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Boundary Conditions and Fresnel Equations for Weakly Spatially Dispersive Media

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Abstract

Although usually negligible for natural materials for optical and lower frequencies, spatial dispersion is a significant effect for metamaterials. In this thesis the electromagnetics of such media are investigated using a second order in \mathbf{k} approximation for the polarisation and assuming centro-symmetric inclusions. Boundary conditions derived by Lange and Raab to electric-octopole - magnetic quadrupole order are taken a step further by also accounting for multipole surface effects. Yaghjian and Silveirinha's boundary conditions and Fresnel equations are taken a step further by also accounting for dipolarisations for a medium with a non-zero electric quadrupolarisation. Lastly, two attempts at modelling interface behaviour for a general second order spatially dispersive medium are made. For one of the attempts, Fresnel equations are obtained.

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1 Introduction

Electromagnetics is an important branch of physics, describing the vast number of phenomena involving electromagnetic waves. In astronomy, the typical range of frequencies practical for measurements are from around 1 kHz (generated in the interstellar medium plasma) to gamma rays with frequencies higher than 10^{20} Hz. There are a lot of instruments and applications utilising waves within this massive spectrum, perhaps most importantly in telecommunications. Together with weak nuclear force, strong nuclear force and gravitation, the electromagnetic force is one of the four fundamental forces shaping nature. In electromagnetics, one is concerned with charged particles and magnetic moments. Charged particles at rest are usually described as an electric charge density, whereas charged particles in motion are usually described as an electric current density. Both of these generate electromagnetic fields, as is described by Maxwell's equations and are therefore called electromagnetic sources. However, they are also influenced by electromagnetic fields themselves, in a way that is described by the Lorentz force. Thus, electromagnetic sources and their effects is a neatly coupled system compactly described by Maxwell's equations, which on the differential form using index notation are as follows;

$$\nabla_i E_i - \frac{1}{\epsilon_0} \rho = 0, \quad (1)$$

$$\epsilon_{ijk} \nabla_j E_k + \dot{B}_i = 0, \quad (2)$$

$$\nabla_i B_i = 0, \quad (3)$$

$$\epsilon_{ijk} \nabla_j B_k - \mu_0 J_i - \mu_0 \epsilon_0 \dot{E}_i = 0. \quad (4)$$

The induced electric current density J_i and the bound electric charge density ρ are given as

$$J_i = \dot{P}_i, \quad (5)$$

$$\rho = -\nabla_i P_i, \quad (6)$$

where P_i is the polarisation. Throughout this paper only dielectrics¹ will be discussed, so there are no free charge or current densities to account for. The Lorentz force is given as

$$\mathbf{F} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B}).$$

¹As can be understood from reading this paper, the name "dielectrics" for describing polarisable media is a somewhat misleading name. It is due to the dipole approximation, which entails that only the electric dipole moment is significant beyond the electric monopole (electric charge). While this is true in most natural materials with negligible spatial dispersion, it is not so for materials with significant spatial dispersion, which is seen in metamaterials. For such media, higher order moments become significant as well, and a name like "multi-electrics" would be more suitable.

Since the observations relating magnetism to electrical current, most notably by Hans Christian Ørsted in 1820, the theory of electromagnetism flourished from the efforts of numerous scientists. To mention some, there was André-Marie Ampère, with his description of the force interaction between two electrically conducting wires. His description was later called Ampère's law, and was motivated by the observation made by Ørsted. Another contributor was Michael Faraday, who in 1821 put forth his description for the generation of current in an electric circuit from a time varying magnetic field. It was named "Faraday's law of induction", and was later reformulated by Maxwell, to give one of Maxwell's four fundamental equations of electromagnetism. Maxwell's equations, published in "A Dynamical Theory of the Electromagnetic Field" in 1865, together with the Lorentz force law, fully describe all classical phenomena of electromagnetism. Through the separate work of these contributors, they laid the foundation of the electromagnetics together.

In order to describe a whole medium (e.g. a gas, a metal or an insulating solid) using the laws of electromagnetism, as opposed to a simple set of discrete charges, one needs a homogenisation method. That is, rather than taking account of every single one of the innumerable charges that constitute the medium of interest, one should find a way to describe the response of the medium as a net or effective response. In order to do so, it is common to separate between the free charges ρ_f and the bound charges ρ_b . In this thesis we only discuss dielectric media, so ρ_f is zero and ρ_b will simply be written ρ . The bound charges are charges that are associated with a molecule (or an inclusion in metamaterial arrays) and induced by an external electric field. Normally this induction is described merely by a dipolarisation obeying the equations (6) and expressed as

$$P_i(\mathbf{r}) = \int_V r_i \rho(\mathbf{r}) dv.$$

where r_j is a position vector from some origin to the dipole at the infinitesimal volume dv and r_i is the induced separation vector within the dipole. The integral is taken over the macroscopic, but small volume V which of the critical dimension is far smaller than the wavelength used, so that the polarisation can be locally related to the electric field. From the definitions (5) and (6) and Maxwell's equations, it can be seen that the dipolarisation is crucial in the description of the total electromagnetic response of polarisable media. For all materials the degree of polarisation is dependent on the magnitude and direction of this external electric field, and for many materials the relation is linear:

$$P_i = \epsilon_0 \chi_{ij} E_j,$$

where ϵ_0 is the vacuum permittivity and χ_{ij} is the electric susceptibility tensor.

However, the dipolarisation model assumes that there are only electric dipole moments

worth considering in the medium, and this is not generally true. In fact, the electric dipole moment is only the second term in a series expansion of the scalar potential from which the fields are derived, the first term being the electric monopole (i.e. electric charge) [5, section 1.1]. The dipole approximation holds well for most normal materials from the combination of two reasons: firstly, the higher order multipoles contain increasing numbers of separation vector factors. For example consider the following multipole moment

$$M = \int_V r_i r_j r_k \dots \rho(\mathbf{r}) dv.$$

M is an electric multipole moment of arbitrary order, \mathbf{r} is a position vector from some origin to the volume element dv and r_i, r_j and so on are the induced separation distance vectors within the multipole. The vector factors r_i, r_j, \dots are on the length scale of the unit cell or molecule. Secondly, for normal materials the unit cells are usually of dimensions much smaller than the wavelength of the electromagnetic waves applied. This means that increasing orders of multipoles are of decreasing importance. For larger unit cells, or for shorter wavelengths, the higher order multipoles beyond the dipole become more important [7]. A non rigorous motivation for the importance of this ratio of between the unit cell and the wavelength, and the consequent higher order moments is the following: for a higher ratio, more change in the electric field associated with the wave happens over the distance of the unit cell or molecule. Therefore, spatial derivatives of increasing order of the electric field become important as the ratio becomes larger [5, section 2.12]. This effect is called spatial dispersion, and because of it we would expect a more complex expression for our total polarisation. This is discussed in the next section.

As fabrication technology is evolving, more advanced materials can be fabricated than before, and materials with structures not seen in nature are becoming feasible to make. An example of such a material is the electromagnetic "cloak" made by Pendry et al in 2006 [6], where they investigated the degree of electromagnetic "footprint" reduction achieved by shielding an object with the cloak for a specific frequency band of radiation. Although development in fabrication technology permits of creating arrays of smaller and smaller inclusions, they will typically be much larger than the unit cell in a natural material ². Therefore, we expect the spatial dispersion in these to be significant, and for a good description of the electromagnetic response of such metamaterials we therefore need updated theory. The modern era of the field properly started off with a publication by J.B. Pendry in 2000 [8], in which it was described how a metamaterial slab with simultaneous negative permittivity and permeability would be a perfect lens [4]. Since then, new interest was found in formulating such new theories for metamaterials, with

²An important point to make is that even if inclusions the size of natural material unit cells were possible, such a metamaterial would not be very interesting as a certain spatial dispersion is needed for the artificial magnetisation and higher order multipoles to contribute significantly, which is the whole purpose of metamaterials.

considerable contributions from Lange and Raab, A.D. Yaghjian and M. Silveirinha among others.

Among the potential applications of metamaterials, there are materials leaving weaker or no electromagnetic traces (given the fancy name of invisibility cloaks). Such an effect is obtained from constructing a metamaterial from which scattering and shadow effects are dramatically reduced as compared to normal materials. Other examples are gradient-index lenses, negative refractive index superlenses with a resolution not limited by the normal diffraction limit, flat lenses that produce highly collimated beams from an embedded antenna or optical source, beam concentrators, polarization rotators and splitters, metamaterials that perfectly absorb electromagnetic radiation and many more [9]. Therefore, there is good reason to study electromagnetic metamaterials not only for the sake of understanding the physics, but also for industrial applications.

In this work, the polarisation model and homogenisation method used are introduced and described in section 2. These must both account for nonlocality as the aim is to model a spatially dispersive medium. More specifically, we want to investigate the electromagnetic behaviour at an interface between such a medium and another, and thus a half-space model must be applied. In works by M. Silveirinha, the half-space model differs slightly in its form from the one applied by Lange and Raab, but in section 3 these are shown to be equivalent. Studying Maxwell's equations for such an interface, boundary conditions for the electric and magnetic fields can be obtained. Furthermore, from the combination of these boundary conditions and an appropriate constitutive relation, the Fresnel equations that govern reflection and refraction can be derived. The method of obtaining the boundary conditions is therefore important. Different methods are used and tested in the sections that follow, and they are largely based on the approaches used by Lange and Raab [10] and Yaghjian and Silveirinha [15]. In the first part of section 4, boundary conditions for media with multipoles to the order of electric-octopole - magnetic-quadrupole are derived in the fashion of Lange and Raab, but where the multipoles are allowed to contain a δ -term to account for surface effects. In the second part, general boundary conditions are derived for a medium with a general polarisation, i.e. for multipole contributions up to an arbitrary order. This is of interest because all spatial dispersive effects to a chosen order would be accounted for, with contributions from all potentially contributing multipoles. In section 4.2 this is done for spatial dispersion to the second order in \mathbf{k} . This approximation is used for the sake of simplicity, but the results obtained would be precise for weakly spatially dispersive media. In section 5, boundary conditions and Fresnel equations are derived for a quadrupolar medium in the fashion of Yaghjian and Silveirinha, but where in addition to the electric quadrupolarisation the medium also exhibits electric and magnetic dipolarisation. Such a medium might be more realistic than a purely quadrupolar medium. Contributions to the second order spatial dispersive effect in that case come from both the magnetic dipolarisation and the electric quadrupolarisa-

tion. In section 6, the attempt in section 4.2 at deriving boundary conditions and Fresnel equations for a general second order spatially dispersive medium is repeated, this time with inspiration from Yaghjian and Silveirinha, but still using the method of Lange and Raab. The findings are then discussed and finally a conclusion is given.

2 Polarisation and Homogenisation of Nonlocal Media

In order to efficiently describe the electromagnetic behaviour of macroscopic media consisting of innumerable charges, one is dependent on a way of averaging out the microscopic field variations that would not contribute significantly to the macroscopic fields. Doing the average renders the macroscopic fields, and this procedure is called a homogenisation method. For normal media, the homogenisation procedure can be carried out as described in Appendix A. As is described at the end of the appendix, the described procedure can also be used for metamaterial media, replacing the normal media unit cell with the metamaterial unit cell. However, this is still only valid under a continuum criterium $d/\lambda \ll 1$, where d is the unit cell dimension. This criterium is described by Yaghjian in [12]. Although it is usually fulfilled for normal media, with unit cell dimensions typically around $d \approx 0.1\text{nm}$ [8, chapter 10.2], for metamaterials the dimension would typically be much larger, even comparable to the wavelength: $d/\lambda \approx 1$ [12]. This causes spatial derivative terms of the electric field to be significant contributions to the polarisation, and therefore the homogenisation theory introduced in Appendix A is generally not adequate. In what follows, we will briefly explain this difference between so-called locality for normal media and nonlocality for spatially dispersive media, and present a current homogenisation theory for nonlocal media as described in [8]. Instead of using the notation of [8] where a capital letter \mathbf{F} is used for microscopic fields and $\langle \mathbf{F} \rangle$ for macroscopic fields, we use instead the notation of [3] where the microscopic fields are denoted by small letters, and the macroscopic fields by capital letters.

For normal polarisable media that are linear, the induced (macroscopic) fields \mathbf{D} and \mathbf{H} at a given point in the medium can be related directly to the macroscopically averaged fields \mathbf{E} and \mathbf{B} (over small volumes of integration) at that same point:

$$\begin{aligned}\mathbf{D}(\mathbf{r}) &= \epsilon_0 \bar{\epsilon}_r \cdot \mathbf{E}(\mathbf{r}) + \sqrt{\epsilon_0 \mu_0} \bar{\boldsymbol{\xi}} \cdot \mathbf{H}(\mathbf{r}) \\ \mathbf{B}(\mathbf{r}) &= \sqrt{\epsilon_0 \mu_0} \bar{\boldsymbol{\zeta}} \cdot \mathbf{E}(\mathbf{r}) + \mu_0 \bar{\boldsymbol{\mu}}_r \cdot \mathbf{H}(\mathbf{r}).\end{aligned}$$

where $\bar{\epsilon}_r$ and $\bar{\boldsymbol{\mu}}_r$ are the relative permittivity and permeability tensors respectively and $\bar{\boldsymbol{\xi}}$ and $\bar{\boldsymbol{\zeta}}$ are the magnetoelectric coupling parameters [8]. If the medium of interest has an inversion symmetry, then the magnetoelectric coupling parameters are zero. If the medium is isotropic as well, then the above equations collapse down to the simpler and often used constitutive relations

$$\begin{aligned}\mathbf{D}(\mathbf{r}) &= \epsilon_0 \epsilon_r \mathbf{E}(\mathbf{r}), \\ \mathbf{B}(\mathbf{r}) &= \mu_0 \mu_r \mathbf{H}(\mathbf{r}).\end{aligned}$$

This one-to-one spatial relation between the induced fields and the source fields is what is meant by the term "local" in the context of homogenisation theory. The locality is possible as for normal media the criterium mentioned above holds, and therefore the spatial variation of the electromagnetic fields over the size of the unit cell is negligible. However, as the ratio of the unit cell dimension to the radiation increases, the importance of the spatial variation increases. A significant spatial variation means that the field values in a neighbourhood around the observation point influence the field value at the observation point, and the medium is said to be "nonlocal". For such a medium, instead of the constitutive relations above, we can write

$$\begin{aligned}D_i &= \epsilon_0 E_i + P_i, \\ H_i &= \frac{1}{\mu_0} B_i,\end{aligned}\tag{7}$$

where

$$\mathbf{P} = \mathbf{P}_{dip} - \nabla \times \frac{1}{i\omega} \bar{\mathbf{M}} + \frac{1}{2} \nabla \cdot \bar{\mathbf{Q}} + \dots$$

In this formulation, all of the polarisation (both electric and magnetic) is included in the definition of the electric response field D_i , and the magnetic field constitutive relation is simply that of vacuum. The first term of \mathbf{P} is the electric dipolarisation, and the second is the magnetic dipolarisation. The third term is the electric quadrupolarisation and the next would be the magnetic quadrupolarisation.

The spatial dispersion of our nonlocal medium is clear from the following expression for the electric response field

$$\mathbf{D}(\mathbf{r}) = \int_V \epsilon_s(\omega, \mathbf{r} - \mathbf{r}') \cdot \mathbf{E}(\mathbf{r}') d^3 \mathbf{r}',$$

where \mathbf{r} is a position vector to an observation point in the medium of interest, \mathbf{r}' is a position vector to an infinitesimal volume within the medium and also the variable of integration and ϵ_s is the space domain electric permittivity accounting for all polarisations. As the Fourier transform of a convolution is simply a product, the equations become simpler in the wave vector domain:

$$\begin{aligned}\tilde{\mathbf{D}} &= \epsilon_0 \tilde{\mathbf{E}} + \tilde{\mathbf{P}} = \epsilon_0 \epsilon(\omega, \mathbf{k}) \cdot \tilde{\mathbf{E}}, \\ \tilde{\mathbf{H}} &= \frac{1}{\mu_0} \tilde{\mathbf{B}},\end{aligned}\tag{8}$$

where the wave vector domain permittivity is given by

$$\epsilon_{ij}(\omega, \mathbf{k}) = I_{ij} + \int_0^\infty \int f_{ij}(\tau, \mathbf{r}) e^{i(\mathbf{k}\cdot\mathbf{r} - \omega\tau)} d^3r d\tau.\tag{9}$$

ϵ_{ij} is a tensor dependent on both the angular frequency and the wave vector [2, chapter 12]. The effective volume of integration is determined by the function $f_{ik}(\tau, \mathbf{r})$, which would typically only be nonzero in some neighbourhood around the observation point. Consequently, the response field at the observation point is dependent on the value of the electric field in this neighbourhood. For most natural materials, the spatial dispersion is a very small effect, negligible compared to the temporal dispersion [2], and the permittivity can be taken as independent of the wave vector. However, for a metamaterial with sizeable inclusions (relative to the wavelength), the spatial dispersion can be significant. This is reasonable as for such a case the electric field associated with the wave would have a significant variation over the length scale of the metamaterial inclusion.

