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# Reflection of plane waves by rough surfaces in the sense of Born approximation

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**Abstract**

The topic of the present paper is the reflection 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' formula 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. A further technical condition is defined, which guarantees the existence of the corresponding far field of the Born approximation. This far field contains plane waves, far-field terms like those for bounded scatterers, and, additionally, a new type of terms. The derived formulas can be used for the fast numerical computations of far fields and for the statistics of random rough surfaces.

# 1 Introduction

The progress of modern technology vitally relies on computer chips or other components with small details processing electromagnetic waves of smaller and smaller wavelength. However, a perfect fabrication in accordance with the guidelines of design becomes either too difficult or is even not possible. Instead, the manufactured components of the technical devices deviate from ideal components by random abberations. In the simplest case, a planar interface separating two different materials has typically a lot of tiny corrugations called roughness. Thus, in the present paper, roughness means 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 range, say of about 13 nm, requires the use of multi-layer systems (MLS) as Bragg mirrors, and each of the interface in this MLS has a specific roughness. To understand the impact of such MLS on the reflection of light, the roughness effects on the reflection and transmission of light at each of the interfaces must be clarified.

One of the models to describe MLS is used in the software of Windt [17] and is based on formulas derived by Stearns [14]. Note that similar models have been proposed for MLS earlier by e.g. Bousquet et al. [5] and Elson et al. [9]. 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 timeharmonic electromagnetic plane wave is incident from above. Manipulating the Maxwell's equations according to Jackson [10, Sect. 10.2.A], the partial differential equation 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 plus the scattered field. Since the scattered field is small in comparison to 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 and by dividing with the coefficient of the Fourier transformed displacement field. Then the inverse Fourier transform yields an explicit formula for the displacement field. This formula is an integral over the three-dimensional space. However, one of the integrations can be computed analytically by the residue theorem. Finally, taking limits, a corresponding far-field formula can be derived.

Of course, the Born approximation is not always justified. For electromagnetic waves in the range of X-rays, 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, then the scattered field is expected to be small in comparison to the incoming wave field. 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 that of an ideal planar interface, in which 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 approximate numerical methods. These results are reported in the monographs by Beckmann et al. [3], Ogilvy [13], and Voronovich [16] as well as in the overview article of DeSanto [8]. One approach is to represent the field by potentials or simplified potentials over the interface, which leads to integral equations. Again, Born approximation can be used to derive simple explicit formulas. On the other hand, to get rigorous formulas, the integral equation or the corresponding transmission problem for the Maxwell's equation is to be solved. Clearly, this can be done only numerically, i.e., upto a small error of the numerical method depending on the computing power. Note, however, that a numerical solution for the rigorous approach will take longer computing times then the evaluation of the approximate formulas. Moreover, the analysis of the numerical algorithms in the rigorous case is difficult. Even for the simpler acoustic case in 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. [7, 6] using a variational approach.

So far, the rough interface has been considered as a single smooth interface. In applications, however, the shape is not known explicitly. Realistically, only a few parameters are given to describe e.g. the size of the corrugations and the smoothness of the interface. On the other hand, the incoming plane wave is in reality a ray with a diameter much larger then the wavelength. 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). In the present paper, the stochastic view will not be considered. Note, however, that a fast approximate formula for the single realisations of the stochastic process is a good starting point for a statistical analysis.

The aim of the present paper 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 paper, 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.
– 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.
– A special variant of the limiting absorption principle is to be applied.
– 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 paper 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 [15], and combinations of Fourier modes play an important role for stochastic processes (cf. e.g. Yaglom [18, Equ. (2.61) in Sect. 8]).

The main result of the present paper is a formula of Born approximation for the electromagnetic field, which is adapted to the above-mentioned class of interfaces. For simplicity, all formulas are restricted to the case of reflection. Formulas for the transmitted fields can be obtained by analogous arguments. Moreover, combining reflections and transmission over several interfaces, the case of MLS can be treated like in e.g. [14]. 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 the solution of the vector Helmholtz equation. To derive the far field of this approximate solution, another technical condition is introduced. However, this can hopefully be relaxed in future investigations. The 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.

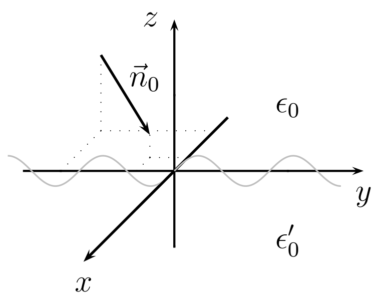


Figure 1: Coordinate system and propagation direction of incident field

The remaining part is organised as follows. The notation and the inhomogeneous vector Helmholtz equation is introduced in Sects. 2.1–2.2. A general formula for its solutions based on the Fourier transform is given in Sect. 2.3.1. This will be simplified in Sects. 2.3.2–2.5. In particular, for these manipulations, a class of special interface functions is defined in Sect. 2.4.1, and the final formula is presented in Theorem 2.1 of Sect. 2.5. The far-field asymptotics of this approximate solution is derived in Sect. 3. In Sect. 3.4 the attenuation formula of Stearns [14] for the efficiency of the specularly reflected plane-wave mode is proved for the special interfaces. Finally, in Sect. 3.5 the resulting formula is compared with a well-known result for sinusoidal gratings.

# 2 Near-field formula of the reflected field

## 2.1 Incident wave

Consider an incident plane wave $\mathcal{E}_0(\vec{x},t) = \vec{E}^0(\vec{x})\, e^{-i\omega t}$, $\vec{E}^0(\vec{x}) = \vec{e}^{\,0}\, e^{i\vec{k}\cdot\vec{x}}$ with a wave vector $\vec{k} := (k_x, k_y, k_z)^\top = k\vec{n}^0$, with $k := \sqrt{\mu_0\epsilon_0}\omega > 0$ real valued, $k_z < 0$ and $\vec{n}^0$ a normalised vector that describes the direction of propagation in the coordinate system shown in Figure 1. The values $\epsilon_0 > 0$ and $\mu_0 > 0$ are the dielectric constant resp. magnetic permeability of the medium above the interface. Note that $\epsilon_0$ and $\mu_0$ are not necessarily the free space values for the vacuum. The symbol $\vec{e}^{\,0}$ stands for a constant vector fixing polarisation and phase. Of course, $\vec{e}^{\,0}$ is perpendicular to $\vec{k}$.

## 2.2 Inhomogeneous vector Helmholtz equation

In this section the Maxwell equations will be used to describe the total field in form of a solution to an inhomogeneous vector Helmholtz equation. Furthermore, this equation will be approximated in the sense of the first order Born approximation. It will also be seen that a similar equation holds for the approximation of the desired scattered field minus the scattered field that results from an ideal interface, which is an interface defined by a plane. Some minor preparations for the following examinations will end this section.

Note that, since $k = \sqrt{\epsilon_0\mu_0}\omega$ is assumed as 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. To incorporate this information into the solution of the subsequently established vector Helmholtz equation, the **limiting absorption principle** is applied. In this sense the examinations in this and the following sections will be done for a 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 $k_{z,\tau} := k_z + i\tau$ and a negative $\tau \in \mathbb{R}$ close to zero. Afterwards the limit $\tau \nearrow 0$ is applied. For technical reasons only the third component of the wave vector instead of the whole vector is chosen complex. Moreover, define $\epsilon_\tau := \epsilon_0 - \frac{\tau^2}{\mu_0\omega^2} + i\,\frac{2\tau k_z}{\mu_0\omega^2}$, with which $k_\tau^2 := \vec{k}_\tau \cdot \vec{k}_\tau = \mu_0\epsilon_\tau\omega^2$ and $\operatorname{Im}\epsilon_\tau > 0$.

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

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

For the time-harmonic case, following [10, Sect. 10.2.A], these equations reduce to the **vector Helmholtz equation** in the sense of distributions

$$\left(\nabla^2 + k_\tau^2\right) \vec{D}^{sc} = -\nabla \times \left[\nabla \times \left(\alpha(\vec{E}^0 + \vec{E}^{sc})\right)\right]. \tag{2.2.2}$$

Here $\vec{E}^{sc} := \vec{E} - \vec{E}^0$ is the scattered electric field, and $\vec{D}^{sc}$ is the scattered displacement field , i.e. $\vec{D}^{sc} := \vec{D} - \vec{D}^0$ with the total displacement field $\vec{D}$ and that of the incoming wave $\vec{D}^0 := \epsilon_\tau \vec{E}^0$. Supposing the interface is the graph $\{(x', f(x')) : x' \in \mathbb{R}^2\}$, the coefficient $\alpha$ is given by $\alpha(\vec{x}) := \epsilon_\tau(\vec{x}) - \epsilon_\tau$ with $\epsilon_\tau(\vec{x}) = \epsilon_\tau$ for $z > f(x')$ and $\epsilon_\tau(\vec{x}) = \epsilon_0'$ for $z < f(x')$.

Now suppose the contrast is small s.t. $\alpha << 1$. Thus the solution $\vec{D}^{sc}$ of (2.2.2) is small, and, thereby, $\vec{E}^{sc}$ is small too. Neglecting the term $\vec{E}^{sc}$ in Equ. (2.2.2), a solution is obtained in the sense of the first order **Born approximation**.

$$\left(\nabla^2 + k_\tau^2\right) \vec{D}^{sc} = -\nabla \times \left[\nabla \times \left(\alpha \vec{E}^0\right)\right] \tag{2.2.3}$$

Of course, this step of Born approximation is heuristic as long as a mathematical model is lacking. Putting it on a rigorous foundation requires a theorem on the transmission value problem for Maxwell's equations in a Sobolev type space, which includes plane-wave incidence and plane-wave solutions. Additional assumptions on the smallness or smoothness of the interface function $f$ might be needed. The Sobolev type space for such a theorem should locally be the $H(\mathrm{curl})$ spaces of electro-magnetic fields with finite energy. Globally, the fields in the space must satisfy a yet unknown radiation condition.

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 (2.2.3). For an arbitrary $f \in L^\infty(\mathbb{R}^2)$, set $\alpha_d(\vec{x}) := \alpha(\vec{x}) - \alpha_Q(\vec{x})$ and $\vec{D}^d(\vec{x}) := \vec{D}^{sc}(\vec{x}) - \vec{D}^{sc}_Q(\vec{x})$ and use (2.2.3) for the difference field $\vec{D}^d$ to get

$$\left(\nabla^2 + k_\tau^2\right) \vec{D}^d(\vec{x}) = -\nabla \times \left[\nabla \times \left(\alpha_d(\vec{x})\vec{E}^0(\vec{x})\right)\right]. \tag{2.2.4}$$

Here, the small terms $\nabla\times\nabla\times(\alpha_d\vec{E}^{sc})$ and $\nabla\times\nabla\times(\alpha_Q[\vec{E}^{sc} - \vec{E}^{sc}_Q])$ have been neglected.

The set of interface functions $f$ can be chosen such that $\alpha_d$ identifies a functional of the space $\mathcal{S}'(\mathbb{R}^3)$ dual to the Schwartz space $\mathcal{S}(\mathbb{R}^3)$. Note that this especially holds 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 $||f||_\infty < \frac{h}{2}$ and $h > 0$. With this the Fourier transform $\hat{\alpha}_d := \mathcal{F}(\alpha_d)$ of $\alpha_d$ is defined in the generalised sense. To be precise, for Schwartz functions $\varphi, \psi \in \mathcal{S}(\mathbb{R}^3)$, the Fourier transform and its inverse are defined by

$$\mathcal{F}\varphi(\vec{s}) := \hat{\varphi}(\vec{s}) := \int\limits_{\mathbb{R}^3} \varphi(\vec{x})\, e^{-i\vec{x}\cdot\vec{s}}\, \mathrm{d}\vec{x}, \quad \mathcal{F}^{-1}\psi(\vec{x}) := \check{\psi}(\vec{x}) := \frac{1}{(2\pi)^3} \int\limits_{\mathbb{R}^3} \psi(\vec{s})\, e^{i\vec{s}\cdot\vec{x}}\, \mathrm{d}\vec{s}, \tag{2.2.5}$$

and $\varphi(\vec{x}) = (\hat{\varphi})\check{}(\vec{x})$. Furthermore, if the duality $\langle f, g\rangle$ of the spaces $\mathcal{S}(\mathbb{R}^3)$ and $\mathcal{S}'(\mathbb{R}^3)$ is the extension of the scalar product $\int f\bar{g}$, then the generalised Fourier transform $\hat{\alpha}_d$ of the Schwartz distribution $\alpha_d \in \mathcal{S}'(\mathbb{R}^3)$ is defined by

$$\langle \hat{\alpha}_d(\vec{s}), \varphi(\vec{s})\rangle := (2\pi)^3 \,\langle \alpha_d(\vec{\eta}), \check{\varphi}(\vec{\eta})\rangle \tag{2.2.6}$$

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

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

## 2.3 Formula for the solution of the Helmholtz equation with a reduction in the dimension of the domain of integration

### 2.3.1 Formula for the solution via Fourier transform

Now follow [14, Formula (6), Section II.A]. Applying the Fourier transform to both sides of (2.2.4), and solving for $\hat{D}^d := (\vec{D}^d)\hat{}$, leads to

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

where $s^2 := ||\vec{s}\,||^2 \neq k_\tau^2$ 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, however, is to be done in the generalised sense. Consequently,

$$\begin{aligned} \left\langle \vec{D}^d(\vec{x}), \varphi(\vec{x}) \right\rangle &= \left\langle \vec{D}^d(\vec{x}), (\hat{\varphi})\check{}\,(\vec{x}) \right\rangle = \frac{1}{(2\pi)^3}\left\langle \hat{\alpha}_d(\vec{s} - \vec{k}_\tau), \overline{\left[\frac{[(\vec{s}\times\vec{e}^{\,0})\times\vec{s}\,]}{s^2 - k_\tau^2}\right]}\,\hat{\varphi}(\vec{s}) \right\rangle \\ &= \int\limits_{\mathbb{R}^3} \alpha_d(\vec{\eta})\, e^{i\vec{k}_\tau\cdot\vec{\eta}} \int\limits_{\mathbb{R}^3} \frac{[(\vec{s}\times\vec{e}^{\,0})\times\vec{s}\,]}{s^2 - k_\tau^2}\, (\bar{\varphi})\check{}\,(\vec{s})\, e^{-i\vec{\eta}\cdot\vec{s}}\, \mathrm{d}\vec{s}\, \mathrm{d}\vec{\eta} \end{aligned} \tag{2.3.1}$$

for all $\varphi \in C_0^\infty(\mathbb{R}^3)$, where the integrals are well defined, since the inverse Fourier transform $\mathcal{F}_{\vec{s}}^{-1}\left(\left[(\vec{s}\times\vec{e}^{\,0})\times\vec{s}\,\right]/(s^2 - k_\tau^2)\; (\bar{\varphi})\check{}\,(\vec{s})\right)(\vec{\eta})$ is a Schwartz function and since $\alpha_d(\vec{\eta})\, e^{i\vec{k}_\tau\cdot\vec{\eta}}$ is uniformly bounded w.r.t. $\eta' := (\eta_x, \eta_y)^\top$ and $\alpha_d(\vec{\eta})$ has a compact support w.r.t. $\eta_z$. Using these arguments, it is also easily seen that the outer integral in (2.3.1) exists absolutely.

It is the overall goal of this section to integrate w.r.t. $s_z$ analytically in (2.3.1) such that only the integrals w.r.t. $s_x$ and $s_y$ remain. Following [14, Section II.B], the order of integration is interchanged and the integral w.r.t. $s_z$ is evaluated applying the residue theorem. In the following section this will be done. Afterwards the limit $\tau \nearrow 0$ will be assessed in Section 2.4.1 for a special type of interface functions.

### 2.3.2 Interchanging the order of integration

In order to change the order of integration and to apply Lebesgue's theorem on dominated convergence, bounded domains of integration are needed. Since the outer integral w.r.t. $\vec{\eta}$ in (2.3.1) exists absolutely for a complex valued $k_\tau^2$ ,

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

where $C_3(\tilde{r}) := B_2(\tilde{r}) \times [-\tilde{r}, \tilde{r}]$ and $B_2(\tilde{r}) := \{\eta' \in \mathbb{R}^2 : |\eta'| \le \tilde{r}\}$. However, for any fixed $\tilde{r}$, the integrals w.r.t. $\vec{\eta}$ and $\vec{s}$ are absolutely integrable. Fubini's theorem implies $\langle \vec{D}^d(\vec{x}), \varphi(\vec{x})\rangle = \lim_{\tilde{r}\to\infty} \langle \vec{D}^d_{\tilde{r}}(\vec{x}), \varphi(\vec{x})\rangle$, where

$$\left\langle \vec{D}^d_{\tilde{r}}(\vec{x}), \varphi(\vec{x}) \right\rangle := \frac{1}{(2\pi)^3} \int\limits_{\mathbb{R}^3} \int\limits_{C_3(\tilde{r})} \alpha_d(\vec{\eta})\, e^{-i\vec{\eta}\cdot(\vec{s}-\vec{k}_\tau)}\, \mathrm{d}\vec{\eta}\, \frac{[(\vec{s}\times\vec{e}^0)\times\vec{s}]}{s^2 - k_\tau^2} \int\limits_{\mathbb{R}^3} \bar{\varphi}(\vec{x})\, e^{i\vec{s}\cdot\vec{x}}\, \mathrm{d}\vec{x}\, \mathrm{d}\vec{s} \tag{2.3.2}$$

will be considered for a fixed $\tilde{r} > h$. The limit $\tilde{r} \to \infty$ will be examined in Section 2.4.1.

Again, since the integral w.r.t. $\vec{s}$ in (2.3.2) is absolutely integrable,

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

with $s' := (s_x, s_y)^\top$. Since $\varphi$ has compact support, the integrands of the integrals w.r.t. $\vec{x}$ and $\vec{s}$ are absolutely integrable for any fixed $r, R \in \mathbb{R}$. Hence, for the bounded domain of integration, Fubini's theorem applies and

$$\left\langle \vec{D}^d_{\tilde{r}}(\vec{x}), \varphi(\vec{x}) \right\rangle = \frac{1}{(2\pi)^3} \lim_{r,R\to\infty} \int\limits_{\mathbb{R}^3} \bar{\varphi}(\vec{x}) \int\limits_{B_2(r)} \int\limits_{-R}^{R} \left\{ \int\limits_{C_3(\tilde{r})} \alpha_d(\vec{\eta})\, e^{-i\vec{\eta}\cdot(\vec{s}-\vec{k}_\tau)}\, \mathrm{d}\vec{\eta}\, \frac{[(\vec{s}\times\vec{e}^0)\times\vec{s}]}{s_z^2 - {\xi_\tau}^2}\, e^{i\vec{s}\cdot\vec{x}} \right\} \mathrm{d}s_z\, \mathrm{d}s'\, \mathrm{d}\vec{x}, \tag{2.3.3}$$

where $\xi_\tau := \sqrt{k_\tau^2 - s_x^2 - s_y^2}$. Here and in the remainder of this paper the square root of a complex number $w$ will be chosen such that the argument of the complex number $\sqrt{w}$ is in $[0, \pi)$. Thus the imaginary part of $\xi_\tau$ is positive and the integrand of the integration w.r.t. $s_z$ in (2.3.3) has no poles for any fixed $s' \in \mathbb{R}^2$.

### 2.3.3 Analytical integration w.r.t. $s_z$ for a fixed $r$

In this section it will be shown that the integrand of the integral w.r.t. $s'$ of (2.3.3) is uniformly bounded on $B_2(r)$ 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, it is sufficient that the integral w.r.t. $s_z$ is absolutely integrable for any $s' \in B_2(r)$ and $\vec{x} \in \mathbb{R}^3$, since $B_2(r)$ is bounded. This will allow to apply Lebesgue's theorem, to evaluate the limit w.r.t. $R$ before evaluating the integrals w.r.t. $s'$. The necessary estimates and the proof of the existence of the pointwise limits will be done for the case $z > h$. Recall that $z$ is the third component of the vector $\vec{x}$.

For convenience, suppose $\tilde{r} > h$ and define

$$\begin{aligned}
\hat{\alpha}_{\tilde{r}}(\vec{s} - \vec{k}_\tau) &:= \int\limits_{C_3(\tilde{r})} \alpha_d(\vec{\eta})\, e^{-i\vec{\eta}\cdot(\vec{s}-\vec{k}_\tau)}\, \mathrm{d}\vec{\eta} = -\Delta \int\limits_{B_2(\tilde{r})} \int\limits_0^{f(\eta')} e^{-i\eta_z(s_z - k_{z,\tau})}\, \mathrm{d}\eta_z\, e^{-i\eta'\cdot(s'-k')}\, \mathrm{d}\eta' \\
&= i\Delta \int\limits_{B_2(\tilde{r})} \frac{1 - e^{-i(s_z - k_{z,\tau})\, f(\eta')}}{s_z - k_{z,\tau}}\, e^{-i\eta'\cdot(s'-k')}\, \mathrm{d}\eta', \qquad (2.3.4) \\
&= -\Delta \int\limits_{B_2(\tilde{r})} \int\limits_0^1 e^{-i(s_z - k_{z,\tau})\,\zeta\, f(\eta')}\, \mathrm{d}\zeta\, f(\eta')\, e^{-i\eta'\cdot(s'-k')}\, \mathrm{d}\eta', \quad \Delta := \epsilon_\tau - \epsilon_0' \qquad (2.3.5)
\end{aligned}$$

which is continuously differentiable and uniformly bounded w.r.t. $\vec{s}$. Following [14, Section II.B], by analytic continuation of $\hat{\alpha}_{\tilde{r}}(\vec{s} - \vec{k}_\tau)\, \frac{[(\vec{s}\times\vec{e}^0)\times\vec{s}]}{s_z^2 - \xi_\tau{}^2}\, e^{is_z z}$ w.r.t. $s_z$ onto $\mathbb{C}$ for all $z > h$, a meromorphic function is obtained. The residue theorem applies to the integration over the closed path $\partial\Omega_R := C_R \cup [-R, R]$, with $C_R := \{z \in \mathbb{C} : \operatorname{Im} z \geq 0, |z| = R\}$. The curve $C_R$ is assumed to be oriented counterclockwise. The integral w.r.t. $s_z$ in (2.3.3) can then be written as

$$\begin{aligned}
\int\limits_{-R}^{R} \hat{\alpha}_{\tilde{r}}(\vec{s} - \vec{k}_\tau)\, \frac{[(\vec{s}\times\vec{e}^0)\times\vec{s}]}{s_z^2 - \xi_\tau{}^2}\, e^{is_z z}\, \mathrm{d}s_z &= -\int\limits_{C_R} \hat{\alpha}_{\tilde{r}}(\vec{s}_w - \vec{k}_\tau)\, \frac{[(\vec{s}_w\times\vec{e}^0)\times\vec{s}_w]}{w^2 - \xi_\tau{}^2}\, e^{iwz}\, \mathrm{d}w \\
&\quad + 2\pi i\, \hat{\alpha}_{\tilde{r}}(\vec{s}_{\xi_\tau} - \vec{k}_\tau)\, \frac{[(\vec{s}_{\xi_\tau}\times\vec{e}^0)\times\vec{s}_{\xi_\tau}]}{2\xi_\tau}\, e^{i\xi_\tau z},
\end{aligned} \qquad (2.3.6)$$

where $\vec{s}_w := (s_x, s_y, w)^\top$ for $w \in \mathbb{C}$. The absolute value of the first summand in (2.3.6) can be estimated as follows

$$\left| \int_{C_R} \hat{\alpha}_{\tilde{r}}(\vec{s}_w - \vec{k}_\tau) \, \frac{[(\vec{s}_w \times \vec{e}^0) \times \vec{s}_w]}{(w-\xi_\tau)(w+\xi_\tau)} \, e^{iwz} \, \mathrm{d}w \right| \leq c_1 c_2(s') \int_0^\pi e^{-\frac{z}{2} R \sin\phi} \, \mathrm{d}\phi \leq \pi \, c_1 c_2(s'), \tag{2.3.7}$$

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

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

where it will be shown that the constant $C(s') := c_1 \, c_2(s')$ is finite for any $s' \in \mathbb{R}^2$.

