \int\limits_0^1\int\limits_{\phi_0-\pi}^{\phi_0+\pi}\frac{f_{\ell,j}(n'(\psi,\phi),\sqrt{1-n'(\psi,\phi)^2}) - f(\nu',0)}{\sqrt{(\phi-\phi_0)^2+\psi^4/4}}\,\mathrm{d}\phi\, e^{ikR\psi}\,\mathrm{d}\psi.$$

Applying integration by parts w.r.t. ψ to this integral leads to

$$\begin{aligned}\tilde{J}_2^0 &= \frac{1}{ikR}\int\limits_{\phi_0-\pi}^{\phi_0+\pi}\frac{f_{\ell,j}(m',1)-f_{\ell,j}(\nu',0)}{\sqrt{(\phi-\phi_0)^2+1/4}}\,\mathrm{d}\phi\, e^{ikR} - \frac{1}{ikR}\int\limits_{\phi_0-\pi}^{\phi_0+\pi}\frac{f_{\ell,j}(n'(0,\phi),0)-f_{\ell,j}(\nu',0)}{|\phi-\phi_0|}\,\mathrm{d}\phi \qquad \text{(B.4.101)} \\ &\quad - \frac{1}{ikR}\int\limits_0^1\int\limits_{\phi_0-\pi}^{\phi_0+\pi}\partial_\psi\left[\frac{f_{\ell,j}(n'(\psi,\phi),\sqrt{1-n'(\psi,\phi)^2}) - f(\nu',0)}{\sqrt{(\phi-\phi_0)^2+\psi^4/4}}\right]\mathrm{d}\phi\, e^{ikR\psi}\,\mathrm{d}\psi.\end{aligned}$$

It is not hard to show that the first integral is finite, since no singularities occur. The second integral is also well defined, since L'Hôpital's rule shows that the quotient behaves like $\partial_\phi[f_{\ell,j}(n'(0,\phi),0)]$ in a neighbourhood of $\phi=\phi_0$, which is at most logarithmically singular. To be precise,

$$\partial_\phi[f_{\ell,j}(n'(0,\phi),0)] = \partial_\phi n'(0,\phi)\cdot\nabla_{n'}f_{\ell,j}(n'(0,\phi),0),$$

where Lemma B.2 shows that $\nabla_{n'}f_{\ell,j}(n'(0,\phi),0)$ has at most a logarithmic singularity. Moreover, it is easily seen that $\partial_\phi n'(0,\phi)$ (cf. (4.2.22)) is bounded in a neighbourhood of $\phi=0$. To show the absolute integrability of the third integral, consider

$$\begin{aligned}\partial_\psi\left[\frac{f_{\ell,j}(n'(\psi,\phi),n_z(\psi,\phi))-f(\nu',0)}{\sqrt{(\phi-\phi_0)^2+\psi^4/4}}\right] &= \frac{\partial_\psi\vec{n}(\psi,\phi)\cdot\nabla_{\vec{n}}f_{\ell,j}(n'(\psi,\phi),n_z(\psi,\phi))}{\sqrt{(\phi-\phi_0)^2+\psi^4/4}}\\ &\quad-\frac{1}{2}\frac{\psi^3\left[f_{\ell,j}(n'(\psi,\phi),n_z(\psi,\phi))-f(\nu',0)\right]}{\sqrt{(\phi-\phi_0)^2+\psi^4/4}^{\,3}}.\end{aligned}\tag{B.4.102}$$

Since the numerator of the first quotient on the right-hand side of (B.4.102) has at most a logarithmic singularity at $(\psi,\phi)^\top=(0,\phi_0)^\top$, the quotient is absolutely integrable. It remains to show that

$$\frac{\psi^3\left[f_{\ell,j}(n'(\psi,\phi),n_z(\psi,\phi))-f(\nu',0)\right]}{(\phi-\phi_0)^2+\psi^4/4}$$

is at most logarithmically singular to prove that (B.4.102) is absolutely integrable. Consider

$$\begin{aligned}\left|\frac{\psi^3\left[f_{\ell,j}(n'(\psi,\phi),n_z(\psi,\phi))-f(\nu',0)\right]}{(\phi-\phi_0)^2+\psi^4/4}\right| &= \frac{\psi^3}{\sqrt{(\phi-\phi_0)^2+\psi^4/4}}\,\frac{|f_{\ell,j}(n'(\psi,\phi),n_z(\psi,\phi))-f(\nu',0)|}{\sqrt{(\phi-\phi_0)^2+\psi^4/4}}\\ &\le c\,\psi\left|\frac{f_{\ell,j}(n'(\psi,\phi),n_z(\psi,\phi))-f(\nu',0)}{\phi-\phi_0}\right|,\end{aligned}$$