In order for the homogenisation method to be successful, we need to obtain the macroscopic Maxwell equations by some means from the microscopic ones. An efficient way to do this is by Floquet theory. To start off, one can assume the standard microscopic Maxwell equations (98) - (101) given in appendix A. transformed to the frequency-wave vector regime. In order to obtain the macroscopic equations, these equations need to be averaged, so that microscopic variations that do not contribute to the macroscopic scale field variation vanish. As described in the appendix, the spatial and temporal derivatives commute with the averaging integral, and therefore the following can be said to hold

$$\begin{aligned}\nabla \cdot \mathbf{E} &= -\nabla \cdot \mathbf{P}/\epsilon_0, \\ \nabla \cdot \mathbf{B} &= 0, \\ \nabla \times \mathbf{E} &= -i\omega\mathbf{B}, \\ \nabla \times \mathbf{B} &= -i\omega\mu_0\mathbf{P} - i\omega\epsilon_0\mu_0\mathbf{E}.\end{aligned}$$

In the above equations, (5) and (6) have also been used, and the capital letters of the fields signify averaged field quantities. The next step is to find expressions for these averaged fields and the general polarisation \mathbf{P} . Firstly, it is assumed that the microscopic fields \mathbf{e} , \mathbf{b} and \mathbf{j} are such that $\mathbf{f}(\mathbf{r})e^{-i\mathbf{k}\cdot\mathbf{r}}$ is periodic, where \mathbf{f} represents either of the microscopic

fields. This means that the fields can be Fourier expanded in the following way

$$\mathbf{f}(\mathbf{r}) = \sum_{\mathbf{J}} \mathbf{f}_{\mathbf{J}} e^{i\mathbf{k}_{\mathbf{J}} \cdot \mathbf{r}}, \quad (10)$$

where $\mathbf{k}_{\mathbf{J}}$ and $\mathbf{f}_{\mathbf{J}}$ are given as

$$\begin{aligned} \mathbf{k}_{\mathbf{J}} &= \mathbf{k} + \mathbf{k}_{\mathbf{J}}^0, \\ \mathbf{f}_{\mathbf{J}} &= \frac{1}{V_{cell}} \int_{cell} \mathbf{f}(\mathbf{r}) e^{-i\mathbf{k}_{\mathbf{J}} \cdot \mathbf{r}} d^3\mathbf{r}, \\ \text{where } \mathbf{k}_{\mathbf{J}}^0 &= j_1 \mathbf{b}_1 + j_2 \mathbf{b}_2 + j_3 \mathbf{b}_3. \end{aligned}$$

The different \mathbf{b} s are reciprocal unit lattice vectors and the j s are integers. For a general averaging integral over all space

$$\mathbf{F}(\mathbf{r}) = \int \mathbf{f}(\mathbf{r} - \mathbf{r}') f(\mathbf{r}') d^3\mathbf{r}',$$

where \mathbf{f} is a macroscopic field to be averaged and f is the weighting function. Its Fourier transform is

$$\tilde{\mathbf{F}}(\mathbf{k}') = \tilde{\mathbf{f}}(\mathbf{k}') \tilde{f}(\mathbf{k}').$$

The $\tilde{}$ is meant to signify the Fourier transformed quantity. $\tilde{\mathbf{f}}$ can be expressed by taking the Fourier transform of (10),

$$\begin{aligned} (2\pi)^3 \int \mathbf{f}(\mathbf{r}) e^{-i\mathbf{k}' \cdot \mathbf{r}} d^3\mathbf{r} &= (2\pi)^3 \int \sum_{\mathbf{J}} \mathbf{f}_{\mathbf{J}} e^{-i(\mathbf{k}_{\mathbf{J}} - \mathbf{k}') \cdot \mathbf{r}} d^3\mathbf{r}, \\ \tilde{\mathbf{f}}(\mathbf{k}') &= (2\pi)^3 \sum_{\mathbf{J}} \int \mathbf{f}_{\mathbf{J}} e^{-i(\mathbf{k}_{\mathbf{J}} - \mathbf{k}') \cdot \mathbf{r}} d^3\mathbf{r}, \\ &= (2\pi)^3 \sum_{\mathbf{J}} \mathbf{f}_{\mathbf{J}} \delta(\mathbf{k}' - \mathbf{k}_{\mathbf{J}}), \end{aligned}$$

where in the last equation the property

$$\int e^{-i(\mathbf{k}_{\mathbf{J}} - \mathbf{k}') \cdot \mathbf{r}} d^3\mathbf{r} = \delta(\mathbf{k}' - \mathbf{k}_{\mathbf{J}})$$

was used. This leads to the following equation for the averaged field in the wave vector domain,

$$\tilde{\mathbf{F}}(\mathbf{k}') = (2\pi)^3 \sum_{\mathbf{J}} \mathbf{f}_{\mathbf{J}} \delta(\mathbf{k}' - \mathbf{k}_{\mathbf{J}}) \tilde{f}(\mathbf{k}_{\mathbf{J}}),$$

where the argument of \tilde{f} has turned into $\mathbf{k}_{\mathbf{J}}$ as the right hand side only is non-zero for $\mathbf{k}' = \mathbf{k}_{\mathbf{J}}$, as dictated by the δ -function. Now doing the inverse Fourier transform of the equation above, we obtain

$$\mathbf{F}(\mathbf{r}) = \sum_{\mathbf{J}} \left(\mathbf{F}_{\mathbf{J}} \tilde{f}(\mathbf{k}_{\mathbf{J}}) e^{i\mathbf{k}_{\mathbf{J}}\mathbf{r}} \right).$$

The weighting function f is the function that expresses the spatial dependency (or non-locality) of the fields. Typically the dependency only reaches out to the unit cell boundary [8], so that $f \approx 0$ for $|\mathbf{r}| > d$, d being the unit cell dimension. The corresponding Fourier transform \tilde{f} is therefore approximately zero for $|\mathbf{k}| > \pi/d$. This means that $\tilde{f}(\mathbf{k}_{\mathbf{J}}) \approx 0$ for $\mathbf{J} \neq 0$, and provided that \mathbf{k} is close to the Brillouin zone origin we also have $\tilde{f}(\mathbf{k}_{\mathbf{J}}) \approx 1$ for $\mathbf{J} = 0$. In other words, only the zero order Floquet harmonic is significantly contributing to the macroscopic field for a realistic choice of the weighting function. Using this, the inverse Fourier transform above simplifies to

$$\mathbf{F} \approx \mathbf{F}_0 e^{i\mathbf{k}\cdot\mathbf{r}},$$

where \mathbf{F}_0 is the zero order Floquet harmonic amplitude given by

$$\mathbf{F}_0 = \frac{1}{V_{cell}} \int_{cell} \mathbf{F}(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} d^3\mathbf{r}.$$

By the procedure described here, the macroscopic fields \mathbf{E} , \mathbf{B} and \mathbf{J} are derived from the microscopic fields \mathbf{e} , \mathbf{b} and \mathbf{j} . The macroscopic current can be expressed in terms of the general polarisation via the relation (5), and thus we have expressed the terms of the macroscopic Maxwell equations above.

As shown above, \mathbf{k} should be close to zero, and therefore a Taylor expansion of a general permittivity $\epsilon(\omega, \mathbf{k})$ with respect to \mathbf{k} around $\mathbf{k} = 0$ can be made. Doing so renders the expression below [1, section 3.1.2]

$$\epsilon_0 \epsilon_{ij}(\omega, \mathbf{k}) \approx \epsilon_0 \delta_{ij} + \epsilon_0 \chi_{ij} + \zeta_{ijk} k_k + \eta_{ijkl} k_k k_l.$$

Here the the factors ζ and η are derivatives of ϵ , and the expansion is written out to the second order in \mathbf{k} [14]. The reason for this choice is that it is a first approximation to the spatial dispersive effects for all media (of any geometry), as for centro-symmetric geometries, the first order term vanishes. This can be seen from the criterium for centro-symmetry $\epsilon_{ij}(\mathbf{k}) = \epsilon_{ij}(-\mathbf{k})^3$.

³Centro-symmetry could be achieved in a metamaterial structure by e.g. using opposed split-ring resonators.

Now using the definition for the response field (7), we can by comparison with (8) – with ϵ_r inserted from (9) – express the polarisation for our linear, spatially dispersive media (weak as such) as

$$P_i = \epsilon_0 \chi_{ij} E_j + \zeta_{ijk} k_k E_j + \eta_{ijkl} k_k k_l E_j.$$

3 Halfspace Model for Analysis of Interface Behaviour of Waves

An interface between two media can be illustrated as in figure 1. The transition layer is the region of space from the surface of medium two to a distance l within the bulk of the medium. In this region the electromagnetic behaviour changes from that characteristic for the medium of incidence to that of the second medium.

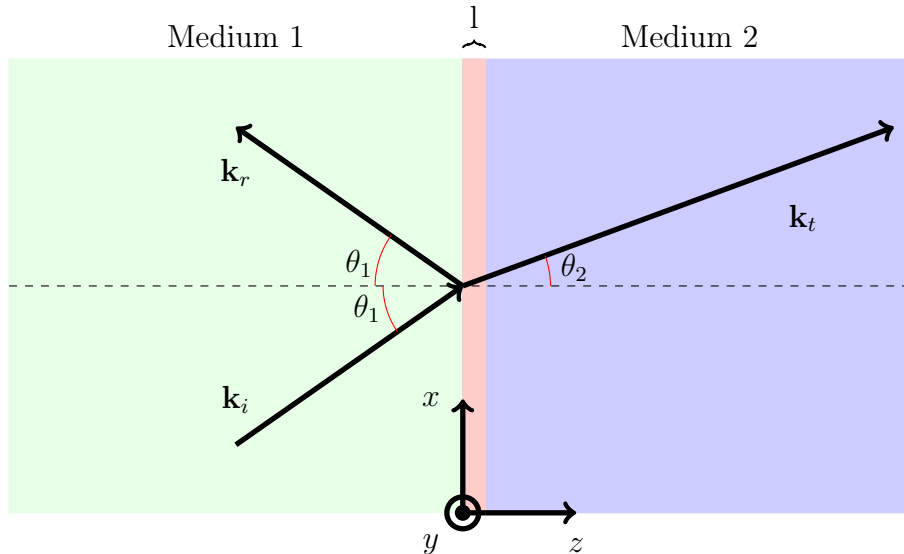


Figure 1: Coordinate system used to model the electromagnetic response across an interface between two media. \mathbf{k}_i and \mathbf{k}_r are the incident and reflected wave vectors respectively, both with an angle θ_1 to the normal. \mathbf{k}_t is the transmitted wave vector with the corresponding refraction angle θ_2 . The transition layer l is the region of space in which the electromagnetic behaviour changes from that characteristic for the medium of incidence (Medium 1) to that of the second medium (Medium 2). For right hand side media with higher order multipole contributions, there might exist additional modes. As is shown in section 5, for a medium with electric quadrupole contribution, there exists an evanescent wave. This mode is confined to the transition layer [12].

For an interface such as that illustrated in figure 1, we want a mathematical model for how the electric fields change across the interface. We expect that for unlike media the electric fields at the different sides of the transition layer are different. Furthermore, we expect this change to be smooth, which is physically reasonable. Thus, demanding that $E_{1,j} = E_{1,j}|_{z=0}$ and $E_{2,j} = E_{2,j}|_{z=l}$ are constants in the transition layer (and otherwise arbitrary functions of z), we can express the net field everywhere as

$$E_j(z) = a(z)E_{1,j} + b(z)E_{2,j}, \quad (11)$$

where $a(z)$ and $b(z)$ are smooth functions. Furthermore, the equation must obey the

following criteria,

$$\begin{aligned} E_j(z=0) &= E_{1,j}, \\ E_j(z=l) &= E_{2,j}. \end{aligned}$$

This formulation complies with the expression for E_j used in [10], as for the limit $l \rightarrow 0$, the criteria above imply that $a(z)$ and $b(z)$ must approach the step functions $u(-z)$ and $u(z)$ respectively. The two field components in (11) are plotted for an arbitrary sine squared form of $a(z)$ and $b(z)$ for illustration.

Writing instead

$$E_j(z) = E_{1,j} + c(z)(E_{2,j} - E_{1,j}), \quad (12)$$

the criteria above can also be met. $c(z)$ is a smooth function obeying the conditions

$$\begin{aligned} c(z=0) &= 0, \\ c(z=l) &= 1. \end{aligned}$$

When the limit $l \rightarrow 0$ is taken, $c(z)$ approaches $u(z)$, and thus equation (12) complies with the formulation of Yaghjian and Silveirinha in [15]. As is seen in this section, the two electric field formulations for the transition layer are equivalent, and the choice of formulation should therefore not affect the expressions of boundary conditions derived using them.

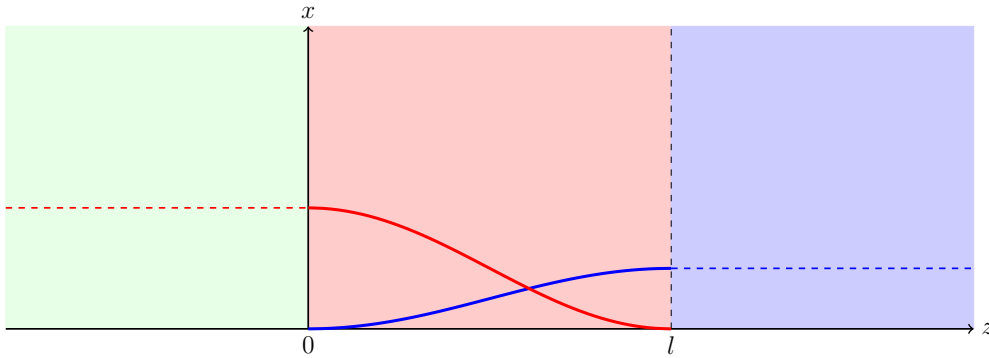


Figure 2: Example plot of the two field components in (11) for an arbitrary sine squared form of $a(z)$ and $b(z)$ (with a $\pi/2$ phase shift between the two functions). The coordinate system is the same as introduced in figure 1 and the same colours represent the same regions of space, but here the transition layer is wider for the sake of illustration. The red curve represents the magnitude of the incident electric field, and the blue the transmitted. These curves are both representing functions that approach step functions (times the factors $E_{1,j}|_{z=0}$ and $E_{2,j}|_{z=l}$, respectively) as the limit $l \rightarrow 0$ is taken. $E_{1,j}|_{z=0}$ and $E_{2,j}|_{z=l}$ represent the values of the electric field at the transition layer boundaries. Note that $E_{1,j}$ is arbitrary (determined by the source and the nature of the medium of incidence) for $z \leq 0$ and similarly for $E_{2,j}$ for $z \geq 0$ in Medium 2.

4 Boundary Conditions for Media with Higher Order Multipoles

4.1 Explicit Polarisation up to Electric Octopole - Magnetic Quadrupole Order, with a δ -term in the Multipoles

Given the charge density ρ^∞ on the form derived in [5],

$$\rho^\infty = -\nabla_i \left(P_i - \frac{1}{2} \nabla_j Q_{ij} + \frac{1}{6} \nabla_j \nabla_k Q_{ijk} + \dots \right),$$

we have an expression for a charge density throughout all of space. However, as we want analyse the electromagnetic behaviour at the boundary of an octopolar medium, we need to modify this expression to be valid for a half-space medium. Rather than just multiplying the multipole moments with the step function $u(z)$, as is done in [10], we allow for the multipole moments to have surface contributions expressed by delta functions to first order. E.g. $P \rightarrow u(z)P + \delta(z)P^{(1)}$, where $P^{(1)}$ is a surface electric dipole. Writing out the terms and grouping them according to the singular functions of increasing order, we obtain for the half-space charge density

$$\begin{aligned} \rho^{\infty/2} = u(z)\rho^\infty - \delta(z) & \left[P_z + \nabla_i P_i^{(1)} - \nabla_i P_i^{(1)} - \nabla_i Q_{iz} - \frac{1}{2} \nabla_i \nabla_j Q_{ij}^{(1)} + \frac{1}{2} \nabla_i \nabla_j Q_{ijz} \right. \\ & \left. + \frac{1}{6} \nabla_i \nabla_j \nabla_k Q_{ijk}^{(1)} \right] + \delta'(z) \left[-P_z^{(1)} + \frac{1}{2} Q_{zz} - \nabla_i Q_{iz}^{(1)} - \frac{1}{2} \left(\nabla_i Q_{izz} + \nabla_i \nabla_j Q_{ijz}^{(1)} \right) \right] \\ & - \delta''(z) \left[-\frac{1}{2} Q_{zz}^{(1)} + \frac{1}{6} Q_{zzz} + \frac{1}{2} \nabla_i Q_{izz}^{(1)} \right] + \delta'''(z) Q_{zzz}^{(1)}. \end{aligned} \quad (13)$$

Equation (13) corresponds to and contains all the terms of equation (5) in [10]. The new terms in the equation above are the surface terms marked by a superscript. Similarly, a new expression for the current density \mathbf{J} can be obtained, and its expression can be found in Appendix B.

As multipoles of order up to the electric octopole - magnetic quadrupole is of concern here, the following expressions for the electric and induction fields are used:

$$\mathbf{E} = u(-z)\mathbf{E}_1 + u(z)\mathbf{E}_2 + \delta(z)\mathbf{E}^{(1)} + \delta(z)\mathbf{E}^{(2)} + \delta'(z)\mathbf{E}^{(3)}, \quad (14)$$

$$\mathbf{B} = u(-z)\mathbf{B}_1 + u(z)\mathbf{B}_2 + \delta(z)\mathbf{B}^{(1)} + \delta(z)\mathbf{B}^{(2)}. \quad (15)$$

The reason for this specific number of terms in the expressions for the fields is that the δ and δ -derivatives terms should match the highest order δ -derivative terms in the charge density ρ and current density \mathbf{J} as dictated by the multipole order. For e.g. the dipole order, a δ in \mathbf{E} would entail an uncompensated δ -derivative term in Gauss' law

and Faraday's law [10], which is easily seen if the Maxwell equations are written out explicitly. The \mathbf{B} -field has one less term than the \mathbf{E} field as otherwise there would be an uncompensated \mathbf{B} -field term in Ampère's law.

Having thus all the expressions for \mathbf{E} , \mathbf{B} , ρ and \mathbf{J} , we can express the left hand sides of Maxwell's equations ((1)-(4)). The left hand side of (1) becomes

$$\begin{aligned} \delta(z) & \left[E_{2z} - E_{1z} + \nabla_i E_i^{(1)} + \frac{1}{\epsilon_0} \left(P_z + \nabla_i P_i^{(1)} - \nabla_i Q_{iz} - \frac{1}{2} \nabla_i \nabla_j Q_{ij}^{(1)} + \frac{1}{2} \nabla_i \nabla_j Q_{ijz} + \frac{1}{6} \nabla_i \nabla_j \nabla_k Q_{ijk}^{(1)} \right) \right] \\ & + \delta'(z) \left[E_z^{(1)} + \nabla_i E_i^{(2)} - \frac{1}{\epsilon_0} \left(-P_z^{(1)} + \frac{1}{2} Q_{zz} + \nabla_i Q_{iz}^{(1)} - \frac{1}{2} [\nabla_i Q_{izz} + \nabla_i \nabla_j Q_{ijz}^{(1)}] \right) \right] \\ & \delta''(z) \left[E_z^{(2)} + \frac{1}{\epsilon_0} \left(-\frac{1}{2} Q_{zz}^{(1)} + \frac{1}{6} Q_{zzz} + \frac{1}{2} \nabla_i Q_{izz}^{(1)} \right) \right] - \delta'''(z) \frac{1}{\epsilon_0} Q_{zzz}^{(1)}. \end{aligned} \quad (16)$$

The equivalent expressions for equations (2)-(4) can be found in Appendix C. With our new expressions for the left hand sides of (1)-(4), we see that we have equations on the form

$$\delta(z)f(x, y, z, t) + \delta'(z)g(x, y, z, t) + \delta''(z)h(x, y, z, t) + \delta'''(z)i(x, y, z, t) = 0. \quad (17)$$

Taking the integral of equation (17) with respect to z results in the condition

$$f_0 - (\nabla_z g)_0 + (\nabla_z^2 h)_0 - (\nabla_z^3 i)_0 = 0. \quad (18)$$

Taking instead the second order derivative of the left hand side (LHS) of equation (17) with respect to x , multiplied with z^2 , and taking the integral of this with respect to z results in the constraint

$$\begin{aligned} \int \nabla_x^2 \text{LHS}(17) z^2 dz & = (\nabla_x^2 h)_0 + 2(\nabla_z \nabla_x^2 i)_0 = 0 \\ \text{so } (\nabla_x^2 h)_0 & = -2(\nabla_z \nabla_x^2 i)_0. \end{aligned} \quad (19)$$

Subjecting (16) to the constraint (18), we obtain an expression for $E_{2z} - E_{1z}$ in terms of multipole and E -field terms. To arrive at an expression solely consisting of multipole terms, consider equation (116) on the form of (17). For this Maxwell equation, the i -term is zero, and taking the integral of the derivative of LHS(17) with respect to x , times z , with respect to z gives the constraint

$$\begin{aligned} \int \nabla_x \text{LHS}(17) z dz & = (\nabla_x g)_0 - 2(\nabla_z \nabla_x h)_0 = 0, \\ \text{so } (\nabla_x g)_0 & = 2(\nabla_z \nabla_x h)_0. \end{aligned} \quad (20)$$

Subjecting (116) to (20), and inserting into the expression for $E_{2z} - E_{1z}$, there are only two E -field terms left. These can be expressed in terms of multipoles by subjecting (16) to the constraint (19), rendering our expression for $E_{2z} - E_{1z}$ only in terms of multipoles. Thus, the first boundary condition is obtained as

$$\begin{aligned}
E_{2z} - E_{1z} = & -\frac{1}{\epsilon_0} \left[P_z + \nabla_x P_x^{(1)} + \nabla_y P_y^{(1)} - \left(\nabla_x Q_{xz} + \nabla_y Q_{yz} + \frac{1}{2} \nabla_z Q_{zz} \right) \right. \\
& \left. + \frac{1}{2} \left(\nabla_x^2 Q_{zz}^{(1)} + \nabla_y^2 Q_{zz}^{(1)} - \nabla_x^2 Q_{xx}^{(1)} - \nabla_y^2 Q_{yy}^{(1)} \right) - \nabla_x \nabla_y Q_{xy}^{(1)} \right. \\
+ \frac{1}{2} \left(\nabla_x^2 Q_{xxz} + \nabla_y^2 Q_{yyz} - \frac{1}{3} \left(\nabla_x^2 + \nabla_y^2 - \nabla_z^2 \right) Q_{zzz} + 2 \nabla_x \nabla_y Q_{xyz} + \nabla_x \nabla_z Q_{xzz} + \nabla_y \nabla_z Q_{yzz} \right) \\
& + \frac{1}{6} \nabla_i \nabla_j \nabla_k Q_{ijk}^{(1)} + \frac{1}{2} \left(\nabla_z^2 \nabla_i Q_{izz}^{(1)} - \nabla_x^2 \nabla_i Q_{izz}^{(1)} - \nabla_y^2 \nabla_i Q_{izz}^{(1)} - \nabla_z \nabla_i \nabla_j Q_{ijz}^{(1)} \right) \\
& \left. + 2 \left(\nabla_z \nabla_x^2 Q_{zzz}^{(1)} + \nabla_z \nabla_y^2 Q_{zzz}^{(1)} \right) + \nabla_z^3 Q_{zzz}^{(1)} \right].
\end{aligned}$$

The other five boundary conditions are found by deriving constraints similar to (19) and (20), and applying the constraints to the appropriate Maxwell equations on the form of (17) (equations ((16), (116), (117) and (118))). The boundary conditions can be found in Appendix D. Note that the terms in the boundary conditions (24)-(29) of [10] are also found in the boundary conditions derived here, but that in here there are additional terms due to the new delta term of the multipole expressions.