The supremum $c_2(s')$ is finite, since the numerator is a polynomial of $Re^{i\phi}$ of order two, while the second order polynomial in the denominator has no zeros. Obviously $c_1$ is finite too. Together with (2.3.4), $c_1$ can be estimated as

$$\begin{aligned} c_1 &\leq \sup_{R \in [|\vec{k}_\tau|, \infty)} \sup_{\phi \in [0,\pi]} \frac{|\Delta| \; R}{|R - |k_{z,\tau}||} \int_{B_2(\tilde{r})} \left[ e^{-\frac{z}{2} R \sin\phi} + e^{-R \sin\phi \left(\frac{z}{2} - f(\eta')\right)} \, e^{-\tau f(\eta')} \right] \mathrm{d}\eta' \\ &\leq \sup_{R \in [|\vec{k}_\tau|, \infty)} \frac{|\Delta| \; R}{|R - |k_{z,\tau}||} \int_{B_2(\tilde{r})} \left[ 1 + e^{-\tau f(\eta')} \right] \mathrm{d}\eta', \end{aligned}$$

where $z > 0$ and $\frac{z}{2} - f(\eta') > 0$ was used and where the last term is bounded for any fixed $\tilde{r}$, since $R > |\vec{k}_\tau| \geq |k_{z,\tau}|$. The second term of (2.3.6) 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 $c_3 := \sup_{s' \in \mathbb{R}^2} |[(\vec{s}_{\xi_\tau} \times \vec{e}^0) \times \vec{s}_{\xi_\tau}] / \xi_\tau^2|$ of a rational function is bounded. Now (2.3.4) implies

$$\begin{aligned} \left| \hat{\alpha}_{\tilde{r}}(\vec{s}_{\xi_\tau} - \vec{k}_\tau) \, \frac{[(\vec{s}_{\xi_\tau} \times \vec{e}^0) \times \vec{s}_{\xi_\tau}]}{\xi_\tau} \, e^{i\xi_\tau z} \right| &\leq c_3 \left| \Delta \int_{B_2(\tilde{r})} \frac{1 - e^{-i(\xi_\tau - k_{z,\tau}) \, f(\eta')}}{\xi_\tau - k_{z,\tau}} \, e^{-i\eta' \cdot (s' - k')} \, \mathrm{d}\eta' \, \xi_\tau \, e^{i\xi_\tau z} \right| \\ &\leq c_3 \left| \frac{\Delta \, \xi_\tau}{\xi_\tau - k_{z,\tau}} \right| \int_{B_2(\tilde{r})} \left[ 1 + \, e^{-\tau \, f(\eta')} \right] \mathrm{d}\eta'. \end{aligned} \tag{2.3.8}$$

Again, the remaining quotient in the last estimate (2.3.8) is uniformly bounded w.r.t. $s'$. Indeed, $\operatorname{Im} \xi_\tau > 0$ and $\operatorname{Im} k_{z,\tau} = \tau < 0$ leading to $\operatorname{Im}(\xi_\tau - k_{z,\tau}) > 0$. Hence the supremum

$$c_4(\tilde{r}) := \sup_{s' \in \mathbb{R}^2} \left| \hat{\alpha}_{\tilde{r}}(\vec{s}_{\xi_\tau} - \vec{k}_\tau) \, \frac{[(\vec{s}_{\xi_\tau} \times \vec{e}^0) \times \vec{s}_{\xi_\tau}]}{\xi_\tau} \, e^{i\xi_\tau z} \right| \tag{2.3.9}$$

is finite for any fixed $\tilde{r} > h$ and $\tau < 0$. Consequently, the integral w.r.t. $s_z$ in (2.3.3) is absolutely bounded by $\pi \, C(s') + 2\pi \, c_4(\tilde{r})$ (cf. (2.3.7)), 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 (2.3.7) it can be shown, that the limit of the integral over $C_R$ tends to zero as $R$ tends to infinity.

Indeed, the limit of this estimate can be found by considering the limit of an upper bound for the non-negative integral for any fixed $z > h \geq 0$. However

$$\lim_{R\to\infty} \int\limits_{\pi/4}^{\pi/2} e^{-\frac{z}{2}R\sin\phi}\,\mathrm{d}\phi \leq \lim_{R\to\infty} \frac{\pi}{4} e^{-\frac{z}{2}R\sin\frac{\pi}{4}} = 0, \tag{2.3.10}$$

$$\lim_{R\to\infty} \int\limits_{0}^{\pi/4} e^{-\frac{z}{2}R\sin\phi}\,\mathrm{d}\phi < \lim_{R\to\infty} \int\limits_{0}^{\pi/4} e^{-\frac{z}{2}R\sin\phi}\, 2\cos\phi\,\mathrm{d}\phi = 0. \tag{2.3.11}$$

Therefore, (2.3.6) leads to

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

Finally, if $\varphi(\vec{x}) = 0$ for all $z \leq h$, it follows that (cf. (2.3.3))

$$\left\langle \vec{D}^d_{\tilde{r}}(\vec{x}), \varphi(\vec{x}) \right\rangle = \frac{i}{8\pi^2} \lim_{r\to\infty} \int\limits_{\mathbb{R}^3} \bar{\varphi}(\vec{x}) \int\limits_{B_2(r)} \hat{\alpha}_{\tilde{r}}(\vec{s}_{\xi_\tau} - \vec{k}_\tau)\, \frac{[(\vec{s}_{\xi_\tau}\times\vec{e}^{0})\times\vec{s}_{\xi_\tau}]}{\xi_\tau}\, e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}}\,\mathrm{d}s'\,\mathrm{d}\vec{x}. \tag{2.3.12}$$

### 2.3.4 Calculation of the limit w.r.t. $r$

The goal of this subsection will be to evaluate the limit $r \to \infty$ in equation (2.3.12). 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 $z > h$. This absolute integral is also uniformly bounded w.r.t. $x' \in \mathbb{R}^2$ and $z > h$. The product of $\varphi \in C_0^\infty(\mathbb{R}^3)$ and the integral w.r.t. $s'$ in equation (2.3.12) is then dominated by a non-negative integrable function. Therefore Lebesgue's applies.

First, the term $\xi_\tau = \sqrt{k_\tau^2 - s'^2}$, with $s'^2 := \|s'\|^2$, $k_{z,\tau} = k_z + i\tau$ and $k_z < 0$, will be examined more closely. Since for $s'^2 > 2|\vec{k}_\tau|^2$, $\mathrm{Re}(k_\tau^2 - s'^2) = k^2 - \tau^2 - s'^2 < 0$ and $\mathrm{Im}(k_\tau^2 - s'^2) = 2k_z\tau > 0$, the argument $\arctan\left(\frac{2k_z\tau}{k^2-\tau^2-s'^2}\right) + \pi$ of the complex number $k_\tau^2 - s'^2$ is in $\left(\frac{\pi}{2}, \pi\right)$. Here $\arctan\colon \mathbb{R} \to \left(-\frac{\pi}{2}, \frac{\pi}{2}\right)$. Hence, the angle $\theta$, the argument of $\sqrt{k_\tau^2 - s'^2}$, is in $\left(\frac{\pi}{4}, \frac{\pi}{2}\right)$ leading to $\sin\theta > \frac{1}{\sqrt{2}}$. With this in mind, with $|z - f(\eta')| > \frac{h}{2}$ for all $z > h$, and with the definition of $c_3$, (2.3.8) and (2.3.9), the splitting of the domain of integration into $B_2(\sqrt{2}|\vec{k}_\tau|)$ and $\mathbb{R}^2 \setminus B_2(\sqrt{2}|\vec{k}_\tau|)$ yields

$$\left| \int\limits_{\mathbb{R}^2} \hat{\alpha}_{\tilde{r}}(\vec{s}_{\xi_\tau} - \vec{k}_\tau)\, \frac{[(\vec{s}_{\xi_\tau}\times\vec{e}^{0})\times\vec{s}_{\xi_\tau}]}{\xi_\tau}\, e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}}\,\mathrm{d}s' \right| \leq 2\pi|\vec{k}_\tau|^2 c_4(\tilde{r}) \tag{2.3.13}$$

$$+ c_3\,\Delta \int\limits_{\mathbb{R}^2\setminus B_2(\sqrt{2}|\vec{k}_\tau|)} \left| \frac{\xi_\tau\,\pi\,\tilde{r}^2}{\xi_\tau - k_{z,\tau}} \right| e^{-\frac{h}{2\sqrt{2}}\sqrt{|k_\tau^2 - s'^2|}}\, e^{\tau h}\,\mathrm{d}s'.$$

Similarly to the estimate (2.3.8), the quotient on the right-hand side is uniformly bounded w.r.t. $s'$. This shows that the integral is finite for any fixed $z > h$ since the integrand decreases exponentially. Thus Lebesgue's theorem can be applied to evaluate the limit $r \to \infty$ and, for a $\varphi$ with $\varphi(\vec{x}) = 0$ for all $z \leq h$,

$$\left\langle \vec{D}^d_{\tilde{r}}(\vec{x}), \varphi(\vec{x}) \right\rangle = \frac{i}{8\pi^2} \int\limits_{\mathbb{R}^3} \bar{\varphi}(\vec{x}) \int\limits_{\mathbb{R}^2} \hat{\alpha}_{\tilde{r}}(\vec{s}_{\xi_\tau} - \vec{k}_\tau) \frac{[(\vec{s}_{\xi_\tau} \times \vec{e}^{\,0}) \times \vec{s}_{\xi_\tau}]}{\xi_\tau} e^{i\vec{s}_{\xi_\tau} \cdot \vec{x}} \, \mathrm{d}s' \, \mathrm{d}\vec{x}. \quad (2.3.14)$$

## 2.4 Limit $\tilde{r} \to \infty$ and limiting absorption for a special interface space

### 2.4.1 Almost periodic and decaying interface functions

In this section the last remaining limits $\tilde{r} \to \infty$ and $\tau \nearrow 0$ will be evaluated for a special choice of interfaces. Unfortunately, the treatment of general bounded and smooth interface functions $f$ seems not to be possible. So our analysis is restricted 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. [4]), and functions of the same type, but with an integer order of decay at infinity.

Consider the space of real valued interface functions $\mathcal{A}_1 := \left\{ f : \mathbb{R}^2 \to \mathbb{R}, f \in \mathcal{A}_1^{\mathbb{C}} \right\}$ taken from the complex valued space

$$\mathcal{A}_1^{\mathbb{C}} := \left\{ f : \mathbb{R}^2 \to \mathbb{C} | \, f(\eta') = \sum_{l=0}^{3} \left[ \frac{1}{\sqrt{1 + |\eta'|^2}^{\,l}} \sum_{j \in \mathbb{Z}} \lambda_{l,j} \, e^{i\omega'_{l,j} \cdot \eta'} \right] + g(\eta') \right.$$
$$\left. \lambda_{l,j} \in \mathbb{C}, \; \omega'_{l,j} \in \mathbb{R}^2, \; ||f||_{\mathcal{A}_1} < \infty \right\}$$

where

$$||f||_{\mathcal{A}_1} := \sum_{l=0}^{3} \sum_{j \in \mathbb{Z}} |\lambda_{l,j}| + ||g||_{1,1} + ||g||_\infty, \quad \big|\big|g(\eta')\big|\big|_{1,1} := \big|\big|(1 + |\eta'|) \, g(\eta')\big|\big|_{L^1(\mathbb{R}^2)}. \quad (2.4.1)$$

Note that the summation over $l$ in the sum for $f$ in the definition of $\mathcal{A}_1^{\mathbb{C}}$ can be restricted to $l \leq 3$ since the $g_{l,j} := \{1 + |\eta'|^2\}^{-l/2} e^{i\omega'_{l,j} \cdot \eta'}, \; l > 3$ have a finite norm $||g_{l,j}||_{1,1}$ and can be included into $g$. Further note that the restrictions $\omega'_{l,j} = -\omega'_{l,-j}$ and $\lambda_{l,j} = \overline{\lambda_{l,-j}}$, $l = 0, 1, 2, 3$, $j \in \mathbb{Z}$ ensure that the function $f$, given as a sum in the definition of $\mathcal{A}_1^{\mathbb{C}}$, is real valued. There holds

**Lemma 2.1.** *The spaces $\mathcal{A}_1$ and $\mathcal{A}_1^{\mathbb{C}}$ together with the norm $||\cdot||_{\mathcal{A}_1}$ and pointwise multiplication form Banach algebras.*

The proof of this lemma consists of a straightforward verification of the properties of a Banach algebra. Since the process is lengthy, but contains no difficulties, the proof is omitted.

**Remark 2.1.** *The coefficients $\lambda_{l,j}$ depend continuously on $f \in \mathcal{A}_1$. Moreover, the term $g$ depends continuously on $f \in \mathcal{A}_1$ w.r.t. to the norm $|| \cdot ||_{1,1} + || \cdot ||_\infty$.*

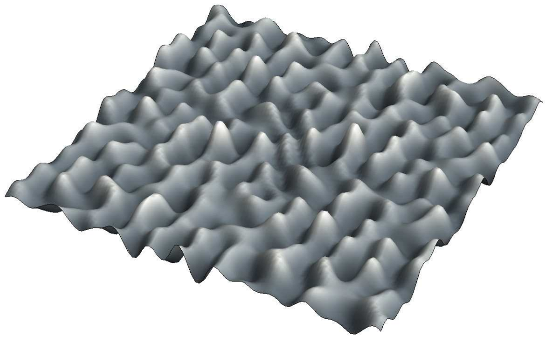

Figure 2: Example of an interface function from $\mathcal{A}_1$ using only the almost periodic portion and choosing a finite number of uniformly distributed random parameters $\lambda_{0,j}$ and $\omega'_{0,j}$.

#### 2.4.2 Existence of the remaining Cauchy principle value and the limit of the limiting absorption principle

Assuming an interface function $f$ from $\mathcal{A}_1$, it will be shown that the limit of (2.3.14)

$$\left\langle \vec{D}^d(\vec{x}), \varphi(\vec{x}) \right\rangle = \frac{i}{8\pi^2} \lim_{\substack{\tau \nearrow 0 \\ \tilde{r}\to\infty}} \int_{\mathbb{R}^3} \bar{\varphi}(\vec{x}) \int_{\mathbb{R}^2} \hat{\alpha}_{\tilde{r}}(\vec{s}_{\xi_\tau} - \vec{k}_\tau) \frac{[(\vec{s}_{\xi_\tau} \times \vec{e}^{\,0}) \times \vec{s}_{\xi_\tau}]}{\xi_\tau} e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}} \,\mathrm{d}s' \,\mathrm{d}\vec{x} \quad (2.4.2)$$

exists. First consider the integral w.r.t. $s'$ for an interface function $f$. Using Equs. (2.3.4) and (2.3.5) for $\hat{\alpha}_{\tilde{r}}$, the integral w.r.t. $s'$ transforms to $i\Delta$ times

$$\int_{\mathbb{R}^2} \int_{B_2(\tilde{r})} \frac{1 - e^{-i(\xi_\tau - k_{z,\tau}) f(\eta')}}{\xi_\tau - k_{z,\tau}} e^{-i\eta'\cdot(s'-k')} \,\mathrm{d}\eta' \, \frac{[(\vec{s}_{\xi_\tau} \times \vec{e}^{\,0}) \times \vec{s}_{\xi_\tau}]}{\xi_\tau} e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}} \,\mathrm{d}s' \quad (2.4.3)$$

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

Here Fubini's theorem applies for any fixed $\tilde{r}$ and $\tau < 0$, since $e^{i\xi_\tau(z - \zeta f(\eta'))}$ decays exponentially as $|s'|$ tends to infinity and since the integrand is uniformly bounded w.r.t. $\eta' \in B_2(\tilde{r})$. Replacing $f(\eta')\, e^{-i(\xi_\tau - i\tau)\zeta\, f(\eta')}$ by $\sum_{n\in\mathbb{N}_0} (-i\zeta)^n \; f(\eta')^{n+1} \frac{(\xi_\tau - i\tau)^n}{n!}$ leads to

$$\int_{\mathbb{R}^2} \int_{B_2(\tilde{r})} \frac{1 - e^{-i(\xi_\tau - k_{z,\tau}) f(\eta')}}{\xi_\tau - k_{z,\tau}} e^{-i\eta'\cdot(s'-k')} \,\mathrm{d}\eta' \, \frac{[(\vec{s}_{\xi_\tau} \times \vec{e}^{\,0}) \times \vec{s}_{\xi_\tau}]}{\xi_\tau} e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}} \,\mathrm{d}s' = i\,\mathrm{I}_1 + i\,\mathrm{I}_2,$$

$$\mathrm{I}_1 := \int_0^1 \int_{\mathbb{R}^2} \Bigg\{ \int_{B_2(\tilde{r})} \sum_{n=0}^{8} (-i\zeta)^n \; f(\eta')^{n+1} \frac{(\xi_\tau - i\tau)^n}{n!} e^{ik_z\zeta\, f(\eta')}\, e^{-i\eta'\cdot(s'-k')} \,\mathrm{d}\eta'$$
$$\frac{[(\vec{s}_{\xi_\tau} \times \vec{e}^{\,0}) \times \vec{s}_{\xi_\tau}]}{\xi_\tau} e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}} \Bigg\} \,\mathrm{d}s' \,\mathrm{d}\zeta, \quad (2.4.4)$$

$$\mathrm{I}_2 := \int\limits_0^1 \int\limits_{\mathbb{R}^2} \Bigg\{ \int\limits_{B_2(\tilde r)} \sum_{n=9}^{\infty} (-i\zeta)^n \ f(\eta')^{n+1} \frac{(\xi_\tau - i\tau)^n}{n!} \, e^{ik_z\zeta\, f(\eta')} \, e^{-i\eta'\cdot(s'-k')} \, \mathrm{d}\eta' \\ \frac{[(\vec{s}_{\xi_\tau} \times \vec{e}^{\,0}) \times \vec{s}_{\xi_\tau}]}{\xi_\tau} \, e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}} \Bigg\} \, \mathrm{d}s' \, \mathrm{d}\zeta. \tag{2.4.5}$$

where $\mathbb{N}_0$ is the set of non-negative integers. First, examine integral (2.4.4) by replacing the exponential $e^{ik_z\zeta\, f(\eta')}$ with its sum leading to

$$\mathrm{I}_1 = \sum_{n=0}^{8} \int\limits_0^1 \frac{(-i\zeta)^n}{n!} \int\limits_{\mathbb{R}^2} \Bigg\{ \frac{(\xi_\tau - i\tau)^n}{\xi_\tau} \int\limits_{B_2(\tilde r)} f(\eta')^{n+1} \sum_{m\in\mathbb{N}_0} \frac{(ik_z\zeta\, f(\eta'))^m}{m!} \, e^{-i\eta'\cdot(s'-k')} \, \mathrm{d}\eta' \\ \left[\left(\vec{s}_{\xi_\tau} \times \vec{e}^{\,0}\right) \times \vec{s}_{\xi_\tau}\right] \, e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}} \Bigg\} \, \mathrm{d}s' \, \mathrm{d}\zeta. \tag{2.4.6}$$

Since $f \in \mathcal{A}_1 \subset \mathcal{A}_1^{\mathbb{C}}$, the term

$$f_n(\eta') := f_{n,k_z,\zeta}(\eta'), \qquad f_{n,k_z,\zeta} := f^{n+1} \, e^{ik_z\zeta\, f} = \sum_{m\in\mathbb{N}_0} \frac{(ik_z\zeta)^m}{m!} \, f^{m+n+1} \tag{2.4.7}$$

is also an element of $A_1^{\mathbb{C}}$. More precisely, there holds

**Lemma 2.2.** *For any function $f$ in $\mathcal{A}_1$, the function $f_n$ (cf. (2.4.7)) is equal to*

$$f_n(\eta') = \sum_{\ell=0}^{3} \left[ \frac{1}{\sqrt{1+|\eta'|^2}^{\,\ell}} \sum_{j\in\mathbb{Z}} \tilde\lambda_{\ell,j}^n \, e^{i\tilde\omega'_{\ell,j}\cdot\eta'} \right] + \tilde g_n(\eta'), \tag{2.4.8}$$

*where the $\tilde\omega'_{\ell,j}$, $\ell = 0, 1, 2, 3$ are defined as the entries of the sets*

$$\left\{\tilde\omega'_{0,j} : j \in \mathbb{Z}\right\} = \left\{ \sum_{\kappa\in\mathbb{Z}} m_\kappa \omega'_{0,\kappa} : \ m_\kappa \in \mathbb{N}_0, \ \sum_{\kappa\in\mathbb{Z}} m_\kappa < \infty \right\}, \tag{2.4.9}$$

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

*and where*

$$\tilde\lambda_{0,j}^n := \sum_{\substack{m_\kappa\in\mathbb{N}_0: \\ \tilde m := \sum_{\kappa\in\mathbb{Z}} m_\kappa \geq n+1, \, \tilde m < \infty \\ \sum_{\kappa\in\mathbb{Z}} m_\kappa \omega'_{0,\kappa} = \tilde\omega'_{0,j}}} (ik_z\zeta)^{\tilde m - n - 1} \, \frac{\tilde m!}{(\tilde m - n - 1)!} \left[ \prod_{\kappa\in\mathbb{Z}} \frac{[\lambda_{0,\kappa}]^{m_\kappa}}{m_\kappa!} \right], \tag{2.4.10}$$

$$\tilde\lambda_{\ell,j}^n := \sum_{\substack{m_\kappa^l\in\mathbb{N}_0: \\ \tilde m := \sum_{l=0}^{\ell} \sum_{\kappa\in\mathbb{Z}} m_\kappa^l \geq n+1, \, \tilde m < \infty \\ \sum_{l=1}^{\ell} l \sum_{\kappa\in\mathbb{Z}} m_\kappa^l = \ell, \, \sum_{l=0}^{\ell} \sum_{\kappa\in\mathbb{Z}} m_\kappa^l \omega'_{l,\kappa} = \tilde\omega'_{\ell,j}}} (ik_z\zeta)^{\tilde m - n - 1} \, \frac{\tilde m!}{(\tilde m - n - 1)!} \left[ \prod_{l=0}^{\ell} \prod_{\kappa\in\mathbb{Z}} \frac{[\lambda_{l,\kappa}]^{m_\kappa^l}}{m_\kappa^l!} \right], \tag{2.4.11}$$

$$\tilde{g}_n(\eta') := \sum_{m\in\mathbb{N}_0} \frac{(m+n+1)!}{m!}\,(ik_z\zeta)^m \sum_{\vec{n}_5\in \mathrm{I}_{m+n+1}\setminus\left(\bigcup\limits_{\ell=0}^{3}\mathrm{I}^\ell_{m+n+1}\right)} \left[ \frac{g(\eta')^{n_4}}{n_4!\,\sqrt{1+|\eta'|^2}^{\left(\sum\limits_{l=1}^{3} l n_l\right)}} \right.$$

$$\left. \prod_{l=0}^{3} \sum_{m_\infty\in \mathrm{J}_{n_l}} \left\{ \left[\prod_{j\in\mathbb{Z}} \frac{[\lambda_{l,j}]^{m_j}}{m_j!}\right] e^{i\eta'\cdot\sum\limits_{j\in\mathbb{Z}} m_j\omega'_{l,j}} \right\} \right], \tag{2.4.12}$$

$$\mathrm{I}_a := \left\{ (n_0,\dots,n_4)\in\mathbb{N}_0^5 \,\middle|\, \sum_{l=0}^{4} n_l = a \right\}, \quad \mathrm{J}_a := \left\{ (m_j)_{j\in\mathbb{Z}} \,\middle|\, m_j\in\mathbb{N}_0,\ \sum_{j\in\mathbb{Z}} m_j = a \right\},$$

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

*Proof.* The existence of representation (2.4.8) is a simple consequence of the algebra structure of $\mathcal{A}_1$. The coefficients and $\tilde{g}_n$ can be found by evaluating (2.4.8) using the multinomial theorem and rearranging the resulting sums. □

Note that $f_n$ also depends on the constant $k_z$ and the variables $\zeta\in[0,1]$ and $n\in\{0,\dots,8\}$. To be precise, $\tilde{\lambda}^n_{\ell,j}$ is dependent on $k_z$, $\zeta$ and $n$, while $\tilde{\omega}'_{\ell,j}$ is a constant for any fixed $\ell = 0,\dots,3$ and $j\in\mathbb{Z}$. Similarly the function $\tilde{g}_n$ depends on $k_z$ and $\zeta$. With this, the limit $\tilde{r}\to\infty$ of (2.4.6) can be evaluated as the sum $\lim_{\tilde{r}\to\infty}\mathrm{I}_1 = \mathrm{I}_{1,1}+\mathrm{I}_{1,2}+\mathrm{I}_{1,3}$, where

$$\mathrm{I}_{1,1} := \lim_{\tilde{r}\to\infty} \sum_{n=0}^{8}\sum_{j\in\mathbb{Z}} \left\{ \int_0^1 \tilde{\lambda}^n_{0,j}\frac{(-i\zeta)^n}{n!}\,\mathrm{d}\zeta \int_{\mathbb{R}^2} \left\{ \frac{(\xi_\tau - i\tau)^n}{\xi_\tau} \int_{B_2(\tilde{r})} e^{i\tilde{\omega}'_{0,j}\cdot\eta'}\, e^{-i\eta'\cdot(s'-k')}\,\mathrm{d}\eta' \right.\right.$$

$$\left.\left. \left[\left(\vec{s}_{\xi_\tau}\times\vec{e}^{\,0}\right)\times\vec{s}_{\xi_\tau}\right]\, e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}} \right\} \mathrm{d}s' \right\}, \tag{2.4.13}$$

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

$$\left.\left. \frac{(\xi_\tau - i\tau)^n}{\xi_\tau} \left[\left(\vec{s}_{\xi_\tau}\times\vec{e}^{\,0}\right)\times\vec{s}_{\xi_\tau}\right]\, e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}} \right\} \mathrm{d}s' \right\}, \tag{2.4.14}$$

$$\mathrm{I}_{1,3} := \lim_{\tilde{r}\to\infty} \sum_{n=0}^{8} \int_0^1 \frac{(-i\zeta)^n}{n!} \int_{\mathbb{R}^2} \left\{ \frac{(\xi_\tau - i\tau)^n}{\xi_\tau} \int_{B_2(\tilde{r})} \tilde{g}_n(\eta')\, e^{-i\eta'\cdot(s'-k')}\,\mathrm{d}\eta' \right.$$

$$\left. \left[\left(\vec{s}_{\xi_\tau}\times\vec{e}^{\,0}\right)\times\vec{s}_{\xi_\tau}\right]\, e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}} \right\} \mathrm{d}s'\,\mathrm{d}\zeta. \tag{2.4.15}$$

Obviously, the limit (2.4.15) exists since for any $n \in \{0, \dots, 8\}$ the function $\tilde{g}_n$ is independent of $s'$ and absolutely integrable w.r.t. $\eta'$, and $\frac{(\xi_\tau - i\tau)^n}{\xi_\tau}\ \left[(\vec{s}_{\xi_\tau} \times \vec{e}^{\,0}) \times \vec{s}_{\xi_\tau}\right]\ e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}}$ is uniformly bounded and absolutely integrable w.r.t. $s'$ for any fixed $\tau < 0$.