where applying L'Hôpital's rule shows that, for any fixed $\psi\in[0,1]$, the remaining quotient behaves like $\partial_\phi[f_{\ell,j}(n'(\psi,\phi),n_z(\psi,\phi))]$ in a neighbourhood of $\phi=\phi_0$. This, however, is at most logarithmically singular, as mentioned above. It follows that (cf. (B.4.102))

$$\left|\partial_\psi\left[\frac{f_{\ell,j}(n'(\psi,\phi),n_z(\psi,\phi))-f(\nu',0)}{\sqrt{(\phi-\phi_0)^2+\psi^4/4}}\right]\right|\le c\frac{\left|\log\left((\phi-\phi_0)^2+\psi^4/4\right)\right|}{\sqrt{(\phi-\phi_0)^2+\psi^4/4}}\tag{B.4.103}$$

is weakly singular and thus absolutely integrable, if first integrated w.r.t ϕ and then w.r.t. ψ. To be precise,

$$\begin{aligned}\int_0^1\int_{\phi_0-\pi}^{\phi_0+\pi}\frac{\left|\log\left((\phi-\phi_0)^2+\psi^4/4\right)\right|}{\sqrt{(\phi-\phi_0)^2+\psi^4/4}}\,\mathrm{d}\phi\,\mathrm{d}\psi &\le \int_0^1\left|\log(\psi^4/4)\right|\int_{\phi_0-\pi}^{\phi_0+\pi}\frac{1}{\sqrt{(\phi-\phi_0)^2+\psi^4/4}}\,\mathrm{d}\phi\,\mathrm{d}\psi\\ &= 2\int_0^1\left|\log(\psi^4/4)\right|\left[\log\left(\pi+\sqrt{\pi^2+\psi^4/4}\right)-\log(\psi^4/4)\right]\mathrm{d}\psi,\end{aligned}$$

which is obviously finite. Finally, applying the Riemann-Lebesgue lemma to the third integral on the right-hand side of (B.4.101) leads to

$$\tilde{J}_2^0=\frac{1}{ikR}\int_{\phi_0-\pi}^{\phi_0+\pi}\frac{f_{\ell,j}(m',1)-f_{\ell,j}(\nu',0)}{\sqrt{(\phi-\phi_0)^2+1/4}}\,\mathrm{d}\phi\,e^{ikR}-\frac{1}{ikR}\int_{\phi_0-\pi}^{\phi_0+\pi}\frac{f_{\ell,j}(n'(0,\phi),0)-f(\nu',0)}{|\phi-\phi_0|}\,\mathrm{d}\phi+o\left(\frac{1}{R}\right).\tag{B.4.104}$$

At last, (cf. (B.4.93) and (B.3.36))

$$\tilde{J}_3^0=\int_0^1\int_{\phi_0-\pi}^{\phi_0+\pi}\frac{1}{\sqrt{(\phi-\phi_0)^2+\psi^4/4}}\,\mathrm{d}\phi\,e^{ikR\psi}\,\mathrm{d}\psi$$

$$= 2\int_0^1 \log\left(2\pi + 2\sqrt{\pi^2+\psi^4/4}\right)\, e^{ikR\psi}\,\mathrm{d}\psi - 4\int_0^1 \log\psi\, e^{ikR\psi}\,\mathrm{d}\psi.$$

Employing integration by parts to the first of these two integrals leads to

$$2\int_0^1 \log\left(2\pi + 2\sqrt{\pi^2+\psi^4/4}\right)\, e^{ikR\psi}\,\mathrm{d}\psi = 2\log\left(2\pi+2\sqrt{\pi^2+1/4}\right)\,\frac{e^{ikR\psi}}{ikR} - 2\log(4\pi)\frac{1}{ikR}$$
$$- \frac{2}{ikR}\int_0^1 \partial_\psi\left[\log\left(2\pi+2\sqrt{\pi^2+\psi^4/4}\right)\right] e^{ikR\psi}\,\mathrm{d}\psi.$$

It is easily seen that

$$\partial_\psi\left[\log\left(2\pi+2\sqrt{\pi^2+\psi^4/4}\right)\right] = \frac{\psi^3}{\sqrt{\pi^2+\psi^4/4}\left(2\pi+2\sqrt{\pi^2+\psi^4/4}\right)}$$

is absolutely integrable w.r.t. $\psi \in [0,1]$. Hence, with the Riemann-Lebesgue lemma, there holds

$$\tilde{J}_3^0 = 2\log\left(2\pi+2\sqrt{\pi^2+1/4}\right)\,\frac{e^{ikR\psi}}{ikR} - 2\log(4\pi)\frac{1}{ikR} - 4\int_0^1 \log\psi\, e^{ikR\psi}\,\mathrm{d}\psi + o\left(\frac{1}{R}\right).$$