4.2 General Polarisation

4.2.1 Derivation of Boundary Conditions

Assuming smooth electric field variation over a transition layer $[0, l]$, in which the fields' behaviour change from that of the incident medium to that of the other medium, we have a case as that illustrated in figure 1 and 2. Assuming now that $l \rightarrow 0$, the fields' variation at the interface is described by step functions. As opposed to in the previous section, the following set of definitions for \mathbf{P} , \mathbf{E} , \mathbf{B} , \mathbf{J} and ρ are used,

$$P_i = u(-z)P_{1,i} + u(z)P_{2,i} + \delta(z)P_i^{(1)} + \delta'(z)P_i^{(2)}, \quad (21)$$

$$E_i = u(-z)E_{1,i} + u(z)E_{2,i}, \quad (22)$$

$$B_i = u(-z)B_{1,i} + u(z)B_{2,i} + \delta(z)B_i^{(1)},$$

$$J_i = \dot{P}_i,$$

$$\rho = -\nabla_i P_i.$$

The motivation for using these definitions is that this way leads to cleaner and more transparent calculations, and to let the general polarisation account for weak spatial dispersion. This is an effect due to the polarisation's dependency on the second order spatial derivative of the electric field as described in section 2, and contributions to this second order effect may come from higher order multipoles in addition to the electric quadrupole and magnetic dipole. Similarly to in the previous section, the reason for the different number of orders in the singular functions of the expressions is due to the nature of the Maxwell equations and that singular functions in the fields should be compensated by singular terms of the same order in other fields or sources. Consequently, the polarisation needs singular terms of one and two orders of differentiation higher than that of the electric field. Also, from (2) it can be seen that the induction field needs a term one order of differentiation higher than the electric field. The model of [10] is used where two separate step functions are used to describe the electric field on each side of the interface.

The left hand sides of Maxwell's equations (1)-(4) thus become

$$\begin{aligned} \nabla \cdot \mathbf{E} - \frac{1}{\epsilon_0} \rho &= \delta(z) \left(E_{2z} - E_{1z} + \frac{1}{\epsilon_0} \left[P_{2z} - P_{1z} + \nabla_i P_i^{(1)} \right] \right) \\ &+ \delta'(z) \frac{1}{\epsilon_0} \left(P_z^{(1)} + \nabla_i P_i^{(2)} \right) + \delta''(z) \frac{1}{\epsilon_0} P_z^{(2)}, \end{aligned} \quad (23)$$

$$\nabla \times \mathbf{E} + \dot{\mathbf{B}} = \delta(z) \left(-E_{2y} + E_{1y} + \dot{B}_x^{(1)}; E_{2x} - E_{1x} + \dot{B}_y^{(1)}; \dot{B}_z^{(1)} \right), \quad (24)$$

$$\nabla \cdot \mathbf{B} = \delta(z) \left(B_{2z} - B_{1z} + \nabla_i B_i^{(1)} \right) + \delta'(z) B_z^{(1)}, \quad (25)$$

$$\begin{aligned} \nabla \times \mathbf{B} - \mu_0 \mathbf{J} - \mu_0 \epsilon_0 \dot{\mathbf{E}} = & \delta(z) \left(-B_{2y} + B_{1y} + \nabla_y B_z^{(1)} - \nabla_z B_y^{(1)} - \mu_0 \dot{P}_x^{(1)}; \right. \\ & B_{2x} - B_{1x} + \nabla_z B_x^{(1)} - \nabla_x B_z^{(1)} - \mu_0 \dot{P}_y^{(1)}; \nabla_x B_y^{(1)} - \nabla_y B_x^{(1)} - \mu_0 \dot{P}_z^{(1)} \left. \right) \\ & + \delta'(z) \left(-B_y^{(1)} - \mu_0 \dot{P}_x^{(2)}; B_x^{(1)} - \mu_0 \dot{P}_y^{(2)}; -\mu_0 \dot{P}_z^{(2)} \right). \end{aligned} \quad (26)$$

Using the same approach as that indicated in 4.1, boundary conditions can be derived from Maxwell's equations (1)-(4) with the left hand sides expressed as in (23)-(26) above, rendering

$$\begin{aligned} E_{2x} - E_{1x} &= \mu_0 \ddot{P}_x^{(2)}, \\ E_{2y} - E_{1y} &= \mu_0 \ddot{P}_y^{(2)}, \\ E_{2z} - E_{1z} &= -\frac{1}{\epsilon_0} \left(P_{2z} - P_{1z} + \nabla_x P_x^{(1)} + \nabla_y P_y^{(1)} - \nabla_z \left[\nabla_x P_x^{(2)} + \nabla_y P_y^{(2)} \right] \right), \\ B_{2x} - B_{1x} &= \mu_0 \left(\dot{P}_y^{(1)} - \nabla_z \dot{P}_y^{(2)} \right) \\ B_{2y} - B_{1y} &= -\mu_0 \left(\dot{P}_x^{(1)} - \nabla_z \dot{P}_x^{(2)} \right) \\ B_{2z} - B_{1z} &= -\mu_0 \left(\nabla \times \dot{\mathbf{P}}^{(2)} \right)_z. \end{aligned}$$

Assuming that our medium is linear and exhibits weak spatial dispersion, the general polarisation can be expressed as

$$P_i = \epsilon_0 \chi_{ij} E_j + \zeta_{ikj} k_k E_j + \eta_{iklj} k_k k_l E_j. \quad (27)$$

This expression comes from a series expansion of the permittivity tensor as described in section 2.

In order to isolate the second order contribution to the spatial dispersion, centro-symmetric inclusions can be assumed in the bulk of the medium. This causes the first order term in \mathbf{k} of equation (27) to be zero, as the polarisation should not change for the transformation $\mathbf{P}(\mathbf{k}) \rightarrow \mathbf{P}(-\mathbf{k})$. The new expression for the polarisation therefore becomes

$$P_i = \epsilon_0 \chi_{ij} E_j - \eta_{iklj} \nabla_k \nabla_l E_j, \quad (28)$$

where the property $\nabla_i = ik_i$ of our plane wave electric field is used. In order to model our

half-space medium, we insert our expression for the electric field (22) into this expression and define $\chi_{ij} = u(-z)\theta_{ij} + u(z)O_{ij}$ and $\eta_{iklj} = u(-z)\gamma_{iklj} + u(z)\zeta_{iklj}$. For the case where the left hand side medium is vacuum, θ_{ij} and γ_{iklj} would be zero, but that is not assumed here for the sake of generality. Grouping the resulting terms in singular functions leads to the expression

$$\begin{aligned} P_i &= u(-z)\left(\epsilon_0\theta_{ij} - \gamma_{iklj}\nabla_k\nabla_l\right)E_{1,j} + u(z)\left(\epsilon_0O_{ij} - \zeta_{iklj}\nabla_k\nabla_l\right)E_{2,j} \\ &+ \delta(z)u(-z)2\gamma_{ikzj}\nabla_k(E_{1,j} - E_{2,j}) + \delta'(z)u(-z)\gamma_{izzj}(E_{1,j} - E_{2,j}). \\ &+ \delta(z)u(z)2\zeta_{ikzj}\nabla_k(E_{1,j} - E_{2,j}) + \delta'(z)u(z)\zeta_{izzj}(E_{1,j} - E_{2,j}). \end{aligned} \quad (29)$$

Comparing this expression with the one in (21), it is clear that $P_{1,i}$ and $P_{2,i}$ are as given below in (34) and (35). Expressions for $P_i^{(1)}$ and $P_i^{(2)}$ can be found by equating the integrals of (21) and (29) with respect to z over some range $[-l, l]$ containing the interface plane $z = 0$. As the two first terms in (29) are already identified as the two first terms in (21), these terms can be left out. Doing this calculation, using the convention that $u(0) = 1/2$, results in an equation

$$\begin{aligned} P_i^{(1)} - \nabla_z P_i^{(2)} &= (\gamma_{ikzj} + \zeta_{ikzj})\nabla_k(E_{1,j} - E_{2,j}) - \int \delta(z)\frac{d}{dz}\left[u(-z)\gamma_{izzj}(E_{1,j} - E_{2,j})\right]dz \\ &\quad - \int \delta(z)\frac{d}{dz}\left[u(z)\gamma_{izzj}(E_{1,j} - E_{2,j})\right]dz \end{aligned} \quad (30)$$

$$\begin{aligned} &= \int \delta^2(z)(\gamma_{izzj} - \zeta_{izzj})(E_{1,j} - E_{2,j})dz + (\gamma_{ikzj} + \zeta_{ikzj})\nabla_k(E_{1,j} - E_{2,j}) \\ &\quad - \frac{1}{2}(\gamma_{izzj} + \zeta_{izzj})\nabla_z(E_{1,j} - E_{2,j}) \end{aligned} \quad (31)$$

$$= \left[(\gamma_{ixzj} + \zeta_{ixzj})\nabla_x + \frac{1}{2}(\gamma_{izzj} + \zeta_{izzj})\nabla_z\right](E_{1,j} - E_{2,j}). \quad (32)$$

In (30), the first term is obtained directly from the integrals in (29) with a δ -function in the integrand, whereas the second and the last terms are obtained from a partial integration of the terms in (29) with a $\delta'(z)$ -function. Evaluating the latter ones gives the first and the last term of (31), and from the first term we must have that

$$(\gamma_{izzj} - \zeta_{izzj})(E_{2,j} - E_{1,j}) = 0, \quad (33)$$

otherwise the integral would be infinite. Using the final form (32), we can define $P_i^{(1)}$ and $P_i^{(2)}$ as in the following set of definitions;

$$P_{1,i} = \left(\epsilon_0 \theta_{ij} - \gamma_{iklj} \nabla_k \nabla_l \right) E_{1,j}, \quad (34)$$

$$P_{2,i} = \left(\epsilon_0 O_{ij} - \zeta_{iklj} \nabla_k \nabla_l \right) E_{2,j}, \quad (35)$$

$$P_i^{(1)} = -(\gamma_{ixzj} + \zeta_{ixzj}) \nabla_x (E_{2,j} - E_{1,j}), \quad (36)$$

$$P_i^{(2)} = \frac{1}{2} (\gamma_{izzj} + \zeta_{izzj}) (E_{2,j} - E_{1,j}). \quad (37)$$

Using these expressions, the phase matching condition $\nabla_x = ik_x$ and the criterion (33) from above the boundary conditions can be expressed as

$$E_{2x} - E_{1x} = \frac{1}{2} \mu_0 (\gamma_{xzzj} - \zeta_{xzzj}) (\ddot{E}_{2,j} - \ddot{E}_{1,j}) = 0, \quad (38)$$

$$E_{2y} - E_{1y} = \frac{1}{2} \mu_0 (\gamma_{yzzj} - \zeta_{yzzj}) (\ddot{E}_{2,j} - \ddot{E}_{1,j}) = 0, \quad (39)$$

$$\begin{aligned} E_{2z} - E_{1z} = & -\frac{1}{\epsilon_0} \left(\left[\epsilon_0 O_{zj} - \zeta_{zklj} \nabla_k \nabla_l \right] E_{2,j} - \left[\epsilon_0 \theta_{zj} - \gamma_{zklj} \nabla_k \nabla_l \right] E_{1,j} \right. \\ & - \left[(\gamma_{xxzj} + \zeta_{xxzj}) \nabla_x^2 + (\gamma_{yxzj} + \zeta_{yxzj}) \nabla_x \nabla_y \right. \\ & \left. \left. + \frac{1}{2} (\gamma_{xzzj} + \zeta_{xzzj}) \nabla_x \nabla_z + \frac{1}{2} (\gamma_{yzzj} + \zeta_{yzzj}) \nabla_y \nabla_z \right] (E_{2,j} - E_{1,j}) \right), \end{aligned} \quad (40)$$

$$B_{2x} - B_{1x} = -\mu_0 \left((\gamma_{yxzj} + \zeta_{yxzj}) \nabla_x + \frac{1}{2} (\gamma_{yzzj} + \zeta_{yzzj}) \nabla_z \right) (\dot{E}_{2,j} - \dot{E}_{1,j}), \quad (41)$$

$$B_{2y} - B_{1y} = \mu_0 \left((\gamma_{xxzj} + \zeta_{xxzj}) \nabla_x + \frac{1}{2} (\gamma_{xzzj} + \zeta_{xzzj}) \nabla_z \right) (\dot{E}_{2,j} - \dot{E}_{1,j}), \quad (42)$$

$$B_{2z} - B_{1z} = \frac{1}{2} \mu_0 \left((\gamma_{xzzj} + \zeta_{xzzj}) \nabla_y \right) (\dot{E}_{2,j} - \dot{E}_{1,j}). \quad (43)$$

4.2.2 Comparison with the Boundary Conditions of Yaghjian and Silveirinha

In [15], Yaghjian and Silveirinha analyse the case of a purely quadrupolar half-space in vacuum, with its interface being the plane $z = 0$ and the plane of incidence the xz -plane. An incident plane wave of transverse magnetic polarisation is assumed, implying that the induction field only has a nonzero y -component: $\mathbf{B}_1 = [0, B_{1y}, 0]$ and the electric field only has nonzero x - and z -components: $\mathbf{E}_1 = [E_{1x}, 0, E_{1z}]$. Furthermore, there is no variation in the y -direction, so spatial derivatives of the fields with respect to y are all zero. As the medium of incidence is vacuum, $\theta_{ij} = 0$ and $\gamma_{iklj} = 0$ in (38)-(43), and the fact that there are no electric dipoles in the quadrupolar medium means that $O_{ij} = 0$. Using this, the tangential boundary conditions (38)-(43) become

$$E_{2x} - E_{1x} = -\frac{1}{2}\zeta_{xzzj}(\ddot{E}_{2,j} - \ddot{E}_{1,j}) = 0, \quad (44)$$

$$E_{2y} - E_{1y} = 0,$$

$$B_{2x} - B_{1x} = 0,$$

$$B_{2y} - B_{1y} = \mu_0 \left(\zeta_{xzzz} \nabla_x (\dot{E}_{2z} - \dot{E}_{1z}) + \frac{1}{2} \zeta_{xzzx} \nabla_z (\dot{E}_{2x} - \dot{E}_{1x}) \right). \quad (45)$$

(44) becomes zero due to the criterium (33) (the temporal periodicity of the electric fields means the temporal derivatives only amount to a linear scaling). Assuming that $E_{2z} - E_{1z} \neq 0$, the same criterium gives $\zeta_{izzz} = 0$. The corresponding tangential boundary conditions derived in [15] are

$$E_{2x} - E_{1x} = 0, \quad (46)$$

$$E_{2y} - E_{1y} = 0,$$

$$B_{2x} - B_{1x} = 0,$$

$$B_{2y} - B_{1y} = -\frac{i\omega\mu_0}{2} \hat{\mathbf{z}} \times (\hat{\mathbf{z}} \cdot \bar{\mathbf{Q}}^2) = \frac{\mu_0}{4} (\nabla_x \dot{E}_{2z} + \nabla_z \dot{E}_{2x}), \quad (47)$$

where the right hand side (47) is obtained using the definition for $\bar{\mathbf{Q}}$ introduced in Silveirinha and Yaghjian's article (and motivated in [13]):

$$\bar{\mathbf{Q}} = \alpha_Q \epsilon_0 \left[\frac{1}{2} (\nabla \mathbf{E} + \mathbf{E} \nabla) - \frac{1}{3} (\nabla \cdot \mathbf{E}) \bar{\mathbf{I}} \right]. \quad (48)$$

The term $\mathbf{E} \nabla$ is meant to signify the transpose of the tensor $\nabla \mathbf{E}$. As can be observed, the general boundary condition (45) cannot express the specific boundary condition (47) of Silveirinha and Yaghjian.

5 Boundary Conditions and Fresnel Equations for a Realistic Quadrupolar Medium

5.1 Fresnel Equations

In [15], Yaghjian and Silveirinha find boundary conditions for a hypothetical material exhibiting only electric quadrupolarisation and no magnetisation, placed in vacuum. In this section we apply their approach for finding the boundary conditions for a TM polarised wave incident on a quadrupolar medium also exhibiting electric and magnetic dipolarisation. This means that instead of having a total polarisation $\mathbf{P} = -(\nabla \cdot \bar{\mathbf{Q}})/2$, we have a total polarisation

$$\mathbf{P} = \left(\epsilon_0 \chi_e + \frac{(1 - \mu_r^{-1})}{\omega^2 \mu_0} \nabla \times \nabla \times \right) \mathbf{E} - \frac{1}{2} \nabla \cdot \bar{\mathbf{Q}}, \quad (49)$$

where the dipolarisation is accounted for by the first term, the magnetisation by the second and the quadrupolarisation is expressed in the third term as in [15] (the definition of $\bar{\mathbf{Q}}$ can also be found in the previous section, equation (48)). With the magnetisation accounted for in the polarisation, the magnetic field is given as for vacuum,

$$\mathbf{H} = \frac{\mathbf{B}}{\mu_0}.$$

The second term of the polarisation above comes from defining the total polarisation of the medium as consisting of an electric and a magnetic part, as is done in [14], equation (17). To arrive at the form above, one can use the definition $\mathbf{M} = (\mu_r - 1)\mathbf{H} = (1 - \mu_r^{-1})\mathbf{B}/\mu_0$, and substitute for \mathbf{B} using the Maxwell equation (2). The polarisation above holds of course only for the multipole medium, which is denoted by a superscript ² in the rest of this section. For the vacuum side, there is no polarisation as there are no polarisable entities. The superscript ¹ refers to the vacuum side.