To evaluate the limits (2.4.13) and (2.4.14) consider $\int_{\mathbb{R}^2} \sqrt{1+|\eta'|^2}^{\,-\ell}\ e^{-i\eta'\cdot\left(s'-(k'+\tilde{\omega}'_{\ell,j})\right)}\,\mathrm{d}\eta'$ for $\ell = 0, 1, 2, 3$, which can be evaluated as a Hankel transform of order zero defined as (cf. [1, Equ. 9.1.18, Sect. 9.1] for the relation between Hankel and Fourier transform)

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

Keeping in mind that the inverse Hankel transform coincides with the Hankel transform, the well-known Fourier transform for the Dirac delta and [12, Equs. 2.19, 2.20 and 2.110, Sect. I.1.2] lead to

$$\int_{\mathbb{R}^2} \frac{e^{-i\eta'\cdot\left(s'-(k'+\tilde{\omega}'_{\ell,j})\right)}}{\sqrt{1+|\eta'|^2}^{\,\ell}}\,\mathrm{d}\eta' = \begin{cases} 4\pi^2\,\delta\left(s'-(k'+\tilde{\omega}'_{0,j})\right) & \text{if } \ell = 0 \\ 2\pi\, e^{-\left|s'-(k'+\tilde{\omega}'_{1,j})\right|} / \left|s'-(k'+\tilde{\omega}'_{1,j})\right| & \text{if } \ell = 1 \\ 2\pi\, K_0\left(\left|s'-(k'+\tilde{\omega}'_{2,j})\right|\right) & \text{if } \ell = 2 \\ 2\pi\, e^{-\left|s'-(k'+\tilde{\omega}'_{3,j})\right|} & \text{if } \ell = 3 \end{cases}, \qquad (2.4.16)$$

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 (2.4.16) with $\ell = 1$ is a weakly singular function, while that of (2.4.16) with $\ell = 3$ is uniformly bounded.

The limits of the integrals (2.4.13) and (2.4.14) are 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 $z > h$. To be more exact, for the function $F_{\tilde{r},\ell,j}(\eta') := \mathbb{1}_{B_2(\tilde{r})}(\eta')\,(1+|\eta'|^2)^{-\ell/2}\, e^{i\eta'\cdot(\tilde{\omega}'_{\ell,j}+k')}$ the limit is evaluated as

$$\lim_{\tilde{r}\to\infty}\int_{\mathbb{R}^2} \mathcal{F}F_{\tilde{r},\ell,j}(s')\,\varphi_n(s')\,\mathrm{d}s' = \lim_{\tilde{r}\to\infty}\int_{\mathbb{R}^2} F_{\tilde{r},\ell,j}(\eta')\,\mathcal{F}\varphi_n(\eta')\,\mathrm{d}\eta' = \int_{\mathbb{R}^2} \frac{e^{i\eta'(\tilde{\omega}'_{\ell,j}+k')}}{\sqrt{1+|\eta'|^2}^{\,\ell}}\mathcal{F}\varphi_n(\eta')\,\mathrm{d}\eta' \qquad (2.4.17)$$

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. $j$. Indeed, switching to absolute values in the formulas for $\mathrm{I}_{1,1}$ and $\mathrm{I}_{1,2}$ will lead to a product of a sum over $j$ independent of $\tilde{r}$ times an integral independent of $j$, which is the right-hand side of Equ. (2.4.17) switched to absolute values. The sum w.r.t. $j$ exists, since $(\tilde{\lambda}^n_{\ell,j})_{j\in\mathbb{Z}}$ is an absolutely summable sequence.

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

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

Inserting this into (2.4.14) leads to

$$
\mathrm{I}_{1,2} = \sum_{\ell=1}^{3} \sum_{n=0}^{8} \sum_{j\in\mathbb{Z}} \int_0^1 \tilde{\lambda}^n_{\ell,j} \frac{(-i\zeta)^n}{n!} \,\mathrm{d}\zeta \int_{\mathbb{R}^2} \mathcal{F}F_{\infty,\ell,j}(s') \,\frac{(\xi_\tau - i\tau)^n}{\xi_\tau} \left[\left(\vec{s}_{\xi_\tau} \times \vec{e}^{\,0}\right) \times \vec{s}_{\xi_\tau}\right] e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}} \,\mathrm{d}s'. \tag{2.4.18}
$$

These integrals exist since the integrands are at most weakly singular, since the $\mathcal{F}F_{\infty,\ell,j}$ are bounded at infinity (cf. [1, Equ. 9.7.2, Sect. 9.1]), and since $e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}}$ is exponentially decreasing and ensures the existence of the integral w.r.t. $s'$.

It remains to examine the limit $\tau \nearrow 0$ of (2.4.18). Note that the integral w.r.t. $s'$ exists even if the singularity points of (2.4.16) with $\ell = 1$ or (2.4.16) with $\ell = 2$ coincide with the singularity point of $\frac{1}{\xi_\tau} = \frac{1}{\sqrt{k_\tau^2 - s'^2}}$ for $\tau = 0$.

**Lemma 2.3.** *For any $k \in \mathbb{R}_+$ and $k' \in \mathbb{R}^2$, the integral $\int_{B_2(2k)} 1/\sqrt{k - |s'|}\; 1/\left|k' - s'\right| \,\mathrm{d}s'$ is finite.*

Changing to local coordinates the proof is straightforward. This lemma can be used to apply Lebesgue's theorem to evaluate the limit $\tau \nearrow 0$ of the integrand w.r.t. $s'$ in (2.4.18) and thus (2.4.14).

On the other hand, for the integral w.r.t $s'$ and $\eta'$ in $\mathrm{I}_{1,1}$ the limit

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

is obtained. In this sense, the limit in (2.4.13) evaluates as

$$
\mathrm{I}_{1,1} = 4\pi^2 \sum_{n=0}^{8} \sum_{j\in\mathbb{Z}} \int_0^1 \tilde{\lambda}^n_{0,j} \,(-i\zeta)^n \,\mathrm{d}\zeta \,\frac{\left(\omega^j_{z,\tau} - \tau\right)^n}{n!\;\omega^j_{z,\tau}} \left[\left(\vec{\omega}^j_\tau \times \vec{e}^{\,0}\right) \times \vec{\omega}^j_\tau\right] e^{i\vec{\omega}^j_\tau\cdot\vec{x}}, \tag{2.4.19}
$$

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. $j$. This is a consequence of $\mathcal{A}_1^{\mathbb{C}}$ being a Banach algebra.

It remains to consider the limit $\tau \nearrow 0$ of the two terms (2.4.19) and (2.4.15). The limit can easily be evaluated since the sum w.r.t. $j$ exists absolutely and the integral w.r.t. $\zeta$ is uniformly bounded w.r.t. $\tau$. However, to obtain a finite limit of $\left(\omega^j_{z,\tau} - \tau\right)^n / \omega^j_{z,\tau}$ for $n = 0$, it has to be assumed that $\omega^j_{z,0} \neq 0$, i.e., (cf. (2.4.9) for the connection between $\omega'_{0,j}$ and $\tilde{\omega}'_{0,j}$)

$$
k \notin \mathrm{cl}\left\{ \left|k' + \sum_{j\in\mathbb{Z}} m_j \omega'_{0,j}\right| :\; m_j \in \mathbb{N}_0 \text{ s.t.} \sum_{j\in\mathbb{Z}} m_j < \infty \right\}. \tag{2.4.20}
$$

**Remark 2.2.** *This condition is not necessary. If $k$ is equal to $\left|k' + \sum_{j\in\mathbb{Z}} m_j \omega'_{0,j}\right|$ for a special sequence $m_j$, if this is an isolated point of the set in Equ.* (2.4.20)*, 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* (2.5.3) *and Theorem 2.1) vanishes, then the limit* $\tau \nearrow 0$ *exists even though* (2.4.20) *is violated.*

Analogously, the limit $\tau \nearrow 0$ of (2.4.15) is easily calculated using Lebesgue's theorem, since the integral $\int_{B_2(\tilde{r})} \tilde{g}_n(\eta')\, e^{-i\eta'\cdot(s'-k')}\,\mathrm{d}\eta'$ is uniformly bounded w.r.t. $s'$ by $||\tilde{g}_n||_{L^1(\mathbb{R}^2)} < \infty$ while the quotient $\frac{(\xi_\tau - i\tau)^n}{\xi_\tau}\,[(\vec{s}_{\xi_\tau}\times\vec{e}^{\,0})\times\vec{s}_{\xi_\tau}]\; e^{i\vec{s}_{\xi_\tau}\cdot\vec{x}}$ is pointwise convergent and uniformly bounded w.r.t. $\tau$ by a function that is integrable w.r.t. $s'$. It follows that the limits $\tilde{r}\to\infty$ and $\tau\nearrow 0$ of (2.4.6) can be evaluated.

Now consider the remaining integral (2.4.5). Using $\frac{1+|\eta'|_*^4}{1+|\eta'|_*^4}\, e^{-i\eta'\cdot(s'-k')} = \frac{\left(1+\nabla^4_{s'}\right) e^{-i\eta'\cdot(s'-k')}}{1+|\eta'|_*^4}$, where $\nabla^4_{s'} := \partial^4_{s_x} + \partial^4_{s_y}$ and $|\eta'|_*^4 := \eta_x^4 + \eta_y^4$, leads to

$$\mathrm{I}_2 = \int_0^1 \int_{\mathbb{R}^2} \Bigg\{ \int_{B_2(\tilde{r})} \sum_{n=9}^{\infty} (-i\zeta)^n\; f(\eta')^{n+1} \frac{(\xi_\tau - i\tau)^n}{n!}\; e^{ik_z\zeta\, f(\eta')}\; \frac{\left(1+\nabla^4_{s'}\right)\, e^{-i\eta'\cdot(s'-k')}}{1+|\eta'|_*^4}\,\mathrm{d}\eta' \\ \frac{[(\vec{s}_{\xi_\tau}\times\vec{e}^{\,0})\times\vec{s}_{\xi_\tau}]}{\xi_\tau}\, e^{is'\cdot x'}\, e^{iz\xi_\tau} \Bigg\}\,\mathrm{d}s'\,\mathrm{d}\zeta. \tag{2.4.21}$$

To further transform this expression, consider the following lemma.

**Lemma 2.4.** *For two complex valued functions* $f, g \in C^4(\mathbb{R}^2)$ *the following equation holds true.*

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

This is easily shown using the Leibniz rule. Naturally, Lemma 2.4 also holds for derivatives w.r.t. $s_y$. Using this and setting $S_9^\infty := S_9^\infty(s',\eta',\zeta) := \sum_{n=9}^\infty (-i\zeta)^n\, f(\eta')^{n+1}\frac{(\xi_\tau - i\tau)^n}{n!}\, e^{i\frac{z}{2}\xi_\tau}$, equation (2.4.21) transforms to

$$\mathrm{I}_2 = \sum_{j=0}^{2}\sum_{m=0}^{M_j} (-1)^m \binom{4}{m} \int_0^1 \int_{\mathbb{R}^2} \Bigg\{ \partial_{s'}^{(4-m)\alpha'_j} \Bigg[ \int_{B_2(\tilde{r})} \partial_{s'}^{m\alpha'_j}\, S_9^\infty \frac{e^{ik_z\zeta\, f(\eta')}}{1+|\eta'|_*^4}\, e^{-i\eta'\cdot(s'-k')}\,\mathrm{d}\eta' \Bigg] \\ \frac{[(\vec{s}_{\xi_\tau}\times\vec{e}^{\,0})\times\vec{s}_{\xi_\tau}]}{\xi_\tau}\, e^{is'\cdot x'}\, e^{i\frac{z}{2}\xi_\tau} \Bigg\}\,\mathrm{d}s'\,\mathrm{d}\zeta, \tag{2.4.22}$$

$$\alpha'_j := \begin{cases} (0,0) & \text{if } j=0 \\ (1,0) & \text{if } j=1 \\ (0,1) & \text{if } j=2 \end{cases}, \qquad M_j := \begin{cases} 0 & \text{if } j=0 \\ 4 & \text{otherwise} \end{cases}.$$

Applying integration by parts $(4-m)$ times to the integral w.r.t. $s'$, the term $\mathrm{I}_2$ takes the form

$$\mathrm{I}_2 = \sum_{j=0}^{2}\sum_{m=0}^{M_j} \binom{4}{m} \int_0^1 \int_{\mathbb{R}^2} \Bigg\{ \int_{B_2(\tilde{r})} \partial_{s'}^{m\alpha'_j}\, S_9^\infty \frac{e^{ik_z\zeta\, f(\eta')}}{1+|\eta'|_*^4}\, e^{-i\eta'\cdot(s'-k')}\,\mathrm{d}\eta' \\ \partial_{s'}^{(4-m)\alpha'_j} \Bigg[ \frac{[(\vec{s}_{\xi_\tau}\times\vec{e}^{\,0})\times\vec{s}_{\xi_\tau}]}{\xi_\tau}\, e^{is'\cdot x'}\, e^{i\frac{z}{2}\xi_\tau} \Bigg] \Bigg\}\,\mathrm{d}s'\,\mathrm{d}\zeta, \tag{2.4.23}$$

where the absolute value of

$$S_9^\infty = f(\eta')\, e^{-i(\xi_\tau - i\tau)\left(\zeta\, f(\eta') - \frac{z}{2}\right)}\, e^{-\tau \frac{z}{2}} - \sum_{n=0}^{8} (-i\zeta)^n\; f(\eta')^{n+1} \frac{\left(\xi_\tau - i\tau\right)^n}{n!}\, e^{i\frac{z}{2}\xi_\tau} \tag{2.4.24}$$

is uniformly bounded w.r.t. $\eta'$ and $\tau$ and decreases exponentially as $|s'|$ tends to infinity. Indeed, $f(\eta')$ is bounded, $|\tau| \leq 1$ and the right-hand side of the last equation is an exponentially decaying function w.r.t. $s'$, since $(\zeta\, f(\eta') - z/2) < 0$. On the other hand, $e^{i\frac{z}{2}\xi_\tau}$ and all its derivatives decay exponentially as $|s'|$ tends 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. $\eta'$ is dominated by the term $\frac{1}{1+|\eta'|_*^4}$. 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 $\frac{1}{\xi_\tau}$ is only weakly singular for $\tau = 0$. To evaluate the limit $\tau \nearrow 0$ for any fixed $j \in \{1, 2\}$ it remains to show that

$$\left| \partial_{s'}^{m\alpha'_j} S_9^\infty \;\; \partial_{s'}^{(4-m)\alpha'_j} \left[ \frac{\left[(\vec{s}_{\xi_\tau} \times \vec{e}^{\,0}) \times \vec{s}_{\xi_\tau}\right]}{\xi_\tau}\, e^{is'\cdot x'}\, e^{i\frac{z}{2}\xi_\tau} \right] \right| \tag{2.4.25}$$

is uniformly bounded w.r.t. $\eta'$ and $-1 < \tau < 0$ 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. $\eta'$ is then ensured by the term $\frac{1}{1+|\eta'|_*^4}$. Before an estimate of (2.4.25) can be found, the derivatives have to be examined. This is done by splitting the domain of integration w.r.t. $s'$ in (2.4.23) into $B_2(2k)$ and $\mathbb{R}^2 \setminus B_2(2k)$ to examine the behaviour of (2.4.25) at the singularity $s'^2 = k^2$ and at infinity separately. To study the behaviour around the singularity, the subsequent lemma is used to show that differentiation and summation can be interchanged in (2.4.25).

**Lemma 2.5.** *The sums $S_9^\infty$ and*

$$\partial_{s'}^{m\alpha'_j} S_9^\infty = \sum_{n=9}^{\infty} \frac{(-i\zeta)^n}{n!}\, f(\eta')^{n+1} \partial_{s'}^{m\alpha'_j} \left[ (\xi_\tau - i\tau)^n\; e^{i\frac{z}{2}\xi_\tau} \right] \tag{2.4.26}$$

*are uniformly bounded w.r.t. $s' \in B_2(2k)$, $\eta' \in B_2(\tilde{r})$ and $\tau \in [-1, 0]$.*

*Proof.* This is obviously true for $j = 0$ or $m = 0$ since no singularities occur. To show this for $m > 0$, the product rule for higher order derivatives and Faà di Bruno's formula are applied to evaluate the derivatives. Afterwards the resulting sums are examined leading to summands, which are uniformly bounded w.r.t. $s'$, times the term $(\xi_\tau - i\tau)^{n-a} / {\xi_\tau}^{(2m-a-b)}$, where $a$ and $b$ are non-negative integers depending on the indices of the sums. Obviously, this quotient is uniformly bounded w.r.t. $s' \in B_2(2k)$ and $\tau \in [-1, 0]$ for any $n \geq 9$, since $m \leq 4$. It can now be shown that there exist functions $q^m_{j,\tilde{l},\vec{\ell}_1}(s', z) := q^m_{j,l,\tilde{l},\vec{\ell}_1}(s', z, \tau)$, uniformly bounded w.r.t. $s'$ and $\tau$, such that

$$\partial_{s'}^{m\alpha'_j} S_9^\infty = \sum_{n=9}^{\infty} (-i\zeta)^n\; f(\eta')^{n+1} \sum_{(l,\vec{\ell}_1,\tilde{l}) \in \mathrm{S}_m} \frac{q^m_{j,\tilde{l},\vec{\ell}_1}(s', z)}{\left(n - s_l(\vec{\ell}_1)\right)!} \frac{\left(\xi_\tau - i\tau\right)^n}{{\xi_\tau}^{(2m-\tilde{l})}}\, e^{i\frac{z}{2}\xi_\tau}, \tag{2.4.27}$$

where $\mathrm{S}_m := \{(l, \vec{\ell}_1, \tilde{l}) : l = 0, \ldots, m, \vec{\ell}_1 \in T_l, \tilde{l} = 0, \ldots, \tilde{l}_b\}$, where the index set $T_l := \{(\ell_1, \ldots, \ell_l) \in \mathbb{N}_0^l : \sum_{o=1}^l o\ell_o = l\}$, where the upper index bound $\tilde{l}_b := \tilde{l}_b(m) := \max_{l=0,\ldots,m} \max_{\vec{\ell}_2 \in T_{m-l}} s_{m-l}(\vec{\ell}_2) \leq m \leq 4$, and where $s_l$: $\mathbb{N}_0^l \to \mathbb{N}_0$, $(\ell_1, \ldots, \ell_l) \mapsto \sum_{o=1}^l \ell_o$. Since the sum over $S_m$ is finite and since $(\xi_\tau - i\tau)^n / {\xi_\tau}^{(2m-\tilde{l})}$ is bounded for bounded $s'$, the boundedness of (2.4.26) follows easily. ☐

The second derivative in (2.4.25) can be evaluated as

$$\partial_{s'}^{(4-m)\alpha'_j} \left[ \frac{[(\vec{s}_{\xi_\tau} \times \vec{e}^0) \times \vec{s}_{\xi_\tau}]}{\xi_\tau} e^{is' \cdot x'} e^{i\frac{z}{2}\xi_\tau} \right] = \frac{\vec{q}_j(s', \xi_\tau)}{{\xi_\tau}^{(9-2m)}} e^{is' \cdot x'} e^{i\frac{z}{2}\xi_\tau}, \tag{2.4.28}$$

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 the product of the derivatives in (2.4.25) is equal to

$$\sum_{n=9}^{\infty} (-i\zeta)^n f(\eta')^{n+1} \sum_{(l,\vec{\ell}_1,\tilde{l}) \in \mathrm{S}_m} \frac{q^m_{j,\tilde{l},\vec{\ell}_1}(s', z)}{\big(n - s_l(\vec{\ell}_1)\big)!} \frac{(\xi_\tau - i\tau)^n}{{\xi_\tau}^{9-\tilde{l}}} \vec{q}_j(s', \xi_\tau) e^{is' \cdot x'} e^{iz\xi_\tau} \tag{2.4.29}$$

for $s' \in B_2(2k)$. However, this is bounded uniformly w.r.t. $\tau$ and $\eta'$ by a function that is integrable w.r.t. $s'$. Hence, Lebesgue's theorem applies to this part of integral (2.4.23), i.e. for the integration w.r.t. $s'$ over $B_2(2k)$.

For all $s' \in \mathbb{R}^2 \setminus B_2(2k)$, the right-hand side of (2.4.27) yields

$$\begin{aligned} \partial_{s'}^{m\alpha'_j} S_9^\infty = \sum_{(l,\vec{\ell}_1,\tilde{l}) \in \mathrm{S}_m} \Bigg\{ & q^m_{j,\tilde{l},\vec{\ell}_1}(s', z) \frac{\big(\xi_\tau - i\tau\big)^{s_l(\vec{\ell}_1)}}{{\xi_\tau}^{\left(2m-\tilde{l}\right)}} f(\eta')^{s_l(\vec{\ell}_1)+1} (-i\zeta)^{s_l(\vec{\ell}_1)} \\ & \left( e^{-i(\xi_\tau - i\tau)\zeta f(\eta')} - \sum_{n=0}^{8-s_l(\vec{\ell}_1)} (-i\zeta)^n f(\eta')^n \frac{\big(\xi_\tau - i\tau\big)^n}{n!} \right) \Bigg\} e^{i\frac{z}{2}\xi_\tau} \end{aligned} \tag{2.4.30}$$

which is uniformly bounded w.r.t. $\tau$ and $\eta'$ by a function that is integrable w.r.t. $s'$. The same holds again for (2.4.28). Note that the integrand in (2.4.23) is uniformly bounded w.r.t. $\eta'$ as well. Hence, Lebesgue's theorem can also be applied to integral (2.4.23) taken for $s' \in \mathbb{R}^2 \setminus B_2(2k)$.

### 2.4.3 Formula for the limit $\tilde{r} \to \infty$ and $\tau \nearrow 0$

Thus it has been shown that the limits $\tau \nearrow 0$ and $\tilde{r} \to \infty$ of the sum $i\mathrm{I}_1 + i\mathrm{I}_2$ (cf. (2.4.4) and (2.4.5)) exist, by showing that they exist for the two summands separately. Note that the splitting of the sum over $n$, leading to $\mathrm{I}_1$ and $\mathrm{I}_2$, can be done for $8$ replaced by any fixed $N \geq 8$. The existence of the limits of (2.4.4) and (2.4.5) will still hold. This will now be used to show that

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

$$= \sum_{n\in\mathbb{N}_0} \lim_{\substack{\tau\nearrow 0\\ \tilde r\to\infty}} \int_0^1 \int_{\mathbb{R}^2}\int_{\mathbb{R}^2} w_n^{\tilde r,\tau}(\zeta,\eta',s')\,\mathrm{d}\eta'\,\mathrm{d}s'\,\mathrm{d}\zeta, \tag{2.4.31}$$

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

where $\lim_{\tau\nearrow 0,\tilde r\to\infty} := \lim_{\tau\nearrow 0}\lim_{\tilde r\to\infty}$. Note that the existence of the limit on the first line of (2.4.31) is what has been shown above. Clearly,

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

for which the existence of the first term on the right-hand side has already been shown. It remains to evaluate the limit of the second term on the right-hand side applying Lebesgue's theorem. To do so, the same transformations that led to (2.4.23) are applied here. Furthermore, the integral w.r.t. $s'$ is again split into the sum 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

$$\lim_{\substack{N\to\infty\\ N\geq 8}} \lim_{\substack{\tau\nearrow 0\\ \tilde r\to\infty}} \int_0^1 \int_{\mathbb{R}^2}\int_{\mathbb{R}^2} \sum_{n=N+1}^{\infty} w_n^{\tilde r,\tau}(\zeta,\eta',s')\,\mathrm{d}\eta'\,\mathrm{d}s'\,\mathrm{d}\zeta$$
$$= \lim_{\substack{N\to\infty\\ N\geq 8}} \int_0^1 \int_{\mathbb{R}^2}\int_{\mathbb{R}^2} \sum_{n=N+1}^{\infty} w_n^{\infty,0}(\zeta,\eta',s')\,\mathrm{d}\eta'\,\mathrm{d}s'\,\mathrm{d}\zeta. \tag{2.4.32}$$

In view of (2.4.23), for $\tau=0$ the limit (2.4.32) transforms to

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

$$+ \lim_{\substack{N\to\infty\\N\geq 8}} \int\limits_0^1 \int\limits_{\mathbb{R}^2\setminus B_2(2k)} \int\limits_{\mathbb{R}^2} \tilde{w}_2(N,\zeta,\eta',s')\,\mathrm{d}\eta'\,\mathrm{d}s'\,\mathrm{d}\zeta,$$

where (cf. (2.4.23) and (2.4.29))

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

and (cf. (2.4.23), (2.4.28) and (2.4.30) with $8$ replaced by $N$ and with the exponential replaced by its Taylor series expansion)

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

using $\xi := \sqrt{k^2-s'^2}$. It remains to apply Lebesgue's theorem to evaluate the limit $N\to\infty$. First, observe

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

However, estimating (2.4.29), it has already be shown that this function is integrable w.r.t. $\eta'$, $s'$ and $\zeta$. Hence, Lebesgue's theorem can be applied. On the other hand, it is easily shown that

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

which is integrable w.r.t. $s'\in\mathbb{R}^2\setminus B_2(2k)$, $\eta'$ and $\zeta$ for $z>h$. Thus Lebesgue's theorem implies

$$\lim_{\substack{N\to\infty\\N\geq 8}}\int\limits_0^1\int\limits_{\mathbb{R}^2}\int\limits_{\mathbb{R}^2}\sum_{n=N+1}^{\infty}w_n^{\infty,0}(\zeta,\eta',s')\,\mathrm{d}\eta'\,\mathrm{d}s'\,\mathrm{d}\zeta$$
$$=\int\limits_0^1\int\limits_{\mathbb{R}^2}\int\limits_{\mathbb{R}^2}\lim_{\substack{N\to\infty\\N\geq 8}}\sum_{n=N+1}^{\infty}w_n^{\infty,0}(\zeta,\eta',s')\,\mathrm{d}\eta'\,\mathrm{d}s'\,\mathrm{d}\zeta = 0$$

since the sum w.r.t. $n$ converges pointwise to zero. Consequently, equation (2.4.31) holds true.

