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Modeling and simulation-based characterization of periodic absorbers for partially coherent fields

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Abstract

The absorption of electromagnetic fields plays an important role in many applications such as the energy collection, using thermal or photovoltaic solar panels, or space observation at infrared and optical frequencies, which is based on bolometers. For all these applications and many others, a complete and efficient characterization of the absorption capabilities of a given structure is required. Moreover, in most applications, the fields absorbed by the structure are only partially spatially coherent, since they originate from thermal random fluctuations.

Usually, the quality of an absorber is assessed by showing the percentage of power absorbed, when it is excited by a plane wave, as a function of the frequency, angle of incidence and polarization of the plane wave. Such information is easily interpretable by human and may provide valuable insights into the phenomena through which the absorption is taking place. However, as shown in this thesis, such a characterization is not self-contained, except in some particular cases: some information is missing to predict the power absorbed by the structure for incident fields consisting of combination of plane-waves.

This thesis is mainly focusing on two objectives. First, an efficient numerical tool is developed to study periodic and non-periodic lossy structures, which is based on the Method of Moments. It is shown that the singular integrals arising for basis and testing functions that are overlapping can be handled fully analytically. Evaluating the integral in this way, a very accurate evaluation of the impedance matrix can be performed in a competitive amount of time.

Then, we propose a spectral method for the computation of the periodic impedance matrix, for the simulation of 2D periodic structures. Using a plane-wave summation, the interaction between distant basis and testing functions is obtained rapidly while the interaction between close basis and testing functions is estimated using a Taylor expansion. It is shown that the presented method is well suited for the simulation of densely packed periodic structures provided that it is excited from many different angles. Some

post-processing techniques are proposed to extend the simulation range of geometries that can be simulated to 2D periodic structures with some defects in the periodicity and to 3D semi-infinite structures. Using the latter, the propagative and evanescent modes of a 3D periodic metamaterial can be found without resorting to back-propagation and therefore without contaminating the results with numerical noise.

To answer to the second objective of the thesis, using the results provided by the previously described software and exploiting the Energy Absorption Interferometry (EAI), a self-contained characterization of periodic absorbing structures is proposed and illustrated through several examples, among which a silver slab and an array of parallel free-standing plasmonic silver nanorods. It is shown that, in the structure studied, the absorption is mainly mediated by evanescent surface modes creeping along the surface of the structure. By adding a scattering layer, the incident fields can be coupled to the surface modes and absorption can be greatly increased. Depending on the exploited mode of absorption, the latter can also be made angularly selective.

Last, an analytical model is provided for the computation of propagating modes inside the so-called wire medium, *i.e.* a regular array of perfectly conducting wires embedded in a dielectric host. It is shown that, inside such a medium, propagative and evanescent modes are naturally orthogonal to each others using a given scalar product.

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Introduction

For more than 15 years, an entire field of research has been developed around the concept of metamaterials. This concept comes from the observation that, provided that the atoms constituting a material are small with respect to the incident wavelength, the material can be treated as being a continuous homogeneous medium. The variations that appear at the scale of the atoms can be modelled using macroscopic parameters, such as the permittivity and permeability. Extending this reasoning, it is possible to engineer meta-atoms smaller than the wavelength of operation such that any periodic arrangement of these meta-atoms can be treated as being homogeneous [1]. The advantage of that approach is that not only the composition but also the shape and size of the meta-atoms can be tuned in order to precisely control the macroscopic parameters of the device.

The applications that can benefit from this concept are numerous, so that, rapidly, a scientific community has emerged around that subject. For example, in [2], the authors propose to use metamaterial-based cloaking to reduce the coupling between densely packed antennas working at different frequencies. In [3, 4], metamaterials based resonant structures are used to enhance the magnetic field in MRI applications. In [5, 6, 7], different kinds of metamaterials were used to improve the resolution that can be achieved in imaging systems. In [8], a metamaterial acts as a waveguiding structure. In [9, 10], a metamaterial based coating was used to improve the radiative power transfer between two surface for thermophotovoltaic applications. For more theoretical purposes, the authors of [11] produced the electromagnetic equivalent of topological insulators (*i.e.* topological band gap structures) to study the surface mode that appears in the surface between two different topological band gap structures. This list of various applications is far from being exhaustive.

Since the only constraint about the meta-atoms is their subwavelength dimensions, the first realizations have been realized at low frequencies. However, since that moment, the concept evolved and many applications have been transposed to infrared and optical frequencies. For example, for

negative-index metamaterials, the first experimental realization was done in [12] at 5 GHz while demonstration of this property at optical frequencies was only demonstrated years later [13].