Now combining the two Maxwell curl equations ((2) and (4)), one obtains

$$\frac{1}{\mu_r} \nabla \times \nabla \times \mathbf{E} - k_0^2 \left(\epsilon_r \mathbf{E} - \frac{1}{2} \nabla \cdot \bar{\mathbf{Q}} / \epsilon_0 \right) = 0. \quad (50)$$

Substituting $\bar{\mathbf{Q}}$ with $\bar{\mathbf{Q}}_0$ from [15] (which is simply defined as $\bar{\mathbf{Q}}$ multiplied with the step function), ϵ_r with $1 + u(z)\chi_e$ and μ_r with $1 + u(z)\chi_m$, we get instead the combined curl equation for the whole system

$$\frac{1}{1 + u(z)\chi_m} \nabla \times \nabla \times \mathbf{E} - k_0^2 \left([1 + u(z)\chi_e] \mathbf{E} - \frac{1}{2} \nabla \cdot \bar{\mathbf{Q}}_0 / \epsilon_0 \right) = 0. \quad (51)$$

The step functions associated with the permittivity and permeability terms in (51) are here taken to be "normal" step functions, abruptly going from 0 to 1 at $z = 0$. This is in contrast to the step function in $\bar{\mathbf{Q}}_0$, defined to smoothly increase from 0 to 1 over the transition layer. Using these normal step functions amounts to assuming that the electric and magnetic dipole effects really can be said to change abruptly at the interface. However, this assumption is not evidently valid as is discussed in section 7.

Taking the integral of the x -component of this equation times z over the transition layer, we get the following

$$\int_0^l \text{LHS}(51)_x z dz = -k_0^2 \epsilon_r \int_0^l E_x z dz - \frac{1}{\mu_r} \left(\int_0^l (\nabla_z^2 E_x) z dz - ik_0 \int_0^l (\nabla_z E_z) z dz \right) + \frac{1}{2} \omega^2 \mu_0 \int_0^l (\nabla \cdot \bar{\mathbf{Q}}_0)_x z dz,$$

where the dipolarisation is accounted for in the first term. This integral is the same as that in [15] (equation (40)), except for the factors ϵ_r and μ_r here. The first and the third integrals above will contain the factor l when evaluated (using integration by parts), and as $l \rightarrow 0$ they become zero. Only the second and the last integral survives, giving similarly to what is obtained in [15] that

$$\left(\frac{1}{8} k_0^2 \alpha_Q - \mu_r^{-1} \right) (E_x^2 - E_x^1) = 0. \quad (52)$$

The second term in the first parentheses was 1 in [15], as there a magnetisation was not considered. The equation above is implying the boundary condition

$$E_x^2 - E_x^1 = 0.$$

In the same fashion, it can be shown that also the additional boundary condition of [15],

$$Q_{zz} = 0, \quad (53)$$

does not change for our case.

On the other hand, the last boundary condition does change. In [15], the derivation of the induction field boundary condition is carried out with Ampère's law as the starting point. We will now use their derivation for showing how the boundary condition becomes for our case which includes dipolarisations. The form of Ampère's law for our case is

$$\nabla \times \mathbf{B} + i\omega \epsilon_0 \epsilon_r \mu_0 \mathbf{E} - \frac{1}{2} i\omega \mu_0 \nabla \cdot \bar{\mathbf{Q}}_0 + \frac{i(1 - \mu_r^{-1})}{\omega} \nabla \times \nabla \times \mathbf{E} = 0. \quad (54)$$

In order for the calculation to be as simple as possible, the last term of the left hand side above can be rewritten as

$$-(1 - \mu_r^{-1})\nabla \times \mathbf{B},$$

using (2). Equation (54) then becomes

$$\frac{1}{\mu_r}\nabla \times \mathbf{B} + i\omega\epsilon_0\epsilon_r\mu_0\mathbf{E} - \frac{1}{2}i\omega\mu_0\nabla \cdot \bar{\mathbf{Q}}_0 = 0.$$

By doing this, we have effectively moved the magnetic dipole contribution from the total polarisation to a responsefield $\mathbf{H} = \mathbf{B}/\mu_0\mu_r$. Now taking the integral of the x -component of this equation with respect to z over the transition layer, we obtain almost the same equation as in [15] (equation (45)), with the difference being the factor μ_r in the denominator of the $B_y^{(2)}$ -term:

$$\frac{1}{\mu_0}\left(\frac{B_y^{(2)}}{\mu_r} - B_y^{(1)}\right) = -\frac{1}{2}i\omega\epsilon_0\alpha_Q\left(\frac{1}{2}\nabla_z E_x^{(2)} + \frac{1}{2}ik_{0x}E_z^{(2)} - \frac{1}{6}ik_{0x}(E_z^{(2)} - E_z^{(1)})\right). \quad (55)$$

Another expression for the difference $\frac{B_y^{(2)}}{\mu_r} - B_y^{(1)}$ can be obtained from taking the difference between the magnetic fields on each side of the transition layer, expressed using (2):

$$\begin{aligned} H_y^{(2)} - H_y^{(1)} &= \frac{1}{\mu_0}\left(\frac{B_y^{(2)}}{\mu_r} - B_y^{(1)}\right) = \frac{1}{i\omega\mu_0}\left(\nabla_z E_x^{(2)} - \nabla_z E_x^{(1)} - ik_{0x}(E_z^{(2)} - E_z^{(1)})\right), \\ \text{so that } i\omega\left(\frac{B_y^{(2)}}{\mu_r} - B_y^{(1)}\right) &= \nabla_z E_x^{(2)} - \nabla_z E_x^{(1)} - ik_{0x}(E_z^{(2)} - E_z^{(1)}). \end{aligned} \quad (56)$$

Inserting (55) into (56), the following equation can be obtained after some algebra

$$\nabla_z E_x^{(2)} - \nabla_z E_x^{(1)} - ik_{0x}(E_z^{(2)} - E_z^{(1)}) = \frac{k_0^2\alpha_Q}{4}\left(\nabla_z E_x^{(2)} + ik_{0x}\left[E_z^{(2)} - \frac{1}{3}(E_z^{(2)} - E_z^{(1)})\right]\right). \quad (57)$$

The left hand side of this equation is now equal to the right hand side of (56), so by substituting our left side for (56)'s left, we obtain the following boundary condition for the induction field

$$\frac{B_y^{(2)}}{\mu_r} - B_y^{(1)} = -\frac{ik_0^2\alpha_Q}{4\omega}\left(\nabla_z E_x^{(2)} + ik_{0x}\left[E_z^{(2)} - \frac{1}{3}(E_z^{(2)} - E_z^{(1)})\right]\right). \quad (58)$$

It is straight forward to show that neglecting the latter term of (57), as is done in [15], we would instead have gotten the boundary condition

$$\frac{B_y^{(2)}}{\mu_r} - B_y^{(1)} = -\frac{i\omega\mu_0}{2}\mathbf{z} \times (\mathbf{z} \cdot \bar{\mathbf{Q}}^{(2)}) \cdot \mathbf{y},$$

which is identical to what is derived in [15], except for the factor μ_r in the denominator of the $B_y^{(2)}$ -term.

Having obtained the boundary conditions, we can now proceed to derive the Fresnel equations governing reflection and refraction. To do this, we need to know what kinds of modes are present in the bulk of the multipole medium. In that region, $\epsilon_r = (1 + \chi_e)$, $\mu_r = (1 + \chi_m)$ and instead of $\bar{\mathbf{Q}}_0$ we can use $\bar{\mathbf{Q}}$ as defined in equation (48)(or equation (9) of [15]). With these changes, and applying the identity

$$\nabla \times (\nabla \times \mathbf{A}) = \nabla(\nabla \cdot \mathbf{A}) - \nabla^2 \mathbf{A}, \quad (59)$$

where \mathbf{A} is a general vector, to equation (51) and then taking the cross product of the resulting equation with \mathbf{E} , we get

$$\frac{1}{\mu_r} \left[\nabla(\nabla \cdot \mathbf{E}) \times \mathbf{E} - (\nabla^2 \mathbf{E}) \times \mathbf{E} \right] - k_0^2 \epsilon_r \mathbf{E} \times \mathbf{E} + \frac{1}{2} \frac{k_0^2}{\epsilon_0} (\nabla \cdot \bar{\mathbf{Q}}) \times \mathbf{E} = 0. \quad (60)$$

For phase matching along the x -axis of the waves on each side of the interface, we have $\nabla_x \mathbf{E} = ik_x \mathbf{E}$. As we also have periodic variation of the electric field in the z -direction, $(\nabla^2 \mathbf{E}) \parallel \mathbf{E}$, and we can write $(\nabla^2 \mathbf{E}) \times \mathbf{E} = 0$. Furthermore, using the definition of the quadrupole moment $\bar{\mathbf{Q}}$, we have that the last term can be rewritten in the following way

$$\frac{1}{2} \frac{k_0^2}{\epsilon_0} (\nabla \cdot \bar{\mathbf{Q}}) \times \mathbf{E} = \frac{1}{2} \alpha_Q k_0^2 \left(\frac{1}{6} (\nabla \cdot \mathbf{E}) (\nabla \times \mathbf{E}) \right).$$

Using this, equation (60) becomes

$$\frac{1}{\mu_r} (\nabla \times \mathbf{E}) (\nabla \cdot \mathbf{E}) - \frac{1}{\mu_r} (\nabla \cdot \nabla) (\mathbf{E} \times \mathbf{E}) - k_0^2 \epsilon_r (\mathbf{E} \times \mathbf{E}) + \frac{1}{2} \alpha_Q k_0^2 \left(\frac{1}{6} (\nabla \cdot \mathbf{E}) (\nabla \times \mathbf{E}) \right) = 0,$$

which can be simplified to

$$(\mu_r^{-1} + \frac{1}{12} \alpha_Q k_0^2) (\mathbf{k} \times \mathbf{E}) (\mathbf{k} \cdot \mathbf{E}) = 0.$$

This implies that

$$(\mathbf{k} \times \mathbf{E}) (\mathbf{k} \cdot \mathbf{E}) = 0.$$

In this implication we have assumed that $\frac{1}{12} \alpha_Q k_0^2 \neq -\mu_r$, which is necessarily true for lossless media as then α_Q should be a positive number (for a material with a non-zero

quadrupolar effect) [12]. From the last equation above we have that in the medium, there can be one mode for which $(\mathbf{k} \times \mathbf{E}) = 0$ which implies that $(\mathbf{k} \cdot \mathbf{E}) \neq 0$, and there can be one where the opposite holds. For the first, $\mathbf{k} \parallel \mathbf{E}$, so this mode is longitudinal, and for the second they are perpendicular, meaning a transverse mode. Both of these must fulfil Maxwell's equations separately. Looking at the longitudinal mode and giving it the subscript e , the corresponding quadrupole moment becomes

$$\bar{\mathbf{Q}}_e = \alpha_Q \epsilon_0 i \left[\mathbf{E}_e \mathbf{k}_e - \frac{1}{3} (\mathbf{k}_e \cdot \mathbf{E}_e) \bar{\mathbf{I}} \right],$$

as for $(\mathbf{k} \times \mathbf{E}) = 0$, $\mathbf{E} \mathbf{k} = \mathbf{k} \mathbf{E}$. For our model, with both a nonzero electric dipolarisation given by $\epsilon_0 \chi_e \mathbf{E}$ and a nonzero quadrupolarisation given by $-\nabla \cdot \bar{\mathbf{Q}}/2$, the correct version of Maxwell's equation (1) becomes

$$\nabla \cdot \mathbf{E} = \frac{1}{2\epsilon_0 \epsilon_r} \nabla \cdot (\nabla \cdot \bar{\mathbf{Q}}), \quad (61)$$

which is obtained by inserting the $\rho = -\nabla_i P_i$ into (1), with P_i as expressed in the beginning of this section. For the longitudinal mode we get

$$\nabla \cdot \bar{\mathbf{Q}}_e = -\frac{2}{3} \alpha_Q \epsilon_0 i (\mathbf{k}_e \cdot \mathbf{E}_e) \mathbf{k}_e,$$

as $\mathbf{k}_e \cdot (\mathbf{E}_e \mathbf{k}_e) = (\mathbf{k}_e \cdot \mathbf{E}_e) \mathbf{k}_e$. Furthermore,

$$\nabla \cdot (\nabla \cdot \bar{\mathbf{Q}}_e) = -\frac{2}{3} \alpha_Q \epsilon_0 i (\mathbf{k}_e \cdot \mathbf{E}_e) (\mathbf{k}_e \cdot \mathbf{k}_e),$$

as $\nabla[(\mathbf{k}_e \cdot \mathbf{E}_e) \mathbf{k}_e] = (\mathbf{k}_e \cdot \mathbf{E}_e) (\mathbf{k}_e \cdot \mathbf{k}_e)$. Now inserting $\nabla \cdot (\nabla \cdot \bar{\mathbf{Q}}_e)$ into equation (61), we get that

$$\mathbf{k}_e \cdot \mathbf{k}_e = -\frac{3\epsilon_r}{\alpha_Q}, \quad (62)$$

which means that k_{ez} must be imaginary as k_x is real and $\alpha_Q \geq 0$, and the longitudinal wave is therefore evanescent.

For the transverse mode $\nabla \cdot \mathbf{E} = 0$ and $\nabla \times \mathbf{E} \neq 0$. Applying (59) to equation (50) and using $k_i^2 = \omega^2 \epsilon_0 \mu_0$ (the incident wave is in vacuum), we obtain

$$-\frac{1}{\mu_r} \nabla^2 \mathbf{E}_t = k_0^2 \left(\epsilon_r \mathbf{E}_t - \frac{1}{2} \nabla \cdot \bar{\mathbf{Q}}_t / \epsilon_0 \right), \quad (63)$$

where $\bar{\mathbf{Q}}_t$ can be expressed as

$$\bar{\mathbf{Q}}_t = \frac{1}{2}\alpha_Q\epsilon_0\left[\nabla\mathbf{E}_t + \mathbf{E}_t\nabla\right].$$

$\nabla \cdot \bar{\mathbf{Q}}_t$ then becomes

$$\frac{1}{2}\alpha_Q\epsilon_0\nabla^2\mathbf{E}_t.$$

Inserting into (63) and doing some algebra results in the following expression

$$\mathbf{k}_t \cdot \mathbf{k}_t = \mathbf{k}_i \cdot \mathbf{k}_i \epsilon_r \left(\frac{1}{\mu_r} - \frac{1}{4}k_0^2\alpha_Q \right)^{-1}. \quad (64)$$

Summarising the three boundary conditions from earlier in this section, choosing the approximated version of the magnetic field boundary condition as in [15], we have

$$E_{tx} + E_{ex} - E_{ix} - E_{rx} = 0 \quad (65)$$

$$B_t/\mu_r - B_i - B_r = -\frac{i\omega\mu_0}{2}\left[\mathbf{z} \times (\mathbf{z} \cdot \bar{\mathbf{Q}}_t + \mathbf{z} \cdot \bar{\mathbf{Q}}_e)\right] \cdot \mathbf{y} \quad (66)$$

$$\mathbf{z} \cdot (\bar{\mathbf{Q}}_t + \bar{\mathbf{Q}}_e) \cdot \mathbf{z} = 0, \quad (67)$$

Writing out $\mathbf{k}_e \times \mathbf{E}_e = 0$ and $\mathbf{k}_t \cdot \mathbf{E}_t = 0$ for the evanescent and transmitted waves respectively, we get

$$k_x E_{ez} = k_{ez} E_{ex} \quad (68)$$

$$k_x E_{tx} = -k_{tz} E_{tz}. \quad (69)$$

Inserting the expression for the electric quadrupole moment (48) into the additional boundary condition (67), we get

$$k_{tz} E_{tz} + \frac{2}{3}k_{ez} E_{ez} - \frac{1}{3}k_x E_{ex} = 0. \quad (70)$$

From (62) we can rewrite to get

$$2k_{ez}^2 - k_x^2 = -\frac{6}{\alpha_Q}\left(\epsilon_r + \frac{1}{2}\alpha_Q k_x^2\right). \quad (71)$$

Now inserting (68) and (69) into (70), and then using (71), we get

$$E_{ex} = -\frac{\alpha_Q k_x^2}{2\epsilon_r + \alpha_Q k_x^2} E_{tx}. \quad (72)$$

To translate equation (65) into an equation with the magnetic field instead of the electric,

we need to find expressions for E_{tx} , E_{rx} and E_{ix} (E_{ex} is already expressed in terms of E_{tx}) in terms of the corresponding magnetic fields. Using $\mathbf{k}_t \times \mathbf{E}_t = \omega \mathbf{B}_t$, (69), recognising $k_{tz}^2 + k_x^2$ as equal to $\mathbf{k}_t \cdot \mathbf{k}_t$ and substituting this latter expression with $k_i^2 \epsilon_r (1/\mu_r - \alpha_Q k_0^2/4)^{-1}$ (from equation (64)), we get for the propagating wave

$$E_{tx} = \frac{\omega k_{tz}}{k_i^2 \epsilon_r} \left(\frac{1}{\mu_r} - \frac{\alpha_Q k_0^2}{4} \right) B_t. \quad (73)$$

Now using $\mathbf{k}_i \times \mathbf{E}_i = \omega \mathbf{B}_i$ for the incident wave, and likewise for the reflected wave, and $\mathbf{k} \cdot \mathbf{E} = 0$ (both of these are transversal) we get the expressions

$$E_{ix} = \frac{\omega k_{1z}}{k_i^2} B_i \quad (74)$$

$$E_{rx} = -\frac{\omega k_{1z}}{k_i^2} B_r. \quad (75)$$

Combining equations (72) and (73), and inserting (72)-(75) into (65), we get

$$B_i - B_r = \frac{k_{tz}}{k_{1z}} \frac{(1/\mu_r - \alpha_Q k_i^2/4)}{(\epsilon_r + \alpha_Q k_x^2/2)} B_t \equiv f B_t \quad (76)$$

From equation (66) we can derive another equation relating B_i , B_r and B_t . The y -component of the vector term in the square brackets of (66) becomes

$$\begin{aligned} \mathbf{z} \times [\mathbf{z} \cdot (\bar{\mathbf{Q}}_t + \bar{\mathbf{Q}}_e)] \cdot \mathbf{y} &= \frac{\alpha_Q \epsilon_0 i}{2} [k_{tz} E_{tx} + k_x E_{tz} + k_{ez} E_{ex} + k_x E_{ez}] \\ &= \frac{\alpha_Q \epsilon_0 i}{2 k_{tz}} \left[(k_t^2 - 2k_x^2) - \frac{\alpha_Q k_x^2 k_{ez} k_{tz}}{\epsilon_r + \alpha_Q k_x^2/2} \right] E_{tx}, \end{aligned}$$

where in the second equation (68), (69), $k_t^2 = k_{tz}^2 + k_x^2$ and (72) have been used. Now inserting the last equation above into (66), and using (73), we get

$$B_i + B_r = \left(\frac{1}{\mu_r} - \frac{\alpha_Q}{4\epsilon_r} \left(\frac{1}{\mu_r} - \alpha_Q k_i^2/4 \right) \left[k_t^2 - 2k_x^2 - \frac{\alpha_Q k_x^2 k_{ez} k_{tz}}{\epsilon_r + \alpha_Q k_x^2/2} \right] \right) B_t \equiv g B_t. \quad (77)$$

From equations (76) and (77), we have

$$B_i - B_r = f B_t,$$

$$B_i + B_r = g B_t,$$

rendering the reflection and transmission coefficients

$$r \equiv \frac{B_r}{B_i} = \frac{g-f}{f+g}, \quad (78)$$

$$t \equiv \frac{B_t}{B_i} = \frac{2}{f+g}, \quad (79)$$

respectively.