Thus it was shown that both limits in (2.4.2) can be evaluated by applying Lebesgue's theorem, integration by parts and generalised Fourier transform, which then leads to a representation of $\vec{D}^d(\vec{x})$ in the sense of a generalised function. Since the integral w.r.t. $s'$ is a locally bounded integrable function w.r.t. $\vec{x}$, the distribution $\vec{D}^d(\vec{x})$ can be identified with the locally integrable function

$$\vec{D}^d(\vec{x}) = \frac{i}{8\pi^2} \int\limits_{\mathbb{R}^2} \hat{\alpha}(\vec{s}_\xi - \vec{k})\, \frac{[(\vec{s}_\xi \times \vec{e}^{\,0}) \times \vec{s}_\xi]}{\xi}\, e^{i\vec{s}_\xi \cdot \vec{x}}\, \mathrm{d}s', \tag{2.4.33}$$

where the above manipulations are needed to define the integral (see the subsequent Equation (2.4.34)). More precisely, the last integral is well defined in the following sense (cf. (2.4.2), (2.4.4), (2.4.5), (2.4.15), (2.4.16) with $\ell = 1, 2, 3$, (2.4.18) and (2.4.19)): For convenience, define the new variable $\vec{n}^r := \vec{s}_{\xi_z}/\sqrt{s_x^2 + s_y^2 + \xi_z^2} = \vec{s}_{\xi_z}/k = (n_x, n_y, n_z^r)^\top$ with $n_z^r := \sqrt{1 - n'^2}$. Observe $\mathrm{d}s' = k^2\, \mathrm{d}n'$ and define $\tilde{\lambda}_{4,j}^n := 1$ for $j = 0$ and all $n \in \mathbb{N}_0$ and $\tilde{\lambda}_{4,j}^n := 0$ for $j \in \mathbb{Z} \setminus \{0\}$ and $n \in \mathbb{N}_0$. Then

$$\begin{aligned}
\vec{D}^d(\vec{x}) = &-i\, \frac{\Delta}{2} \sum_{n \in \mathbb{N}_0} \sum_{j \in \mathbb{Z}} \int\limits_0^1 \tilde{\lambda}_{0,j}^n \frac{(-i\zeta)^n}{n!}\, \mathrm{d}\zeta\, \left[ \left( \vec{\omega}^j \times \vec{e}^{\,0} \right) \times \vec{\omega}^j \right] \left( \omega_z^j \right)^{n-1} e^{i\vec{\omega}^j \cdot \vec{x}} \\
&- \epsilon_0 \sum_{\ell=1}^4 \sum_{n \in \mathbb{N}_0} \sum_{j \in \mathbb{Z}} \int\limits_0^1 \tilde{\lambda}_{\ell,j}^n \frac{(-ik\zeta)^n}{n!} \int\limits_{\mathbb{R}^2} \frac{\vec{h}_{\ell,j}(n')}{n_z^r}\, e^{ik\vec{n}^r \cdot \vec{x}}\, \mathrm{d}n'\, \mathrm{d}\zeta, 
\end{aligned}\tag{2.4.34}$$

$$\vec{\omega}^j := \left( k' + \tilde{\omega}'_{0,j}, \omega_z^j \right)^\top, \quad \omega_z^j := \sqrt{k^2 - \left| k' + \tilde{\omega}'_{0,j} \right|^2} \tag{2.4.35}$$

with $\Delta := \epsilon_0 - \epsilon'_0$, with $\tilde{\lambda}_{\ell,j}^n$, $\tilde{\omega}'_{\ell,j}$ and $\tilde{g}_n$ as in Lemma 2.2 and with $\vec{h}_{\ell,j} := \vec{h}_{\ell,j,n}$,

$$\vec{h}_{\ell,j,n} := i\, \frac{\Delta\, k^3}{4\pi\epsilon_0} [n_z^r]^n \left[ \left( \vec{n}^r \times \vec{e}^{\,0} \right) \times \vec{n}^r \right] \begin{cases} e^{-\left|kn' - (k' + \tilde{\omega}'_{1,j})\right|} / \left| kn' - (k' + \tilde{\omega}'_{1,j}) \right|, & \text{if } \ell = 1 \\ K_0 \left( \left| kn' - (k' + \tilde{\omega}'_{2,j}) \right| \right), & \text{if } \ell = 2 \\ e^{-\left|kn' - (k' + \tilde{\omega}'_{1,j})\right|}, & \text{if } \ell = 3 \\ 1/(2\pi)\, \int_{\mathbb{R}^2} \tilde{g}_n(\eta')\, e^{-i\eta' \cdot (kn' - k')}\, \mathrm{d}\eta', & \text{if } \ell = 4, j = 0 \end{cases} \tag{2.4.36}$$

Recall $\vec{D}^{sc}(\vec{x}) = \vec{D}^d(\vec{x}) + \vec{D}^{sc}_{\mathcal{Q}}(\vec{x})$. For $z > f(x')$ [10, Boundary conditions (7.37), Sect. 7.3] implies $\vec{D}^{sc}_{\mathcal{Q}}(\vec{x}) = \epsilon_0\, \vec{r}(\vec{k}, \vec{e}^{\,0})\, e^{i\vec{k}^r \cdot \vec{x}}/|k'|^2$, where $\vec{k}^r := (k_x, k_y, -k_z)^\top = (k', -k_z)^\top$ is the wave vector of the reflected wave mode, $\tilde{k} := \sqrt{\mu_0 \epsilon'_0}\, \omega$ the wave number beneath the interface, $\vec{e}^{\,0} = (e_x^0, e_y^0, e_z^0)^\top$ the vector of polarisation, and

$$\begin{aligned}
\vec{r}(\vec{k}, \vec{e}^{\,0}) := &\frac{k_z + \sqrt{\tilde{k}^2 - |k'|^2}}{k_z - \sqrt{\tilde{k}^2 - |k'|^2}} (k_y e_x^0 - k_x e_y^0) \begin{pmatrix} k_y \\ -k_x \\ 0 \end{pmatrix} \\
&+ \frac{\tilde{k}^2 k_z + k^2 \sqrt{\tilde{k}^2 - |k'|^2}}{\tilde{k}^2 k_z - k^2 \sqrt{\tilde{k}^2 - |k'|^2}}\, \frac{k_z (k_x e_x^0 + k_y e_y^0) - |k'|^2 e_z^0}{k^2} \begin{pmatrix} -k_x k_z \\ -k_y k_z \\ -|k'|^2 \end{pmatrix}.
\end{aligned}\tag{2.4.37}$$

## 2.5 Scattered electric field

Following the definitions and notation introduced in Section 2.2 the reflected displacement field $\vec{D}^d(\vec{x})$ for $z > h$ can be reduced to its underlying electric fields, Hence, when applying this to (2.4.33), the component of the scattered electric field with polarisation $\vec{e}$ is represented by

$$\vec{e}^* \cdot \vec{E}_d^{sc}(\vec{x}) = \frac{i}{8\pi^2 \epsilon(\vec{x})} \int\limits_{\mathbb{R}^2} \hat{\alpha}(\vec{s}_\xi - \vec{k}) \, \frac{\vec{e}^* \cdot [(\vec{s}_\xi \times \vec{e}^0) \times \vec{s}_\xi]}{\xi} \, e^{i\vec{s}_\xi \cdot \vec{x}} \, \mathrm{d}s',$$

for all $\vec{x} \in \mathbb{R}^3$ with $z > h$, where $\vec{e}^*$ is the complex conjugate of the polarisation vector $\vec{e}$.

**Theorem 2.1.** *Assume the interface, described by the graph of a function $f \in \mathcal{A}_1$ that satisfies condition* (2.4.20)*, is illuminated by an incoming plane wave as in Subsection 2.1. Then the Born approximation of the reflected polarised electric field for $z > 2h$ can be written as*

$$\vec{e}^* \cdot \vec{E}^r(\vec{x}) = \vec{e}^* \cdot \left( \vec{E}_d^r(\vec{x}) + \vec{E}_Q(\vec{x}) \right) = E_Q - E_0 - E_1 - E_2 - E_3 - E_4, \qquad (2.5.1)$$

$$E_Q := r(\vec{k}, \vec{e}^0, \vec{e}^*) \, \frac{e^{i\vec{k}^r \cdot \vec{x}}}{|k'|^2}, \qquad (2.5.2)$$

$$E_0 := i \, \frac{\Delta}{2\epsilon_0} \sum_{n \in \mathbb{N}_0} \sum_{j \in \mathbb{Z}} \int\limits_0^1 \tilde{\lambda}_{0,j}^n \frac{(-i\zeta)^n}{n!} \, \mathrm{d}\zeta \;\; \vec{e}^* \cdot \left[ \left( \vec{\omega}^j \times \vec{e}^0 \right) \times \vec{\omega}^j \right] \, \left( \omega_z^j \right)^{n-1} \, e^{i\vec{\omega}^j \cdot \vec{x}}, \qquad (2.5.3)$$

$$E_\ell := \sum_{n \in \mathbb{N}_0} \sum_{j \in \mathbb{Z}} \int\limits_0^1 \tilde{\lambda}_{\ell,j}^n \frac{(-ik\zeta)^n}{n!} \int\limits_{\mathbb{R}^2} \frac{h_{\ell,j}(n')}{n_z^r} \, e^{ik\vec{n}^r \cdot \vec{x}} \, \mathrm{d}n' \, \mathrm{d}\zeta, \quad \ell = 1, \ldots, 4, \qquad (2.5.4)$$

*where $r(\vec{k}, \vec{e}^0, \vec{e}^*) := \vec{e}^* \cdot \vec{r}(\vec{k}, \vec{e}^0)$ (cf.* (2.4.37)*) and $\vec{k}^r := (k_x, k_y, -k_z)^\top$. The numbers $\tilde{\lambda}_{\ell,j}^n$ and $\tilde{\omega}_{\ell,j}'$ are defined in Lemma 2.2, the symbols $\vec{\omega}^j$ and $\omega_z^j$ in* (2.4.35)*. For a two-dimensional vector $n'$, the vector $\vec{n}^r := (n', n_z^r)^\top$ is defined with $n_z^r := \sqrt{1 - n'^2}$, and $h_{\ell,j} := \vec{e}^* \cdot \vec{h}_{\ell,j}$ for $\ell = 1, \ldots, 4$ (cf.* (2.4.36)*). Furthermore, there exists a $z_0 > 0$ such that the sums in $E_\ell$, $\ell = 0, \ldots, 4$, are absolutely and uniformly convergent for any $z \geq z_0$.*

*Proof.* As already stated above, Equ. (2.5.2) can be deduced from [10, Sect. 7.3]. Furthermore, taking the derivations in the previous subsections into account (cf. (2.4.34)), it remains to show the absolute convergence. To do so, the definition of the algebra norm in (2.4.1) implies that, for any $0 \leq \zeta \leq 1$,

$$\sum_{j \in \mathbb{Z}} \left| \tilde{\lambda}_{\ell,j}^n \right| \leq \left| \left| f^{n+1} \, e^{ik_z \zeta \, f} \right| \right|_{\mathcal{A}_1} \leq c \, ||f||_{\mathcal{A}_1}^n \, , \qquad (2.5.5)$$

with a constant $c > 0$ independent of $n$. Furthermore, for any $\ell = 0, \ldots, 3$, the function $\tilde{\lambda}_{\ell,j}^n(\zeta) := \tilde{\lambda}_{\ell,j}^n$ (cf. (2.4.10) and (2.4.11)) is continuous w.r.t. $\zeta$ by the algebra property of $\mathcal{A}_1^{\mathbb{C}}$.

Split $E_0$ according to $E_0 = E_0^a + E_0^b$,

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

and $E_0^b := E_0 - E_0^a$. With this, first consider $E_0^a$, leading to $\omega_z^j \in \mathbb{R}$. Thus, (2.5.5) implies

$$|E_0^a| \le c \sum_{n\in\mathbb{N}_0} \frac{1}{n!} \int_0^1 \sum_{\substack{j\in\mathbb{Z} \\ |\tilde{\omega}'_{0,j}|<k}} \left|\tilde{\lambda}_{0,j}^n(\zeta_0)\right| \,\mathrm{d}\zeta\, k^{n+1} \le c \sum_{n\in\mathbb{N}_0} \frac{k^n\;\|f\|_{\mathcal{A}_1}^n}{n!} < \infty.$$

For $E_0^b$ define a $z_0$ with $z_0 > \|f\|_{\mathcal{A}_1}$, and assume $z > z_0$. It follows that

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

The supremum of $|\omega_z^j|^n \; e^{-\left|\omega_z^j\right| z_0}$ is $\left(\frac{n}{e}\right)^n z_0^{-n}$. Stirling's formula (cf. [2, Sect. 2.5.2]) implies $\left(\frac{n}{e}\right)^n z_0^{-n} \sim \frac{n!}{\sqrt{2\pi\, n}}\, z_0^{-n}$ for $n \to \infty$. Using once more (2.5.5), it follows that

$$\left|E_0^b\right| \le c \sum_{n\in\mathbb{N}_0} \frac{1}{\sqrt{n}} \sum_{\substack{j\in\mathbb{Z} \\ |\tilde{\omega}'_{0,j}|\ge k}} \int_0^1 \left|\tilde{\lambda}_{0,j}^n\right| \,\mathrm{d}\zeta\, z_0^{-n} \le c \sum_{n\in\mathbb{N}_0} \frac{1}{\sqrt{n}} \left(\frac{\|f\|_{\mathcal{A}_1}}{z_0}\right)^n < \infty$$

for $z_0 > \|f\|_{\mathcal{A}_1}$. Hence, $E_0^b$ and thereby $E_0$ is absolutely and uniformly convergent for any $z \ge z_0$.

The $E_\ell$, with $\ell = 1, \ldots, 4$ (cf. (2.4.36)) can be treated similarly. This time the domain of integration of the integral w.r.t. $s'$ is split into the two parts $B_2(k)$ and $\mathbb{R}^2 \setminus B_2(k)$. Moreover, it has to be taken into account that the integrands w.r.t. $s' \in B_2(k)$ are at most weakly singular. □

# 3 Far-field formula

## 3.1 Plane-wave modes in the far field

The goal of this section will be to find the far-field pattern for the Born solution of the transmitted electric field in the case of interface functions from $\mathcal{A}_1$.

To obtain this far field, the terms on the right-hand side of (2.5.1) will be treated separately, starting with the first, i.e. (2.5.3). Examining the exponent of $e^{i\vec{\omega}_z^j\cdot\vec{x}} = e^{i(k'+\tilde{\omega}'_{0,j})\cdot x'} e^{iz(k^2-|k'+\tilde{\omega}'_{0,j}|^2)^{1/2}}$, 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 $(k^2-|k'+\tilde{\omega}'_{0,j}|^2)^{\frac{1}{2}}$ being either real or purely imaginary with a non-negative imaginary part. To evaluate the far field, fix the far-field direction by a unit vector $\vec{m}$ with $m_z > 0$ and consider the far-field asymptotics at the points $\vec{x} =: R\vec{m}$, where $R$ tends to infinity. In (2.5.3) all summands, for which $\left|k' + \tilde{\omega}'_{0,j}\right|^2 > k^2$, decay exponentially as $R$ tends to infinity and are thus negligible evanescent modes of the electric field. Only the remaining terms contribute as the plane-wave modes $e^{iR\vec{\omega}_z^j\cdot\vec{m}}$ to the far field.

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

### 3.2.1 Splitting of the field

Continue by considering the remaining terms (2.5.4) for $\ell = 1, \ldots, 4$. 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. To further study the integrals, the technical condition $|k' + \tilde{\omega}'_{1,j}| \neq k$ or $|k' + \tilde{\omega}'_{2,j}| \neq k$ is assumed. The integral w.r.t. $n'$ will thus be separated into

$$\int\limits_{\mathbb{R}^2} \frac{h_{\ell,j}(n')}{n_z^r}\, e^{ik\vec{n}^r\cdot\vec{x}}\, \mathrm{d}n' = W^1_{\ell,j} + W^2_{\ell,j} + W^3_{\ell,j}, \tag{3.2.1}$$

$$W^1_{\ell,j} := \int\limits_{B_2(1)} \Big(1 - \chi_\epsilon(kn' - k' - \tilde{\omega}'_{\ell,j})\Big) \frac{h_{\ell,j}(n')}{n_z^r}\, e^{ik\vec{n}^r\cdot\vec{x}}\, \mathrm{d}n', \tag{3.2.2}$$

$$W^2_{\ell,j} := \int\limits_{\mathbb{R}^2\setminus B_2(1)} \Big(1 - \chi_\epsilon(kn' - k' - \tilde{\omega}'_{\ell,j})\Big) \frac{h_{\ell,j}(n')}{n_z^r}\, e^{ik\vec{n}^r\cdot\vec{x}}\, \mathrm{d}n', \tag{3.2.3}$$

$$W^3_{\ell,j} := \int\limits_{\mathbb{R}^2} \chi_\epsilon(kn' - k' - \tilde{\omega}'_{\ell,j})\, \frac{h_{\ell,j}(n')}{n_z^r}\, e^{ik\vec{n}^r\cdot\vec{x}}\, \mathrm{d}n'. \tag{3.2.4}$$

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

### 3.2.2 Far field generated by 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 leads to

$$W^2_{\ell,j} = \int_0^{2\pi}\int_1^{\infty} \Big(1 - \chi_\epsilon(k\rho n'_0 - k' - \tilde{\omega}'_{\ell,j})\Big)\, h_{\ell,j}(\rho n'_0)\, e^{ik\rho R n'_0\cdot m'}\, \rho\, \frac{e^{-kRm_z\sqrt{\rho^2-1}}}{\sqrt{1-\rho^2}}\,\mathrm{d}\rho\,\mathrm{d}\phi$$

$$= \frac{1}{ikRm_z}\, W^{2,1}_{\ell,j} + \frac{1}{ikRm_z}\, W^{2,2}_{\ell,j}, \tag{3.2.5}$$

$$W^{2,1}_{\ell,j} := \int_0^{2\pi} \Big(1 - \chi_\epsilon(kn'_0 - k' - \tilde{\omega}'_{\ell,j})\Big)\, h_{\ell,j}(n'_0)\, e^{ikRn'_0\cdot m'}\,\mathrm{d}\phi, \tag{3.2.6}$$

$$W^{2,2}_{\ell,j} := \int_0^{2\pi}\int_1^{\infty} \partial_\rho \Big[\Big(1 - \chi_\epsilon(k\rho n'_0 - k' - \tilde{\omega}'_{\ell,j})\Big)\, h_{\ell,j}(\rho n'_0)\, e^{ik\rho Rn'_0\cdot m'}\Big]\, e^{-kRm_z\sqrt{\rho^2-1}}\,\mathrm{d}\rho\,\mathrm{d}\phi. \tag{3.2.7}$$

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

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

$$n'_{0,j}(u) := \begin{pmatrix} \cos\Big[(-1)^{j+1}\arccos\Big(\frac{u}{k|m'|}\Big) + \phi' + (j-1)2\pi\Big] \\ \sin\Big[(-1)^{j+1}\arccos\Big(\frac{u}{k|m'|}\Big) + \phi' + (j-1)2\pi\Big] \end{pmatrix}$$

for $j = 1, 2$. Note that the integrand of both integrals is integrable w.r.t. $u$ on the compact set $[-k\,|m'|\,, k\,|m'|]$. 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 (3.2.5) tends to zero faster than $1/R$ as $R$ tends to infinity. In the case of $m' = (0,0)^\top$ the term (3.2.6) is independent of $R$ and remains. Later on, when examining $W^1_{\ell,j}$, it will be seen that this term also occurs for the integral over $B_2(1)$ but with opposite sign. The sum of the two is thus zero.

For $W^{2,2}_{\ell,j}$ examine the derivative

$$\begin{aligned}
&\partial_\rho \Big[\Big(1 - \chi_\epsilon(k\rho n'_0 - k' - \tilde{\omega}'_{\ell,j})\Big)\, h_{\ell,j}(\rho n'_0)\, e^{ik\rho Rn'_0\cdot m'}\Big] \\
&\quad = -kn'_0 \cdot \nabla\chi_\epsilon(k\rho n'_0 - k' - \tilde{\omega}'_{\ell,j})\, h_{\ell,j}(\rho n'_0)\, e^{ik\rho Rn'_0\cdot m'} \\
&\qquad + \Big(1 - \chi_\epsilon(k\rho n'_0 - k' - \tilde{\omega}'_{\ell,j})\Big)\, n'_0 \cdot \nabla h_{\ell,j}(\rho n'_0)\, e^{ik\rho Rn'_0\cdot m'} \\
&\qquad + ikRn'_0 \cdot m' \Big(1 - \chi_\epsilon(k\rho n'_0 - k' - \tilde{\omega}'_{\ell,j})\Big)\, h_{\ell,j}(\rho n'_0)\, e^{ik\rho Rn'_0\cdot m'}.
\end{aligned} \tag{3.2.8}$$

Since

$$|\nabla_{n'}[n_z^r(n')]| = \frac{\rho}{\sqrt{\rho^2-1}}, \quad \left|\nabla_{n'}\left[\frac{1}{|n'-\nu'|}\right]\right| \le \frac{c}{|n'-\nu'|^2}, \quad \left|\nabla_{n'}\left[e^{-k|n'-\nu'|}\right]\right| \le c \tag{3.2.9}$$

it follows, for $\ell = 1$, (cf. (2.4.36) for $\ell = 1$) that

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

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

$$\left|\left(1-\chi_\epsilon(k\rho n_0' - k' - \tilde\omega_{\ell,j}')\right) n_0'\cdot\nabla h_{\ell,j}(\rho n_0')\right|\, e^{-\frac{k}{2}Rm_z\sqrt{\rho^2-1}} \le c\left(1+\frac{\rho}{\sqrt{\rho^2-1}}\right). \tag{3.2.10}$$

It follows that (cf. (3.2.8))

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

for $\rho\in[1,\infty)$ and substituting $u=R\sqrt{\rho^2-1}$ and $\mathrm{d}\rho=\frac{1}{R}\frac{u}{\sqrt{R^2+u^2}}\,\mathrm{d}u$ (cf. (3.2.7))

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

Consequently the second term on the right-hand side of (3.2.5) has an asymptotic behaviour of $o\left(\frac{1}{R}\right)$ and

$$W_{\ell,j}^2 = o\left(\frac{1}{R}\right). \tag{3.2.11}$$

### 3.2.3 Far field generated by smooth integrands of plane waves

To examine the integral in Formula (3.2.2), observe that the mapping $n' = (n_x, n_y)^\top \mapsto \vec{n}^r = (n_x, n_y, \sqrt{1-n_x^2-n_y^2})^\top$ 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 now be transformed to spherical coordinates $(\theta,\phi)$, 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

$$\vec{m} = (\sin\alpha\cos\beta, \sin\alpha\sin\beta, \cos\alpha)^\top, \tag{3.2.12}$$

then $\vec{n}^r$ can be represented as

$$\vec{n}^r(\theta,\phi) := \begin{pmatrix} \sin\alpha\cos\beta\cos\theta + (\cos\alpha\cos\beta\cos\phi - \sin\beta\sin\phi)\sin\theta \\ \sin\alpha\sin\beta\cos\theta + (\cos\alpha\sin\beta\cos\phi + \cos\beta\sin\phi)\sin\theta \\ \cos\alpha\,\cos\theta - \sin\alpha\cos\phi\sin\theta \end{pmatrix} \tag{3.2.13}$$