Using (B.4.81) then gives

$$\tilde{J}_3^0 = 2\log\left(2\pi+2\sqrt{\pi^2+1/4}\right)\,\frac{e^{ikR\psi}}{ikR} - 2\log(4\pi)\frac{1}{ikR} - 4\left[\tilde{\gamma} + \log(kR) - i\frac{\pi}{2}\right]\,\frac{1}{ikR} + o\left(\frac{1}{R}\right). \tag{B.4.105}$$

Finally, all the terms for $\alpha = 0$ can be added up, (cf. (B.4.91))

$$\mathcal{J}_1 = \tilde{J}_1^0 + \tilde{J}_2^0 + f_{\ell,j}(\nu',0)\,\tilde{J}_3^0.$$

Therefore, using that

$$\int_{\phi_0-\pi}^{\phi_0+\pi} \frac{1}{\sqrt{(\phi-\phi_0)^2+1/4}}\,\mathrm{d}\phi = 2\log\left(2\pi+2\sqrt{\pi^2+1/4}\right)$$

and that m' is a constant independent of ϕ such that

$$\frac{1}{ikR}\int_{\phi_0-\pi}^{\phi_0+\pi} f_{\ell,j}(m',1)\frac{1}{|m'-\nu'|}\,\mathrm{d}\phi\, e^{ikR} = 2\pi\frac{f_{\ell,j}(m',1)}{|m'-\nu'|}\,\frac{e^{ikR}}{ikR},$$

it follows that (cf. (B.4.100), (B.4.104) and (B.4.105))

$$\begin{aligned}
\mathcal{J}_1 = {} & \frac{1}{ikR}\int_{\phi_0-\pi}^{\phi_0+\pi} f_{\ell,j}(m',1)\left[\frac{1}{|m'-\nu'|} - \frac{1}{\sqrt{(\phi-\phi_0)^2+1/4}}\right]\mathrm{d}\phi\, e^{ikR} \\
& + \frac{1}{ikR}\int_{\phi_0-\pi}^{\phi_0+\pi} \frac{f_{\ell,j}(m',1)-f_{\ell,j}(\nu',0)}{\sqrt{(\phi-\phi_0)^2+1/4}}\,\mathrm{d}\phi\, e^{ikR} + 2f_{\ell,j}(\nu',0)\,\log\left(2\pi+2\sqrt{\pi^2+1/4}\right)\,\frac{e^{ikR\psi}}{ikR} \\
& - \frac{1}{ikR}\int_{\phi_0-\pi}^{\phi_0+\pi} f_{\ell,j}(n'(0,\phi),0)\left[\frac{1}{|n'(0,\phi)-\nu'|} - \frac{1}{|\phi-\phi_0|}\right]\mathrm{d}\phi - \frac{1}{ikR}\int_{\phi_0-\pi}^{\phi_0+\pi} \frac{f_{\ell,j}(n'(0,\phi),0) - f(\nu',0)}{|\phi-\phi_0|}\,\mathrm{d}\phi \\
& - 2\log(4\pi)\frac{f_{\ell,j}(\nu',0)}{ikR} - 4f_{\ell,j}(\nu',0)\,\left[\tilde{\gamma}+\log(kR) - i\frac{\pi}{2}\right]\,\frac{1}{ikR} + o\left(\frac{1}{R}\right)
\end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{ikR} \int\limits_{\phi_0-\pi}^{\phi_0+\pi} f_{\ell,j}(m',1) \frac{1}{|m'-\nu'|} \,\mathrm{d}\phi\, e^{ikR} \\
&\quad - f_{\ell,j}(\nu',0) \int\limits_{\phi_0-\pi}^{\phi_0+\pi} \frac{1}{\sqrt{(\phi-\phi_0)^2+1/4}} \,\mathrm{d}\phi\, \frac{e^{ikR}}{ikR} + 2 f_{\ell,j}(\nu',0)\, \log\left(2\pi + 2\sqrt{\pi^2+1/4}\right) \frac{e^{ikR\psi}}{ikR} \\
&\quad - \frac{1}{ikR} \int\limits_{\phi_0-\pi}^{\phi_0+\pi} f_{\ell,j}(n'(0,\phi),0) \left[\frac{1}{|n'(0,\phi)-\nu'|} - \frac{1}{|\phi-\phi_0|}\right] \mathrm{d}\phi - \frac{1}{ikR} \int\limits_{\phi_0-\pi}^{\phi_0+\pi} \frac{f_{\ell,j}(n'(0,\phi),0) - f(\nu',0)}{|\phi-\phi_0|} \,\mathrm{d}\phi \\
&\quad + f_{\ell,j}(\nu',0) \frac{2\pi}{kR} - 2 f_{\ell,j}(\nu',0) \left[2\tilde{\gamma} + 2\log(kR) + \log(4\pi)\right] \frac{1}{ikR} + o\left(\frac{1}{R}\right) \\
&= 2\pi \frac{f_{\ell,j}(m',1)}{|m'-\nu'|} \frac{e^{ikR}}{ikR} + f_{\ell,j}(\nu',0) \frac{2\pi}{kR} \\
&\quad - \frac{1}{ikR} \int\limits_{\phi_0-\pi}^{\phi_0+\pi} f_{\ell,j}(n'(0,\phi),0) \left[\frac{1}{|n'(0,\phi)-\nu'|} - \frac{1}{|\phi-\phi_0|}\right] \mathrm{d}\phi - \frac{1}{ikR} \int\limits_{\phi_0-\pi}^{\phi_0+\pi} \frac{f_{\ell,j}(n'(0,\phi),0) - f(\nu',0)}{|\phi-\phi_0|} \,\mathrm{d}\phi, \\
&\quad - 2 f_{\ell,j}(\nu',0) \left[2\tilde{\gamma} + 2\log(kR) + \log(4\pi)\right] \frac{1}{ikR} + o\left(\frac{1}{R}\right). \qquad \text{(B.4.106)}
\end{aligned}
$$