5.2 Energy Conservation

To evaluate further the validity of the expressions for the transmission and reflection coefficients derived in the previous section, one can check for energy conservation of radiative energy in the two media by investigating the normal component of Poynting's vector on both sides of the transition layer, assuming the evanescent mode is confined there [15]. These should equal each other, as we are considering a lossless material. Mathematically expressed, $S_{iz} + S_{rz} = S_{tz}$ must be fulfilled, where \mathbf{S} is Poynting's vector,

$$S_k = \frac{1}{2\mu_0} \text{Re}\{\varepsilon_{ijk} E_i^* B_j\} - \frac{\omega}{4} \frac{\partial \varepsilon_{ij}}{\partial k_k} E_i^* E_j, \quad (80)$$

as defined by Landau and Lifshitz [2, equation 103.15]. The equation is here given in SI units instead of CGS units. ε is the Levi Civita symbol, so that $\{\varepsilon_{ijk} E_i^* B_j\} = \mathbf{E}^* \times \mathbf{B}$, and ε_{ij} is the permittivity. The second term comes from the spatial dispersion in the quadrupolar medium: $D_i(\mathbf{k}) = \varepsilon_{ij}(\mathbf{k}) E_j$. Equating this expression for the response field to the expression in (7) (where P_i is given as in (49)), we have

$$\bar{\varepsilon} \mathbf{E} = \varepsilon_0 \bar{\varepsilon}_r \mathbf{E} + \frac{(1 - \mu_r^{-1})}{\omega^2 \mu_0} \nabla \times \nabla \times \mathbf{E} - \frac{1}{2} \nabla \cdot \bar{\mathbf{Q}}.$$

Using the vector identity (59), the identities

$$\begin{aligned} \nabla \cdot (\mathbf{E} \nabla) &= \nabla \cdot (\nabla \mathbf{E})^T = \nabla (\nabla \cdot \mathbf{E}), \\ \nabla \cdot (\nabla \mathbf{E}) &= (\nabla \cdot \nabla) \mathbf{E}, \end{aligned}$$

and writing out $\nabla \cdot \bar{\mathbf{Q}}$, we obtain the following:

$$\frac{\varepsilon_{ij} E_j}{\varepsilon_0} = \bar{\varepsilon}_r E_i - \left(\frac{1 - \mu_r^{-1}}{k_0^2} + \frac{\alpha_Q}{4} \right) \nabla_l^2 E_i + \left(\frac{1 - \mu_r^{-1}}{k_0^2} - \frac{\alpha_Q}{12} \right) \nabla_i (\nabla_j E_j).$$

However, as the evanescent mode is left out, the property $\nabla \cdot \mathbf{E} = 0$ associated with the propagating modes can be applied, and therefore the last term above is zero. Using that

$\nabla \cdot \mathbf{E} = i\mathbf{k} \cdot \mathbf{E}$ and dividing both sides by \mathbf{E} , the equation above thus reduces to

$$\frac{\epsilon_{ij}}{\epsilon_0} = \bar{\epsilon}_r - \left[\frac{1 - \mu_r^{-1}}{k_0^2} + \frac{\alpha_Q}{4} \right] k_l k_l.$$

Differentiating with respect to k_k and using $\partial k_\alpha / \partial k_\beta = \delta_{\alpha\beta}$, this becomes

$$\begin{aligned} \frac{1}{\epsilon_0} \frac{\partial \epsilon_{ij}}{\partial k_k} &= -2 \left(\frac{1 - \mu_r^{-1}}{k_0^2} + \frac{\alpha_Q}{4} \right) k_l \delta_{lk} \\ &= -2 \left(\frac{1 - \mu_r^{-1}}{k_0^2} + \frac{\alpha_Q}{4} \right) k_k. \end{aligned}$$

For our transmitted propagating mode, the first term of (80) can be expressed as

$$\frac{1}{2\mu_0\omega} |\mathbf{E}_t|^2 \mathbf{k}_t,$$

as $\mathbf{k} \perp \mathbf{E} \perp \mathbf{B}$ and the direction of $\mathbf{E} \times \mathbf{B}$ is in the \mathbf{k}_t -direction. In the above (2) has also been used.

Now inserting this into equation (80), we get for Poynting's vector in the right hand side medium

$$\mathbf{S}_t = \frac{1/\mu_r - \alpha_Q k_i^2/4}{2\mu_0\omega} |\mathbf{E}_t|^2 \mathbf{k}_t. \quad (81)$$

From equation (80) we can also find the expressions for \mathbf{S}_i and \mathbf{S}_r . The incident and reflected waves are on the vacuum side of our two media space, and ϵ_{ij} is simply equal to ϵ_0 . This means that the second term in (80) is zero. Using again (2), $\mathbf{k} \perp \mathbf{E} \perp \mathbf{B}$ and that $\mathbf{E}^* \times \mathbf{B}$ is in the direction of \mathbf{k} , we can express Poynting's vector for the incident and reflected waves as

$$\begin{aligned} \mathbf{S}_i &= \frac{\omega}{2\mu_0 k_i^2} B_i^2 \mathbf{k}_i \\ \mathbf{S}_r &= \frac{\omega}{2\mu_0 k_i^2} B_r^2 \mathbf{k}_r. \end{aligned}$$

Equating the z-components of the above vectors with the z-component of (81), recalling that $k_{rz} = -k_{iz} = -k_{1z}$, we get

$$\frac{\omega k_{1z}}{2\mu_0 k_i^2} (B_i^2 - B_r^2) = \frac{1/\mu_r - \alpha_Q k_i^2/4}{2\mu_0\omega} E_t^2 k_{tz}.$$

Expressing E_t^2 as $E_{tx}^2 + E_{tz}^2$, inserting the expressions derived earlier for E_{tx}^2 and E_{tz}^2 , using (64) and dividing by B_i , we get after some simplifications that

$$1 - |r|^2 = a|t|^2, \quad (82)$$

$$\text{where } a = \frac{k_{tz}}{k_{1z}\epsilon_r} (1/\mu_r - \alpha_Q k_i^2/4)^2.$$

Plotting the difference between the left and right hand sides of equation 82 using the script in appendix F, it can be verified that the difference is zero with deviations on the order of the computer's numerical uncertainty. The equation is therefore seen to hold, and the energy is conserved.

5.3 Dipolar Behaviour for a Negligible Quadrupolarisation

For a negligible quadrupolarisation ($\alpha_Q \approx 0$), the expressions for f and g become

$$f = \frac{k_{tz}}{k_{1z}} \frac{1}{\epsilon_r \mu_r},$$

$$g = \frac{1}{\mu_r}.$$

Using the definitions of the reflection and transmission coefficients (78) and (79), we obtain by some algebra that

$$r = \frac{k_{1z}\epsilon_r - k_{tz}}{\epsilon_r k_{1z} + k_{tz}},$$

$$t = \frac{2\epsilon_r \mu_r k_{1z}}{\epsilon_r k_{1z} + k_{tz}}.$$

which are the normal Fresnel equations for the reflection and transmission of a dipolar medium in vacuum. Using the script in appendix F with a very small value for α_Q , this can be plotted. For an angle of incidence of 0° , the coefficients for an air-water interface are plotted in figure 3 as a function of the incident wavenumber times the critical dimension d of the hypothetical inclusions. In figure 4, the transmission and reflection coefficients are plotted for the same interface, but this time at an incidence angle of 53° , which is the Brewster angle for water.

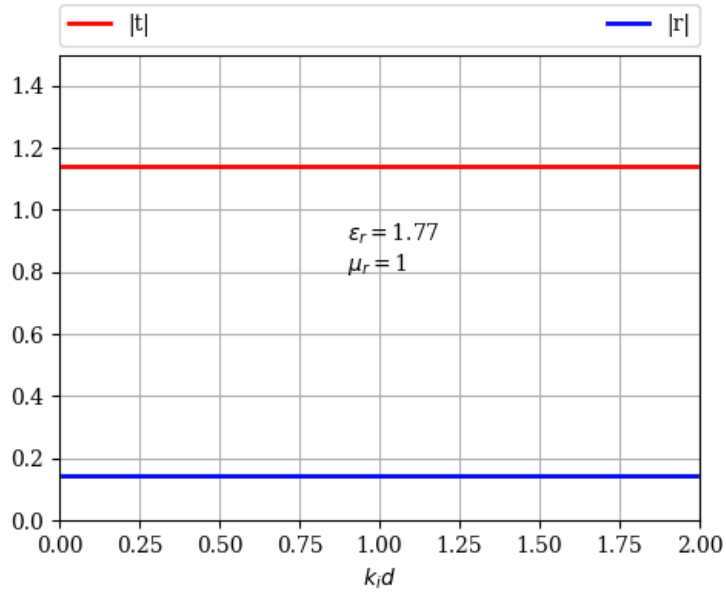


Figure 3: Absolute values of transmission and reflection coefficients (t and r respectively) for air-water as a function of the incident wavenumber times the critical dimension d of the hypothetical inclusions, for an incidence angle of 0° .

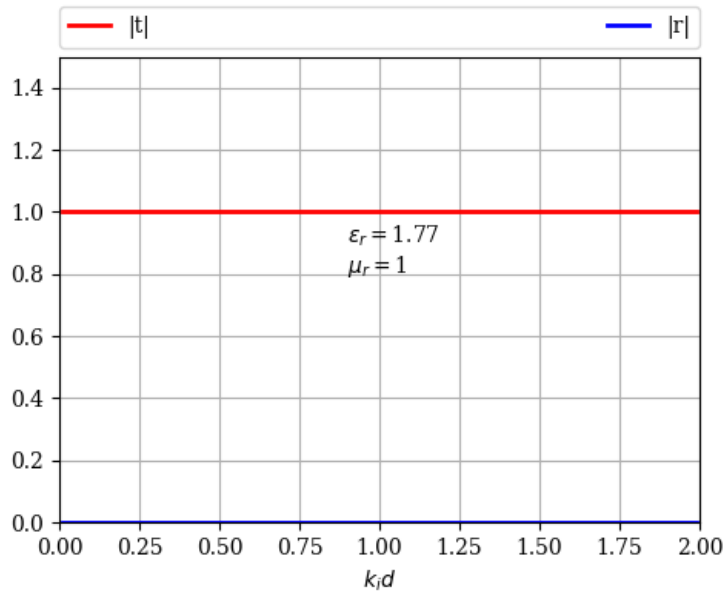


Figure 4: Absolute values of transmission and reflection coefficients (t and r respectively) for air-water as a function of the incident wavenumber times the critical dimension d of the hypothetical inclusions, at the Brewster angle (53°).

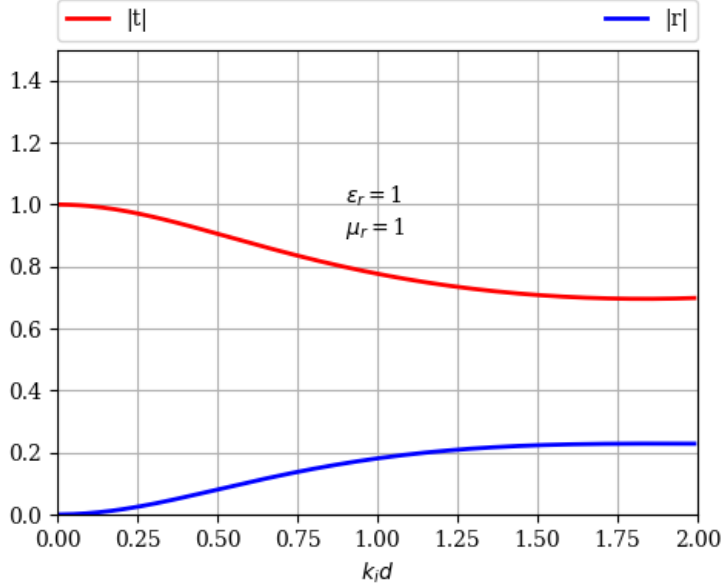


Figure 5: The absolute values of the transmission and reflection coefficients are plotted above as a function of the incident wavenumber times the critical dimension d of the hypothetical inclusions. Both the angle of incidence and the quadrupolarisation density α_Q are set to be the same as that in [15], namely 80° and $0.27d^2$ respectively, for easy comparison.

5.4 Purely Quadrupolar Medium

For a purely quadrupolar medium, the dipolar permittivity and permeability have to have the value of one, and we obtain from the script in appendix F the plot seen in figure 5. As can be observed from comparison with the plots above, the quadrupolarisation is the only source of frequency dependence in the model used.

5.5 Evanescent Transmission Wave Vector

As can be observed from equation (64), the transmission wave vector \mathbf{k}_t becomes imaginary for when

$$\left(\frac{1}{\mu_r} - \frac{1}{4}k_0^2\alpha_Q\right) < 0,$$

and is ill-defined for when the left hand side above equals zero. From the inequation above, the following inequation can easily be derived using the definition of [15] for the quadrupolarisation density ($\alpha_Q = 0.27d^2$),

$$k_0d > \sqrt{\frac{4}{0.27\mu_r}}.$$

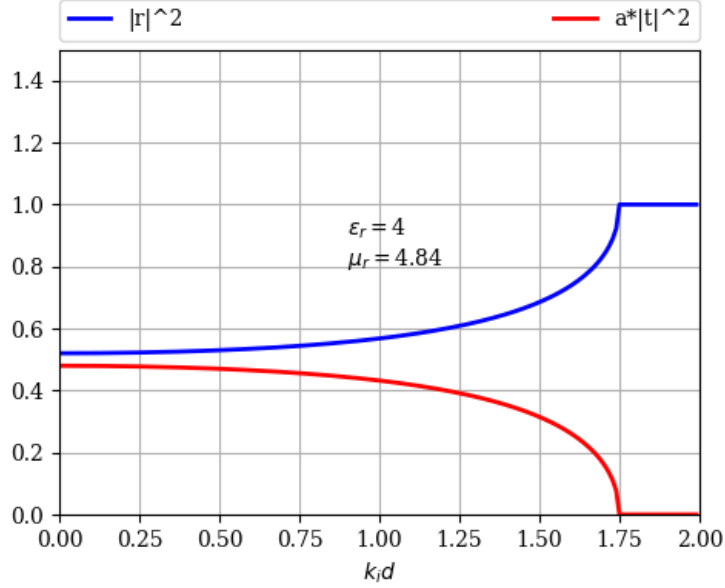


Figure 6: Plot of the absolute values of the reflection and transmission coefficients squared, normalised with the use of Poynting's vector (giving the scaling factor a), as a function of the incident wavenumber times the critical dimension d of the hypothetical inclusions. In this plot an incidence angle of 80° was used.

As an example, for the electric permittivity $\epsilon_r = 4$ and magnetic permeability $\mu_r = 4.84$, it can be calculated from the last equation that the transmission wave vector is evanescent for frequencies $k_0 d > 1.75$. The scaled and squared transmission and reflection coefficients for this example are plotted in figure 6 using the script in appendix F.

5.6 Yaghjian and Silveirinha's Exact Fresnel Equations

In order to arrive at the boundary condition (66) above, an approximation of (58) was done as in [15]. There it is stated that "For a highly accurate continuum, $k_0^2 \alpha_Q \ll 1$ and, thus, the $k_0^2 \alpha_Q / 12$ -term in (47) can be neglected". This assumption is not necessarily valid, or at least might be a very rough approximation, as the comparable $k_0^2 \alpha_Q / 4$ -term is kept. Expressing $E_x^{(2)}$ as $E_{tx} + E_{ex}$ and $E_x^{(1)}$ as $E_{ix} + E_{rx}$, and going through the same calculations as those following (65)-(67) for this exact B -field boundary condition instead of the approximated (66), the exact Fresnel equations can be derived. This is possible as the different electric field components are related to each other through (68), (69) and (72) (with the incident and reflection waves being related in the same way as the transmitted one, as they are all propagating modes) and these components can further be related to the induction fields through equations (73), (74) and (75). Doing this, one obtains a coefficient g that is different to the one in (78) and (79), and reads

$$g = \frac{1/\mu_r - \frac{\alpha_Q k_0^2}{4\omega} A \left[(k_{tz} + k_x + k_{tz}^2/3) + (2k_{ez}/3 + k_x) B \right]}{1 - \alpha_Q k_x^2/12},$$

where A is the total factor in (73) so that $E_{tx} = AB_t$ and B is the total factor in (72) so that $E_{ex} = BE_{tx}$. Using this expression for g in our formulae for the reflection and transmission coefficients, the exact Fresnel equations (according to the derivation of Yaghjian and Silveirinha) are obtained. Applying these coefficients in the equation for the energy conservation (82) and plotting the difference between the left and right hand sides using the script in appendix F, we can obtain a plot such as that in figure 7. As can be seen from the green curve in the plot, the difference is non-zero, so energy conservation is violated.

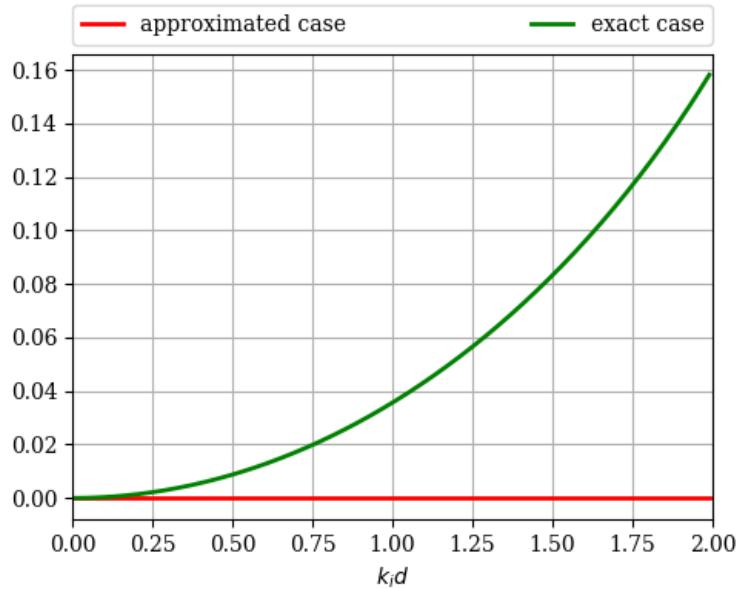


Figure 7: Plot of the absolute value of the difference between the left and right hand sides of equation (82) for the exact expressions for the reflection and transmission coefficients (the green curve) and for the approximated expressions (the red curve). This plot was obtained for an angle of incidence about 60° , with an electric permittivity of 3, a permeability of 2 and a quadrupolarisation density of $0.27d^2$. The angle was chosen so that the deviation from zero would be maximised (given the values of the other parameters used).