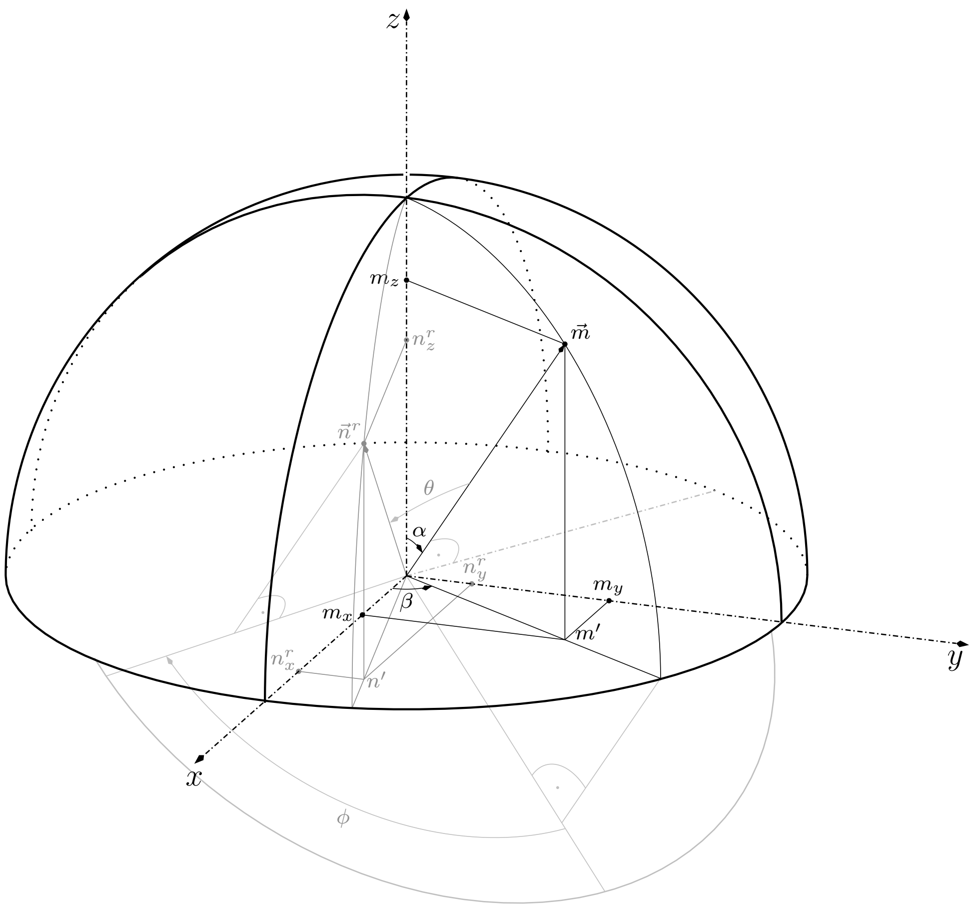


Figure 3: Spherical coordinates w.r.t. $\vec{m}$

as visualised in Figure 3. Now $n_x$ and $n_y$ can be substituted in integral (3.2.3). For this, the determinant of the Jacobian matrix $\partial(n_x, n_y)/\partial(\theta, \phi)$ is $|\partial(n_x, n_y)/\partial(\theta, \phi)| = n_z^r(\theta, \phi)\sin\theta$. Hence the differential $\mathrm{d}n'$ is replaced by $n_z^r(\theta, \phi)\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi$. Thus

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

where $\theta(\phi) \le \pi$ is the angle for which $\vec{n}^r(\theta(\phi), \phi)$ is contained in the $x-y$ plane and $n'(\theta, \phi)$ is defined as $(n_x^r(\theta,\phi), n_y^r(\theta,\phi))^\top$. Substituting $\cos\theta$ by $\psi$ and applying integration by parts to the integral over $\psi$ leads to the following expression.

$$\begin{aligned} W^1_{\ell,j} &= \int_0^{2\pi}\int_{\cos\theta(\phi)}^{1} \Big(1 - \chi_\epsilon(kn'(\psi,\phi) - k' - \tilde{\omega}'_{\ell,j})\Big)\, h_{\ell,j}\Big(n'(\psi,\phi)\Big)\, e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi \qquad (3.2.14)\\ &= 2\pi\Big(1 - \chi_\epsilon(km' - k' - \tilde{\omega}'_{\ell,j})\Big)\, h_{\ell,j}(m')\,\frac{e^{ikR}}{ikR} - \frac{1}{ikR}W^{1,1}_{\ell,j} - \frac{1}{ikR}W^{1,2}_{\ell,j} \end{aligned}$$

$$W^{1,1}_{\ell,j} := \int_0^{2\pi} \Big(1 - \chi_\epsilon(kn_0'(\phi) - k' - \tilde\omega'_{\ell,j})\Big)\, h_{\ell,j}\Big(n_0'(\phi)\Big)\, e^{ikR\cos\theta(\phi)}\, \mathrm{d}\phi$$

$$W^{1,2}_{\ell,j} := \int_0^{2\pi} \int_{\cos\theta(\phi)}^{1} \partial_\psi \left[\Big(1 - \chi_\epsilon(kn'(\psi,\phi) - k' - \tilde\omega'_{\ell,j})\Big)\, h_{\ell,j}\Big(n'(\psi,\phi)\Big)\right] e^{ikR\psi}\, \mathrm{d}\psi\, \mathrm{d}\phi, \tag{3.2.15}$$

where

$$n'(\psi,\phi) := \begin{pmatrix} \sin\alpha\cos\beta\ \psi + (\cos\alpha\cos\beta\cos\phi - \sin\beta\sin\phi)\sqrt{1-\psi^2} \\ \sin\alpha\sin\beta\ \psi + (\cos\alpha\sin\beta\cos\phi + \cos\beta\sin\phi)\sqrt{1-\psi^2} \end{pmatrix} \tag{3.2.16}$$

and $n_0'(\phi) := n'\big(\cos\theta(\phi), \phi\big)$. To examine $W^{1,1}_{\ell,j}$ a closer look at $\cos\theta(\phi)$ is necessary. Since $\theta(\phi)$ is the solution of

$$n_z^r(\theta(\phi),\phi) = \cos\alpha\cos\theta(\phi) - \sin\alpha\sin\theta(\phi)\cos\phi = 0, \tag{3.2.17}$$

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

$$\cos\theta(\phi) = \begin{cases} \cos\left(\arctan\left(\frac{\cot\alpha}{\cos\phi}\right)\right) & \text{if } \phi \neq \frac{\pi}{2}, \frac{3}{2}\pi,\ \alpha \neq 0 \text{ and } \frac{\cot\alpha}{\cos\phi} > 0 \\ \cos\left(\pi + \arctan\left(\frac{\cot\alpha}{\cos\phi}\right)\right) & \text{if } \phi \neq \frac{\pi}{2}, \frac{3}{2}\pi,\ \alpha \neq 0 \text{ and } \frac{\cot\alpha}{\cos\phi} < 0\ , \\ 0 & \text{if } \phi = \frac{\pi}{2}, \frac{3}{2}\pi \text{ or } \alpha = 0 \end{cases} \tag{3.2.18}$$

or $\cos\theta(\phi) = \tan\alpha\cos\phi/\sqrt{1+\tan^2\alpha\cos^2\phi}$. From this it is easily deduced that $\cos\theta(\phi)$ is monotone for $0 \le \phi < \pi$ and for $\pi \le \phi < 2\pi$. Thus, unless $\alpha = 0$, for these two cases the substitution $t := \cos\theta(\phi)$ is possible. It is easily calculated that $\phi(t) = \arccos\big(\cot\alpha\,\frac{t}{\sqrt{1-t^2}}\big)$, $\mathrm{d}\phi = -\cos\alpha/(1-t^2)\ 1/(\sin^2\alpha - t^2)^{1/2}\mathrm{d}t$ and $-\sin\alpha < \cos\theta(\phi) \le \sin\alpha$ for $0 \le \phi < \pi$. After this transformation the integrands are only weakly singular at $t = \pm\sin\alpha$ and thus absolutely integrable for $0 < \alpha < \pi/2$. 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 (3.2.14) follows from the Riemann-Lebesgue lemma. In the case $\alpha = 0$, the value $\cos\theta(\phi)$ is identically zero and

$$-\frac{1}{ikR} \int_0^{2\pi} \Big(1 - \chi_\epsilon(kn_0'(\phi) - k' - \tilde\omega'_{\ell,j})\Big)\, h_{\ell,j}\Big(n_0'(\phi)\Big)\, \mathrm{d}\phi, \tag{3.2.19}$$

with (cf. (3.2.16)) $n_0'(\phi) = (\cos(\beta+\phi), \sin(\beta+\phi))^\top$ remains. Note that with this, (3.2.19) is the negative of (3.2.6) for $m' = (0,0)^\top$. Thus the two terms cancel when $W^1_{\ell,j}$ is added to $W^2_{\ell,j}$.

Next $W^{1,2}_{\ell,j}$ (cf. (3.2.15)) is examined. Note that the function $h_{\ell,j}(n')$ can also be written as $\tilde h_{\ell,j}(n', n_z^r)$, with $n_z^r := \sqrt{1-n'^2}$ and a function $\tilde h_{\ell,j}$ analytic for $kn' \neq k' + \tilde\omega'_{\ell,j}$ (cf. (2.4.36)). Using this, it can easily be shown that the derivative

$$\partial_\psi \left[\Big(1 - \chi_\epsilon(kn'(\psi,\phi) - k' - \tilde\omega'_{\ell,j})\Big)\, h_{\ell,j}\Big(n'(\psi,\phi)\Big)\right]$$

is weakly singular and thus integrable on $\{(\phi,\psi)\colon\ 0 \le \phi \le 2\pi,\ \cos\theta(\phi) \le \psi \le 1\}$. Thus the absolute value of the integral w.r.t. $\psi$ is uniformly bounded w.r.t. $R$ by a function that is integrable w.r.t. $\phi$. Additionally, it follows from the Riemann-Lebesgue lemma that the integral w.r.t. $\psi$ 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. (3.2.14))

$$W^1_{\ell,j} = 2\pi \left(1 - \chi_\epsilon(km' - k' - \tilde{\omega}'_{\ell,j})\right) h_{\ell,j}(m') \,\frac{e^{ikR}}{ikR} + o\left(\frac{1}{R}\right). \tag{3.2.20}$$

### 3.2.4 Far field generated by a singular integrand

**Main term for weakly singular integrand over unit disc**

To examine the integral in (3.2.4), three cases will be considered separately. At first, the support of the cut-off function is supposed to be located outside of the unit disk. Then, for the support inside the unit disk, we distinguish the case $0 \le \alpha < \pi/2$ for $km' \ne k' + \tilde{\omega}'_{\ell,j}$ and the case $0 \le \alpha < \pi/2$ for $km' = k' + \tilde{\omega}'_{\ell,j}$. These distinctions are necessary to apply different substitutions to show the asymptotic behaviour of $W^3_{\ell,j}$. The second case is considered first.

Assume $km' \ne k' + \tilde{\omega}'_{\ell,j}$ and that the $\epsilon$ of the cut-off function (cf. Sect. 3.2.1) is small enough such that $m'$ is not an element of the support of $\chi_\epsilon\left(k(\,\cdot\,,\,\cdot\,)^\top - k' - \tilde{\omega}'_{\ell,j}\right)$. Apply the same substitution as in Section 3.2.3. Thus, (cf. the first line of (3.2.14))

$$W^3_{\ell,j} = \int\limits_0^{2\pi} \int\limits_{\cos\theta(\phi)}^{1} \chi_\epsilon\big(kn'(\psi,\phi) - k' - \tilde{\omega}'_{\ell,j}\big)\, h_{\ell,j}\big(n'(\psi,\phi)\big)\, e^{ikR\psi}\, \mathrm{d}\psi\, \mathrm{d}\phi. \tag{3.2.21}$$

In the case $\ell > 1$ the same approach as for $W^1_{\ell,j}$ can be applied, since in this case $h_{\ell,j}$ has at most a logarithmic singularity at the point $kn' = k' + \tilde{\omega}'_{\ell,j}$. For $\ell = 2, 3$ it follows that even the derivative w.r.t. $\psi$ of $h_{\ell,j}$, occurring when applying integration by parts w.r.t. $\psi$ (cf. (3.2.14)), 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. $\psi$ of $h_{4,0}$ is also integrable w.r.t. $\psi \in [\cos\theta(\phi), 1]$ and $\phi \in [0, 2\pi)$, since $\partial_\psi n'(\psi,\phi)$ is weakly singular and since (cf. (2.4.36) for $\ell = 4$)

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

is uniformly bounded w.r.t. $n'(\psi,\phi) \in B_2(1)$. Indeed the function $\tilde{g}_n(\eta')$, as an element of the algebra $\mathcal{A}^{\mathbb{C}}_1$, was defined such that $||(1 + |\eta'|)\, \tilde{g}_n(\eta')||_{L^1(\mathbb{R}^2)}$ is finite.

Next the case $\ell = 1$ is examined. Define

$$f_j(\psi,\phi) := h_{1,j}\big(n'(\psi,\phi)\big)\ |n'(\psi,\phi) - \nu'|\,, \tag{3.2.22}$$

where $\nu' := \frac{k' + \tilde{\omega}'_{\ell,j}}{k}$. Moreover, the cut-off function is further specified as the tensor product of two cut-off functions $\tilde{\chi}^1_\epsilon = \tilde{\chi}^2_\epsilon \in C^\infty_0(\mathbb{R})$ with the same epsilon as before. Thus, by defining

$(\psi_0, \phi_0)^\top$ such that $n'(\psi_0, \phi_0) = \nu'$,

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

For $0 \le \alpha < \pi/2$, the integral is now split into

$$W^3_{1,j} = W^{3,1}_j + g_j(\psi_0, \phi_0)\, W^{3,2}_j, \tag{3.2.23}$$

$$W^{3,1}_j := \int\limits_0^{2\pi} \int\limits_{\psi_0-\epsilon}^{1} \frac{\tilde{\chi}^1_\epsilon(\phi - \phi_0)\, \tilde{\chi}^2_\epsilon(\psi - \psi_0)\, \big[g_j(\psi, \phi) - g_j(\psi_0, \phi_0)\big]}{\sqrt{\tilde{a}\,(\psi - \psi_0)^2 + \tilde{b}\,(\phi - \phi_0)^2 + \tilde{c}\,(\psi - \psi_0)\,(\phi - \phi_0)}}\, e^{ikR\psi}\, \mathrm{d}\psi\, \mathrm{d}\phi,$$

$$W^{3,2}_j := \int\limits_0^{2\pi} \int\limits_{\psi_0-\epsilon}^{1} \frac{\tilde{\chi}^1_\epsilon(\phi - \phi_0)\, \tilde{\chi}^2_\epsilon(\psi - \psi_0)}{\sqrt{\tilde{a}\,(\psi - \psi_0)^2 + \tilde{b}\,(\phi - \phi_0)^2 + \tilde{c}\,(\psi - \psi_0)\,(\phi - \phi_0)}}\, e^{ikR\psi}\, \mathrm{d}\psi\, \mathrm{d}\phi, \tag{3.2.24}$$

$$g_j(\psi, \phi) := f_j(\psi, \phi)\, \frac{\sqrt{\tilde{a}\,(\psi - \psi_0)^2 + \tilde{b}\,(\phi - \phi_0)^2 + \tilde{c}\,(\psi - \psi_0)\,(\phi - \phi_0)}}{|n'(\psi, \phi) - \nu'|} \tag{3.2.25}$$

$$\tilde{a} := \Big|\partial_\psi \Big[n'(\psi, \phi)\Big]_{\substack{\psi=\psi_0\\ \phi=\phi_0}}\Big|^2 \qquad \tilde{b} := \Big|\partial_\phi \Big[n'(\psi, \phi)\Big]_{\substack{\psi=\psi_0\\ \phi=\phi_0}}\Big|^2, \tag{3.2.26}$$

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

Note that $g_j$ is continuous if $g_j(\psi_0, \phi_0)$ is defined as the limit of $\psi \longrightarrow \psi_0$ and $\phi \longrightarrow \phi_0$, which is finite as will be shown now. Obviously $\lim_{(\psi,\phi)\to(\psi_0,\phi_0)} f_j(\psi, \phi) = f_j(\psi_0, \phi_0)$ since the function $f_j$ is defined by removing the singularity of $h_{1,j}$. For the limit $(\psi, \phi) \to (\psi_0, \phi_0)$ of the remaining factor in $g_j$, transform $(\psi - \psi_0, \phi - \phi_0)$ to the polar coordinates $\tilde{\rho}(\cos\tilde{\theta}, \sin\tilde{\theta})$ and consider the limit $\tilde{\rho} \longrightarrow 0$. Clearly all these radial limits exist and are independent of the angle $\tilde{\theta}$ for $\tilde{a}\cos^2\tilde{\theta} + \tilde{b}\sin^2\tilde{\theta} + \tilde{c}\cos\tilde{\theta}\sin\tilde{\theta} \neq 0$. This, however, follows if and only if the two vectors $\partial_\psi n'$ and $\partial_\phi n'$ are not parallel. To be precise, if the determinant $\tilde{d} := |\partial n'(\psi, \phi)/\partial(\psi, \phi)|_{\psi=\psi_0, \phi=\phi_0}$ is non-zero for $\psi_0 > \cos\theta(\phi_0)$. Evaluating $\tilde{d}$, leads to $\tilde{d} = -n^r_z(\psi_0, \phi_0) \neq 0$ for $\psi_0 \neq \cos\theta(\phi_0)$, since $n^r_z(\psi, \phi)$ is by construction only zero for $\psi = \cos\theta(\phi)$. 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. $\psi$ or $\phi$ (cf. (3.2.26)) would be zero and thus $\tilde{d} = 0$.

Using an approach similar to the one used for $W^1_{1,j}$, it will now be shown that $W^{3,1}_j$ has an asymptotic behaviour of $o(1/R)$ as $R$ tends to infinity. Apply integration by parts w.r.t. $\psi$ to $W^{3,1}_j$, keeping in mind that $\tilde{\chi}^2_\epsilon(1 - \psi_0) = \tilde{\chi}^2_\epsilon(-\epsilon) = 0$. Then

$$\begin{aligned} W^{3,1}_j = &-\frac{1}{ikR} \int\limits_0^{2\pi} \int\limits_{\psi_0-\epsilon}^{1} \frac{\tilde{\chi}^1_\epsilon(\phi - \phi_0)\, [\tilde{\chi}^2_\epsilon]'(\psi - \psi_0)\, \big[g_j(\psi, \phi) - g_j(\psi_0, \phi_0)\big]}{\sqrt{\tilde{a}\,(\psi - \psi_0)^2 + \tilde{b}\,(\phi - \phi_0)^2 + \tilde{c}\,(\psi - \psi_0)\,(\phi - \phi_0)}}\, e^{ikR\psi}\, \mathrm{d}\psi\, \mathrm{d}\phi \\ &- \frac{1}{ikR} \int\limits_0^{2\pi} \int\limits_{\psi_0-\epsilon}^{1} \frac{\tilde{\chi}^1_\epsilon(\phi - \phi_0)\, \tilde{\chi}^2_\epsilon(\psi - \psi_0)\, \partial_\psi g_j(\psi, \phi)}{\sqrt{\tilde{a}\,(\psi - \psi_0)^2 + \tilde{b}\,(\phi - \phi_0)^2 + \tilde{c}\,(\psi - \psi_0)\,(\phi - \phi_0)}}\, e^{ikR\psi}\, \mathrm{d}\psi\, \mathrm{d}\phi \end{aligned}$$

$$+\frac{1}{ikR}\int\limits_0^{2\pi}\int\limits_{\psi_0-\epsilon}^{1}\left\{\frac{\tilde{\chi}_\epsilon^1(\phi-\phi_0)\,\tilde{\chi}_\epsilon^2(\psi-\psi_0)\,\big[g_j(\psi,\phi)-g_j(\psi_0,\phi_0)\big]}{\sqrt{\tilde{a}\,(\psi-\psi_0)^2+\tilde{b}\,(\phi-\phi_0)^2+\tilde{c}\,(\psi-\psi_0)\,(\phi-\phi_0)}^{\,3}}\right.$$
$$\left.\left[\tilde{a}\,(\psi-\psi_0)+\frac{\tilde{c}}{2}\,(\phi-\phi_0)\right]\,e^{ikR\psi}\right\}\,\mathrm{d}\psi\,\mathrm{d}\phi, \qquad (3.2.27)$$

where

$$\partial_\psi g_j(\psi,\phi)=\partial_\psi\left[\frac{f_j(\psi,\phi)}{\sqrt{1+\sum\limits_{\substack{(l_1,l_2)\in\mathbb{N}_0^2\\ l_1+l_2\geq 3}} b_{l_1,l_2}\,\frac{(\psi-\psi_0)^{l_1}\,(\phi-\phi_0)^{l_2}}{\tilde{a}\,(\psi-\psi_0)^2+\tilde{b}\,(\phi-\phi_0)^2+\tilde{c}\,(\psi-\psi_0)\,(\phi-\phi_0)}}}\right] \qquad (3.2.28)$$

is uniformly bounded in a neighbourhood of $(\psi,\phi)=(\psi_0,\phi_0)$. Indeed, for $\partial_\psi f_j(\psi,\phi)$ this can be seen by considering (3.2.22), (2.4.36) for $\ell=1$, the third equation of (3.2.9) and (3.2.13) for $\cos\theta=\psi, \sin\theta=\sqrt{1-\psi^2}$ and $\psi_0<1$. Furthermore, by using radial coordinates as before, it can be proven that

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

is bounded for $(\psi,\phi)\to(\psi_0,\phi_0)$. In fact the existence of radial limits can be shown. This limit can be evaluated using the fact that the gradient of $f_j$ is uniformly bounded for $\psi_0<1$ and that $\tilde{a}\cos^2\tilde{\theta}+\tilde{b}\sin^2\tilde{\theta}+\tilde{c}\cos\tilde{\theta}\sin\tilde{\theta}\neq 0$.

Hence, using this and the fact that (3.2.28) is uniformly bounded in a neighbourhood of $(\psi,\phi)=(\psi_0,\phi_0)$, it is easily seen that all the integrands on the right-hand side of (3.2.27) are at most weakly singular and thus absolutely integrable w.r.t. $\psi$. Thus the integrals w.r.t. $\psi$ are uniformly bounded w.r.t. $R$ by a function that is integrable w.r.t. $\phi$. Therefore, using Lebesgue's theorem and the Riemann-Lebesgue lemma shows that $W_j^{3,1}=o(1/R)$.

To examine $W_j^{3,2}$ (cf. (3.2.24)) interchange the order of integration and substitute $\psi$ and $\phi$ by introducing the new variables $\tilde{\psi}-\tilde{\psi}_0:=\tilde{d}\tilde{b}^{1/2}\,(\psi-\psi_0)$ and $\tilde{\phi}-\tilde{\phi}_0:=\tilde{b}^{1/2}\frac{\tilde{c}}{2}\,(\psi-\psi_0)+\tilde{b}^{3/2}\,(\phi-\phi_0)$, where $\tilde{d}=(\tilde{a}\,\tilde{b}-\frac{\tilde{c}^2}{4})^{1/2}$, $\tilde{\psi}_0:=\tilde{d}\tilde{b}^{1/2}\,\psi_0$ and $\tilde{\phi}_0:=\tilde{b}^{1/2}(\frac{\tilde{c}}{2}\,\psi_0+\tilde{b}\,\phi_0)$. Thus $\mathrm{d}\phi\,\mathrm{d}\psi=\frac{1}{\tilde{d}\,\tilde{b}^2}\,\mathrm{d}\tilde{\phi}\,\mathrm{d}\tilde{\psi}$,

$$\sqrt{\tilde{a}\,(\psi-\psi_0)^2+\tilde{b}\,(\phi-\phi_0)^2+\tilde{c}\,(\psi-\psi_0)(\phi-\phi_0)}=\frac{\sqrt{(\tilde{\psi}-\tilde{\psi}_0)^2+(\tilde{\phi}-\tilde{\phi}_0)^2}}{\tilde{b}}.$$

Defining $\tilde{d}_1:=\frac{1}{\tilde{d}\sqrt{\tilde{b}}}$ and $\tilde{d}_2:=\frac{\tilde{c}}{2\tilde{d}}$, it follows that (cf. (3.2.24))

$$W_j^{3,2}=\frac{1}{\tilde{d}\tilde{b}}\int\limits_{\frac{\psi_0-\epsilon}{\tilde{d}_1}}^{\frac{1}{\tilde{d}_1}}\tilde{\chi}_\epsilon^2\left(\tilde{d}_1(\tilde{\psi}-\tilde{\psi}_0)\right)\int\limits_{\tilde{d}_2\tilde{\psi}}^{\tilde{d}_2\tilde{\psi}+2\pi\sqrt{\tilde{b}}^3}\frac{\tilde{\chi}_\epsilon^1\left(\frac{\tilde{\phi}-\tilde{\phi}_0-\tilde{d}_2(\tilde{\psi}-\tilde{\psi}_0)}{\sqrt{\tilde{b}}^3}\right)}{\sqrt{(\tilde{\psi}-\tilde{\psi}_0)^2+(\tilde{\phi}-\tilde{\phi}_0)^2}}\,\mathrm{d}\tilde{\phi}\,e^{ik\tilde{d}_1R\tilde{\psi}}\,\mathrm{d}\tilde{\psi} \qquad (3.2.29)$$

Recall that $\epsilon$ was chosen such that $\tilde{\chi}^1_\epsilon([\tilde{\phi}-\tilde{\phi}_0-\tilde{d}_2(\tilde{\psi}-\tilde{\psi}_0)]/\tilde{b}^{3/2})$ is zero for $\tilde{\phi}$ equal to the boundaries of the domain of integration w.r.t. $\tilde{\phi}$. Thus, integrating by parts leads to

$$\int\limits_{\tilde{d}_2\tilde{\psi}}^{\tilde{d}_2\tilde{\psi}+2\pi\sqrt{\tilde{b}}^3} \frac{\tilde{\chi}^1_\epsilon\left(\frac{\tilde{\phi}-\tilde{\phi}_0-\tilde{d}_2(\tilde{\psi}-\tilde{\psi}_0)}{\sqrt{\tilde{b}}^3}\right)}{\sqrt{(\tilde{\psi}-\tilde{\psi}_0)^2+(\tilde{\phi}-\tilde{\phi}_0)^2}}\,\mathrm{d}\tilde{\phi} = -\int\limits_{\tilde{d}_2\tilde{\psi}}^{\tilde{d}_2\tilde{\psi}+2\pi\sqrt{\tilde{b}}^3} \frac{[\tilde{\chi}^1_\epsilon]'\big(t(\tilde{\psi},\tilde{\phi})\big)}{\sqrt{\tilde{b}}^3}\,\log\Big(s(\tilde{\psi},\tilde{\phi})\Big)\,\mathrm{d}\tilde{\phi}, \tag{3.2.30}$$

where the two functions $t$ and $s$ are defined as $t(\tilde{\psi},\tilde{\phi}) := [\tilde{\phi}-\tilde{\phi}_0-\tilde{d}_2(\tilde{\psi}-\tilde{\psi}_0)]/\tilde{b}^{3/2}$ and $s(\tilde{\psi},\tilde{\phi}) := \tilde{\phi}-\tilde{\phi}_0+[(\tilde{\psi}-\tilde{\psi}_0)^2+(\tilde{\phi}-\tilde{\phi}_0)^2]^{1/2}$. Note that the integrand of the integral on the right-hand side is uniformly bounded since $[\tilde{\chi}^1_\epsilon]'(\phi)$ is zero in a neighbourhood of $\phi=0$.