At these high frequencies, the fields are generally thermal in origin, so that the concept of spatial coherence, which is usually irrelevant at low frequencies, become unavoidable at infrared and optical frequencies for most applications. That concept is particularly relevant for absorption applications, where the power absorbed by the structure is a quadratic quantity of the fields, preventing the use of the superposition principle. Nowadays, absorbing metamaterials are still being characterized by the percentage of power they absorb for propagative plane waves coming from different angles of incidence (see e.g: [14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28]). Different physical phenomena are exploited to engineer surfaces with high plane wave absorption, such as the strong localization of the fields in random scattering media [26, 24, 19], the simultaneous and balanced excitation of electric and magnetic dipolar resonant modes [25, 22], the asymmetry in incident and reflected modes inside a lossy medium used for light trapping [28], the creation of Fabry-Perot like cavities to suppress the reflected fields [18, 17] or the exploitation of evanescent surface modes using periodic corrugations [27, 21, 20]. A good review of the different phenomena exploited for absorption and their peculiar characteristics can be found in [23].

However, as illustrated in this thesis, providing the way the surface absorbs plane waves coming from different angles of incidence is not sufficient to provide a complete and self-consistent description of the absorption capabilities of the structure for far-field excitations. Moreover, these metrics fail to deal with near-field excitations, which involve evanescent plane waves. These limitations are unacceptable in some applications, such as the near-field radiative heat transfer [9, 10], in which the evanescent part of the spectrum plays a critical role, or the space observation at infrared and optical frequencies, in which the incident fields are detected by bolometers and a precise model is required to retrieve the incident fields from the output of the detectors [29].

A method that can deal with these problems has been theoretically presented in [30] and numerically implemented for 2D geometries in [31]. One goal of this thesis is to extend this formalism to realistic 3D geometries that are periodic along two directions.

Another important aspect in the study of metamaterials is the new numerical challenges that arise, especially at high frequencies. Indeed, metamaterials are made of deeply subwavelength densely packed inclusions. Moreover, for some applications, these inclusions are tailored to be resonant or strongly coupled. Last, at high frequencies, the metals are exhibiting plasmonic behaviour, so that high contrasts in the permittivity at

very small scales must be handled [32]. Without a proper numerical tool, such metamaterials cannot be simulated without imposing strong hypotheses (*e.g.* perfect 2D periodic infinite structures [33, 34], dipole-like response of the scatterers [35, 36, 37], etc.).

When these hypotheses are no longer valid, the Method of Moments (MoM) shows a great potential [32, 38, 39] due to its high modularity, which leaves plenty of room for physics-based or purely mathematical acceleration techniques (*e.g.* the Fast Multipole Method (FMM) [40], the Macro-Basis Functions (MBF) [41], etc.).

The goal of this thesis is to develop numerical and conceptual tools to efficiently study the absorption of incident fields by metamaterials taking into account the spatial coherence of the fields.

In a first instance, in order to compute the response of dense periodic structures, a numerical method capable to efficiently simulate such geometries is essential. Second, a method to characterize the absorption capabilities of the structure taking into account the spatial coherence of the incident fields is needed. The relevant quantities required by this method should be obtainable using the full-wave solver previously developed, which can only deal with fully coherent excitations.

Outline of the Thesis

This dissertation is divided into four distinct chapters. The content of each of them is detailed in this section. The original contributions are highlighted.

Non-periodic Method of Moments

The first chapter focuses on the Method of Moments (MoM) for the simulation of non-periodic structures [42, 43]. This method can be used to compute the response of a non-periodic structure to any incident fields and for the computation of the power absorbed. In this section, we re-derive the MoM starting from Maxwell's equations to reach the final formulation. During that development, it is recalled that some singular integrals need to be routinely evaluated.

There are mainly two different approaches that have been proposed in the literature to deal with these singular integrals. The first approach consists in the analytical evaluation of the singular part of the function, and a numerical computation of the part that could not be evaluated analytically. The second approach proposes to deal with the integral in a purely numerical way, using specialized quadratures that are tailored to compensate for the singularity.

After a literature review of these methods, we propose an extension to existing analytical-based methods to provide the value of the integral in an entirely analytical way. The method is extensively tested and compared with existing techniques. It is shown to be competitive with state-of-the-art techniques in terms of accuracy and computation time.

Periodic Method of Moments

In the second chapter, the MoM is extended to the simulation of 2D periodic structures using a spectral formulation. Traditionally, the periodic Green's function is rapidly evaluated, *e.g.* using the Ewald method [44] or the Levin acceleration scheme [45], and then integrated numerically on the basis and testing functions. An alternative method is proposed in the second chapter which does not require to spatially integrate the periodic Green's function. It is based on a plane wave expansion of the fields emitted by the basis function. A detailed error analysis of the method is conducted. A special treatment of near interactions is also proposed. The presented method appears to be particularly well suited for the simulation of densely packed 2D periodic structures made of 3D inclusions, such as metamaterials.

Several post-processing techniques applied to the periodic impedance matrix are also presented. First, an iterative method is proposed to simulate semi-infinite 3D periodic structures, which is essential for the study of surface-related effects. This method relies on the use of fictitious interfaces [46]. Using these fictitious interfaces, each layer can be treated separately. These layers can be stacked in an iterative way, doubling their number at each iteration. This technique can also be used to compute the eigenmodes inside a 3D periodic structure without involving back-propagation. It is an important feature of the proposed method since most of the other methods proposed in the literature are entailing at some point back-propagation, which is known to be ill-conditioned.