Note that (cf. (4.2.22) with $\alpha = 0$)

$$
n'(0,\phi) = \begin{pmatrix} \cos\beta\cos\phi - \sin\beta\sin\phi \\ \sin\beta\cos\phi + \cos\beta\sin\phi \end{pmatrix} = \begin{pmatrix} \cos(\beta+\phi) \\ \sin(\beta+\phi) \end{pmatrix},
$$

where ϕ is measured starting not at zero degrees but at β. Thus, $\beta+\phi$ is equal to a $\tilde{\phi}$ in standard polar coordinates, which shows that $n'(0,\phi)$ is equal to the n_0' (cf. substitution in (4.2.9)) used in (B.3.104). With this, it is easily shown that most of the terms on the right-hands side of (B.4.106) will vanish when $\mathcal{J}_1$ is added to $\mathcal{J}_2$ (cf. (B.3.104)) for $\alpha = 0$ or equivalently $m' = (0,0)^\top$. To be precise,

$$
\begin{aligned}
\mathcal{J}_2 = &\frac{1}{ikR} \int\limits_{\phi_0-\pi}^{\phi_0+\pi} f_{\ell,j}(n_0',0) \left[\frac{1}{|n_0'-\nu'|} - \frac{1}{|\phi-\phi_0|}\right] \mathrm{d}\phi + \frac{1}{ikR} \int\limits_{\phi_0-\pi}^{\phi_0+\pi} \frac{f_{\ell,j}(n_0',0) - f_{\ell,j}(\nu',0)}{|\phi-\phi_0|} \,\mathrm{d}\phi \\
&+ 2 f_{\ell,j}(\nu',0) \left(2\tilde{\gamma} + 2\log(kR) + \log(4\pi)\right) \frac{1}{ikR} + o\left(\frac{1}{R}\right),
\end{aligned}
$$

such that (cf. (B.2.4) and (B.4.106))

$$
\mathcal{J} = \mathcal{J}_1 + \mathcal{J}_2 = 2\pi \frac{f_{\ell,j}(m',1)}{|m'-\nu'|} \frac{e^{ikR}}{ikR} + f_{\ell,j}(\nu',0) \frac{2\pi}{kR} + o\left(\frac{1}{R}\right)
$$

for $m' = (0,0)^\top$.

At last, the formulas for the four cases of $m' = (0,0)^\top$, $m'/|m'| \neq \pm\nu'$ (cf. (B.4.83)), $m'/|m'| = \nu'$ (cf. (B.4.38)) and $m'/|m'| = -\nu'$ (cf. (B.4.87)) can be put together to get

$$
\mathcal{J} = \frac{2\pi}{ikR} \frac{f_{\ell,j}(m',m_z)}{|m'-\nu'|} e^{ikR} + f_{\ell,j}(\nu',0) \frac{2\pi}{kRm_z} e^{ikR\nu'\cdot m'} + o\left(\frac{1}{R}\right).
$$

As was already stated in the paragraph before Section B.3.1, the constant $f_{\ell,j}(\nu',0) = f_{\ell,j,n}(\nu',0)$ is zero in the case of $\ell \geq 2$. Additionally, the definition of $f_{1,j,n}(n',n_z^r)$ (cf. (B.2.1)) gives that $f_{1,j,n}(\nu',0)$ is also zero for $n > 0$. It follows that

$$
\mathcal{J} = \frac{2\pi}{ikR} \frac{f_{\ell,j}(m',m_z)}{|m'-\nu'|} e^{ikR} + \mathbb{1}_{(1,0)}(\ell,n)\, f_{\ell,j}(\nu',0) \frac{2\pi}{kRm_z} e^{ikR\nu'\cdot m'} + o\left(\frac{1}{R}\right),
$$

which concludes the proof of Theorem B.1.