Applying (3.2.30) and taking into account that $\partial_{\tilde{\psi}}[\log s(\tilde{\psi},\tilde{\phi})] = -(\tilde{\psi}-\tilde{\psi}_0)\,\partial_{\tilde{\phi}}[1/s(\tilde{\psi},\tilde{\phi})]$, another integration by parts w.r.t. $\tilde{\phi}$ implies

$$\partial_{\tilde{\psi}}\left[\int\limits_{\tilde{d}_2\tilde{\psi}}^{\tilde{d}_2\tilde{\psi}+2\pi\sqrt{\tilde{b}}^3} \frac{\tilde{\chi}^1_\epsilon\Big(t(\tilde{\psi},\tilde{\phi})\Big)}{\sqrt{(\tilde{\psi}-\tilde{\psi}_0)^2+(\tilde{\phi}-\tilde{\phi}_0)^2}}\,\mathrm{d}\tilde{\phi}\right] \tag{3.2.31}$$

$$= \frac{\tilde{d}_2}{\tilde{b}^3}\int\limits_{\tilde{d}_2\tilde{\psi}}^{\tilde{d}_2\tilde{\psi}+2\pi\sqrt{\tilde{b}}^3} [\tilde{\chi}^1_\epsilon]''\Big(t(\tilde{\psi},\tilde{\phi})\Big)\,\log s(\tilde{\psi},\tilde{\phi})\,\mathrm{d}\tilde{\phi} - \frac{1}{\tilde{b}^3}\int\limits_{\tilde{d}_2\tilde{\psi}}^{\tilde{d}_2\tilde{\psi}+2\pi\sqrt{\tilde{b}}^3} [\tilde{\chi}^1_\epsilon]''\Big(t(\tilde{\psi},\tilde{\phi})\Big)\,\frac{\tilde{\psi}-\tilde{\psi}_0}{s(\tilde{\psi},\tilde{\phi})}\,\mathrm{d}\tilde{\phi}.$$

Again, all integrands on the right-hand side of (3.2.31) are uniformly bounded, since $[\tilde{\chi}^1_\epsilon]''(\phi)$ is zero in a neighbourhood of $\phi=0$.

With this in mind integration by parts w.r.t. $\tilde{\psi}$ is applied to integral $W^{3,2}_j$ (cf. (3.2.29)). Once more $\tilde{\chi}^2_\epsilon(\tilde{d}_1\,(\tilde{\psi}-\tilde{\psi}_0))$ is zero at the boundaries of the domain of integration w.r.t. $\tilde{\psi}$, and $W^{3,2}_j = o(1/R)$. Indeed, since the remaining integrand is uniformly bounded on the domain of integration, the Riemann-Lebesgue lemma applies. Hence (cf. (3.2.23))

$$W^3_{1,j} = o\left(\frac{1}{R}\right). \tag{3.2.32}$$

**Main term for asymptotics in the direction of the weak singularity**

It is now assumed that $km' = k\nu' = k' + \tilde{\omega}'_{\ell,j}$ and $\epsilon < 1-\sin\alpha$ such that $n^r_z = \sqrt{1-n'^2} > 0$ for all $n' \in \mathrm{supp}\chi_\epsilon(k(\,\cdot\,,\,\cdot\,)^\top - km')$. 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 prove an asymptotic behaviour of $o(1/R)$ for $W^3_{\ell,j}$ (compare with the beginning of Section 3.2.4). The same substitution as in Section 3.2.3 is applied. Thus, (compare with (3.2.4) and perform the substitution of variables leading to the first line of (3.2.14))

$$W^3_{\ell,j} = \int\limits_0^{2\pi}\int\limits_0^1 \chi_\epsilon\big(kn'(\psi,\phi)-k\nu'\big)\,h_{\ell,j}\big(n'(\psi,\phi)\big)\,e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi. \tag{3.2.33}$$

First $W^3_{1,j}$ is examined by using (3.2.22). Moreover, this time the cut-off function is further specified as $\chi_\epsilon\big(kn'(\psi,\phi) - k\nu'\big) = \tilde{\chi}_\epsilon\big(\psi - 1\big)$, where $\tilde{\chi}_\epsilon \equiv 1$ in a neighbourhood of zero and where $\tilde{\chi}_\epsilon \in C_0^\infty(\mathbb{R})$ is defined with the same epsilon as before (cf. Sect. 3.2.1). Note that $n'(1,\phi_0) = \nu'$ for any $\phi_0 \in [0, 2\pi)$,

$$W^3_{1,j} = \int_0^{2\pi}\int_0^1 \frac{\tilde{\chi}_\epsilon\big(\psi - 1\big)\, f_j(\psi,\phi)}{|n'(\psi,\phi) - \nu'|}\, e^{ikR\psi}\, \mathrm{d}\psi\, \mathrm{d}\phi = \int_0^{2\pi}\int_0^1 \frac{g_j(\psi,\phi)}{\sqrt{1-\psi}}\, e^{ikR\psi}\, \mathrm{d}\psi\, \mathrm{d}\phi, \quad (3.2.34)$$

$$g_j(\psi,\phi) := \tilde{\chi}_\epsilon\big(\psi - 1\big)\, f_j(\psi,\phi)\, \frac{\sqrt{1-\psi}}{|n'(\psi,\phi) - \nu'|} \quad (3.2.35)$$

For $0 \le \alpha < \pi/2$, (3.2.16) implies

$$\begin{aligned} |n'(\psi,\phi) - \nu'|^2 = (1-\psi)\, \Big[& 2\left(1 - \sin^2\alpha\cos^2\phi\right) - 2\sin\alpha\cos\alpha\cos\phi\,\sqrt{1-\psi^2} \\ & + (1-\psi)\, \left(\sin^2\alpha\cos^2\phi - \cos^2\alpha\right)\Big], \end{aligned} \quad (3.2.36)$$

$$\begin{aligned} g_j(\psi,\phi) = \tilde{\chi}_\epsilon\big(\psi - 1\big)\, f_j(\psi,\phi)\Big(& 2 - 2\sin^2\alpha\cos^2\phi - 2\sin\alpha\cos\alpha\cos\phi\,\sqrt{1-\psi^2} \\ & + (1-\psi)\left(\sin^2\alpha\cos^2\phi - \cos^2\alpha\right)\Big)^{-\frac{1}{2}}. \end{aligned} \quad (3.2.37)$$

Note that $g_j(1,\phi) = \frac{f_j(1,\phi_0)}{\sqrt{2}\sqrt{1-\sin^2\alpha\cos^2\phi}} < \infty$, 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 $\alpha \in \big[0, \frac{\pi}{2}\big)$. Furthermore the function $f_j(\psi,\phi)$ has the form (cf. (3.2.22) and (2.4.36) for $\ell = 1$)

$$\begin{aligned} f_j(\psi,\phi) &= c_h\left[n^r_z(\psi,\phi)\right]^n e^{-k\sqrt{1-\psi}\,\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}} \\ &\qquad \Big(D(\phi) + E(\phi)\,\psi\sqrt{1-\psi^2} + F(\phi)\,\psi^2\Big) \\ &= c_h\left(\big[\cos\alpha\,\psi\big]^n + G(\psi,\phi) + \mathbb{1}_{[1,\infty)}(n)\, H(\phi)\,\psi^{n-1}\sqrt{1-\psi^2}\right) \\ &\qquad e^{-k\sqrt{1-\psi}\,\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}}\, \Big(D(\phi) + E(\phi)\,\psi\sqrt{1-\psi^2} + F(\phi)\,\psi^2\Big). \end{aligned} \quad (3.2.38)$$

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

$$c_h := i\,\frac{\Delta k^2}{4\pi\epsilon_0}. \quad (3.2.39)$$

Similarly $D(\phi)$, $E(\phi)$ and $F(\phi)$ are second order polynomials of $\sin\phi$ and $\cos\phi$ defined such that (cf. (3.2.13))

$$D(\phi) + E(\phi)\psi\sqrt{1-\psi^2} + F(\phi)\psi^2 = \vec{e}^{\,*}\cdot\left[\left(\vec{n}^r(\psi,\phi)\times\vec{e}^{\,0}\right)\times\vec{n}^r(\psi,\phi)\right]. \quad (3.2.40)$$

Finally, $G$ and $H$ are defined by the binomial formula for $(\cos\alpha\,\psi - \sin\alpha\cos\phi\sqrt{1-\psi^2})^n$ as

$$\begin{aligned} G(\psi,\phi) &:= \sum_{m=2}^{n}\binom{n}{m}\big[\cos\alpha\,\psi\big]^{n-m}\left[-\sin\alpha\cos\phi\sqrt{1-\psi^2}\right]^m, \\ H(\phi) &:= -\frac{n!}{(n-1)!}\,\sin\alpha\,\cos\phi\,\big[\cos\alpha\big]^{n-1}. \end{aligned} \quad (3.2.41)$$

This shows that $\partial_\psi G(\psi,\phi)$ and $G(\psi,\phi)/\sqrt{1-\psi}$ are uniformly bounded w.r.t. $(\psi,\phi) \in \mathrm{supp}\tilde{\chi}_\epsilon(\cdot-1)\times[0,2\pi]$ for any fixed $n$.

Later on, the following lemma for the function $g_j$ (cf. (3.2.35)) is needed.

**Lemma 3.1.** *There exist a continuous function $g_j^0(\phi)$ such that, for any $0\le\phi<2\pi$, the limit $\lim_{\psi\to1}\{\partial_\psi[g_j(\psi,\phi)]-g_j^0(\phi)/\sqrt{1-\psi}\}$ exists and is uniformly bounded w.r.t. $\phi$.*

*Proof.* Using (3.2.38) it can be shown that $\partial_\psi[f_j(\psi,\phi)] = f_j^s(\psi,\phi)/\sqrt{1-\psi}+f_j^r(\psi,\phi)$, where both $f_j^s$ and $f_j^r$ are continuous functions. Moreover, with this it can be shown that (cf. (3.2.37))

$$\partial_\psi\left[g_j(\psi,\phi)\right]=\frac{g_j^s(\psi,\phi)}{\sqrt{1-\psi}}+g_j^r(\psi,\phi), \tag{3.2.42}$$

where again both $g_j^s$ and $g_j^r$ are continuous functions. In order to get the limit behaviour of $\partial_\psi\left[g_j(\psi,\phi)\right]$ at $\psi=1$, evaluate the limit $\psi\to1$ of the two functions $f_j^s(\psi,\phi)$ and $f_r^s(\psi,\phi)$. A lengthy but simple calculation reveals

$$\begin{aligned}f_j^0(\phi) &:= f_j^s(1,\phi)=c_h\,\cos^n\alpha\left\{-\frac{E(\phi)}{\sqrt2}+\frac{k}{2}\sqrt{A(\phi)}\left(D(\phi)+F(\phi)\right)\right\}\\&\qquad\qquad+c_h\,\mathbb{1}_{[1,\infty)}(n)\,\frac{H(\phi)}{\sqrt2}\left(D(\phi)+F(\phi)\right),\end{aligned} \tag{3.2.43}$$

$$\begin{aligned}f_j^1(\phi) &:= f_j^r(1,\phi)\\&=c_h\,\cos^n\alpha\left\{\frac{k}{\sqrt2}\,E(\phi)\,\sqrt{A(\phi)}+2F(\phi)+\frac{k\,C(\phi)}{2\sqrt2\,\sqrt{A(\phi)}}\left(D(\phi)+F(\phi)\right)\right\}\\&\quad+c_h\,\mathbb{1}_{[1,\infty)}(n)\left\{\left[\frac{n!}{2(n-2)!}\sin^2\alpha\cos^2\phi\left[\cos\alpha\right]^{n-2}\right.\right.\\&\qquad\qquad\left.\left.\frac{k}{\sqrt2}\,H(\phi)\,\sqrt{A(\phi)}-n\,\cos^n\alpha\right]\Big(D(\phi)+F(\phi)\Big)\right\}.\end{aligned} \tag{3.2.44}$$

Consequently (cf. 3.2.37), the limit $\psi\to1$ of the functions $g_j^s(\psi,\phi)$ and $g_j^r(\psi,\phi)$ evaluates as

$$g_j^0(\phi):=g_j^s(1,\phi)=\frac{f_j^0(\phi)}{\sqrt2\sqrt{1-\sin^2\alpha\cos^2\phi}}-\frac{f_j(1,\phi_0)\,\sin\alpha\cos\alpha\cos\phi}{4\sqrt{1-\sin^2\alpha\cos^2\phi}^3}, \tag{3.2.45}$$

$$g_j^1(\phi):=g_j^r(1,\phi)=\frac{f_j^1(\phi)}{\sqrt2\sqrt{1-\sin^2\alpha\cos^2\phi}}-\frac{f_j(1,\phi_0)\left(\cos^2\alpha-\sin^2\alpha\cos^2\phi\right)}{4\sqrt2\,\sqrt{1-\sin^2\alpha\cos^2\phi}^3}. \tag{3.2.46}$$

To evaluate the limit $\lim_{\psi\to1}\{\partial_\psi[g_j(\psi,\phi)]-g_j^0(\phi)/\sqrt{1-\psi}\}$ it is necessary to take a closer look at $\partial_\psi f_j^s(\psi,\phi)$ and $\partial_\psi g_j^s(\psi,\phi)$. For the first, there exist two continuous functions $F_j^r$ and $F_j^s$ such that

$$\partial_\psi f_j^s(\psi,\phi)=F_j^r(\psi,\phi)+\frac{F_j^s(\psi,\phi)}{\sqrt{1-\psi}}. \tag{3.2.47}$$

Similarly (cf. 3.2.37)), two continuous functions $G_j^r$ and $G_j^s$ can be found such that

$$\partial_\psi g_j^s(\psi,\phi) = G_j^r(\psi,\phi) + \frac{\tilde{\chi}_\epsilon(\psi-1)\,\partial_\psi\left[f_j^s(\psi,\phi)\right]}{\sqrt{A(\phi)+B(\phi)\,(1-\psi)+C(\phi)\sqrt{1-\psi^2}}} + \frac{G_j^s(\psi,\phi)}{\sqrt{1-\psi}}. \tag{3.2.48}$$

Using l'Hospital's rule, it can now be seen that (cf. (3.2.42), (3.2.48) and (3.2.47))

$$\begin{aligned}
\lim_{\psi\to 1}\left\{\partial_\psi\left[g_j(\psi,\phi)\right] - \frac{g_j^0(\phi)}{\sqrt{1-\psi}}\right\} &= \lim_{\psi\to 1}\left[\frac{g_j^s(\psi,\phi)-g_j^0(\phi)}{\sqrt{1-\psi}}\right] + g_j^1(\phi)\\
&= \lim_{\psi\to 1}\left[\partial_\psi g_j^s(\psi,\phi)\,(-2)\sqrt{1-\psi}\right] + g_j^1(\phi)\\
&= g_j^1(\phi) - 2\left\{\frac{\lim_{\psi\to 1}\left[\partial_\psi f_j^s(\psi,\phi)\sqrt{1-\psi}\right]}{\sqrt{A(\phi)}} + G_j^s(1,\phi)\right\}\\
&= g_j^1(\phi) - 2\left\{\frac{F_j^s(1,\phi)}{\sqrt{A(\phi)}} + G_j^s(1,\phi)\right\},
\end{aligned} \tag{3.2.49}$$

which (cf. (3.2.46)) is uniformly bounded w.r.t. $\phi \in [0, 2\pi)$. □

Now $W_{1,j}^3$ (cf. (3.2.34), (3.2.35) and (3.2.45)) is split into $W_{1,j}^3 = W_j^{3,5} + W_j^{3,6} + W_j^{3,7}$, where

$$W_j^{3,5} := \int_0^{2\pi}\int_0^1 \frac{g_j(\psi,\phi) - g_j(1,\phi) + 2\,g_j^0(\phi)\,\sqrt{1-\psi}}{\sqrt{1-\psi}}\,e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi, \tag{3.2.50}$$

$$W_j^{3,6} := \int_0^{2\pi} g_j(1,\phi)\,\mathrm{d}\phi \int_0^1 \frac{e^{ikR\psi}}{\sqrt{1-\psi}}\,\mathrm{d}\psi, \tag{3.2.51}$$

$$W_j^{3,7} := -2\int_0^{2\pi} g_j^0(\phi)\,\mathrm{d}\phi \int_0^1 e^{ikR\psi}\,\mathrm{d}\psi = -2\int_0^{2\pi} g_j^0(\phi)\,\mathrm{d}\phi\,\frac{e^{ikR}-1}{ikR}. \tag{3.2.52}$$

Transform $W_j^{3,5}$ by applying integration by parts w.r.t. $\psi$. For this, note that by once more using l'Hospital's rule it can be shown that (cf. (3.2.49))

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

Moreover, since $g_j(\psi,\phi)$ (cf. (3.2.37)) is an analytic function of $\sqrt{1-\psi}$ for $\psi$ close to one, it can even be concluded that

$$\left|g_j(\psi,\phi) - g_j(1,\phi) + 2\,g_j^0(\phi)\,\sqrt{1-\psi}\right| \sim |1-\psi|\,. \tag{3.2.53}$$

Thus integration by parts in (3.2.50) provides

$$W_j^{3,5} = \frac{1}{ikR} \int_0^{2\pi} \Big[ g_j(1,\phi) - 2\, g_j^0(\phi) \Big] \, \mathrm{d}\phi - \frac{1}{ikR} \int_0^{2\pi} \int_0^1 \left\{ \frac{\partial_\psi \, g_j(\psi,\phi) - \frac{g_j^0(\phi)}{\sqrt{1-\psi}}}{\sqrt{1-\psi}} + \frac{1}{2} \frac{g_j(\psi,\phi) - g_j(1,\phi) + 2\, g_j^0(\phi) \sqrt{1-\psi}}{\sqrt{1-\psi}^3} \right\} e^{ikR\psi} \, \mathrm{d}\psi \, \mathrm{d}\phi,$$

where the integrand of the second integral on the right-hand side is absolutely integrable w.r.t. $\psi$ and $\phi$ (cf. (3.2.49) and (3.2.53)). Hence, the Riemann-Lebesgue lemma applies, and

$$W_j^{3,5} = \frac{1}{ikR} \int_0^{2\pi} \Big[ g_j(1,\phi) - 2\, g_j^0(\phi) \Big] \, \mathrm{d}\phi + o\left(\frac{1}{R}\right). \tag{3.2.54}$$

It remains to consider $W_j^{3,6}$ (cf. (3.2.51)). Using [11, Equ. 16, Sects. I.1 and II.1] as well as [1, Equs. 7.3.9, 7.3.10, 7.3.27 and 7.3.28, Sect. 7.3] leads to

$$\int_0^1 \frac{e^{ikR\psi}}{\sqrt{1-\psi}} \, \mathrm{d}\psi = \sqrt{\pi} \, \frac{1-i}{\sqrt{2k}} \, \frac{e^{ikR}}{\sqrt{R}} + o\left(\frac{1}{R}\right).$$

Thus (cf. (3.2.54), (3.2.51) and (3.2.52))

$$W_{1,j}^3 = \frac{1}{ikR} \int_0^{2\pi} g_j(1,\phi) \, \mathrm{d}\phi + \sqrt{\pi} \int_0^{2\pi} g_j(1,\phi) \, \mathrm{d}\phi \, \frac{1-i}{\sqrt{2k}} \, \frac{e^{ikR}}{\sqrt{R}} - 2 \int_0^{2\pi} g_j^0(\phi) \, \mathrm{d}\phi \, \frac{e^{ikR}}{ikR} + o\left(\frac{1}{R}\right). \tag{3.2.55}$$

Using $f_j(1,\phi) = f_j(1,\phi_0)$ (cf. (3.2.22) and (3.2.16)), [1, Equ. 17.2.6, Sect. 17.2] and (3.2.37) leads to

$$\int_0^{2\pi} g_j(1,\phi) \, \mathrm{d}\phi = \frac{f_j(1,\phi_0)}{\sqrt{2}} \int_0^{2\pi} \frac{1}{\sqrt{1 - \sin^2\alpha \cos^2\phi}} \, \mathrm{d}\phi = 2\sqrt{2} \, f_j(1,\phi_0) \, \tilde{F}(\frac{\pi}{2} \setminus \alpha) \tag{3.2.56}$$

where $\tilde{F}$ denotes the elliptic integral of the first kind (cf. [1, Equ. 17.2.6]). For the last remaining integral $\int_0^{2\pi} g_j^0(\phi) \, \mathrm{d}\phi$, a closer look at $g_j^0$ yields (cf. (3.2.45), (3.2.43), (3.2.38) and (3.2.41))

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

With (3.2.13), $\vec{n}^r(\psi,\phi) = \vec{v}_0(\alpha,\beta,\psi) + \cos\phi\,\vec{v}_1(\alpha,\beta,\sqrt{1-\psi^2}) + \sin\phi\,\vec{v}_2(\alpha,\beta,\sqrt{1-\psi^2})$. Equ. (3.2.40) implies that $D(\phi) + F(\phi) = \vec{e}^{\,*}\cdot[(\vec{m}\times\vec{e}^{\,0})\times\vec{m}]$. For the coefficient $E(\phi)$ of $\psi\sqrt{1-\psi^2}$ in (3.2.40), it is concluded that $E(\phi) = E_1\,\sin\phi + E_2\,\cos\phi$, with constants $E_1$ and $E_2$ only dependent on $\alpha$, $\beta$, $\vec{e}^{\,*}$ and $\vec{e}^{\,0}$. Indeed, due to (3.2.13) the coefficient of $\cos^2\phi$ can arise only from those terms in $\vec{e}^{\,*}\cdot[(\vec{v}_1\times\vec{e}^{\,0})\times\vec{v}_1]$, 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 $\int_0^{2\pi} g_j^0(\phi)\,\mathrm{d}\phi = c_h\,\pi k\cos^n\alpha\;\;\vec{e}^{\,*}\cdot[(\vec{m}\times\vec{e}^{\,0})\times\vec{m}]$, since for any fixed $m\in\mathbb{R}$ the integrals $\int_0^{2\pi}\sin\phi/(1-\sin^2\alpha\cos^2\phi)^{-m/2}\,\mathrm{d}\phi$ and $\int_0^{2\pi}\cos\phi/(1-\sin^2\alpha\cos^2\phi)^{-m/2}\,\mathrm{d}\phi$ are zero. Consequently, since $m_z = \cos\alpha$ (cf. (3.2.12)) and in view of (3.2.39), (3.2.55) and (3.2.56),

$$
\begin{aligned}
W^3_{1,j} &= f_j(1,\phi_0)\,\tilde{F}(\pi\setminus\alpha)\left(\frac{\sqrt{2}}{ikR} + \sqrt{\pi}\,\frac{1-i}{\sqrt{k}}\,\frac{e^{ikR}}{\sqrt{R}}\right) \\
&\quad - i\,\frac{\Delta k^3}{2\epsilon_0}\,m_z^n\;\vec{e}^{\,*}\cdot\big[(\vec{m}\times\vec{e}^{\,0})\times\vec{m}\big]\;\frac{e^{ikR}}{ikR} + o\left(\frac{1}{R}\right), \\
&= i\,\frac{\Delta k^2}{4\pi\epsilon_0}\,m_z^n\;\vec{e}^{\,*}\cdot\big[(\vec{m}\times\vec{e}^{\,0})\times\vec{m}\big]\left\{2\tilde{F}(\frac{\pi}{2}\setminus\alpha)\left(\frac{\sqrt{2}}{ikR} + \sqrt{\pi}\,\frac{1-i}{\sqrt{k}}\,\frac{e^{ikR}}{\sqrt{R}}\right) - 2k\pi\,\frac{e^{ikR}}{ikR}\right\} \\
&\quad + o\left(\frac{1}{R}\right),
\end{aligned}
\tag{3.2.57}
$$

where $f_j(1,\phi_0) = i\,\frac{\Delta\,k^2}{4\pi\epsilon_0}\,m_z^n\;\vec{e}^{\,*}\cdot[(\vec{m}\times\vec{e}^{\,0})\times\vec{m}]$ was used (cf. (2.4.36) for $\ell=1$ and (3.2.22)).