Last, the Fictitious Source Superposition Method [47] is extended to the MoM formalism in order to simulate defective 2D periodic structures made of 3D penetrable objects, *i.e.* structures that are 2D periodic except for few defects or additional scatterers.

Energy Absorption Interferometry

In the third chapter, the EAI formalism [30, 29], which was extended to 1D periodic structures in 2D geometries and single polarization in [31], is extended to 2D periodic structures made of realistic 3D scatterers and the two possible polarizations of the fields. This formalism is illustrated through several examples.

It is shown that, characterizing a structure through this formalism using near-field sources, absorbing phenomena confined to the near-field can be highlighted, such as the presence of surface waves with high transverse wavenumber. Making use of the method developed in Chapter 2, a scattering layer is added on the top of the plasmonic structure. Through this scattering layer, the near-field absorption mechanisms can be coupled to propagating incident fields. In this way, the absorption can be improved by one order of magnitude.

Analytical modelling of the Wire Medium

One promising candidate for the absorption of partially coherent fields at infrared and optical frequencies is the so-called Wire Medium. In the last chapter, we present a review of the different models that have been developed in the literature to compute the modes that can propagate inside this medium is presented, and an original model is developed. This model is modular, since different ways to circumvent the simplifying hypotheses are presented. Last, it is shown that the modes inside a lossless wire medium possess an orthogonality property using a specially devised scalar product.

Answer to the objectives

Concerning the first object, namely the simulation toolbox, chapters 1 and 2 are proposing different methods to deal with different kind of problems. Combining these methods, most of the periodic metamaterials that have already been proposed in the literature can be simulated, ranging from waveguides based on defective photonic crystals [48] to the surface modes of topological insulators [11] or the absorbers made of non-periodic scatterers on top of hyperbolic metamaterials [49].

The second objective is the characterization of the absorption capabilities of periodic structures. This problem is tackled in chapter 3, where the formalism used is first developed theoretically and then applied to relevant examples, as a proof of concept.

The last chapter corresponds to a lead that was followed, due to the appealing properties of the wire medium for absorption [49], but abandoned too early to provide results directly correlated to the original objectives, mainly for time reasons.

Chapter 1

Numerical modelling of non-periodic structures

Except for few canonical structures for which an analytical solution for electromagnetic radiation, scattering and absorption exists, complex structures are generally studied using numerical techniques. Among the numerous methods available, it is important to choose carefully the one to be used depending on the problem to be solved. In this work, it was essentially the Method of Moments (MoM) that was used [43]. It enables the solution of frequency-domain surface integral equations (SIE). With respect to other methods, it offers several advantages: only the surfaces need to be discretized, reducing the total number of unknowns one has to deal with; the radiation boundary conditions are implicitly satisfied (in the non-periodic case); the results are robust against high variations of the constitutive parameters [38] and the method is very flexible, meaning that physics-based acceleration techniques can be easily incorporated at every step of the method. Those techniques include the use of Macro-Basis Functions (MBF) [50], the fast matrix-vector multiplication using multipoles [40], the rapid inversion of the impedance matrix using the band-limited characteristic of far-field interactions [51], etc.

The method also has several fundamental drawbacks. First, since the MoM is an integral method, it means that the system of equations one eventually has to solve is generally dense. Moreover, since it is a frequency-domain method, one simulation is only providing the response of a structure for a single frequency. Last, the Method of Moments can only be used for geometries that are homogeneous by part. Techniques have already been developed in the literature to partly relieve these constraints (see, for example, [51, 52]).

This Chapter is devoted to the formulation of the MoM. It can be divided into two parts. First, the MoM formulation used in this thesis is re-derived starting from Maxwell's equations. As well known, it is shown that singular integrals have to be routinely evaluated in order to compute the impedance matrix. In the second part, an original technique is proposed to evaluate analytically these integrals, providing the value of the integral with a machine-precision accuracy despite the singular integrand.

1.1 Derivation of the surface integral equations

1.1.1 From Maxwell's to Helmholtz equations in an homogeneous medium

The behaviour of electromagnetic fields within a homogeneous and isotropic material is described using the four Maxwell's equations. In the spectral domain, using a phasor notation, they read:

$$\nabla \cdot \mathbf{D} = \rho_J, \quad (1.1a)$$

$$\nabla \cdot \mathbf{B} = 0, \quad (1.1b)$$

$$\nabla \times \mathbf{E} = -j\omega\mathbf{B}, \quad (1.1c)$$

$$\nabla \times \mathbf{H} = \mathbf{J} + j\omega\mathbf{D}, \quad (1.1d)$$

with $\mathbf{B} = \mu\mathbf{H}$, $\mathbf{D} = \varepsilon\mathbf{E}$, μ and ε the local permeability and permittivity, ρ_J the local charge density and $\mathbf{J}$ the local current density. Note that a phasor notation has been used, so that the actual value of field $\mathcal{A}$ at time t is given by $\mathcal{R}\{\mathbf{A} \exp(j\omega t)\}$, with ω the angular frequency for which the calculations are done and $\mathcal{R}\{a\}$ the real part of a . These equations can be extended to a non-isotropic material using tensors to describe the permittivity and permeability. However, this case will not be considered hereafter.