Appendix C

Definitions & Theorems

In this chapter, fundamental definitions and theorems are introduced, which are employed in this thesis. The purpose of this is to introduce the used notation and to make the definitions and theorems easily accessible to the reader.

Definition C.1 (Schwartz space[1]). *The space*

$$\mathcal{S}(\mathbb{R}^n) := \left\{ f \in C^\infty(\mathbb{R}^n) \middle| \lim_{\|x\| \to \infty} x^\alpha \, \partial_x^\beta f(x) = 0 \text{ for all } \alpha \in \mathbb{N}_0^n \text{ and for all } \beta \in \mathbb{N}_0^n \right\},$$

where α and β are multi-indices such that $x^\alpha = x_1^{\alpha_1} \cdots x_n^{\alpha_n}$ and $\partial_x^\beta = \partial_{x_1}^{\beta_1} \cdots \partial_{x_n}^{\beta_n}$, is called Schwartz space. This space is a subspace of the space of smooth function $C^\infty(\mathbb{R}^n)$, inheriting its vector space operations, and is induced by the family of the seminorms $\|f\|_N := \sup_{x \in \mathbb{R}^n} \max_{|\alpha|,|\beta| < N} |x^\alpha \, \partial_x^\beta f(x)|$. The elements of this space are called Schwartz functions.

Theorem C.2. *The Fourier transform is a bijective mapping from $\mathcal{S}(\mathbb{R}^n)$ to $\mathcal{S}(\mathbb{R}^n)$. (cf. [39, Theorem V.2.8])*

Theorem C.3 (Lebesgue's dominated convergence theorem[2]). *Let (S, Σ, μ) be a measure space and $T \in \Sigma$ a μ-measurable set. Assume all functions $f_1, f_2, \ldots : T \to \mathbb{K}$ are absolutely integrable and there is a measurable function $f : T \to \mathbb{K}$ with $f(t) = \lim_{n \to \infty} f_n(t)$, almost everywhere. If an integrable function $g : T \to \mathbb{K}$ exists, such that for all $n \in \mathbb{N}$*

$$|f_n| < g$$

almost everywhere, then f is integrable and

$$\lim_{n \to \infty} \int_T f_n \, \mathrm{d}\mu = \int_T f \, \mathrm{d}\mu.$$

Theorem C.4 (Fubini's theorem[3]). *If $(X \times Y, \mathcal{M} \otimes \mathcal{N}, \mu \otimes \nu)$ is a product measure space, $f : X \times Y \to \mathbb{C}$ is $\mathcal{M} \otimes \mathcal{N}$-measurable and one of the integrals*

$$\int\limits_{X \times Y} |f| \, \mathrm{d}\mu \otimes \nu, \qquad \int\limits_X \left(\int\limits_Y |f(x,y)| \, \mathrm{d}\nu(y) \right) \mathrm{d}\mu(x), \qquad \int\limits_Y \left(\int\limits_X |f(x,y)| \, \mathrm{d}\mu(x) \right) \mathrm{d}\nu(y)$$

is finite, then all integrals are finite and equal, i.e., f is $\mu \otimes \nu$-integrable, and

$$\int\limits_X \left(\int\limits_Y f(x,y) \, \mathrm{d}\nu(y) \right) \mathrm{d}\mu(x) = \int\limits_Y \left(\int\limits_X f(x,y) \, \mathrm{d}\mu(x) \right) \mathrm{d}\nu(y)$$

is finite.

[1] cf. [39, Definition V.2.3]
[2] cf. [39, Theorem A.3.2]
[3] cf. [17, Theorem 2.1 in Chapter V]

Definition C.5 (Holomorphic functions[4]). *A function $f : D \subset \mathbb{C}^n \to \mathbb{C}$ is called holomorphic on an open set D, if the function is continuously differentiable w.r.t. the complex variable in D.*

Definition C.6 (Meromorphic functions[5]). *A function $f : D \subset \mathbb{C}^n \to \mathbb{C}$ is called meromorphic on an open set D, if the function is holomorphic except on a set of isolated points, which are poles of f.*

Theorem C.7 (Residue theorem[6]). *Let C be a positively oriented simple closed piecewise smooth curve. Moreover, let the function f be continuous in $\mathrm{In}(C) \cup C$ and meropmorphic on $\mathrm{In}(C)$, where the poles $z_1, \ldots, z_n$ of f lie in the interior $\mathrm{In}(C)$ of C. There holds*

$$\int_C f(z)\,\mathrm{d}z = 2\pi i \sum_{j=1}^{n} \operatorname*{Res}_{z=z_j} f(z),$$

where $\mathrm{Res}_{z=z_j} f(z)$ denotes the residue of f at point z_j.