6 Boundary Conditions and Fresnel Equations for a Medium with an Asymmetric Quadrupole Moment

In section 5, a medium exhibiting both electric and magnetic dipolarisation and also electric quadrupolarisation was analysed in order to investigate the weak spatial dispersion of a hypothetical metamaterial. By weak spatial dispersion is meant contributions to the total polarisation that are second order in \mathbf{k} or lower, in reciprocal space. In the case of section 5, the second order effect consists of contributions from the magnetic dipolarisation and electric quadrupolarisation. However, there might also be second order contributions from higher order multipoles, and these would be missed in the case of section 5. Defining instead a general multipole $\bar{\mathbf{Q}}$ that is asymmetric, all second order effects can be included in $\bar{\mathbf{Q}}$. Using the same reference system as in 5 (that described in section 3), the polarisation of an infinite medium of such kind can therefore be expressed as

$$P_i^\infty = P_i^d - \frac{1}{2}\nabla_j Q_{ij}, \quad (83)$$

where P_i^d is the electric dipolarisation. In order to model an interface, the half-space equivalent expression should be used, which is obtained simply by multiplying the moments with the step function $u(z)$. Using (5) and (6), the source densities thus become

$$\begin{aligned} \rho &= u(z)\rho^\infty - \delta(z)P_z + \frac{1}{2}\delta(z)\left(\nabla_i Q_{iz} + \nabla_j Q_{zj}\right) + \frac{1}{2}\delta'(z)Q_{zz}. \\ J_i &= u(z)J_i^\infty - \frac{1}{2}\delta(z)\dot{Q}_{iz}. \end{aligned}$$

Just as argued in [10], it is reasonable to assume that the fields must have a form so that in Maxwell's equations, there are field terms in singular order that match those of the sources above. Consequently, just as for the electric quadrupole - magnetic dipole order we can write

$$\begin{aligned} \mathbf{E} &= u(-z)\mathbf{E}_1 + u(z)\mathbf{E}_2 + \delta(z)\mathbf{E}^{(1)}, \\ \mathbf{B} &= u(-z)\mathbf{B}_1 + u(z)\mathbf{B}_2. \end{aligned}$$

The boundary conditions can be derived with the sources and fields as expressed above. The first step to obtaining these is to insert the expressions for the fields and sources into Maxwell's equations (equations (1)-(4)). Doing this and grouping the resulting terms in singular functions of increasing order, one can observe that the step functions are associated with Maxwell's equations for the bulk of the media, and these terms are zero. The remaining terms are then terms in δ and its derivative, as shown below;

$$\delta(z) \left[E_{2z} - E_{1z} + \nabla \cdot \mathbf{E}^{(1)} + \frac{1}{\epsilon_0} \left(P_z - \frac{1}{2} [\nabla_i Q_{iz} + \nabla_j Q_{zj}] \right) \right] + \delta'(z) \left(E_z^{(1)} - \frac{1}{2\epsilon_0} Q_{zz} \right) = 0, \quad (84)$$

$$\delta(z) \left(\left[-E_{2y} + E_{1y}, E_{2x} - E_{1x}, 0 \right] + \nabla \times \mathbf{E}^{(1)} \right) + \delta'(z) \left[-E_y^{(1)}, E_x^{(1)}, 0 \right] = 0, \quad (85)$$

$$\delta(z) (B_{2z} - B_{1z}) = 0, \quad (86)$$

$$\delta(z) \left[-B_{2y} + B_{1y} + \frac{1}{2} \mu_0 \dot{Q}_{xz} - \epsilon_0 \mu_0 \dot{E}_x^{(1)}, B_{2x} - B_{1x} + \frac{1}{2} \mu_0 \dot{Q}_{yz} - \epsilon_0 \mu_0 \dot{E}_y^{(1)}, \frac{1}{2} \mu_0 \dot{Q}_{zz} - \epsilon_0 \mu_0 \dot{E}_z^{(1)} \right] = 0. \quad (87)$$

These equations are on the form

$$\delta(z)f(z) + \delta'(z)g(z) = 0,$$

from which one can derive two criteria for f and g . The first is gotten from taking the integral of (6) with respect to z over some range containing $z = 0$. The second is gotten from multiplying (6) with z , and then doing the same procedure. The criteria are found to be

$$f_0 - (\nabla_z g)_0 = 0, \quad (88)$$

$$g_0 = 0, \quad (89)$$

where the subscript means that the expressions are evaluated at zero. Applying (89) to the two equations (84) and (85), it can be seen that the surface term of the electric field can be expressed as

$$\mathbf{E}^{(1)} = \left[0, 0, \frac{1}{2\epsilon_0} Q_{zz} \right].$$

Using this, the fact that a TM wave is modelled (so that E_y is zero everywhere) and applying the criterium (88) to all of the equations (84)-(87), the following boundary conditions are obtained;

$$E_{2x} - E_{1x} = \frac{1}{\epsilon_0} \nabla_x Q_{zz}, \quad (90)$$

$$E_{2y} - E_{1y} = 0,$$

$$E_{2z} - E_{1z} = -\frac{1}{\epsilon_0} \left(P_z - \frac{1}{2} \left[\nabla_x Q_{xz} + \nabla_x Q_{zx} + \nabla_z Q_{zz} \right] \right),$$

$$B_{2x} - B_{1x} = 0,$$

$$B_{2y} - B_{1y} = -\frac{i\omega\mu_0}{2} Q_{xz}, \quad (91)$$

$$B_{2z} - B_{1z} = 0.$$

In [15], the additional boundary condition (53) ($Q_{zz} = 0$) was derived. There, $\bar{\mathbf{Q}}$ was the symmetric electric quadrupole moment, but here we are dealing with a general $\bar{\mathbf{Q}}$ with also an antisymmetric part. By comparison between the expression for the polarisation (83) and the general expression for polarisation of a centro-symmetric weakly dispersive medium (equation (28)), we can express $\bar{\mathbf{Q}}$ as

$$Q_{ik} = -2i\eta_{iklj}k_l E_j.$$

Having thus a relation between $\bar{\mathbf{Q}}$ and the electric field, the updated versions of the boundary conditions (90), (91) and (67) from which the Fresnel equations will be derived can now be written

$$E_{tx} - E_{ix} - E_{rx} = 0, \quad (92)$$

$$B_t - B_i - B_r = -\omega\mu_0\eta_{xzlj}k_l E_j, \quad (93)$$

$$\eta_{zzlj}k_l E_j = 0, \quad (94)$$

respectively. The evanescent mode is neglected for simplicity, and the validity of the expressions can be verified by carrying out the same derivation as in [15], but using instead the $\bar{\mathbf{Q}}$ as defined above.

The expression for the polarisation of the medium of interest is

$$P_i = \epsilon_0\chi_{ij}E_j + \eta_{iklj}k_k k_l E_j,$$

and consequently the induced current density can be written

$$J_i = -i\omega\epsilon_0\chi_{ij}E_j - i\omega\eta_{iklj}k_k k_l E_j.$$

In order to find an expression for the transmission wavenumber squared ($\mathbf{k}_t \cdot \mathbf{k}_t$), the curl equations for the bulk of the medium can be combined. Using the expression above for the current density and the property for propagating modes $\nabla \cdot \mathbf{E} = 0$, the equation below is found,

$$k_t^2 = k_0^2 \epsilon_r + \frac{k_0^2}{\epsilon_0} \eta_{iklj} k_k k_l.$$

When the index $l = k$, the rightmost term can be grouped with the left hand side term as $k_k k_k = k_t^2$. Also, the fact that the order in which the spatial derivatives ∇_k and ∇_l of (28) appear is unimportant, means that $\eta_{iklj} = \eta_{ilkj}$. Thus, the equation above can be further manipulated to give the expression

$$k_t^2 = \frac{k_0^2 \left(\epsilon_r + \frac{2}{\epsilon_0} \eta_{ixzj} k_x k_{tz} \right)}{\left(1 - \frac{k_0^2}{\epsilon_0} (\eta_{ixxl} + \eta_{izzl}) \right)}. \quad (95)$$

Proceeding now to express the terms of (92) in terms of the induction field \mathbf{B} , a relation between $B_i - B_r$ and B_t can be found. Just as in 5, we use Faraday's law (equation (2)) and $\nabla \cdot \mathbf{E} = 0$ to express E_{tx} , E_{ix} and E_{rx} in terms of B_t , B_i and B_r and thus obtain

$$E_{tx} = \frac{\omega k_{tz}}{k_t^2} B_t, \quad (96)$$

$$= \frac{\omega k_{tz}}{k_0^2} \frac{\left(1 - \frac{k_0^2}{\epsilon_0} (\eta_{ixxl} + \eta_{izzl}) \right)}{\left(\epsilon_r + \frac{2}{\epsilon_0} \eta_{ixzj} k_x k_{tz} \right)} B_t, \quad (97)$$

where in the second equation (95) was used. The expressions for E_{ix} and E_{rx} remain identical to the expressions (74) and (75) of section 5. Now inserting into the boundary condition (92) and applying the boundary condition (94), it is found that

$$f = \frac{k_{tx}}{k_{1z}} \frac{\left(1 - \frac{k_0^2}{\epsilon_0} (\eta_{ixxl} + \eta_{zzzl}) \right)}{\left(\epsilon_r + \frac{2}{\epsilon_0} \eta_{ixzj} k_x k_{tz} \right)},$$

where f has the same role as in section 5 of being the factor relating $B_i - B_r$ to B_t .

A second factor g also relating B_t , B_i and B_r can be found from the boundary condition (93). Writing out $\eta_{xzlj} k_l E_j$ yields

$$B_t - B_i - B_r = -\omega \mu_0 \left(\eta_{xzxz} k_x E_{tx} + \eta_{xzxz} k_x E_{tz} + \eta_{xzzx} k_{tz} E_{tx} + \eta_{xzzz} k_{tz} E_{tz} \right).$$

Using $\nabla \cdot \mathbf{E}_t = 0$, inserting for E_{tx} using (96) and applying (94), the expression for g becomes as follows,

$$g = 1 + \frac{\left(1 - \frac{k_0^2}{\epsilon_0}(\eta_{ixxl} + \eta_{xzzl})\right)}{\epsilon_0 \left(\epsilon_r + \frac{2}{\epsilon_0} \eta_{ixzj} k_x k_{tz}\right)} \left((\eta_{xzzx} - \eta_{xzzz}) k_x k_{tz} + \eta_{xzzx} k_{tz}^2 - \eta_{xzzz} k_x^2 \right).$$

From this, the reflection and transmission coefficients are found as the simple functions of f and g in equations (78) and (79), just as in section 5.

7 Discussion

Throughout this thesis, the permittivity, permeability and quadrupolarisation density have been treated as frequency independent, which is why the reflection and transmission coefficient curves in the plots of section 5.3 are constant. This is not true, but in order to investigate the spatial dispersion it is a practical assumption as this effect is then the only source of wavenumber dependency.

The derivation of the boundary conditions for the case of explicit polarisation up to electric octopole - magnetic quadrupole order in section 4.1 is relatively straight forward and interesting for two reasons. Firstly, the electric and magnetic moments are allowed to have a δ -function term. This leads to more complex boundary conditions with the capability of accounting for surface effects in case these exist. Secondly, a polarisation to electric octopole - magnetic quadrupole order would account for weak spatial dispersion quite well by its magnetic dipole and electric quadrupole contribution, as well as the potential contribution from the electric octopole and magnetic quadrupole. However, to obtain the Fresnel equations from these would be a quite cumbersome task and is not attempted in section 4.1. A more appealing way to handle media with higher order multipoles would be the model chosen in 4.2, where the different orders are not expressed explicitly, but rather implicitly contributing to the general polarisation. Furthermore, this general polarisation is in 4.2 taken as a second order approximation in \mathbf{k} , and therefore all second order contributions from all multipoles can be accounted for. Since in [15] the polarisation consists solely of the electric quadrupolarisation, and this is a second order effect, the general polarisation of 4.2 should be able to express the quadrupolarisation. Consequently, also the boundary conditions of section 4.2 should be able to express those of [15]. However, as is seen in that section, the y -direction boundary condition of the induction field derived in [15] cannot be expressed by the corresponding general boundary condition derived in 4.2. One obvious reason one might suspect is the cause of this is that the general boundary conditions of section 4.2 were derived using the half-space model of Lange and Raab [5] for the fields, whereas the boundary conditions derived in [15] relied on another model. However, as reasoned in section 3, these half-space field models turn out to be equivalent. This can also be seen from inserting the definition of the electric field used in [15] into equation (28). This gives exactly the same four last terms as in (29), and therefore the same general boundary conditions follow. Instead, the difference is likely due to the location of the step functions in the expressions for the polarisations. In [15], the polarisation can be expressed as proportional to $\nabla \cdot [u(z)\bar{\mathbf{Q}}]$, whereas in the term $\eta_{iklj}\nabla_k\nabla_l E_j$ the corresponding step function is found in the η -factor and thus outside the scope of the nabla operator.

In section 5, dipolarisations were added to Yaghjian's quadrupole medium, thus resulting in the description of a more complex medium that might be closer to what a realistic medium

would actually be like. In the derivation of the boundary condition for the x -component of the electric field, an assumption was made concerning the step functions associated with the permittivity and permeability. These were assumed to change abruptly at $z = 0$. Although this might hold for the permittivity, the permeability is associated with the magnetic dipolarisation, which is of second order in \mathbf{k} just as the electric quadrupolarisation. Thus, if the electric quadrupolarisation needs to be modelled using smooth step functions over the transition layer, this must also be the case for the magnetic dipolarisation. In order to do this properly, the permittivity and permeability step functions should also be taken as smooth step functions. Multiplying the whole of equation (51) with $(1 + u(z)\chi_m)$ and z and integrating over the transition layer would then imply a contribution from an integral term $-\frac{1}{2}\omega^2\mu_0\int_0^l u(z)(\nabla \cdot Q_0)_x z dz$. This integral must be evaluated in order to know whether the assumption used in section 5 is really valid. Most likely, this would only lead to a somewhat different first factor of equation (52), and therefore the derived boundary condition would still hold.

Although the analysis of the medium and the derivation of its Fresnel coefficients in section 5 seem successful, contributions to the second order spatial dispersion only come from the magnetisation and the electric quadrupolarisation. As higher order multipoles beyond the electric quadrupole and magnetic dipole might also contribute towards the second order spatial dispersion, these possible contributions are not accounted for in the model of section 5 and this possible limitation should be kept in mind.

As can be seen from section 5.3, the expressions for the reflection and transmission coefficients for our realistic quadrupolar medium collapse down to the normal dipolar coefficients for when the quadrupolarisation density is set to be of a negligible magnitude. The normal TM reflection effects such as the Brewster angle (figure 4) and the zero reflection at normal incidence for an impedance matched medium ($\epsilon_r = \mu_r$) can then be obtained using the script in appendix F. Thus, in the limit where $\alpha_Q \rightarrow 0$, dipolar behavior is obtained as expected.

Assuming instead that the medium of interest is purely quadrupolar ($\epsilon_r = \mu_r = 1$), the electromagnetic response exhibits a significant wavenumber dependency as can be seen from figure 5. Comparing with the corresponding plot in [15], it can be observed that the two plots are in agreement, disregarding the evanescent mode free curve and accounting for the fact that it is a slab medium that is modeled in [15].

The validity of equation (82) for the case where exact expressions for the reflection and transmission coefficients are used, can be discussed based on the green curve of figure 7. The red curve shows the difference for the case of the approximated expressions, and plotting this separately it can be verified that the deviation from zero is about 15 orders of magnitude smaller than the values of the left and right hand sides. Thus, the difference is only due to intrinsic numerical uncertainty and the energy is conserved from

the first medium to the second along the normal over the frequency range of interest, as needed⁴. The green curve, on the other hand, shows a different situation. At $k_i d = 0.5$, the deviation is about 1% of the values of the left and right hand sides of (82), and it increases proportionally to the incident wavenumber squared. At lower frequencies, the deviation is negligible as stated in [15].

In section 5.6 the exact expression for g is derived, and it is found that using this g leads to violation of energy conservation across the boundary condition. Inserting the expressions for the reflection and transmission coefficients (equations (78) and (79)) into the energy conservation criterium (82), it can be seen that the equality requires

$$a = gf.$$

As the expression for g for the exact case is different to the approximated case, but the same expression for a is used in both calculations, it is not surprising that energy conservation is violated for one of the two cases. However, it is not obvious how the expression of a should change, or why it apparently results in energy conservation for the case that after all is only an approximation. This apparent problem was not mentioned in [15], but it was claimed that the energy conservation was demonstrated (for the approximated case) in [11]. However, clarity on this matter has not been achieved by the author of this thesis, and the issue remains unsolved.

In section 6, Fresnel coefficients for the case of a general second order polarisation were derived. This is the same as what was attempted in section 4.2, but due to the fact that the derived general boundary conditions could not be unified with the specific boundary conditions of [10] and [15] it could not be carried through. In section 6 the second order term of the polarisation is expressed as the divergence of a general moment $\bar{\mathbf{Q}}$ to which the second order effect of all multipoles is attributed. Thus, the form $\nabla \cdot [u(z)\bar{\mathbf{Q}}]$ can be used in the fashion of [10] and [15] instead of the form $\eta_{ijkl}\nabla_k\nabla_l E_j$ of section 4.2, but for a $\bar{\mathbf{Q}}$ that accounts for all second order contributions and not only those from the magnetic dipole and electric quadrupole. The motivation for this choice is based on the difference between these two forms discussed earlier in this section. As shown in section 5 and in [15], for a non-negligible quadrupole contribution there will exist an additional mode in the quadrupole medium. This means that an additional boundary condition was needed in order to derive the Fresnel coefficients, and the derivation of that boundary condition depended on the quadrupole moment's expression in terms of the fields, i.e. on the constitutive relation $\bar{\mathbf{Q}}(\mathbf{E})$. For multipole orders beyond those of section 5 or [15], there might be more modes present, implying the need for more additional boundary conditions. However, as we want to limit ourselves to weakly spatial dispersive media, we operate with the second order approximation in \mathbf{k} and may assume that the number of

⁴The evanescent wave in the transition layer does not carry energy.

modes remains the same. This way, one can go through with the derivation as done in section 6. The reflection and transmission coefficients obtained are expressed in terms of η -coefficients. These coefficients are defined as the factors that multiplied with the second order spatial derivative of the electric field constitute the second order effect in \mathbf{k} of the polarisation.

As is described in section 2 and in [12], the criterium $|k_0|d \ll 1$ must hold in order for the fundamental Floquet mode approximation to the macroscopic Maxwell equations to be valid, and thus for the medium to be considered a continuum. The problem with this is that the approximation prevents us from modelling the case of sizeable inclusions ($d \leq \lambda$) precisely, which is the case for metamaterials and the reason for them exhibiting significant spatial dispersion. However, the results obtained here and in [15] can still be of importance for materials with a less strict frequency criterium. According to [12], the criterium $|k_0|d < 1$ can sometimes be permitted, and even $|k_0|d > 1$ for special inclusion arrays.

Another point worth mentioning concerning the plot domain is that depending on the given values of μ_r and α_Q , the transmission wave vector might become negative within the plot domain, as described in 5.5. This means that there is no propagating mode in the medium of interest, and therefore there is only reflection. This is seen in figure 6 for $k_0d > 1.75$.

8 Conclusion

In [15], Yaghjian and Silveirinha modelled a purely electric quadrupolar medium in order to look at the quadrupole response isolated. In section 5, the quadrupolarisation is modelled together with electric and magnetic dipolarisation in order to describe a medium closer to what would be the case for a realistic material. As the Fresnel equations derived here are in agreement with the standard Fresnel equations for the dipole approximation, and likewise in agreement with [15] for the purely quadrupolar case when the dipolarisations are negligible, it is likely that we have been successful in our derivation of the Fresnel equations for a medium with both dipolarisations and electric quadrupolarisation.