At the interface between two different homogeneous media, the value of the fields on both sides of the interface are linked through the Boundary Conditions (BC). The BC between two media, designated as 1 and 2, are

$$\hat{\mathbf{n}} \cdot (\mathbf{D}_1 - \mathbf{D}_2) = \rho_S, \quad (1.2a)$$

$$\hat{\mathbf{n}} \cdot (\mathbf{B}_1 - \mathbf{B}_2) = 0, \quad (1.2b)$$

$$\hat{\mathbf{n}} \times (\mathbf{E}_1 - \mathbf{E}_2) = \mathbf{0}, \quad (1.2c)$$

$$\hat{\mathbf{n}} \times (\mathbf{H}_1 - \mathbf{H}_2) = \mathbf{J}_S, \quad (1.2d)$$

with ρ_S the surface charge density, $\mathbf{J}_S$ the surface current density, $\mathbf{A}_i$ the value of the field $\mathbf{A}$ in medium i and $\hat{\mathbf{n}}$ the normal to the interface pointing toward medium 1. Note that the charge conservation is consistent with

Maxwell's equations: substituting (1.1a) into the divergence of (1.1d) provides:

$$\nabla \cdot \mathbf{J} = -j\omega\rho_J. \quad (1.3)$$

In most problems, the current and the charge densities ($\mathbf{J}$ and ρ_J) are known, and one is interested in finding the electric and magnetic fields generated by these sources. Therefore, it would be interesting to re-formulate the Maxwell's equations to ease their solution.

One possibility is to use the Helmholtz theorem [53]. It states that any vector field that is twice continuously differentiable and vanishes sufficiently rapidly toward infinity can be decomposed into an irrotational part (curl-free) and a solenoidal part (div-free). Equation (1.1b) tells us that the $\mathbf{B}$ field is only made of a solenoidal part, so that there exists a vector field $\mathbf{A}$, called the vector potential, such that

$$\mathbf{B} = \nabla \times \mathbf{A} \quad (1.4)$$

Using this identity and substituting it into (1.1c), we obtain that

$$\nabla \times (\mathbf{E} + j\omega\mathbf{A}) = \mathbf{0}. \quad (1.5)$$

The latter tells us that the solenoidal part of $\mathbf{E}$ corresponds to the solenoidal part of $\mathbf{A}$, so that both differ only through an irrotational component. Mathematically, it means that there exists a scalar field φ , called potential, such that

$$\mathbf{E} = -j\omega\mathbf{A} - \nabla\varphi. \quad (1.6)$$

To summarize, the $\mathbf{B}$ and $\mathbf{E}$ unknown vector fields can be reformulated in terms of an unknown vector field $\mathbf{A}$ and an unknown scalar field φ . Moreover, only the solenoidal part of $\mathbf{A}$ has been constrained so far. Indeed, consider scalar fields ψ and ϕ such that

$$\varphi = \phi + \psi \quad (1.7)$$

Then, it can be shown that if $\mathbf{A}$ and φ are a possible solution for given $\mathbf{E}$ and $\mathbf{B}$ fields, then $\mathbf{A}'$ and ϕ are also a possible solution, with

$$\mathbf{A}' = \mathbf{A} + \frac{\nabla\psi}{j\omega}. \quad (1.8)$$

This degree of freedom can be fixed at will since it has no impact on the solution. It will be used later.

Considering that the medium is homogeneous, so that ε and μ do not depend on the position, substituting (1.4) and (1.6) into (1.1a) and (1.1d)

and using the vector calculus identity $\nabla \times \nabla \times \mathbf{A} = \nabla(\nabla \cdot \mathbf{A}) - \nabla^2 \mathbf{A}$ leads to

$$-j\omega \nabla \cdot \mathbf{A} - \nabla^2 \varphi = \frac{\rho_J}{\varepsilon}, \quad (1.9a)$$

$$\nabla \nabla \cdot \mathbf{A} - \nabla^2 \mathbf{A} = \mu \mathbf{J} + \omega^2 \varepsilon \mu \mathbf{A} - j\omega \varepsilon \nabla \varphi. \quad (1.9b)$$

This expression can be simplified using the degree of freedom mentioned in Equation (1.8) and imposing the so-called *Lorentz Gauge*:

$$\nabla \cdot \mathbf{A} + j\omega \mu \varepsilon \varphi = 0, \quad (1.10)$$

which only constrains the irrotational part of $\mathbf{A}$. Using this gauge, (1.9) becomes

$$\nabla^2 \varphi + k_0^2 \varphi = -\frac{\rho_J}{\varepsilon}, \quad (1.11a)$$

$$\nabla^2 \mathbf{A} + k_0^2 \mathbf{A} = -\mu \mathbf{J}, \quad (1.11b)$$

with $k_0^2 \equiv \omega^2 \mu \varepsilon$.