Theorem C.8 (Multinomial theorem[7]). *For any $n, m \in \mathbb{N}$ and $x \in \mathbb{C}^m$,*

$$(x_1 + \cdots + x_m)^n = \sum_{\{\alpha \in \mathbb{N}_0^m \,|\, \alpha_1 + \ldots + \alpha_m = k\}} \binom{k}{\alpha} x^{\alpha},$$

where α is a multi-index and

$$\binom{k}{\alpha} := \frac{k!}{\alpha_1! \cdots \alpha_m!}$$

the multinomial coefficient.

Theorem C.9 (Leibniz rule[8]). *For two n-times differentiable functions f and g,*

$$(f\,g)^{(n)} = \sum_{j=0}^{n} \binom{n}{j} f^{(j)}\, g^{(n-j)}.$$

Theorem C.10 (Faà di Bruno's formula[9]). *If f and g are functions with a sufficient number of derivatives, then*

$$\frac{\mathrm{d}^{(n)}}{\mathrm{d}t} g\big(f(t)\big) = \sum_{\substack{\{(a_1,\ldots,a_m) \in \mathbb{N}_0: \\ \sum_{j=1}^{n} j\, a_j = n\}}} \frac{n!}{\prod_{j=1}^{n} a_j!} \frac{\mathrm{d}^{(a_1+\ldots+a_n)}}{\mathrm{d}f} g\big(f(t)\big) \prod_{j=1}^{n} \frac{\left[\frac{\mathrm{d}^{(j)}}{\mathrm{d}t} f(t)\right]^{a_j}}{j!}.$$

Theorem C.11 (Riemann-Lebesgue lemma[10]). *Assuming $s \in \mathbb{R}^n$, for any absolutely integrable function f, any fixed $n \in \mathbb{N}$ and any non-zero and real valued constant c,*

$$\lim_{\|s\| \to \infty} \int_{\mathbb{R}^n} f(x)\, e^{ics\cdot x}\,\mathrm{d}x = 0.$$

Theorem C.12 (Binomial theorem[11]). *For any $n \in \mathbb{N}$ and $x, y \in \mathbb{C}$,*

$$(x+y)^n = \sum_{j=0}^{n} \binom{n}{j} x^{n-j}\, y^j.$$

[4]cf. [8, Definition 2.2]
[5]cf. [8, Definition 3.3]
[6]cf. [8, Theorem 3.8]
[7]cf. [6, Theorem 2.2]
[8]cf. [3, p. 375]
[9]cf. [25]
[10]cf. [2, Theorem 9.9]
[11]cf. [3, p. 59]