Next $W^3_{2,j}$ of (3.2.33) is examined. The cut-off function is defined the same way as for $\ell=1$. Recall that the modified Bessel function $K_0\big(k\;|n'-\nu'|\,\big)$ in $h_{2,j}\big(n'(\psi,\phi)\big)$ (cf. (2.4.36) for $\ell = 2$) has a logarithmic singularity of the form $\log\big(\frac{k}{2}\,|n'-\nu'|\,\big)$. This, as seen above (cf. (3.2.36)), can be transformed to

$$
\begin{aligned}
\log\left(\frac{k}{2}\,|n'-\nu'|\right) &= \frac{1}{2}\,\log(1-\psi) + \frac{1}{2}\,\log\Bigg[\frac{k^2}{4}\Big((1-\psi)\,\big(\sin^2\alpha\cos^2\phi - \cos^2\alpha\big) \\
&\qquad + 2 - 2\sin^2\alpha\cos^2\phi - 2\sin\alpha\cos\alpha\cos\phi\,\sqrt{1-\psi^2}\Big)\Bigg].
\end{aligned}
\tag{3.2.58}
$$

Furthermore, using [1, Equs. 9.6.13 and 9.6.12, Sect. 9.6] and (3.2.58), we arrive at

$$
\begin{aligned}
K_0\left(k\,|n'-\nu'|\right) &= -\frac{1}{2}\log\left(1-\psi\right) - \tilde{\gamma} + \mathcal{O}\left(\log|n'-\nu'|\;|n'-\nu'|^2\right) - \frac{1}{2}\log\Bigg[\frac{k^2}{4}\Big(2 \\
&\quad - 2\sin^2\alpha\cos^2\phi - 2\sin\alpha\cos\alpha\cos\phi\,\sqrt{1-\psi^2} + (1-\psi)\,\big(\sin^2\alpha\cos^2\phi - \cos^2\alpha\big)\Big)\Bigg]
\end{aligned}
\tag{3.2.59}
$$

where $\tilde{\gamma}$ is Euler's constant. Define (cf. (2.4.36) for $\ell = 2$)

$$h_j(\psi,\phi) := c_h k\, \tilde{\chi}_\epsilon(\psi-1)\sqrt{1-n'^2}^{n}\ \vec{e}^{*}\cdot\left[\left(\vec{n}^{r}\times\vec{e}^{0}\right)\times\vec{n}^{r}\right]\ K_0\left(k\ |n'-\nu'|\right) + c_h k\, m_z^n\ \vec{e}^{*}\cdot\left[\left(\vec{m}\times\vec{e}^{0}\right)\times\vec{m}\right]\ \frac{1}{2}\log\left(1-\psi\right), \tag{3.2.60}$$

where $c_h$ is as in (3.2.39). It follows with $h_j(1,\phi) := \lim_{\psi\nearrow 1} h_j(\psi,\phi)$ that

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

Again the integral $W_{2,j}^{3}$ is split as

$$W_{2,j}^{3} = W_j^{3,8} + W_j^{3,9}, \qquad W_j^{3,8} := \int_0^{2\pi}\int_0^{1} h_j(\psi,\phi)\, e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi, \tag{3.2.61}$$

$$W_j^{3,9} := -c_h k\,\pi\, m_z^n\ \vec{e}^{*}\cdot\left[\left(\vec{m}\times\vec{e}^{0}\right)\times\vec{m}\right]\int_0^1 \log(1-\psi)\, e^{ikR\psi}\,\mathrm{d}\psi. \tag{3.2.62}$$

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

$$W_j^{3,8} = -c_h k\, m_z^n\ \vec{e}^{*}\cdot\left[\left(\vec{m}\times\vec{e}^{0}\right)\times\vec{m}\right]\int_0^{2\pi}\left\{\tilde{\gamma} + \frac{1}{2}\log\left(\frac{k^2}{2}\right) + \frac{1}{2}\log\left(1-\sin^2\alpha\cos^2\phi\right)\right\}\mathrm{d}\phi\,\frac{e^{ikR}}{ikR} - \frac{1}{ikR}\int_0^{2\pi}\int_0^{1}\partial_\psi h_j(\psi,\phi)\, e^{ikR\psi}\,\mathrm{d}\psi\,\mathrm{d}\phi. \tag{3.2.63}$$

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 the derivative $\partial_\psi h_j(\psi,\phi)$ is absolutely integrable w.r.t. $\psi \in [0,1]$. Consider (cf. (3.2.60) and [1, Equ. 9.6.27, Sect. 9.6])

$$\begin{aligned}
&\partial_\psi h_j(\psi,\phi)\\
&= c_h k\, \tilde{\chi}_\epsilon'(\psi-1)\sqrt{1-n'^2}^{n}\ \vec{e}^{*}\cdot\left[\left(\vec{n}^{r}\times\vec{e}^{0}\right)\times\vec{n}^{r}\right]\ K_0\left(k\ |n'-\nu'|\right)\\
&\quad + c_h k\, \tilde{\chi}_\epsilon(\psi-1)\partial_\psi\left[n'(\psi,\phi)\right]\cdot\nabla_{n'}\left[\sqrt{1-n'^2}^{n}\ \vec{e}^{*}\cdot\left[\left(\vec{n}^{r}\times\vec{e}^{0}\right)\times\vec{n}^{r}\right]\right] K_0\left(k\,|n'-\nu'|\right)\\
&\quad - c_h k\, \tilde{\chi}_\epsilon(\psi-1)\sqrt{1-n'^2}^{n}\ \vec{e}^{*}\cdot\left[\left(\vec{n}^{r}\times\vec{e}^{0}\right)\times\vec{n}^{r}\right]\ k\,\partial_\psi\left[\,|n'-\nu'|\,\right] K_1\left(k\ |n'-\nu'|\right)\\
&\quad - c_h \frac{k}{2}\, m_z^n\ \vec{e}^{*}\cdot\left[\left(\vec{m}\times\vec{e}^{0}\right)\times\vec{m}\right]\ \frac{1}{1-\psi},
\end{aligned} \tag{3.2.64}$$

where (cf. (3.2.16))

$$\partial_\psi\left[n'(\psi,\phi)\right] = \begin{pmatrix}\sin\alpha\cos\beta + (\cos\alpha\cos\beta\cos\phi - \sin\beta\sin\phi)\ \frac{-\psi}{\sqrt{1-\psi^2}}\\ \sin\alpha\sin\beta + (\cos\alpha\sin\beta\cos\phi + \cos\beta\sin\phi)\ \frac{-\psi}{\sqrt{1-\psi^2}}\end{pmatrix}.$$

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 (3.2.64) is uniformly bounded w.r.t. $\psi \in [0,1]$ and thus absolutely integrable. The second term, on the other hand, is bounded for $\psi \in [0,1]$ by the integrable function (cf. (3.2.59)) $c\,(1 + 1/\sqrt{1-\psi} + \log(1-\psi)/\sqrt{1-\psi})$, since $\nabla_{n'}[\sqrt{1-n'^2}^n\ \vec{e}^* \cdot [(\vec{n}^r \times \vec{e}^0) \times \vec{n}^r]]$ is uniformly bounded w.r.t. $\psi$ and $\phi$. 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 (3.2.64). For this the series expansion of $K_1$ is needed (cf. [1, Equs. 9.6.11 and 9.6.10, Sect. 9.6] and [1, Equ. 6.3.2, Sect. 6.3])

$$K_1(k\,|n'-\nu'|) = \frac{1}{k\,|n'-\nu'|} + \frac{1}{4}\left[2\log\left(\frac{k}{2}\,|n'-\nu'|\right) + 2\tilde{\gamma} - 1\right] k\,|n'-\nu'| + o\Big(|n'-\nu'|^2\Big), \tag{3.2.65}$$

as well as the derivative (cf. (3.2.36))

$$\begin{aligned}\partial_\psi\big[\,|n'-\nu'|\,\big] = &-\frac{1}{2}\,\frac{|n'-\nu'|}{1-\psi} \\ &+ \frac{1}{2}\,\frac{2\sin\alpha\cos\alpha\cos\phi\,\frac{\psi}{\sqrt{1+\psi}} - \sqrt{1-\psi}\,\left(\sin^2\alpha\cos^2\phi - \cos^2\alpha\right)}{|n'(\psi,\phi)-\nu'|\,/\sqrt{1-\psi}}\end{aligned} \tag{3.2.66}$$

is needed. Note that the last denominator on the right-hand side is bounded. Indeed, $\sqrt{1-\psi}$ is the singular factor in $|n'(\psi,\phi) - \nu'|$ in the neighbourhood not cut-off by the factor $\tilde{\chi}_\epsilon(\psi-1)$, and the denominator equals $\frac{|n'(\psi,\phi)-\nu'|}{\sqrt{1-\psi}}$ (cf. (3.2.36)). Since the last two terms on the right-hand side of (3.2.64) are bounded for any $\psi \in [0,1)$, it remains to examine the asymptotics of the two for $\psi \nearrow 1$ using (3.2.65) and (3.2.66). For $\psi \nearrow 1$, this leads to

$$\begin{aligned}&- c_h k\,\tilde{\chi}_\epsilon(\psi-1)\sqrt{1-n'^2}^n\ \vec{e}^* \cdot \big[\big(\vec{n}^r \times \vec{e}^0\big) \times \vec{n}^r\big]\ k\,\partial_\psi\big[\,|n'-\nu'|\,\big]\,K_1\left(k\ |n'-\nu'|\right) \\ &- c_h\frac{k}{2}\,m_z^n\ \vec{e}^* \cdot \big[\big(\vec{m} \times \vec{e}^0\big) \times \vec{m}\big]\ \frac{1}{1-\psi} \\ &\qquad \sim -c_h\frac{k}{2}\,m_z^n\ \vec{e}^* \cdot \big[\big(\vec{m} \times \vec{e}^0\big) \times \vec{m}\big]\ \left\{\frac{1}{1-\psi} + 2k\,\partial_\psi\big[\,|n'-\nu'|\,\big]\,K_1\left(k\,|n'-\nu'|\right)\right\} \\ &\qquad = -c_h\frac{k}{2}\,m_z^n\ \vec{e}^* \cdot \big[\big(\vec{m} \times \vec{e}^0\big) \times \vec{m}\big]\ \mathcal{O}\left(\frac{1}{\sqrt{1-\psi}}\right).\end{aligned}$$

Thus the derivative $\partial_\psi h_j(\psi,\phi)$ is absolutely integrable w.r.t. $\psi \in [0,1]$. Furthermore, using the Riemann-Lebesgue lemma, this shows that the integral w.r.t. $\psi$ on the right-hand side of (3.2.63) multiplied by $1/R$ converges to zero with the order $o\left(\frac{1}{R}\right)$. Since the integral w.r.t. $\psi$ is also uniformly bounded w.r.t. $R$ and $\phi$, Lebesgue's theorem can be applied to show that this convergence order also holds for the integral w.r.t. $\phi$. Hence

$$\begin{aligned}W_j^{3,8} = -c_h k\,m_z^n\,\vec{e}^* \cdot \big[\big(\vec{m} \times \vec{e}^0\big) \times \vec{m}\big] &\left\{2\pi\tilde{\gamma} + \pi\log\left(\frac{k^2}{2}\right)\right. \\ &\left. + \int_0^\pi \log\big(1 - \sin^2\alpha\cos^2\phi\big)\,\mathrm{d}\phi\right\}\frac{e^{ikR}}{ikR} + o\left(\frac{1}{R}\right)\end{aligned}$$

$$= -c_h k\, m_z^n\, \vec{e}^{\,*} \cdot \left[ \left( \vec{m} \times \vec{e}^{\,0} \right) \times \vec{m} \right] \left\{ 2\pi\tilde{\gamma} + \pi \log\left( \frac{k^2}{2} \right) + 4\pi \log\left( \cos\frac{\alpha}{2} \right) \right\} \frac{e^{ikR}}{ikR}$$
$$+ o\left( \frac{1}{R} \right). \tag{3.2.67}$$

Finally $W_j^{3,9}$ (cf. (3.2.62)) is evaluated using [11, Equ. 116, Sects. I.4 and II.4] and [1, Equations 5.2.8, 5.2.9, 5.2.34 and 5.2.35, Sect. 5.2] leading to

$$W_j^{3,9} = -c_h k\, \pi\, m_z^n\; \vec{e}^{\,*} \cdot \left[ \left( \vec{n}^r \times \vec{e}^{\,0} \right) \times \vec{n}^r \right] \left[ -\tilde{\gamma} - \log(kR) - i\frac{\pi}{2} \right] \frac{e^{ikR}}{ikR} + o\left( \frac{1}{R} \right).$$

It follows that (cf. the first equation of (3.2.61), (3.2.67) and (3.2.39))

$$W_{2,j}^3 = i\, \frac{\Delta\, k^3}{4\, \epsilon_0}\, m_z^n\; \vec{e}^{\,*} \cdot \left[ \left( \vec{m} \times \vec{e}^{\,0} \right) \times \vec{m} \right]$$
$$\left[ \log R - \tilde{\gamma} - \log\left( \frac{k}{2} \right) - 4 \log\left( \cos\frac{\alpha}{2} \right) + i\frac{\pi}{2} \right] \frac{e^{ikR}}{ikR} + o\left( \frac{1}{R} \right) \tag{3.2.68}$$

**Main term for weakly singular integrand outside the unit disc**

The substitution used in the first line of (3.2.5) leads to (cf. (3.2.4))

$$W_{1,j}^3 = \int\limits_{\phi_0-\pi}^{\phi_0+\pi} \int\limits_1^{\infty} \chi_\epsilon(k\rho n_0' - k\nu')\, \frac{\tilde{f}_j(\rho n_0')}{|\rho n_0' - \nu'|}\, \frac{\rho}{\sqrt{1-\rho^2}}\, e^{ik\rho R n_0' \cdot m'}\, e^{-kRm_z\sqrt{\rho^2-1}}\, \mathrm{d}\rho\, \mathrm{d}\phi,$$

where (cf. (2.4.36) for $\ell = 1$) $\tilde{f}_j(\rho n_0') := h_{1,j}(\rho n_0')\ |\rho n_0' - \nu'|$ is uniformly bounded w.r.t. $\rho$ and $\phi$ on a compact set. Note that, since the support of $(\rho, n_0') \mapsto \chi_\epsilon(k\rho n_0' - k\nu')$ is completely outside the unit circle around zero, there exists a constant $\delta > 0$ such that $\sqrt{\rho^2 - 1} \geq \delta$ for all $k\rho n_0' - k\nu' \in \mathrm{supp}\chi_\epsilon$. Thus for $R \geq 1$

$$\left| W_{1,j}^3 \right| \leq \frac{c}{\delta} \int\limits_{\phi_0-\pi}^{\phi_0+\pi} \int\limits_1^{\infty} \frac{|\chi_\epsilon(k\rho n_0' - k\nu')|}{|\rho n_0' - \nu'|}\, \mathrm{d}\rho\, \mathrm{d}\phi\, e^{-kRm_z\delta} = o\left( \frac{1}{R} \right), \tag{3.2.69}$$

since $|\rho n_0' - \nu'|^{-1}$ is locally integrable w.r.t. $\rho$ and $\phi$.

**The three cases together**

Finally, combining (3.2.4), (3.2.32), (3.2.57), (3.2.68), (3.2.69) and the argument after (3.2.21),

$$
W^3_{\ell,j} = \begin{cases} \mathbb{1}_{k'+\tilde\omega'_{1,j}}(km') \Big\{ i\, \frac{\Delta\, k^2}{4\pi\epsilon_0}\, m^n_z\ \vec e^{\,*}\cdot [(\vec m \times \vec e^{\,0}) \times \vec m] \Big[ 2\tilde F(\frac{\pi}{2}\setminus\alpha) \\ \qquad \Big( \frac{\sqrt2}{ikR} + \sqrt\pi \frac{1-i}{\sqrt k}\, \frac{e^{ikR}}{\sqrt R} \Big) - 2\pi k\, \frac{e^{ikR}}{ikR} \Big] \Big\}, & \text{if } \ell = 1 \\ \mathbb{1}_{k'+\tilde\omega'_{2,j}}(km') \Big\{ i\, \frac{\Delta\, k^3}{4\,\epsilon_0}\, m^n_z\ \vec e^{\,*}\cdot [(\vec m \times \vec e^{\,0}) \times \vec m] \\ \qquad \Big[ \log R - \tilde\gamma - \log \frac{k}{2} - 4 \log\cos\frac{\alpha}{2} + i\frac{\pi}{2} \Big] \frac{e^{ikR}}{ikR} \Big\}, & \text{if } \ell = 2 \\ 2\pi\, \chi_\epsilon(km' - k' - \tilde\omega'_{\ell,j})\, h_{\ell,j}(m')\, \frac{e^{ikR}}{ikR}, & \text{if } \ell = 3,4 \end{cases}
$$
$$
+\, o(1/R) \tag{3.2.70}
$$

no matter if the point $n'$ with $kn' = k' + \tilde\omega'_{\ell,j}$ is located inside or outside the unit circle. Note that the terms for $\ell = 3,4$ are obtained similarly to (3.2.20), but with $1 - \chi_\epsilon(km' - k' - \tilde\omega'_{\ell,j})$ replaced by $\chi_\epsilon(km' - k' - \tilde\omega'_{\ell,j})$ and with $W^1_{\ell,j}$ replaced by $W^3_{\ell,j}$. Furthermore, 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 else. For a singleton $M = \{\mathtt{m}_0\}$, $\mathbb{1}_M(\mathtt{m})$ is shortly written as $\mathbb{1}_{\mathtt{m}_0}(\mathtt{m})$.

## 3.3 The final formula for the reflected field

In conclusion this shows that (cf. (3.2.1), (3.2.11), (3.2.20) and (3.2.70))

$$
\begin{aligned}
&\int_{\mathbb{R}^2} \frac{h_{\ell,j}(n')}{n^r_z}\, e^{ik\vec n^r\cdot\vec x}\, \mathrm{d}n' \\
&= 2\pi\, \mathbb{1}_{\{1,2\}}(\ell) \Big( 1 - \mathbb{1}_{k'+\tilde\omega'_{\ell,j}}(km') \Big)\, h_{\ell,j}(m')\, \frac{e^{ikR}}{ikR} + 2\pi\, \mathbb{1}_{\{3,4\}}(\ell)\, h_{\ell,j}(m')\, \frac{e^{ikR}}{ikR} \\
&\quad - i\, \mathbb{1}_1(\ell)\, \mathbb{1}_{k'+\tilde\omega'_{1,j}}(km')\, \frac{\Delta\, k^2}{2\epsilon_0}\, m^n_z\ \vec e^{\,*}\cdot \big[ (\vec m \times \vec e^{\,0}) \times \vec m \big] \Bigg\{ k\, \frac{e^{ikR}}{ikR} \\
&\qquad\qquad - \frac{1}{\pi}\, \tilde F(\frac{\pi}{2}\setminus\alpha) \left( \frac{\sqrt2}{ikR} + \sqrt\pi \frac{1-i}{\sqrt k}\, \frac{e^{ikR}}{\sqrt R} \right) \Bigg\} \\
&\quad + i\, \mathbb{1}_2(\ell)\, \mathbb{1}_{k'+\tilde\omega'_{2,j}}(km')\, \frac{\Delta\, k^3}{4\,\epsilon_0}\, m^n_z\ \vec e^{\,*}\cdot \big[ (\vec m \times \vec e^{\,0}) \times \vec m \big] \qquad (3.3.1) \\
&\qquad\qquad \left[ \log R - \tilde\gamma - \log\left(\frac{k}{2}\right) - 4 \log\left( \cos\frac{\alpha}{2} \right) + i\frac{\pi}{2} \right] \frac{e^{ikR}}{ikR} + o\left(\frac{1}{R}\right).
\end{aligned}
$$

This gives the asymptotics of one term in (2.5.4). From the uniform and absolute convergence of the sum in (2.5.4) (cf. Theorem 2.1), it is obvious that the asymptotic limit and the summation in (2.5.4) can be interchanged.

**Theorem 3.1.** *Assume the interface is the graph of a function $f \in \mathcal{A}_1$ that satisfies condition* (2.4.20) *and $\left|k' + \tilde\omega'_{\ell,j}\right| \neq k$ for $\ell = 1,2$ and all $j \in \mathbb{Z}$. Suppose this interface is* *illuminated by an incoming plane wave described in Subsection 2.1. Then the far-field asymptotics of the reflected polarised electric field for* $z > \max\left\{2\,\|f\|_{\mathcal{A}_1}, 2\,\|f\|_\infty\right\}$ *in the direction* $\vec{m} = (m', m_z)^\top = (\sin\alpha\cos\beta, \sin\alpha\sin\beta, \cos\alpha)^\top$ *is*

$$
\begin{aligned}
&\vec{e}^{\,*}\!\cdot \vec{E}^r(R\vec{m}) \\
&\quad = r(\vec{k}, \vec{e}^{\,0}, \vec{e}^{\,*})\,\frac{e^{ikR\vec{n}_0^r\cdot\vec{m}}}{|k'|^2} \\
&\quad - i\,\frac{\Delta}{2\epsilon_0}\sum_{n\in\mathbb{N}_0}\sum_{j\in\mathbb{Z}}\int_0^1 \tilde{\lambda}^n_{0,j}\frac{(-i\zeta)^n}{n!}\,\mathrm{d}\zeta\;\; \vec{e}^{\,*}\!\cdot\left[\left(\vec{\omega}^j\times\vec{e}^{\,0}\right)\times\vec{\omega}^j\right]\,\left(\omega_z^j\right)^{n-1} e^{iR\vec{\omega}^j\cdot\vec{m}} \\
&\quad - \sum_{n\in\mathbb{N}_0}\sum_{j\in\mathbb{Z}}\Bigg\{2\pi\sum_{\ell=1}^{2}\left[\int_0^1 \tilde{\lambda}^n_{\ell,j}\,\frac{(-ik\zeta)^n}{n!}\,\mathrm{d}\zeta\,\left(1-\mathbb{1}_{k'+\tilde{\omega}'_{\ell,j}}(km')\right)h_{\ell,j}(m')\right]\frac{e^{ikR}}{ikR} \\
&\qquad\qquad - 2\pi\sum_{\ell=3}^{4}\int_0^1 \tilde{\lambda}^n_{\ell,j}\,\frac{(-ik\zeta)^n}{n!}\,\mathrm{d}\zeta\, h_{\ell,j}(m')\,\frac{e^{ikR}}{ikR} \qquad\qquad (3.3.2)\\
&\qquad\qquad - i\,\frac{\Delta\,k^2}{2\pi\epsilon_0}\,\mathbb{1}_{k'+\tilde{\omega}'_{1,j}}(km')\,m_z^n\int_0^1 \tilde{\lambda}^n_{1,j}\,\frac{(-ik\zeta)^n}{n!}\,\mathrm{d}\zeta\;\;\vec{e}^{\,*}\!\cdot\left[\left(\vec{m}\times\vec{e}^{\,0}\right)\times\vec{m}\right] \\
&\qquad\qquad\qquad \left[\tilde{F}\!\left(\frac{\pi}{2}\setminus\alpha\right)\left(\frac{\sqrt{2}}{ikR}+\sqrt{\pi}\frac{1-i}{\sqrt{k}}\,\frac{e^{ikR}}{\sqrt{R}}\right)-\pi k\frac{e^{ikR}}{ikR}\right] \\
&\qquad\qquad - i\,\frac{\Delta\,k^3}{4\,\epsilon_0}\mathbb{1}_{k'+\tilde{\omega}'_{2,j}}(km')\,m_z^n\int_0^1 \tilde{\lambda}^n_{2,j}\,\frac{(-ik\zeta)^n}{n!}\,\mathrm{d}\zeta\;\;\vec{e}^{\,*}\!\cdot\left[\left(\vec{m}\times\vec{e}^{\,0}\right)\times\vec{m}\right] \\
&\qquad\qquad\qquad \left[\log R - \tilde{\gamma} - \log\frac{k}{2} - 4\log\cos\frac{\alpha}{2} + i\frac{\pi}{2}\right]\frac{e^{ikR}}{ikR}\Bigg\} + o\left(\frac{1}{R}\right),
\end{aligned}
$$

*where* $\vec{n}_0^r := (n_x^0, n_y^0, -n_z^0)^\top$ *for the incoming direction* $\vec{n}^0 = (n_x^0, n_y^0, n_z^0)^\top := \vec{k}/k$ *and where* $r(\vec{k}, \vec{e}^{\,0}, \vec{e}^{\,*}) := \vec{e}^{\,*}\cdot\vec{r}(\vec{k}, \vec{e}^{\,0})$ *with* $\vec{r}(\vec{k}, \vec{e}^{\,0})$ *defined in* (2.4.37). *The numbers* $\tilde{\lambda}^n_{\ell,j}$ *and* $\tilde{\omega}'_{\ell,j}$ *are defined in Lemma 2.2, the symbols* $\vec{\omega}^j$, $\omega_z^j$ *in* (2.4.35), *and* $h_{\ell,j} := \vec{e}^{\,*}\cdot\vec{h}_{\ell,j}$ *with* $\vec{h}_{\ell,j}$ *given in* (2.4.36). *The symbol* $\tilde{\gamma}$ *stands for Euler's constant, and* $\tilde{F}$ *is the elliptic integral of the first kind.*

## 3.4 Reduced efficiency in specular reflection

In this subsection it will be shown that the results, derived in [14, Sect.II.E.1] without fixing any sufficient assumption on the interface, hold for interface functions in $\mathcal{A}_1$. To be precise, it will be proven that the efficiency of the plane wave reflected in specular direction can be represented as the efficiency for reflection at an ideal interface multiplied by an explicit correction term.