Equations of (1.11) correspond to four scalar Helmholtz equations which are mathematically identical. Only the source term (corresponding to the right-hand side) is changing from one equation to the other. Therefore, (1.11) will be much easier to solve than the original Maxwell's equations.

1.1.2 Solution of the Helmholtz equation for a given source distribution in a homogeneous medium

The next step is to solve the Helmholtz equation, *i.e.* for a given distribution of currents $\mathbf{J}$ and charges ρ_J , find the fields that are produced.

First of all, it can be noticed that the Helmholtz equations are linear with respect to the source term, which enables the use of the Green's function formalism (see Appendix A.1). We write $G(\mathbf{r}, \mathbf{r}')$ the value of a solution to the scalar Helmholtz equation at position $\mathbf{r}$ when there is a unit point source at position $\mathbf{r}'$:

$$\nabla^2 G(\mathbf{r}, \mathbf{r}') + k^2 G(\mathbf{r}, \mathbf{r}') = -\delta(\mathbf{r} - \mathbf{r}'), \quad (1.12)$$

with δ the Dirac delta. Then, a possible solution of (1.11a) is

$$\varphi(\mathbf{r}) = \iiint G(\mathbf{r}, \mathbf{r}') \frac{\rho_J(\mathbf{r}')}{\varepsilon} dV(\mathbf{r}'), \quad (1.13)$$

where the integration is performed over the whole space. Note that throughout this thesis, when the limits of an integral are not specified, they implicitly correspond to $-\infty$ and ∞ .

Second, it can be noticed that the solution to a given source distribution is not unique. Indeed, the Helmholtz equation admits homogeneous solutions $H_{\text{hom}}(\mathbf{r})$ of the type

$$H_{\text{hom}}(\mathbf{r}) = A \exp(-j\mathbf{k} \cdot \mathbf{r}) \quad (1.14)$$

with possibly complex $\mathbf{k}$ such that $\mathbf{k} \cdot \mathbf{k} = k_0^2$. However, among all the possible mathematical solutions, only one has a physical meaning. In order to find this physical solution, one can resort to extra boundary conditions called the Sommerfeld radiation condition [54]:

$$\lim_{|\mathbf{r}| \rightarrow \infty} |\mathbf{r}| \left(\frac{\partial}{\partial |\mathbf{r}|} - jk_0 \right) G(\mathbf{r}, \mathbf{r}') = 0. \quad (1.15)$$

Equation (1.15) imposes that the energy transported by the fields propagate away from the source to infinity, and that no energy is coming from infinity.

Combining (1.15) with (1.12), the Green's function for the Helmholtz equation reads

$$G(\mathbf{r}, \mathbf{r}') = \frac{\exp(-jk_0 R)}{4\pi R}, \quad (1.16)$$

with $R = R(\mathbf{r}, \mathbf{r}') = |\mathbf{r}' - \mathbf{r}|$.

Using the Green's function of (1.16) in (1.11), the scalar and vector potentials φ and $\mathbf{A}$ for given charge and current distributions ρ_J and $\mathbf{J}$ are corresponding to

$$\varphi(\mathbf{r}) = \frac{1}{4\pi\epsilon} \iiint \frac{\exp(-jk_0 R)}{R} \rho_J(\mathbf{r}') dV(\mathbf{r}') \quad (1.17a)$$

$$\mathbf{A}(\mathbf{r}) = \frac{\mu}{4\pi} \iiint \frac{\exp(-jk_0 R)}{R} \mathbf{J}(\mathbf{r}') dV(\mathbf{r}'). \quad (1.17b)$$

Finally, substituting these results into Equations (1.4) and (1.6), using the identity $\nabla \times (G\mathbf{J}) = \nabla G \times \mathbf{J} + G\nabla \times \mathbf{J}$, noticing that $\nabla \times \mathbf{J}(\mathbf{r}') = 0$ since ∇ correspond to the derivative with respect to the position $\mathbf{r}$ and $\mathbf{J}(\mathbf{r}')$ is independent from the $\mathbf{r}$ position, and substituting (1.3) to get rid of the charge density, one obtains that

$$\mathbf{H}(\mathbf{r}) = \frac{1}{4\pi} \iiint \nabla \left(\frac{\exp(-jk_0 R)}{R} \right) \times \mathbf{J}(\mathbf{r}') dV(\mathbf{r}'), \quad (1.18a)$$

$$\begin{aligned} \mathbf{E}(\mathbf{r}) = & \frac{-jk_0\eta_0}{4\pi} \iiint \frac{\exp(-jk_0 R)}{R} \mathbf{J}(\mathbf{r}') dV(\mathbf{r}') \\ & - \frac{j\eta_0}{4\pi k_0} \iiint \nabla \left(\frac{\exp(-jk_0 R)}{R} \right) \nabla' \cdot \mathbf{J}(\mathbf{r}') dV(\mathbf{r}'). \end{aligned} \quad (1.18b)$$

∇' indicates that the derivative is applied to the $\mathbf{r}'$ coordinates. Note that the following identities have been used and will be routinely used hereafter:

$$\omega\mu = k_0\eta_0, \quad (1.19a)$$

$$\omega\varepsilon = \frac{k_0}{\eta_0}, \quad (1.19b)$$

with $\eta_0 = \sqrt{\mu/\varepsilon}$ the impedance of the medium.