A goal for this thesis was to derive Fresnel equations for weakly dispersive media, defined as a second order approximation in \mathbf{k} to the polarisation. In section 5, the magnetic dipolarisation and electric quadrupolarisation contribute to the second order effect. However, as it might be that also higher order multipoles contribute significantly to the second order effect, it was of interest to investigate whether it is possible to obtain Fresnel equations for a general second order approximation to the spatial dispersion of a hypothetical multipole medium. This was successfully done in section 6 under the assumption that higher order multipole contributions to the second order effect do not entail additional modes. The evanescent mode was also neglected for simplicity.

For further development of the field that has been the topic of this thesis, it would be productive to repeat the derivation of the tangential electric field boundary condition in section 5 without using the assumption stated there. Furthermore, it would be profitable to gain clarity in the issue concerning the energy conservation discussed above. A first step in order to do so would be to more thoroughly go through the article by Silveirinha [11] to see whether the normal component of the Poynting vector for the approximated case is really shown to be continuous across the transition layer. However, the answer to this question will not explain the lacking energy conservation for the exact case, so this should also be investigated. A last point for further improvement would be to derive the Fresnel equations in section 6 without neglecting the evanescent mode.

Appendices

Appendix A: Homogenisation theory for local media [3, section 6.6]

The microscopic Maxwell equations read

$$\nabla \cdot \mathbf{e} = \rho / \epsilon_0 \quad (98)$$

$$\nabla \cdot \mathbf{b} = 0 \quad (99)$$

$$\nabla \times \mathbf{e} = -\frac{\partial \mathbf{b}}{\partial t} \quad (100)$$

$$\nabla \times \mathbf{b} - \frac{1}{c^2} \frac{\partial \mathbf{e}}{\partial t} = \mu_0 \mathbf{j}, \quad (101)$$

where ρ is the microscopic charge density, \mathbf{j} is the microscopic current density and the macroscopic equations (equations (111)-(114)) can be derived from these through an averaging operation of the form

$$\langle F(\mathbf{x}, t) \rangle = \int f(\mathbf{x}^*) F(\mathbf{x} - \mathbf{x}^*, t) d^3 x^*, \quad (102)$$

where $f(\mathbf{x})$ is a test function and $F(\mathbf{x}, t)$ is the function to be averaged. From the equation it can be seen that the averaging operation commutes with the spatial and temporal derivatives, mathematically expressed as

$$\begin{aligned} \frac{\partial}{\partial x_i} \langle F(\mathbf{x}, t) \rangle &= \left\langle \frac{\partial F}{\partial x_i} \right\rangle \\ \frac{\partial}{\partial t} \langle F(\mathbf{x}, t) \rangle &= \left\langle \frac{\partial F}{\partial t} \right\rangle. \end{aligned}$$

Applying the averaging function to the microscopic Maxwell equations (98) - (101), we get directly to the macroscopic ones for the homogenous equations (99) and (100). On the other hand, the inhomogenous equations become

$$\epsilon_0 \nabla \cdot \mathbf{E} = \langle \rho(\mathbf{x}, t) \rangle \quad (103)$$

$$\frac{1}{\mu_0} \nabla \times \mathbf{B} - \epsilon_0 \frac{\partial \mathbf{E}}{\partial t} = \langle \mathbf{j}(\mathbf{x}, t) \rangle. \quad (104)$$

To continue, one will need to find expressions for $\langle \rho(\mathbf{x}, t) \rangle$ and $\langle \mathbf{j}(\mathbf{x}, t) \rangle$. The microscopic

charge density can be expressed as

$$\rho(\mathbf{x}, t) = \sum_j q_j \delta(\mathbf{x} - \mathbf{x}_j) + \sum_n \rho_n(\mathbf{x}, t), \quad (105)$$

where

$$\rho_n(\mathbf{x}, t) = \sum_{j(n)} q_j \delta(\mathbf{x} - \mathbf{x}_j).$$

The first term in equation (105) is the contribution from the free charge carriers in the medium, whereas the second term is the contribution from bound molecular charges. Applying the averaging function to $\rho_n(\mathbf{x}, t)$ gives

$$\begin{aligned} \langle \rho_n(\mathbf{x}, t) \rangle &= \int f(\mathbf{x}^*) \rho_n(\mathbf{x} - \mathbf{x}^*, t) d^3 x^* \\ &= \sum_{j(n)} q_j \int f(\mathbf{x}^*) \delta(\mathbf{x} - \mathbf{x}^* - \mathbf{x}_{jn} - \mathbf{x}_n) \\ &= \sum_{j(n)} q_j f(\mathbf{x} - \mathbf{x}_n - \mathbf{x}_{jn}), \end{aligned} \quad (106)$$

where $\mathbf{x}_j = \mathbf{x}_n + \mathbf{x}_{jn}$ is the j th charge of the n th molecule. As $f(\mathbf{x}, t)$ changes significantly for small deviations of the argument $(\mathbf{x} - \mathbf{x}_n - \mathbf{x}_{jn})$ from $(\mathbf{x} - \mathbf{x}_n)$ (\mathbf{x}_{jn} on the atomic scale), a valid Taylor expansion of $\langle \rho_n(\mathbf{x}, t) \rangle$ around $(\mathbf{x} - \mathbf{x}_n)$ can be made;

$$\begin{aligned} \langle \rho_n(\mathbf{x}, t) \rangle &= \sum_{j(n)} q_j \left[f(\mathbf{x} - \mathbf{x}_n) - \mathbf{x} \cdot \nabla f(\mathbf{x} - \mathbf{x}_n) + \frac{1}{2} \sum_{ij} (\mathbf{x}_{jn})_i (\mathbf{x}_{jn})_j \frac{\partial^2}{\partial x_i \partial x_j} f(\mathbf{x} - \mathbf{x}_n) + \dots \right] \\ &= q_n f(\mathbf{x} - \mathbf{x}_n) - \mathbf{p}_n \cdot \nabla f(\mathbf{x} - \mathbf{x}_n) + \frac{1}{2} \sum_{ij} (Q_n^*)_{ij} \frac{\partial^2 f(\mathbf{x} - \mathbf{x}_n)}{\partial x_i \partial x_j} + \dots, \end{aligned} \quad (107)$$

where the second equation is obtained by identifying the microscopic multipole moments in the first;

$$\begin{aligned} q_n &= \sum_{j(n)} q_j \\ \mathbf{p}_n &= \sum_{j(n)} q_j \mathbf{x}_{jn} \\ (Q_n^*)_{ij} &= \sum_{j(n)} q_j (\mathbf{x}_{jn})_i (\mathbf{x}_{jn})_j. \end{aligned} \quad (108)$$

Rewriting equation (107), we get

$$\langle \rho_n(\mathbf{x}, t) \rangle = \langle q_n \delta(\mathbf{x} - \mathbf{x}_n) \rangle - \nabla \cdot \langle \mathbf{p}_n \delta(\mathbf{x} - \mathbf{x}_n) \rangle + \frac{1}{2} \sum_{ij} \frac{\partial^2}{\partial x_i \partial x_j} \langle (Q_n^*)_{ij} \delta(\mathbf{x} - \mathbf{x}_n) \rangle,$$

and it can be seen from this equation that we can interpret the averaged charge density as a collection of point multipoles (located at the same point) in the place of the molecule. Now summing up over all the molecules, and adding the average of the free and mobile monopole charge carriers, we get the following expression

$$\langle \rho(\mathbf{x}, t) \rangle = \rho(\mathbf{x}, t) - \nabla \cdot \mathbf{P}(\mathbf{x}, t) + \frac{1}{2} \sum_{ij} Q_{ij}^*(\mathbf{x}, t) + \dots \quad (109)$$

with

$$\begin{aligned} \rho(\mathbf{x}, t) &= \left\langle \sum_j q_j \delta(\mathbf{x} - \mathbf{x}_j) + \sum_n q_n \delta(\mathbf{x} - \mathbf{x}_n) \right\rangle \\ \mathbf{P}(\mathbf{x}, t) &= \left\langle \sum_n \mathbf{p}_n \delta(\mathbf{x} - \mathbf{x}_n) \right\rangle \\ Q_{ij}^*(\mathbf{x}, t) &= \left\langle \sum_n (Q_n^*)_{ij} \delta(\mathbf{x} - \mathbf{x}_n) \right\rangle, \end{aligned}$$

being the first three macroscopic electric multipoles. The index j counts the free monopole charges and n counts molecules. Note that the definition for the macroscopic quadrupole moment in (108) used here is different to the one used by Jackson [3], by a factor 3. The reason for this choice is to get the equations on the same form as those used by Lange and Raab [5, 10] and Silveirinha and Yagjian [15].

Inserting equation (109) into equation (103), we get

$$\sum_i \frac{\partial}{\partial x_i} \left[\epsilon_0 E_i + P_i - \frac{1}{2} \sum_j \frac{\partial}{\partial x_j} Q_{ij}^* + \dots \right] = \rho$$

This is now the macroscopic Maxwell equation corresponding to (98),

$$\nabla \cdot \mathbf{D} = \rho,$$

with

$$D_i = \epsilon_0 E_i + P_i - \frac{1}{2} \sum_j \frac{\partial Q_{ij}^*}{\partial x_j} + \dots \quad (110)$$

The derivation for the macroscopic current density $\mathbf{J}(\mathbf{x}, t)$ is done the same way, but is more complicated due to its vector nature. The starting point is the expression for the

microscopic current density

$$\mathbf{j}(\mathbf{x}, t) = \sum_j q_j \mathbf{v}_j \delta(\mathbf{x} - \mathbf{x}_j(t)).$$

Doing the average of this function (for the sum of the molecules and free charges), and inserting that expression into equation (101), we get

$$\nabla \times \mathbf{H} - \frac{\partial \mathbf{D}}{\partial t} = \mathbf{J},$$

with the response field \mathbf{H} given through the relation

$$\begin{aligned} \left(\frac{1}{\mu_0} \mathbf{B} - \mathbf{H} \right)_i &= M_i + \left\langle \sum_n (\mathbf{p} \times \mathbf{v}_n)_i \delta(\mathbf{x} - \mathbf{x}_n) \right\rangle \\ &- \frac{1}{6} \sum_{j\gamma\delta} \epsilon_{ij\gamma} \frac{\partial}{\partial x_\delta} \left\langle \sum_n (Q_n^*)_{\delta j} (\mathbf{v}_n)_\gamma \delta(\mathbf{x} - \mathbf{x}_n) \right\rangle + \dots \end{aligned}$$

The last two terms are normally very small, as the velocities of the molecules \mathbf{v}_n are low and fluctuate. However, if the whole medium moves ($\mathbf{v}_n = \mathbf{v}$ for all n), then the expression for \mathbf{H} is simplified to

$$\mathbf{H} = \frac{1}{\mu_0} \mathbf{B} - \mathbf{M} - (\mathbf{D} - \epsilon_0 \mathbf{E}) \times \mathbf{v},$$

and if $\mathbf{v} = 0$ we get the familiar relation

$$H = \frac{1}{\mu_0} \mathbf{B} - \mathbf{M}.$$

Thus, we've finally arrived at the macroscopic Maxwell equations:

$$\nabla \cdot \mathbf{D} = \rho \tag{111}$$

$$\nabla \cdot \mathbf{B} = 0 \tag{112}$$

$$\nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0 \tag{113}$$

$$\nabla \times \mathbf{H} - \frac{\partial \mathbf{D}}{\partial t} = \mathbf{J}, \tag{114}$$

where ρ and \mathbf{J} are the free monopole charge density (static ions included) and current density respectively. Although the above derivation is done for a natural material, it also holds for a metamaterial where the metamaterial unit cell replaces the molecules of the natural material and the criterium $d/\lambda \ll 1$ still holds, where d is the dimension of the metamaterial unit cell. [14, section 2].

Appendix B

We use the definition of the current density \mathbf{J} in [10] (equation (2)). Redefining the multipoles as consisting of a step function term and a surface delta term, e.g. $Q_{ij} \rightarrow u(z)Q_{ij} + \delta(z)Q_{ij}^{(1)}$, we can express the half-space current density as

$$\begin{aligned}
\mathbf{J}^{\infty/2} = & u(z) \left[\dot{P}_i - \frac{1}{2} \nabla_j \dot{Q}_{ij}^{(1)} + \epsilon_{ijk} \nabla_j M_k + \frac{1}{6} \nabla_j \nabla_k \dot{Q}_{ijk} - \frac{1}{2} \epsilon_{ijl} \nabla_j \nabla_k M_{lk} \right] \\
& - \delta(z) \left[-P_i^{(1)} + \frac{1}{2} (\dot{Q}_{iz} + \nabla_j \dot{Q}_{ij}^{(1)}) - (\epsilon_{izk} M_k + \epsilon_{ijk} \nabla_j M_k^{(1)}) - \frac{1}{6} (2 \nabla_j \dot{Q}_{ijz} + \nabla_j \nabla_k \dot{Q}_{ijk}^{(1)}) \right. \\
& \quad \left. + \frac{1}{2} (\epsilon_{ijl} \nabla_j M_{lz} + \epsilon_{izl} \nabla_k M_{lk} + \epsilon_{ijl} \nabla_j \nabla_k M_{lk}^{(1)}) \right] \\
& + \delta'(z) \left[-\frac{1}{2} \dot{Q}_{iz}^{(1)} + \epsilon_{izk} M_k^{(1)} + \frac{1}{6} (\dot{Q}_{izz} + 2 \nabla_j \dot{Q}_{ijz}^{(1)}) - \frac{1}{2} (\epsilon_{izl} M_{lz} + \epsilon_{ijl} \nabla_j M_{lz}^{(1)} + \epsilon_{izl} \nabla_k M_{lk}^{(1)}) \right] \\
& \quad - \delta''(z) \left[-\frac{1}{6} \dot{Q}_{izz}^{(1)} + \frac{1}{2} \epsilon_{izl} M_{lz}^{(1)} \right]. \quad (115)
\end{aligned}$$

Appendix C

The expressions for the left hand sides of Maxwell's equations (2)-(4) are given below. Using (14) and (15), the following is obtained for (2):

$$\begin{aligned}
\delta(z) \left(\left[E_{1y} - E_{2y}; E_{2x} - E_{1x}; 0 \right] + \nabla \times \mathbf{E}^{(1)} + \dot{\mathbf{B}}^{(1)} \right) + \delta'(z) \left(\left[-E_y^{(1)}; E_x^{(1)}; 0 \right] + \nabla \times \mathbf{E}^{(2)} \right) \\
+ \delta''(z) \left(\left[-E_y^{(2)}; E_x^{(2)}; 0 \right] \right). \quad (116)
\end{aligned}$$

Equation (3) is obtained by simply taking the divergence of (15), and this gives

$$\delta(z) \left(B_{2z} - B_{1z} + \nabla_i B_i^{(1)} \right) + \delta' B_z^{(1)}. \quad (117)$$

Lastly, (14), (15) and (115) are used to express (4),

$$\begin{aligned}
& \delta(z) \left[B_{1y} - B_{2y} + (\nabla_y B_z^{(1)} - \nabla_z B_y^{(1)}) + \mu_0 \left(-P_x^{(1)} + \frac{1}{2} \dot{Q}_{xz} + \nabla_j \dot{Q}_{xj}^{(1)} + M_y - (\nabla_y M_z^{(1)} - \nabla_z M_y^{(1)}) \right. \right. \\
& - \frac{1}{3} \nabla_j \dot{Q}_{xjz} - \frac{1}{6} \nabla_j \nabla_k \dot{Q}_{xjk}^{(1)} + \frac{1}{2} (\nabla_y M_{zz} - \nabla_z M_{yz} - \nabla_k M_{yk} + \nabla_y \nabla_k M_{zk}^{(1)} - \nabla_z \nabla_k M_{yk}^{(1)}) - \epsilon_0 \dot{E}_x^{(1)} \Big); \\
& B_{2x} - B_{1x} + \nabla_z B_x^{(1)} - \nabla_x B_z^{(1)} + \mu_0 \left(-P_y^{(1)} + \frac{1}{2} \dot{Q}_{yz} + \nabla_j \dot{Q}_{yj}^{(1)} - M_x - \nabla_z M_x^{(1)} - \nabla_x M_z^{(1)} \right. \\
& - \frac{1}{3} \nabla_j \dot{Q}_{yjk} - \frac{1}{6} \nabla_j \nabla_k \dot{Q}_{yjk}^{(1)} + \frac{1}{2} (\nabla_z M_{xz} - \nabla_x M_{zz} + \nabla_k M_{xk} + \nabla_z \nabla_k M_{zk}^{(1)} - \nabla_x \nabla_k M_{zk}^{(1)}) - \epsilon_0 \dot{E}_y^{(1)} \Big); \\
& \nabla_x B_y^{(1)} - \nabla_y B_x^{(1)} + \mu_0 \left(-P_z^{(1)} + \frac{1}{2} \dot{Q}_{zz} + \nabla_j \dot{Q}_{zj}^{(1)} - \frac{1}{3} \nabla_j \dot{Q}_{zjz} - \frac{1}{6} \nabla_j \nabla_k \right. \\
& \left. \dot{Q}_{zjk}^{(1)} + \frac{1}{2} (\nabla_x M_{yz} - \nabla_y M_{xz} + \nabla_x \nabla_k M_{yk}^{(1)} - \nabla_y \nabla_k M_{xk}^{(1)}) - \epsilon_0 \dot{E}_z^{(1)} \right) \Big] \\
& + \delta'(z) \left[-B_y^{(1)} - \mu_0 \left(-\frac{1}{2} \dot{Q}_{xz}^{(1)} - M_y^{(1)} + \frac{1}{6} (\dot{Q}_{xzz} + 2\nabla_j \dot{Q}_{xjz}^{(1)}) \right. \right. \\
& \left. \left. - \frac{1}{2} (-M_{yz} + \nabla_y M_{zz}^{(1)} - \nabla_z M_{yz}^{(1)} - \nabla_k M_{yk}^{(1)}) + \epsilon_0 \dot{E}_x^{(2)} \right); \right. \\
& B_x^{(1)} - \mu_0 \left(-\frac{1}{2} \dot{Q}_{yz}^{(1)} + M_x^{(1)} + \frac{1}{6} (\dot{Q}_{yzz} + 2\nabla_j \dot{Q}_{yjk}^{(1)}) - \frac{1}{2} (M_{xz} + \nabla_z M_{xz}^{(1)} - \nabla_x M_{zz}^{(1)} + \nabla_k M_{xk}^{(1)}) + \epsilon_0 \dot{E}_y^{(2)} \right); \\
& \left. - \mu_0 \left(-\frac{1}{2} \dot{Q}_{zz}^{(1)} + \frac{1}{6} (\dot{Q}_{zzz} + 2\nabla_j \dot{Q}_{zjz}^{(1)}) - \frac{1}{2} (\nabla_x M_{yz}^{(1)} - \nabla_y M_{xz}^{(1)}) + \epsilon_0 \dot{E}_z^{(2)} \right) \right] \\
& + \delta''(z) \left[\mu_0 \left(-\frac{1}{6} \dot{Q}_{xzz}^{(1)} - \frac{1}{2} M_{yz}^{(1)} \right); \mu_0 \left(-\frac{1}{6} \dot{Q}_{yzz}^{(1)} + \frac{1}{2} M_{xz}^{(1)} \right); -\mu_0 \frac{1}{6} \dot{Q}_{zzz}^{(1)} \right]. \quad (118)
\end{aligned}$$