List of Definitions

Variable	**Definition**	**Page**
$\vec{k}$	$(k_x, k_y, k_z)^\top \in \mathbb{R}^3$	12
$\vec{n}^0$	$(n_x^0, n_y^0, n_z^0)^\top = \vec{k}/\Vert\vec{k}\Vert$	12
k	$\Vert\vec{k}\Vert = \sqrt{\mu_0\epsilon_0}\omega$	12
$\vec{k}_\tau$	$(k_x, k_y, k_{z,\tau})^\top$	13
$k_{z,\tau}$	$k_z + i\tau$	13
ϵ_τ	$\epsilon_0 - \frac{\tau^2}{\mu_0\omega^2} + i\,\frac{2\tau k_z}{\mu_0\omega^2}$	13
k_τ^2	$\vec{k}_\tau \cdot \vec{k}_\tau = \mu_0\epsilon_\tau\omega^2$	13
$\vec{E}^0(\vec{x})$	$\vec{e}^0 e^{i\vec{k}_\tau\cdot\vec{x}}$	13
$\vec{E}^r(\vec{x})$	$\vec{E}(\vec{x}) - \vec{E}^0(\vec{x})$ for all $\vec{x}$ above the interface	13
$\vec{D}^0(\vec{x})$	$\epsilon_\tau\vec{E}^0(\vec{x})$	13
$\vec{D}(\vec{x})$	$\varepsilon_\tau(\vec{x})\vec{E}(\vec{x})$	13
$\vec{D}^r(\vec{x})$	$\vec{D}(\vec{x}) - \vec{D}^0(\vec{x})$	14
$\alpha(\vec{x})$	$\varepsilon_\tau(\vec{x}) - \epsilon_\tau$	14
$\alpha_{\mathcal{Q}}(\vec{x})$	$\alpha(\vec{x})$ in the case of $f_{\mathcal{Q}} \equiv 0$	15
$\vec{D}^r_{\mathcal{Q}}(\vec{x})$	$\vec{D}^r(\vec{x})$ in the case of $f_{\mathcal{Q}} \equiv 0$	15
$\alpha_d(\vec{x})$	$\alpha(\vec{x}) - \alpha_{\mathcal{Q}}(\vec{x})$	15
$\vec{D}^d(\vec{x})$	$\vec{D}^r(\vec{x}) - \vec{D}^r_{\mathcal{Q}}(\vec{x})$	15
h	$2\,\Vert f\Vert_\infty$	15
$\mathbb{N}_0$	set of non-negative integers	17
k'	$(k_x, k_y)^\top$	17
ξ	$\sqrt{k^2 - s'^2}$	18
$\vec{s}_w$	$(s_x, s_y, w)^\top$	18
$\vec{\omega}_j$	$\left(k' + \tilde{\omega}'_{0,j}, \omega_z^j\right)^\top$	18
ω_z^j	$\sqrt{k^2 - \left\lvert k' + \tilde{\omega}'_{0,j}\right\rvert^2}$	18
$r(\vec{k}, \vec{e}^0)$	$\Big[\frac{k_z+\sqrt{\tilde{k}^2-\lvert k'\rvert^2}}{k_z-\sqrt{\tilde{k}^2-\lvert k'\rvert^2}}\,(k_y e_x^0 - k_x e_y^0)\,(k_y, -k_x, 0)^\top + \frac{\tilde{k}^2 k_z + k^2\sqrt{\tilde{k}^2-\lvert k'\rvert^2}}{\tilde{k}^2 k_z - k^2\sqrt{\tilde{k}^2-\lvert k'\rvert^2}}\,\frac{k_z(k_x e_x^0 + k_y e_y^0) - \left\lvert k'\right\rvert^2 e_z^0}{k^2}\,(-k_x k_z, -k_y k_z, -\lvert k'\rvert^2)^\top\Big]$	18
$\tilde{k}$	$\sqrt{\mu_0\epsilon'_0}\omega$	18
$\vec{k}^r$	$(k_x, k_y, -k_z)^\top$	18
k'^2	$k_x^2 + k_y^2$	18
$\hat{D}^d(\vec{s})$	$\mathcal{F}\left(\vec{D}^d(\cdot)\right)(\vec{s})$	19
s^2	$\Vert\vec{s}\Vert^2$	19
φ	$\in C_0^\infty(\mathbb{R}^3)$	19
$C_3(\tilde{r})$	$B_2(\tilde{r}) \times [-\tilde{r}, \tilde{r}]$	20
$B_2(\tilde{r})$	$\left\{\eta' \in \mathbb{R}^2 : \lvert\eta'\rvert \le \tilde{r}\right\}$	20
ξ_τ	$\sqrt{k_\tau^2 - s_x^2 - s_y^2}$	20
Δ_τ	$\epsilon_\tau - \epsilon'_0$	21
$\hat{\alpha}_{\tilde{r}}(\vec{s} - \vec{k}_\tau)$	$\int_{C_3(\tilde{r})} \alpha_d(\vec{\eta})\, e^{-i\vec{\eta}\cdot(\vec{s}-\vec{k}_\tau)}\,\mathrm{d}\vec{\eta}$	21