1.1.3 Magnetic sources in Maxwell's equations

It can be seen in (1.1) that there is some asymmetry in the way the electric and magnetic fields behave. It is due to the fact that no magnetic charge nor magnetic current has been observed so far, and therefore probably none of them exists. However, one may introduce some mathematical tools, the magnetic current ($\mathbf{M}$) and charge (ρ_m) densities, mimicking the way in which such magnetic sources would act on the electromagnetic field. The generalized Maxwell's equations then read [43]

$$\nabla \cdot \mathbf{D} = \rho_J, \quad (1.20a)$$

$$\nabla \cdot \mathbf{B} = \rho_m, \quad (1.20b)$$

$$\nabla \times \mathbf{E} = -\mathbf{M} - j\omega\mathbf{B}, \quad (1.20c)$$

$$\nabla \times \mathbf{H} = \mathbf{J} + j\omega\mathbf{D}, \quad (1.20d)$$

and the associated boundary conditions correspond to

$$\hat{\mathbf{n}} \cdot (\mathbf{D}_1 - \mathbf{D}_2) = \rho_S, \quad (1.21a)$$

$$\hat{\mathbf{n}} \cdot (\mathbf{B}_1 - \mathbf{B}_2) = \rho_{m,S}, \quad (1.21b)$$

$$\hat{\mathbf{n}} \times (\mathbf{E}_1 - \mathbf{E}_2) = -\mathbf{M}_S, \quad (1.21c)$$

$$\hat{\mathbf{n}} \times (\mathbf{H}_1 - \mathbf{H}_2) = \mathbf{J}_S, \quad (1.21d)$$

with $\rho_{m,s}$ and $\mathbf{M}_S$ the surface magnetic charge and current densities.

The fields generated by the magnetic sources can be obtained considering that the generalized Maxwell's equations are linear with respect to the sources (electric and magnetic) and following the reasoning used for electric sources. The solution of the generalized Maxwell's equations is:

$$\begin{aligned} \mathbf{E}(\mathbf{r}) = & \frac{-jk_0\eta_0}{4\pi} \iiint \frac{\exp(-jk_0R)}{R} \mathbf{J}(\mathbf{r}') dV(\mathbf{r}') \\ & - \frac{j\eta_0}{4\pi k_0} \iiint \nabla \left(\frac{\exp(-jk_0R)}{R} \right) \nabla' \cdot \mathbf{J}(\mathbf{r}') dV(\mathbf{r}') \end{aligned} \quad (1.22a)$$

$$\begin{aligned}
\mathbf{H}(\mathbf{r}) = & -\frac{1}{4\pi} \iiint \nabla \left(\frac{\exp(-jk_0 R)}{R} \right) \times \mathbf{M}(\mathbf{r}') dV(\mathbf{r}') \\
& -\frac{jk_0}{4\pi\eta_0} \iiint \frac{\exp(-jk_0 R)}{R} \mathbf{M}(\mathbf{r}') dV(\mathbf{r}') \\
& -\frac{j}{4\pi k_0 \eta_0} \iiint \nabla \left(\frac{\exp(-jk_0 R)}{R} \right) \nabla' \cdot \mathbf{M}(\mathbf{r}') dV(\mathbf{r}') \\
& +\frac{1}{4\pi} \iiint \nabla \left(\frac{\exp(-jk_0 R)}{R} \right) \times \mathbf{J}(\mathbf{r}') dV(\mathbf{r}')
\end{aligned} \tag{1.22b}$$

In addition, similarly to (1.3), the magnetic charge conservation law can be derived:

$$\nabla \cdot \mathbf{M} = -j\omega\rho_m. \tag{1.23}$$

1.1.4 Contrast sources and the equivalence principle

Equations of (1.22) provide the value of the electric and magnetic fields due to electric and magnetic sources in an infinite homogeneous and isotropic space. This specific solution has therefore a very limited range of applications. Before extending this range of applications to a medium that is homogeneous by parts, two new tools are required: the contrast sources and the equivalence principle, which leads to Kottler's formulas.