**Theorem 3.2.** *Assuming an interface function* $f \in \mathcal{A}_1$, *the reflected field* $\vec{E}^r$ *in the Born approximation of Theorem 2.1 contains a plane-wave mode propagating in the specular direction*

*$\vec{n}^r := (n_x, n_y, -n_z^0)^\top := \vec{k}^r/k$ with $\vec{k}^r := (k_x, k_y, -k_z)^\top$ of the form*

$$\frac{\Delta}{4\epsilon_0\,[n_z^0]^2}\,\hat{w}(-2k_z)\;\left[(\vec{n}^r\times\vec{e}^{\,0})\times\vec{n}^r\right]\,e^{i\vec{k}^r\cdot\vec{x}} + \mathcal{O}\left(\left[\frac{\Delta}{[n_z^0]^2}\right]^2\right), \tag{3.4.1}$$

$$\hat{w}(-2k_z) := \int_{-\frac{h}{2}}^{\frac{h}{2}} \partial_\zeta\left[\lim_{R\to\infty}\tfrac{1}{4R^2}\int_{-R}^{R}\int_{-R}^{R}\mathbb{1}_{[f(\eta'),\infty)}(\zeta)\,\mathrm{d}\eta_x\,\mathrm{d}\eta_y\right]e^{-i2|k_z|\zeta}\,\mathrm{d}\zeta. \tag{3.4.2}$$

**Remark 3.1.** *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, Equ.* (3.4.1) *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 $\hat{w}(-2k_z)$. Consequently, 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 $p(\zeta) := \lim_{R\to\infty}\frac{1}{4R^2}\int_{-R}^{R}\int_{-R}^{R}\mathbb{1}_{[f(\eta'),\infty)}(\zeta)\,\mathrm{d}\eta_x\,\mathrm{d}\eta_y$ satisfying $p(\infty) = 1$ and $p(-h/2) = 0$.*

**Remark 3.2.** *Applying the formula for the Fourier transform of a derivative to Equ.* (3.4.2) *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.* Examining Equ. (2.5.3) and the definition of $\vec{\omega}_z^j$, it is easily seen that a plane wave in specular direction appears if $\tilde{\omega}'_{0,j} = (0,0)^\top$. The corresponding index $j$ will be denoted by $j_0$. Note that the corresponding $\tilde{\lambda}_{0,j_0}^n$ is the mean value of $f^{n+1}(\eta')\,e^{ik_z\zeta\,f(\eta')}$. To be precise it can be represented as (cf. (2.4.8))

$$\tilde{\lambda}_{0,j_0}^n = \Phi_{0,j_0}^n(f^{n+1}) := \lim_{R\to\infty}\frac{1}{4R^2}\int_{-R}^{R}\int_{-R}^{R} f^{n+1}(\eta')\,e^{ik_z\zeta\,f(\eta')}\,\mathrm{d}\eta_x\,\mathrm{d}\eta_y. \tag{3.4.3}$$

By $\vec{E}^{sp}$ denote the specular part of $\vec{E}^r$ (cf. (2.5.1) and (2.5.3) without scalar product by $\vec{e}^{\,*}$) minus the summand $\vec{E}_Q$, corresponding to the reflection at an ideal interface. Picking up the corresponding terms of (2.5.3) and replacing $\tilde{\lambda}_{0,j_0}^n$ by (3.4.3) leads to

$$\vec{E}^{sp} := -i\,\frac{\Delta}{2\epsilon_0}\sum_{n\in\mathbb{N}_0}\int\limits_0^1 \tilde{\lambda}^n_{0,j_0}\frac{(-i\zeta)^n}{n!}\,\mathrm{d}\zeta\;\;\Big[\Big(\vec{k}^r\times\vec{e}^0\Big)\times\vec{k}^r\Big]\;|k_z|^{n-1}\,e^{i\vec{k}^r\cdot\vec{x}}$$
$$= -i\,\frac{\Delta}{2\epsilon_0}\sum_{n\in\mathbb{N}_0}\int\limits_0^1 \lim_{R\to\infty}\frac{1}{4R^2}\int\limits_{-R}^{R}\int\limits_{-R}^{R} f^{n+1}(\eta')\,e^{ik_z\zeta\,f(\eta')}\,\mathrm{d}\eta_x\,\mathrm{d}\eta_y\frac{(-i\zeta)^n}{n!}\,\mathrm{d}\zeta\,|k_z|^{n-1}$$
$$\Big[\Big(\vec{k}^r\times\vec{e}^0\Big)\times\vec{k}^r\Big]\;e^{i\vec{k}^r\cdot\vec{x}}.$$

Clearly, the $\Phi^n_{0,j_0}$ is a continuous linear functional on the Banach algebra $\mathcal{A}^{\mathbb{C}}_1$. Hence, the functional evaluation can be interchanged with the summation over $n$ and the integration w.r.t. $\zeta$, which themselves are continuous operations in $\mathcal{A}^{\mathbb{C}}_1$.

$$\vec{E}^{sp} = -i\,\frac{\Delta}{2\epsilon_0}\lim_{R\to\infty}\frac{1}{4R^2}\int\limits_{-R}^{R}\int\limits_{-R}^{R}\int\limits_0^1\sum_{n\in\mathbb{N}_0}\frac{(-i|k_z|\zeta\,f(\eta'))^n}{n!}\;e^{ik_z\zeta\,f(\eta')}\,\mathrm{d}\zeta\,\frac{f(\eta')}{|k_z|}\,\mathrm{d}\eta_x\,\mathrm{d}\eta_y$$
$$\Big[\Big(\vec{k}^r\times\vec{e}^0\Big)\times\vec{k}^r\Big]\;e^{i\vec{k}^r\cdot\vec{x}}$$
$$= -i\,\frac{\Delta}{2\epsilon_0}\lim_{R\to\infty}\frac{1}{4R^2}\int\limits_{-R}^{R}\int\limits_{-R}^{R}\int\limits_0^1 e^{-i2|k_z|\zeta\,f(\eta')}\,\mathrm{d}\zeta\,\frac{f(\eta')}{|k_z|}\,\mathrm{d}\eta_x\mathrm{d}\eta_y\;\Big[\Big(\vec{k}^r\times\vec{e}^0\Big)\times\vec{k}^r\Big]\;e^{i\vec{k}^r\cdot\vec{x}}, \tag{3.4.4}$$

since $k_z < 0$. Note that

$$\int\limits_0^1 e^{-i2|k_z|\zeta\,f(\eta')}\,\mathrm{d}\zeta\,f(\eta') = \int\limits_0^{f(\eta')} e^{-i2|k_z|\zeta}\,\mathrm{d}\zeta = \int\limits_{-\frac{h}{2}}^{\frac{h}{2}}\chi(f,\eta',\zeta)\,e^{-i2|k_z|\zeta}\,\mathrm{d}\zeta,$$
$$\chi(f,\eta',\zeta) := \begin{cases} \mathbb{1}_{[0,f(\eta')]}(\zeta) & \text{if } 0\le f(\eta') \\ -\mathbb{1}_{[f(\eta'),0]}(\zeta) & \text{if } f(\eta')<0 \end{cases}.$$

Applying this to the right-hand side of (3.4.4) and using Fubini's theorem leads to

$$\vec{E}^{sp} = -i\,\frac{\Delta}{2\epsilon_0}\lim_{R\to\infty}\int\limits_{-\frac{h}{2}}^{\frac{h}{2}}\frac{1}{4R^2}\int\limits_{-R}^{R}\int\limits_{-R}^{R}\chi(f,\eta',\zeta)\,\mathrm{d}\eta_x\,\mathrm{d}\eta_y\,e^{-i2|k_z|\zeta}\,\mathrm{d}\zeta\,\frac{\big[\big(\vec{k}^r\times\vec{e}^0\big)\times\vec{k}^r\big]}{|k_z|}\,e^{i\vec{k}^r\cdot\vec{x}}. \tag{3.4.5}$$

In order to apply Lebesgue's theorem in (3.4.5), it must be shown that the limit

$$\lim_{R\to\infty}\frac{1}{4R^2}\int\limits_{-R}^{R}\int\limits_{-R}^{R}\chi(f,\eta',\zeta)\,\mathrm{d}\eta_x\,\mathrm{d}\eta_y \tag{3.4.6}$$

exists a.e. for $\zeta$ s.t. $-h/2 \leq \zeta \leq h/2$. Note that $\mu(f,\zeta,R) := \int_{-R}^{R}\int_{-R}^{R}\chi(f,\eta',\zeta)\,\mathrm{d}\eta_x\,\mathrm{d}\eta_y$ is the measure for the set of points $\eta' \in [-R,R]^2$ with $0 \leq \zeta \leq f(\eta')$ minus the measure for the set of points $\eta' \in [-R,R]^2$ with $0 \geq \zeta \geq f(\eta')$ . Hence, $-1 \leq \mu(f,\zeta,R)/(4R^2) \leq 1$ for all $R > 0$. Furthermore, for $\zeta \neq 0$ and for any decaying function $\tilde{f} \in \mathcal{A}_1$, the integral $\mu(\tilde{f},\zeta,R)/(4R^2)$ tends to zero as $R$ tends to infinity. Consequently, only the non-decaying part of $f$ is significant for the limit in (3.4.6). Finally, by density arguments it can be assumed that $f$ is only a finite sum of Fourier modes. However, the existence of the limit in (3.4.6) for such a biperiodic function is easy to see.

Now Lebesgue's theorem for (3.4.5) and the formula for a differentiated generalised Fourier transform yield

$$\begin{aligned}\vec{E}^{sp} &= -i\,\frac{\Delta}{2\epsilon_0|k_z|}\int_{\mathbb{R}}\left[\lim_{R\to\infty}\frac{1}{4R^2}\int_{-R}^{R}\int_{-R}^{R}\chi(f,\eta',\zeta)\,\mathrm{d}\eta_x\mathrm{d}\eta_y\right]e^{-i2|k_z|\zeta}\,\mathrm{d}\zeta\,\left[\left(\vec{k}^r\times\vec{e}^{\,0}\right)\times\vec{k}^r\right]e^{i\vec{k}^r\cdot\vec{x}} \\ &= \frac{-\Delta}{4\epsilon_0|k_z|^2}\int_{\mathbb{R}}\partial_\zeta\left[\lim_{R\to\infty}\frac{1}{4R^2}\int_{-R}^{R}\int_{-R}^{R}\chi(f,\eta',\zeta)\,\mathrm{d}\eta_x\mathrm{d}\eta_y\right]e^{-i2|k_z|\zeta}\,\mathrm{d}\zeta\,\left[\left(\vec{k}^r\times\vec{e}^{\,0}\right)\times\vec{k}^r\right]e^{i\vec{k}^r\cdot\vec{x}}.\end{aligned} \tag{3.4.7}$$

In correspondence with [14, Equ. (12)] define $p$ as in Remark 3.1 and set

$$p_{\mathcal{Q}}(\zeta) := \lim_{R\to\infty}\frac{1}{4R^2}\int_{-R}^{R}\int_{-R}^{R}\mathbb{1}_{[0,\infty)}(\zeta)\,\mathrm{d}\eta_x\,\mathrm{d}\eta_y = \mathbb{1}_{[0,\infty)}(\zeta).$$

It is easily confirmed that $\lim_{R\to\infty}\int_{-R}^{R}\int_{-R}^{R}\chi(f,\eta',\zeta)\,\mathrm{d}\eta_x\,\mathrm{d}\eta_y = \lim_{R\to\infty}\mu(f,\zeta,R)/(4R^2)$ $= p_{\mathcal{Q}}(\zeta) - p(\zeta)$ and that the Fourier transform $\hat{w}_Q(-2|k_z|) = \int_{\mathbb{R}}\partial_\zeta[p_{\mathcal{Q}}(\zeta)]\,e^{-i2|k_z|\zeta}\,\mathrm{d}\zeta$ is equal to one, by using results for generalised Fourier transforms. Furthermore, $\mathrm{supp}(\partial_\zeta p) \subseteq [-h/2,h/2]$. Thus, substituting $\lim_{R\to\infty}\int_{-R}^{R}\int_{-R}^{R}\chi(f,\eta',\zeta)\,\mathrm{d}\eta_x\mathrm{d}\eta_y$ by $p_{\mathcal{Q}}(\zeta)-p(\zeta)$ in Equation (3.4.7) and writing the integral of the difference as a difference of integrals, there holds

$$\vec{E}^{sp} = \frac{\Delta}{4\epsilon_0|k_z|^2}\hat{w}(-2k_z)\,\left[(\vec{k}^r\times\vec{e}^{\,0})\times\vec{k}^r\right]e^{i\vec{k}^r\cdot\vec{x}} - \frac{\Delta}{4\epsilon_0|k_z|^2}\left[(\vec{k}^r\times\vec{e}^{\,0})\times\vec{k}^r\right]e^{i\vec{k}^r\cdot\vec{x}}, \tag{3.4.8}$$

where $\hat{w}(-2k_z)$ is defined in (3.4.2). Finally, the theorem is a consequence of the following asymptotics, which is not hard to prove (compare Stearns [14, Equ. (36), Sect. II.E.1]).

$$\vec{E}_Q(\vec{x}) = \vec{r}\,(\vec{k},\vec{e}^{\,0})\,\frac{e^{i\vec{k}^r\cdot\vec{x}}}{|k'|^2} = \frac{\Delta}{4\,\epsilon_0[k_z]^2}\left[(\vec{k}^r\times\vec{e}^{\,0})\times\vec{k}^r\right]\,e^{i\vec{k}^r\cdot\vec{x}} + \mathcal{O}\left(\left[\frac{\Delta}{[n_z^0]^2}\right]^2\right). \tag{3.4.9}$$

□

## 3.5 The special case of a sinusoidal grating

### 3.5.1 Applied far-field formula

Now consider the reflected electric field for a sinusoidal grating, which is constant in $y$-direction. First Equ. (3.3.2) will be applied, and in the next subsection it is compared with that of Stearns [14].

Assume

$$f(x') := \lambda_{0,-1}\, e^{i\omega'_{0,-1}} + \lambda_{0,1}\, e^{i\omega'_{0,1}} = \frac{h}{2}\cos x, \quad \lambda_{0,\pm 1} := \frac{h}{4},\ \omega'_{0,\pm 1} := \begin{pmatrix} \pm 1 \\ 0 \end{pmatrix}. \tag{3.5.1}$$

To evaluate the second term on the right-hand side of (3.3.2) it is necessary to determine the values of $\tilde{\lambda}^n_{0,j}$ and $\tilde{\omega}'_{0,j}$ for the interface (3.5.1). For $\ell = 1, \ldots, 4$ the $\tilde{\lambda}^n_{\ell,j}$ are zero. To do so, consider Equs. (2.4.9) and (2.4.10). Note that the index set $\mathbb{Z}$ in this equation is reduced to $\{-1, 1\}$ for the interface function (3.5.1). Thus (cf. (3.5.1)) $\tilde{\omega}'_{0,j} = (j, 0)^\top$ for $j \in \mathbb{Z}$. Consequently, (cf. the definition of $\vec{\omega}^j_z$ after (2.4.34)) $\vec{\omega}^j_z = (k_x + j, k_y, (k^2 - (k_x + j)^2 - k_y^2)^{1/2})^\top$. From now on classical diffraction will be assumed, which means that $k_y = 0$, leading to

$$\vec{\omega}^j_z = \Big(k_x + j, 0, \sqrt{k^2 - (k_x + j)^2}\Big)^\top. \tag{3.5.2}$$

The factor $\tilde{\lambda}^n_{0,j}$ can further be transformed to

$$\begin{aligned}
\tilde{\lambda}^n_{0,j} &= \sum_{\substack{\tilde{m}=\max\{n+1,|j|\} \\ \tilde{m}+j \equiv 0 \bmod 2}}^{\infty} (ik_z\zeta)^{\tilde{m}-n-1} \frac{\tilde{m}!}{(\tilde{m}-n-1)!} \frac{h^{\tilde{m}}}{4^{\tilde{m}} \left(\frac{\tilde{m}-j}{2}\right)! \left(\frac{\tilde{m}+j}{2}\right)!} \\
&= \sum_{\substack{\tilde{m}=\max\{0,|j|-n-1\} \\ \tilde{m}+n+1+j \equiv 0 \bmod 2}}^{\infty} (ik_z\zeta)^{\tilde{m}} \frac{(\tilde{m}+n+1)!}{\tilde{m}!} \frac{h^{\tilde{m}+n+1}}{4^{(\tilde{m}+n+1)} \left(\frac{\tilde{m}+n+1-j}{2}\right)! \left(\frac{\tilde{m}+n+1+j}{2}\right)!}.
\end{aligned}$$

It follows that

$$\begin{aligned}
\vec{E}^r(\vec{x}) &= -i\,\frac{\Delta}{2\epsilon_0} \sum_{n\in\mathbb{N}_0} \sum_{j\in\mathbb{Z}} \sum_{\substack{\tilde{m}=\max\{0,|j|-n-1\} \\ \tilde{m}+n+1+j \equiv 0 \bmod 2}}^{\infty} \left\{ \frac{(-i)^n}{n!} \int_0^1 \zeta^{n+\tilde{m}}\, \mathrm{d}\zeta\, (ik_z)^{\tilde{m}} \frac{(\tilde{m}+n+1)!}{\tilde{m}!} \right. \\
&\qquad \left. \frac{h^{\tilde{m}+n+1} \left[(\vec{\omega}^j \times \vec{e}^{\,0}) \times \vec{\omega}^j\right] (\omega^j_z)^{n-1}}{4^{(\tilde{m}+n+1)} \left(\frac{\tilde{m}+n+1-j}{2}\right)! \left(\frac{\tilde{m}+n+1+j}{2}\right)!} e^{i\vec{\omega}^j\cdot\vec{x}} \right\} + \vec{E}^r_{\mathcal{Q}}(\vec{x}) \\
&= -i\,\frac{\Delta}{2\epsilon_0} \sum_{n\in\mathbb{N}_0} \sum_{j\in\mathbb{Z}} \sum_{\substack{\tilde{m}=\max\{0,|j|-n-1\} \\ \tilde{m}+n+1+j \equiv 0 \bmod 2}}^{\infty} \left\{ \frac{(-i)^n}{n!} (ik_z)^{\tilde{m}} \frac{(\tilde{m}+n)!}{\tilde{m}!} \right. \\
&\qquad \left. \frac{h^{\tilde{m}+n+1} \left[(\vec{\omega}^j \times \vec{e}^{\,0}) \times \vec{\omega}^j\right] (\omega^j_z)^{n-1}}{4^{(\tilde{m}+n+1)} \left(\frac{\tilde{m}+n+1-j}{2}\right)! \left(\frac{\tilde{m}+n+1+j}{2}\right)!} e^{i\vec{\omega}^j\cdot\vec{x}} \right\} + \vec{E}^r_{\mathcal{Q}}(\vec{x}).
\end{aligned}$$

Furthermore, in view of the absolute convergence of (2.5.3) these sums can be rearranged in such a way that

$$\vec{E}^r(\vec{x}) = -i\,\frac{\Delta}{2\epsilon_0} \sum_{j\in\mathbb{Z}\setminus\{0\}} \sum_{\substack{n=|j| \\ n+j \equiv 0 \bmod 2}}^{\infty} \sum_{\tilde{m}=0}^{n-1} \left[ \frac{(-i)^{(n-1)}\, h^n (n-1)!\, (-k_z)^{\tilde{m}}}{4^n\, \tilde{m}!\, (n-\tilde{m}-1)!} \left(\omega^j_z\right)^{n-\tilde{m}-2} \right.$$

$$
\frac{\left[(\vec{\omega}^{j}\times\vec{e}^{\,0})\times\vec{\omega}^{j}\right]}{\left(\frac{n-j}{2}\right)!\ \left(\frac{n+j}{2}\right)!}\, e^{i\vec{\omega}^{j}\cdot\vec{x}}\Bigg] \tag{3.5.3}
$$

$$
-\, i\,\frac{\Delta}{2\epsilon_0}\sum_{\substack{n=1\\ n\equiv 0 \bmod 2}}^{\infty}\ \sum_{\tilde{m}=0}^{n-1}\frac{(-i)^{(n-1)}h^{n}(n-1)!}{4^{n}\,\tilde{m}!\,(n-\tilde{m}-1)!}\,(-k_z)^{n-2}\,\frac{\left[\left(\vec{k}^{r}\times\vec{e}^{\,0}\right)\times\vec{k}^{r}\right]}{\left[\left(\frac{n}{2}\right)!\right]^{2}}\, e^{i\vec{k}^{r}\cdot\vec{x}}+\vec{E}^{r}_{\mathcal{Q}}(\vec{x}),
$$

where $\vec{k}^r = \vec{\omega}^0_z = (k_x, 0, -k_z)$ for $k_y = 0$ and $k_z < 0$.

### 3.5.2 Near-field formula of Stearns

According to Stearns (cf. [14, Equ. (19), Sect. II.B])

$$
\vec{E}^{r}(\vec{x}) = \frac{\Delta k^2}{8\pi^2\epsilon_0}\int\limits_{\mathbb{R}^2}\frac{\hat{g}(k\vec{n}^{r}-\vec{k})}{n^{r}_z(n^{r}_z-n^{0}_z)}\ \left[\left(\vec{n}^{r}\times\vec{e}^{\,0}\right)\times\vec{n}^{r}\right]\ e^{ik\vec{n}^{r}\cdot\vec{x}}\,\mathrm{d}n',
$$

where $\vec{n}^r := \left(n_x, n_y, \sqrt{1-n'^2}\right)^{\top}$, $n' := (n_x, n_y)^{\top}$, $n'^2 := n_x^2 + n_y^2$, $n_z^0 := \frac{k_z}{k}$, $\Delta := \epsilon_0 - \epsilon_0'$ 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. (2.2.6)). Formally applying the Fourier transform to $g$ and the Taylor-series expansion of the exponential function leads to

$$
\hat{g}(\vec{s}) := 4\pi^2\,\delta(s_y)\sum_{n\in\mathbb{N}_0}\frac{(-ihs_z)^n}{4^n}\sum_{m=0}^{n}\frac{1}{m!\,(n-m)!}\,\delta(s_x+n-2m)
$$

$$
\vec{E}^{r}(\vec{x}) = \frac{\Delta k}{2\epsilon_0}\sum_{n\in\mathbb{N}_0}\sum_{m=0}^{n}\frac{(-ih)^n(kw_z^{n,m}-k_z)^n}{4^n\,m!\,(n-m)!}\frac{\left[(\vec{w}^{n,m}\times\vec{e}^{\,0})\times\vec{w}^{n,m}\right]}{w_z^{n,m}\,(kw_z^{n,m}-k_z)}\,e^{ik\vec{w}^{n,m}\cdot\vec{x}},
$$

where $\vec{w}^{n,m} := \left(\frac{k_x}{k} + \frac{2m-n}{k}, \frac{k_y}{k}, w_z^{n,m}\right)$ and $w_z^{n,m} := \sqrt{1 - \left(\frac{k_x}{k} + \frac{2m-n}{k}\right)^2 - \frac{k_y^2}{k^2}}$ with $k_y = 0$. Applying the binomial theorem to $(kw_z^{n,m} - k_z)^n$, rearranging the resulting sum and performing a few simple transformations leads to

$$
\vec{E}^{r}(\vec{x}) = -i\,\frac{\Delta}{2\epsilon_0}\sum_{j\in\mathbb{Z}\setminus\{0\}}\ \sum_{\substack{n=|j|\\ n+j\equiv 0 \bmod 2}}^{\infty}\ \sum_{\tilde{m}=0}^{n-1}\Bigg[\frac{(-i)^{n-1}h^{n}\,(n-1)!\ (-k_z)^{\tilde{m}}}{4^{n}\,\tilde{m}!\,(n-\tilde{m}-1)!}\left(\omega_z^{j}\right)^{n-\tilde{m}-2}
$$

$$
\frac{\left[(\vec{\omega}_z^{j}\times\vec{e}^{\,0})\times\vec{\omega}_z^{j}\right]}{\left(\frac{n-j}{2}\right)!\ \left(\frac{n+j}{2}\right)!}\, e^{i\vec{\omega}_z^{j}\cdot\vec{x}}\Bigg]
$$

$$
-\, i\frac{\Delta}{2\epsilon_0}\sum_{\substack{n=1\\ n\equiv 0 \bmod 2}}^{\infty}\ \sum_{\tilde{m}=0}^{n-1}\frac{(-i)^{n-1}h^{n}\,(n-1)!}{4^{n}\,\tilde{m}!\,(n-\tilde{m}-1)!}\,(-k_z)^{n-2}\ \frac{\left[\left(\vec{k}^{r}\times\vec{e}^{\,0}\right)\times\vec{k}^{r}\right]}{\left[\left(\frac{n}{2}\right)!\right]^{2}}\, e^{i\vec{k}^{r}\cdot\vec{x}}
$$

$$
+\ \frac{\Delta}{4\,\epsilon_0[n_z^0]^2}\ \left[\left(\vec{n}_0^{r}\times\vec{e}^{\,0}\right)\times\vec{n}_0^{r}\right]\ e^{ik\vec{n}_0^{r}\cdot\vec{x}} \tag{3.5.4}
$$

for $k_z = k\vec{n}_z^0$, where $\vec{\omega}_z^j$ is defined by (3.5.2) and $\vec{k}^r$ as at the end of Section 3.5.1. Thus the two equations (3.5.3) and (3.5.4) are approximately equal for $\frac{\Delta}{[n_z^0]^2} \ll 1$ (cf. Equ. (3.4.9) and compare Stearns [14, Equ. (36), Sect. II.E.1]).

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