C_R	$\{z \in \mathbb{C} : \operatorname{Im} z \geq 0, \lvert z\rvert = R\}$	21
s'^2	$\lvert s'\rvert^2 = s_x^2 + s_y^2$	23
$\mathbb{1}_M(\mathtt{m})$	one if $\mathtt{m} \in M$ and zero otherwise	29
$\mathbb{1}_{\mathtt{m}_0}(\mathtt{m})$	$\mathbb{1}_{\{\mathtt{m}_0\}}(\mathtt{m})$	29
Δ	$\epsilon_0 - \epsilon_0'$	30
J_a	$\left\{m_\infty := (m_j)_{j\in\mathbb{Z}} \,\middle\vert\, m_j \in \mathbb{N}_0,\ \sum_{j\in\mathbb{Z}} m_j = a\right\}$	32
J_0	Bessel function of the first kind	36
K_0	Modified Bessel function of the second kind	36
$\vec{\omega}_\tau^j$	$\big(k' + \tilde{\omega}_{0,j}', \omega_{z,\tau}^j\big)^\top$	40
$\omega_{z,\tau}^j$	$\sqrt{k_\tau^2 - \big\lvert k' + \tilde{\omega}_{0,j}'\big\rvert^2}$	40
S_m	$\{(l, \vec{\ell}_1, \tilde{l}) : l = 0, \ldots, m,\ \vec{\ell}_1 \in T_l,\ \tilde{l} = 0, \ldots, \tilde{l}_b\}$	47
$\vec{n}_0^r$	$\big(n_x^0, n_y^0, -n_z^0\big)^\top$	57
$\tilde{F}$	elliptic integral of the first kind	57
$\vec{n}^r$	$\frac{\vec{s}_\xi}{\sqrt{s_x^2+s_y^2+\xi^2}}$	58
n_z^r	$\sqrt{1 - n'^2}$	58
$h_{1,j}(n')$	$i\,\frac{\Delta\, k^3}{4\pi\epsilon_0}\,[n_z^r]^n\,\frac{e^{-\lvert kn' - (k'+\tilde{\omega}_{1,j}')\rvert}}{\lvert kn' - (k'+\tilde{\omega}_{1,j}')\rvert}\ \big[\big(\vec{n}^r \times \vec{e}^{\,0}\big) \times \vec{n}^r\big]$	58
$h_{2,j}(n')$	$i\,\frac{\Delta\, k^3}{4\pi\epsilon_0}\,[n_z^r]^n K_0\left(\big\lvert kn' - (k' + \tilde{\omega}_{2,j}')\big\rvert\right)\ \big[\big(\vec{n}^r \times \vec{e}^{\,0}\big) \times \vec{n}^r\big]$	58
$h_{3,j}(n')$	$i\,\frac{\Delta\, k^3}{4\pi\epsilon_0}\,[n_z^r]^n\, e^{-\lvert kn' - (k'+\tilde{\omega}_{1,j}')\rvert} \cdot \big[\big(\vec{n}^r \times \vec{e}^{\,0}\big) \times \vec{n}^r\big]$	59
$h_{4,0}(n')$	$i\,\frac{\Delta\, k^3}{8\pi^2\epsilon_0}\,[n_z^r]^n \int\limits_{\mathbb{R}^2} \tilde{g}_n(\eta', \zeta)\, e^{-i\eta'\cdot\left(kn' - k'\right)}\, \mathrm{d}\eta'\ \big[\big(\vec{n}^r \times \vec{e}^{\,0}\big) \times \vec{n}^r\big]$	59
χ_ϵ	$\chi_\epsilon \in C_0^\infty(\mathbb{R}^2)$, $\operatorname{supp}\chi_\epsilon \subset B_2(\epsilon)$, $\chi_\epsilon(n') = 1$ for $n' \in B_2\left(\frac{\epsilon}{2}\right)$, $1 >> \epsilon > 0$ with $\epsilon < \Big\lvert k - \big\lvert k' + \tilde{\omega}_{\ell,j}'\big\rvert\Big\rvert$ for $\ell = 1, 2$	59
$f_j(\psi, \phi)$	$k\, h_{1,j}\big(n'(\psi, \phi)\big)\ \lvert n'(\psi, \phi) - \nu'\rvert$	67
ν'	$\frac{k'+\tilde{\omega}_{\ell,j}'}{k}$	67
$(\psi_0, \phi_0)^\top$	defined such that $n'(\psi_0, \phi_0) = \nu'$	68
$g_j(\psi, \phi)$	$f_j(\psi, \phi)\,\frac{\sqrt{\tilde{a}\,(\psi-\psi_0)^2+\tilde{b}\,(\phi-\phi_0)^2+\tilde{c}\,(\psi-\psi_0)\,(\phi-\phi_0)}}{\lvert n'(\psi,\phi)-\nu'\rvert}$	68
$\tilde{a}$	$\left\lvert \partial_\psi \Big[n'(\psi, \phi)\Big]_{\psi=\psi_0,\, \phi=\phi_0}\right\rvert^2$	68
$\tilde{b}$	$\left\lvert \partial_\phi \Big[n'(\psi, \phi)\Big]_{\psi=\psi_0,\, \phi=\phi_0}\right\rvert^2$	68
$\tilde{c}$	$2\Big\{\partial_\psi\big[n'(\psi, \phi)\big] \cdot \partial_\phi\big[n'(\psi, \phi)\big]\Big\}_{\psi=\psi_0,\, \phi=\phi_0}$	68
$\tilde{d}$	$\det\left(\frac{\partial n'(\psi,\phi)}{\partial(\psi,\phi)}\right)_{\psi=\psi_0,\, \phi=\phi_0}$	69
$g_j(\psi, \phi)$	$\tilde{\chi}_\epsilon\big(\psi - 1\big)\, f_j(\psi, \phi)\, \frac{\sqrt{1-\psi}}{\lvert n'(\psi,\phi)-\nu'\rvert}$	75
$\tilde{\gamma}$	Euler's constant	83
$\delta_{m\ell}$	Kronecker delta	87
$\vec{k}^t$	$(k', k_z^t)^\top$	106
k_z^t	$-\sqrt{\tilde{k}^2 - \lvert k'\rvert^2}$	106
ν'	$\frac{k'+\tilde{\omega}_{\ell,j}'}{k}$ for $\ell = 1, \ldots, 4$	131
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