The contrast sources are used to model a change in the permittivity or the permeability. Indeed, consider a medium which is homogeneous everywhere excepted on a given volume Ω . In the homogeneous part, the permittivity and permeability are given by ε_h and μ_h , while on the non-homogeneous volume, they are given by $\varepsilon(\mathbf{r}) = \varepsilon_h + \Delta\varepsilon(\mathbf{r})$ and $\mu(\mathbf{r}) = \mu_h + \Delta\mu(\mathbf{r})$. The generalized Maxwell's equations of (1.20) becomes:

$$\nabla \cdot ((\varepsilon_h + \Delta\varepsilon)\mathbf{E}) = \rho_J, \tag{1.24a}$$

$$\nabla \cdot ((\mu_h + \Delta\mu)\mathbf{H}) = \rho_m, \tag{1.24b}$$

$$\nabla \times \mathbf{E} = -\mathbf{M} - j\omega(\mu_h + \Delta\mu)\mathbf{H}, \tag{1.24c}$$

$$\nabla \times \mathbf{H} = \mathbf{J} + j\omega(\varepsilon_h + \Delta\varepsilon)\mathbf{E}. \tag{1.24d}$$

Using the electric and magnetic charge conservation (1.3) and (1.23) and rearranging the expressions, one obtains

$$\nabla \cdot (\varepsilon_h \mathbf{E}) = \frac{j}{\omega} \nabla \cdot (\mathbf{J} + j\omega\Delta\varepsilon\mathbf{E}), \tag{1.25a}$$

$$\nabla \cdot (\mu_h \mathbf{H}) = \frac{j}{\omega} \nabla \cdot (\mathbf{M} + j\omega\Delta\mu\mathbf{H}), \tag{1.25b}$$

$$\nabla \times \mathbf{E} = -(\mathbf{M} + j\omega\Delta\mu\mathbf{H}) - j\omega\mu_h\mathbf{H}, \quad (1.25c)$$

$$\nabla \times \mathbf{H} = (\mathbf{J} + j\omega\Delta\varepsilon\mathbf{E}) + j\omega\varepsilon_h\mathbf{E}. \quad (1.25d)$$

Introducing equivalent electric and magnetic current distributions

$$\mathbf{J}' = j\omega\Delta\varepsilon\mathbf{E}, \quad (1.26a)$$

$$\mathbf{M}' = j\omega\Delta\mu\mathbf{H}, \quad (1.26b)$$

it can be seen that the fields generated by currents $\mathbf{J}$ and $\mathbf{M}$ in the presence of the inhomogeneity correspond to the fields generated inside a homogeneous medium by the superposition of the original currents $\mathbf{J}$ and $\mathbf{M}$ and contrast currents $\mathbf{J}'$ and $\mathbf{M}'$. The amplitude of the contrast currents depends on the local value of the fields.

The important conclusion of (1.25) is that, outside of Ω , the fields are behaving as if there were no inhomogeneity and some additional current sources confined within the volume Ω .

The equivalence principle, whose mathematical formulation and full proof can be found in [55], tells us that for any current distribution within a volume Ω , an equivalent current distribution on the surface of the volume $\partial\Omega$ can be found such that the fields generated by the original currents and the equivalent surface currents outside Ω are identical. From this equivalence principle the Kottler's formulas can be derived [43]; they read

$$\mathbf{E}(\mathbf{r}) = \iiint_{\Omega} \left[-j\omega\mu \frac{\exp(-jk_0R)}{4\pi R} \mathbf{J}(\mathbf{r}') \right. \quad (1.27a)$$

$$\left. - \mathbf{M}(\mathbf{r}') \times \nabla' \left(\frac{\exp(-jk_0R)}{4\pi R} \right) + \frac{\rho_J(\mathbf{r}')}{\varepsilon} \nabla' \left(\frac{\exp(-jk_0R)}{4\pi R} \right) \right] dV(\mathbf{r}')$$

$$\begin{aligned} & - \iint_{\partial\Omega} \left[-j\omega\mu \frac{\exp(-jk_0R)}{4\pi R} (\hat{\mathbf{n}} \times \mathbf{H}(\mathbf{r}')) + (\hat{\mathbf{n}} \times \mathbf{E}(\mathbf{r}')) \right. \\ & \left. \times \nabla' \left(\frac{\exp(-jk_0R)}{4\pi R} \right) + (\hat{\mathbf{n}} \cdot \mathbf{E}(\mathbf{r}')) \nabla' \left(\frac{\exp(-jk_0R)}{4\pi R} \right) \right] dS(\mathbf{r}'), \end{aligned}$$

$$\mathbf{H}(\mathbf{r}) = \iiint_{\Omega} \left[-j\omega\varepsilon \frac{\exp(-jk_0R)}{4\pi R} \mathbf{M}(\mathbf{r}') \right. \quad (1.27b)$$

$$\left. + \mathbf{J}(\mathbf{r}') \times \nabla' \left(\frac{\exp(-jk_0R)}{4\pi R} \right) + \frac{\rho_m(\mathbf{r}')}{\mu} \nabla' \left(\frac{\exp(-jk_0R)}{4\pi R} \right) \right] dV(\mathbf{r}')$$