Appendix D

$$\begin{aligned}
E_{2x} - E_{1x} &= \frac{1}{2\epsilon_0} \left(\nabla_x Q_{zz} - \nabla_x \left[\nabla_x Q_{xzz} + \nabla_y Q_{yzz} + \frac{1}{3} \nabla_z Q_{zzz} \right] \right) \\
&+ \frac{1}{\epsilon_0} \left(-\nabla_x P_z^{(1)} + \nabla_x^2 Q_{xz}^{(1)} + \nabla_x \nabla_y Q_{yz}^{(1)} - \frac{1}{2} \nabla_x \nabla_i \nabla_j Q_{ijz}^{(1)} + \nabla_z \nabla_x \nabla_i Q_{izz}^{(1)} + 3\nabla_z^2 \nabla_x Q_{zzz}^{(1)} \right) \\
&+ \mu_0 \left(\frac{1}{6} \ddot{Q}_{xzz} + \frac{1}{2} \dot{M}_{yz} - \frac{1}{2} \dot{Q}_{xz}^{(1)} - \dot{M}_y^{(1)} + \frac{1}{3} \nabla_j \ddot{Q}_{xjz}^{(1)} + \frac{1}{2} \left[\nabla_x \dot{M}_{yx}^{(1)} + \nabla_y \dot{M}_{yy}^{(1)} - \nabla_z \dot{M}_z z^{(1)} \right] \right).
\end{aligned}$$

$$\begin{aligned}
E_{2y} - E_{1y} &= \frac{1}{2\epsilon_0} \left(\nabla_y Q_{zz} - \nabla_y \left[\nabla_x Q_{xzz} + \nabla_y Q_{yzz} + \frac{1}{3} \nabla_z Q_{zzz} \right] \right) \\
&+ \frac{1}{\epsilon_0} \left(-\nabla_y P_z^{(1)} + \nabla_y \nabla_i Q_{iz}^{(1)} - \frac{1}{2} \nabla_y \nabla_i \nabla_j Q_{ijz}^{(1)} - \nabla_z \nabla_y Q_{zz}^{(1)} + \nabla_z \nabla_y \nabla_i Q_{izz}^{(1)} + 3\nabla_z^2 \nabla_y Q_{zzz}^{(1)} \right) \\
&+ \mu_0 \left(\frac{1}{6} \ddot{Q}_{yzz} - \frac{1}{2} \dot{M}_{xz} - \frac{1}{2} \ddot{Q}_{yz}^{(1)} + \dot{M}_x^{(1)} + \frac{1}{3} \nabla_j \ddot{Q}_{yjk}^{(1)} + \frac{1}{2} \left[\nabla_x \dot{M}_z z^{(1)} - \nabla_z \dot{M}_x z^{(1)} - \nabla_k \dot{M}_{xk}^{(1)} \right] \right).
\end{aligned}$$

$$\begin{aligned}
B_{2z} - B_{1z} &= \frac{1}{2}\mu_0 \left(\frac{1}{3}\nabla_y \dot{Q}_{xzz} - \frac{1}{3}\nabla_x \dot{Q}_{yzz} + \nabla_x M_{xz} + \nabla_y M_{yz} \right) \\
&+ \mu_0 \left(\frac{1}{3} \left[\nabla_z \nabla_x \dot{Q}_{yzz}^{(1)} - \nabla_z \nabla_y \dot{Q}_{xzz}^{(1)} + \nabla_y \nabla_j \dot{Q}_{xjz}^{(1)} - \nabla_x \nabla_j \dot{Q}_{yjj}^{(1)} \right] \right. \\
&+ \frac{1}{2} \left[\nabla_x \dot{Q}_{yz}^{(1)} - \nabla_y \dot{Q}_{xz}^{(1)} + \nabla_x^2 (M_{xx}^{(1)} - M_{zz}^{(1)}) - \nabla_y^2 M_{zz}^{(1)} \right] \\
&\quad \left. - \nabla_x M_x^{(1)} - \nabla_y M_y^{(1)} - \nabla_z \nabla_x M_{xz}^{(1)} - \nabla_z \nabla_y M_{yz}^{(1)} - \nabla_y^2 M_{yy}^{(1)} \right).
\end{aligned}$$

$$\begin{aligned}
B_{2x} - B_{1x} &= -\mu_0 \left[\frac{1}{2}\dot{Q}_{yz} - M_x - \frac{1}{3} \left(\nabla_x \dot{Q}_{xyz} + \nabla_y \dot{Q}_{yyz} + \frac{1}{2}\nabla_z \dot{Q}_{yzz} - \frac{1}{2}\nabla_y \dot{Q}_{zzz} \right) \right. \\
&+ \frac{1}{2} \left(\nabla_k M_{xk} - \nabla_x M_{zz} \right) - P_y^{(1)} + \nabla_j \dot{Q}_{yj}^{(1)} - \nabla_x M_z^{(1)} + 2\nabla_z \nabla_y \dot{Q}_{zzz}^{(1)} \\
&- \frac{1}{2} \left(\nabla_x^2 M_{zx}^{(1)} + \nabla_x \nabla_y M_{zy}^{(1)} + \nabla_y \dot{Q}_{zz}^{(1)} - \nabla_y \nabla_i \dot{Q}_{izz}^{(1)} + \nabla_z \dot{Q}_{yz}^{(1)} \right) \\
&\quad \left. + \frac{1}{3}\nabla_z \nabla_i \dot{Q}_{yiz}^{(1)} - \frac{1}{6} \left(\nabla_j \nabla_k \dot{Q}_{yjk}^{(1)} + \nabla_z^2 \dot{Q}_{yzz}^{(1)} \right) \right].
\end{aligned}$$

$$\begin{aligned}
B_{2y} - B_{1y} &= \mu_0 \left[\frac{1}{2}\dot{Q}_{xz} + M_y - \frac{1}{3} \left(\nabla_x \dot{Q}_{xxz} + \nabla_y \dot{Q}_{xyz} + \frac{1}{2}\nabla_z \dot{Q}_{xzz} - \frac{1}{2}\nabla_x \dot{Q}_{zzz} \right) \right. \\
&- \frac{1}{2} \left(\nabla_k M_{yk} - \nabla_y M_{zz} \right) - P_x^{(1)} + \nabla_j \dot{Q}_{xj}^{(1)} - \nabla_y M_z^{(1)} + 2\nabla_z \nabla_x \dot{Q}_{zzz}^{(1)} \\
&+ \frac{1}{2} \left(\nabla_y \nabla_x M_{zx}^{(1)} + \nabla_y^2 M_{zy}^{(1)} - \nabla_x \dot{Q}_{zz}^{(1)} + \nabla_x \nabla_i \dot{Q}_{izz}^{(1)} - \nabla_z \dot{Q}_{xz}^{(1)} \right) \\
&\quad \left. + \frac{1}{3}\nabla_z \nabla_i \dot{Q}_{xiz}^{(1)} - \frac{1}{6} \left(\nabla_j \nabla_k \dot{Q}_{xjk}^{(1)} + \nabla_z^2 \dot{Q}_{xzz}^{(1)} \right) \right].
\end{aligned}$$

Appendix E

$$\begin{aligned}
\nabla \times \mathbf{E} + \dot{\mathbf{B}} &= \delta(z) \left[E_{1y} - E_{2y} + \nabla_y E_z^{(1)} - \nabla_z E_y^{(1)} + \dot{B}_x^{(1)}; E_{2x} - E_{1x} + \nabla_z E_x^{(1)} - \nabla_x E_z^{(1)} + \dot{B}_y^{(1)}; \right. \\
&\quad \left. \nabla_x E_y^{(1)} - \nabla_y E_x^{(1)} + \dot{B}_z^{(1)} \right] \\
+ \delta'(z) &\left[-E_y^{(1)} + \nabla_y E_z^{(2)} - \nabla_z E_y^{(2)}; E_x^{(1)} + \nabla_z E_x^{(2)} - \nabla_x E_z^{(2)}; \nabla_x E_y^{(2)} - \nabla_y E_x^{(2)} \right] + \delta''(z) \left[-E_y^{(2)}; E_x^{(2)}; 0 \right].
\end{aligned}$$

$$\nabla \cdot \mathbf{B} = \delta(z) \left(B_{2z} - B_{1z} + \nabla_i B_i^{(1)} \right) + \delta'(z) B_z^{(1)}.$$

$$\begin{aligned} \nabla \times \mathbf{B} - \mu_0 \mathbf{J} - \mu_0 \epsilon_0 \dot{\mathbf{E}} = \delta(z) & \left[-B_{2y} + B_{1y} + \nabla_y B_z^{(1)} - \nabla_z B_y^{(1)} - \mu_0 \dot{P}_x^{(1)} - \mu_0 \epsilon_0 \dot{E}_x^{(1)}; \right. \\ B_{2x} - B_{1x} + \nabla_z B_x^{(1)} - \nabla_x B_z^{(1)} - \mu_0 \dot{P}_y^{(1)} - \mu_0 \epsilon_0 \dot{E}_y^{(1)}; & \nabla_x B_y^{(1)} - \nabla_y B_x^{(1)} - \mu_0 \dot{P}_z^{(1)} - \mu_0 \epsilon_0 \dot{E}_z^{(1)} \left. \right] \\ + \delta'(z) & \left[-B_y^{(1)} - \mu_0 \dot{P}_x^{(2)} - \mu_0 \epsilon_0 \dot{E}_x^{(2)}; B_x^{(1)} - \mu_0 \dot{P}_y^{(2)} - \mu_0 \epsilon_0 \dot{E}_y^{(2)}; -\mu_0 \dot{P}_z^{(2)} - \mu_0 \epsilon_0 \dot{E}_z^{(2)} \right]. \end{aligned}$$

Appendix F

```

1 from numpy import pi, sin
2 import numpy as np
3 import math
4 import matplotlib.pyplot as plt
5 from matplotlib.widgets import Slider, Button, RadioButtons
6 from matplotlib import rc
7 from numpy.lib import scimath
8
9 # Constants and definitions
10
11 global mu_0, mu_r, epsilon_0, epsilon_r, B_i, d, alpha_Q #, k_e_dot_k_e
12
13 epsilon_r = 3 # relative permittivity
14 mu_0 = 4*pi*1e-7 # vacuum permeability
15 mu_r = 2 # relative permeability
16 epsilon_0 = 8.85418782*1e-12 # vacuum permittivity
17 #B_i = 1e-6
18 d = 100*1e-9 # dimension of inclusions
19 alpha_Q = 0.27*d**2 # quadrupolarisation density
20
21 def transmission(angle, k_i):
22     #allocating global variables
23     global k_e_dot_k_e, mu_r_, k_x, k_2x, k_ex, k_1z, k_t, k_tz, ...
24         k_ez, f, g, a, \
25         g_exact_no_evan, E_tx_B_t_ratio, E_ex_E_tx_ratio, g_exact
26     k_e_dot_k_e = -3*epsilon_r/alpha_Q
27     mu_r_ = 1/(1/mu_r-alpha_Q*k_i**2/4)
28     k_x = (math.sin(math.radians(angle))) * (k_i)
29     k_2x = k_x
30     k_ex = k_x
31     k_1z = (math.cos(math.radians(angle))) * (k_i)
32     k_t = scimath.sqrt((k_i)**2*epsilon_r*mu_r_)
33     k_tz = np.sqrt(k_t**2 - k_2x**2)
34     k_ez = 1j * np.sqrt(k_ex**2 - k_e_dot_k_e)

```



```

34     f = (k_tz/k_lz)*(1/mu_r_)/(epsilon_r + alpha_Q*k_x**2/2)
35     g = (1/mu_r)-alpha_Q*(1/mu_r_)*(k_t**2-2*k_x**2-\
36         (alpha_Q*k_x**2*k_ez*k_tz)/(epsilon_r + ...
37         alpha_Q*k_x**2/2))/\
38         (4*epsilon_r)
39     g_exact_no_evan = (1/mu_r-(alpha_Q/4)*(k_i**2/3 + ...
40         k_tz*mu_r_/epsilon_r))/\
41         (1-k_x**2*alpha_Q/12)
42     E_tx_B_t_ratio = k_tz/(k_i**2*epsilon_r*mu_r_)
43     E_ex_E_tx_ratio = -alpha_Q*k_x**2/(2*epsilon_r + alpha_Q*k_x**2)
44     g_exact = (1/mu_r-E_tx_B_t_ratio*(k_i**2*alpha_Q/4)*\
45         ((k_tz+k_x+k_x**2/(3*k_tz))\
46         + (2*k_ez/3+k_x)*E_ex_E_tx_ratio))/\
47         (1-k_x**2*alpha_Q/12)
48     a = k_tz*(1/mu_r_)**2/(k_lz*epsilon_r)
49     return (2/(f+g))
50
51 def reflection(angle, k_i):
52     return ((g-f)/(f+g))
53
54 def transmission_exact_no_evan(angle, k_i):
55     return (2/(f+g_exact_no_evan))
56
57 def reflection_exact_no_evan(angle, k_i):
58     return ((g_exact_no_evan-f)/(f+g_exact_no_evan))
59
60 def transmission_exact(angle, k_i):
61     return (2/(f+g_exact))
62
63 def reflection_exact(angle, k_i):
64     return ((g_exact-f)/(f+g_exact))
65
66 axis_color = 'lightgoldenrodyellow'
67 fig = plt.figure()
68 plt.rc('font', family='serif')
69 plt.xlabel('$k_i$ d$')
70 fig2 = plt.figure()
71 plt.rc('font', family='serif')
72 plt.xlabel('$k_i$ d$')
73 fig3 = plt.figure()
74 plt.rc('font', family='serif')
75 plt.xlabel('$k_i$ d$')
76
77 # Draw the plot
78 ax = fig.add_subplot(111)

```

```

79 ax.text(0.9, 0.9, '$\epsilon_r = $' + str(epsilon_r) + '\n' + \
80         '$\mu_r = $' + str(mu_r))
81
82 fig.subplots_adjust(left=0.25, bottom=0.25)
83 ax2 = fig2.add_subplot(111)
84 ax2.text(0.9, 0.8, '$\epsilon_r = $' + str(epsilon_r) + '\n' + \
85         '$\mu_r = $' + str(mu_r))
86 fig2.subplots_adjust(left=0.25, bottom=0.25)
87 ax3 = fig3.add_subplot(111)
88 ax3.text(0.9, 0.8, '$\epsilon_r = $' + str(epsilon_r) + '\n' + \
89         '$\mu_r = $' + str(mu_r))
90 fig3.subplots_adjust(left=0.25, bottom=0.25)
91 k_i = np.arange(0.01/d, 2/d, 0.01/d)
92 angle_0 = 80
93 [line] = ax.plot(k_i*d, abs(transmission(angle_0, k_i)), linewidth=2, ...
94                 color='red', label="|t|")
95 [line2] = ax.plot(k_i*d, abs(reflection(angle_0, k_i)), linewidth=2, ...
96                 color='blue', label="|r|")
97 [line3] = ax2.plot(k_i*d, abs(reflection(angle_0, k_i))**2, ...
98                 linewidth=2, color='blue', label="|r|^2")
99 [line4] = ax2.plot(k_i*d, a*abs(transmission(angle_0, k_i))**2, ...
100                 linewidth=2, color='red', label="a*|t|^2")
101 [line5] = ax3.plot(k_i*d, abs(reflection(angle_0, ...
102                 k_i))**2+a*abs(transmission(angle_0, k_i))**2-1, linewidth=2, ...
103                 color='red', label="approximated case") # label="diff"
104 #[line6] = ax.plot(k_i*d, abs(transmission_exact_no_evan(angle_0, ...
105                 k_i)), linewidth=2, color='black', label="|t|")
106 #[line7] = ax.plot(k_i*d, abs(reflection_exact_no_evan(angle_0, ...
107                 k_i)), linewidth=2, color='orange', label="|r|")
108 [line8] = ax.plot(k_i*d, abs(transmission_exact(angle_0, k_i)), ...
109                 linewidth=2, color='green', label="|t| exact")
110 [line9] = ax.plot(k_i*d, abs(reflection_exact(angle_0, k_i)), ...
111                 linewidth=2, color='purple', label="|r| exact")
112 [line10] = ax2.plot(k_i*d, abs(reflection_exact(angle_0, k_i))**2, ...
113                 linewidth=2, color='purple', label="|r|^2 exact")
114 [line11] = ax2.plot(k_i*d, a*abs(transmission_exact(angle_0, ...
115                 k_i))**2, linewidth=2, color='green', label="a*|t|^2 exact")
116 [line12] = ax3.plot(k_i*d, abs(abs(reflection_exact(angle_0, ...
117                 k_i))**2+a*abs(transmission_exact(angle_0, k_i))**2-1), ...
118                 linewidth=2, color='green', label="exact case")
119
120
121
122 ax.set_xlim([0, 2])
123 ax.set_ylim([0, 1.5])
124 ax2.set_xlim([0, 2])
125 ax2.set_ylim([0, 1.5])
126 ax.legend(bbox_to_anchor=(0., 1.02, 1., .102), loc=3,

```

```

112         ncol=2, mode="expand", borderaxespad=0.)
113 ax.grid()
114 ax2.legend(bbox_to_anchor=(0., 1.02, 1., .102), loc=3,
115           ncol=2, mode="expand", borderaxespad=0.)
116 ax2.grid()
117
118 plt.legend(bbox_to_anchor=(0., 1.02, 1., .102), loc=3,
119           ncol=2, mode="expand", borderaxespad=0.)
120 ax3.set_xlim([0, 2])
121 #plt.legend(bbox_to_anchor=(0.8, 0.95), loc=2, borderaxespad=0.)
122
123
124 # Add two sliders for tweaking the parameters
125 angle_slider_ax = fig.add_axes([0.25, 0.10, 0.65, 0.03], ...
126                               facecolor=axis_color)
127 angle_slider = Slider(angle_slider_ax, 'angle', 0.0, 90.0, ...
128                       valinit=angle_0)
129
130 def sliders_on_changed(val):
131     line.set_ydata(abs(transmission(angle_slider.val, k_i)))
132     line2.set_ydata(abs(reflection(angle_slider.val, k_i)))
133     line3.set_ydata(abs(reflection(angle_slider.val, k_i))**2)
134     line4.set_ydata(a*abs(transmission(angle_slider.val, k_i))**2)
135     line5.set_ydata(abs(reflection(angle_slider.val, ...
136                       k_i))**2+a*abs(transmission(angle_slider.val, k_i))**2-1)
137     #line6.set_ydata(abs(transmission_exact_no_evan(angle_slider.val, ...
138                       k_i)))
139     #line7.set_ydata(abs(reflection_exact_no_evan(angle_slider.val, ...
140                       k_i)))
141     line8.set_ydata(abs(transmission_exact(angle_slider.val, k_i)))
142     line9.set_ydata(abs(reflection_exact(angle_slider.val, k_i)))
143     line10.set_ydata(abs(reflection_exact(angle_slider.val, k_i))**2)
144     line11.set_ydata(a*abs(transmission_exact(angle_slider.val, k_i))**2)
145     line12.set_ydata(abs(abs(reflection_exact(angle_slider.val, ...
146                       k_i))**2+a*abs(transmission_exact(angle_slider.val, k_i))**2-1))
147     fig.canvas.draw_idle()
148     fig2.canvas.draw_idle()
149     fig3.canvas.draw_idle()
150 angle_slider.on_changed(sliders_on_changed)
151
152
153 # Add a button for resetting the parameters
154 reset_button_ax = fig.add_axes([0.8, 0.025, 0.1, 0.04])
155 reset_button = Button(reset_button_ax, 'Reset', color=axis_color, ...
156                      hovercolor='0.975')
157
158 def reset_button_on_clicked(mouse_event):
159     #freq_slider.reset()

```

```
152     angle_slider.reset ()
153
154 reset_button.on_clicked(reset_button_on_clicked)
155 plt.grid()
156 plt.show()
```

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