$$- \iint_{\partial\Omega} \left[j\omega\varepsilon \frac{\exp(-jk_0R)}{4\pi R} (\hat{\mathbf{n}} \times \mathbf{E}(\mathbf{r}')) + (\hat{\mathbf{n}} \times \mathbf{H}(\mathbf{r}')) \right]$$

$$\times \nabla' \left(\frac{\exp(-jk_0 R)}{4\pi R} \right) + (\hat{\mathbf{n}} \cdot \mathbf{H}(\mathbf{r}')) \nabla' \left(\frac{\exp(-jk_0 R)}{4\pi R} \right) \Big] dS(\mathbf{r}'),$$

for any $\mathbf{r} \in \Omega$, with $\mathbf{n}$ the normal to $\partial\Omega$ pointing outside Ω . These formulas have a very deep meaning. Indeed, the value of the fields in a given point of a finite volume is uniquely defined by the sources within this volume and the value of the fields along the boundary of this volume (*i.e.* the value of the fields on $\partial\Omega$ provides all the necessary information about the sources that may exist outside Ω to compute the fields inside Ω). Moreover, since an inhomogeneity can be modeled as an equivalent contrast source, the value of the fields inside Ω is independent of the material parameters (permittivity and permeability) outside of Ω . These formulas can be extended to unbounded volumes by considering that the unbounded volume correspond to a bounded volume with a boundary that goes to infinity [55]. It can be shown that the contribution of this additional boundary vanishes using the Sommerfeld radiation condition of (1.15).

In (1.27), it can be noticed that the operator applied to the rotated tangential fields $(\hat{\mathbf{n}} \times \mathbf{H})$ and $(\hat{\mathbf{n}} \times \mathbf{E})$ is similar to the operator applied to the current densities $\mathbf{J}$ and $\mathbf{M}$. Indeed, multiplying (1.20c) and (1.20d) by $\hat{\mathbf{n}}$, considering that no forced source is crossing the boundary of the volume (*i.e.* $\hat{\mathbf{n}} \cdot \mathbf{M} = 0$ and $\hat{\mathbf{n}} \cdot \mathbf{J} = 0$ on the boundary), and using the identity $\hat{\mathbf{n}} \cdot (\nabla \times \mathbf{A}) = -\nabla \cdot (\hat{\mathbf{n}} \times \mathbf{A})$, the following identities can be found:

$$\hat{\mathbf{n}} \cdot \mathbf{H} = \frac{-j}{\omega\mu} \nabla \cdot (\hat{\mathbf{n}} \times \mathbf{E}), \quad (1.28a)$$

$$\hat{\mathbf{n}} \cdot \mathbf{E} = \frac{j}{\omega\varepsilon} \nabla \cdot (\hat{\mathbf{n}} \times \mathbf{H}). \quad (1.28b)$$

Substituting (1.28) into (1.27), one can see that the fields only depends on the *tangential* component of the fields at the interface. Denoting $\mathbf{J}_{\text{eq}}$ and $\mathbf{M}_{\text{eq}}$ the equivalent surface currents, one obtains:

$$\mathbf{J}_{\text{eq}} = -\hat{\mathbf{n}} \times \mathbf{H} \quad (1.29a)$$

$$\mathbf{M}_{\text{eq}} = \hat{\mathbf{n}} \times \mathbf{E} \quad (1.29b)$$

1.1.5 Solution for a medium homogeneous by parts

Now, all the tools required to treat a space filled with a medium that is homogeneous by parts are available. Consider a volume Ω_2 of permittivity ε_2 and permeability μ_2 inside a host medium of permittivity ε_1 and permeability μ_1 . The geometry is illustrated in Fig. 1.1.

Some impressed sources $\mathbf{J}_1$ and $\mathbf{M}_1$ are located in the host medium and generating fields that are scattered by the inclusion. Some other impressed

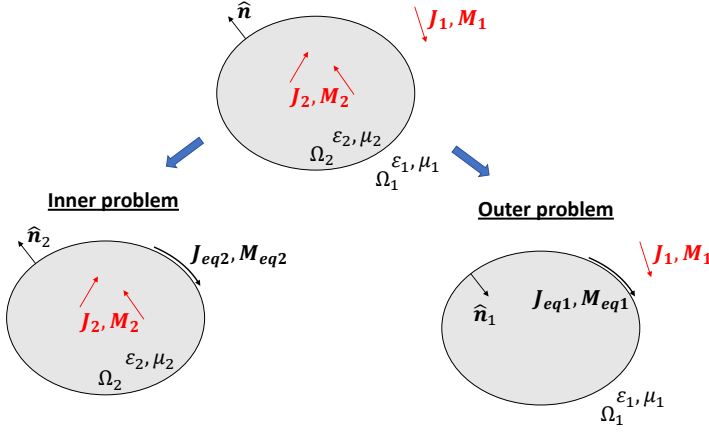


Figure 1.1: Illustration of the equivalence principle. The whole space filled with two different dielectrics is decomposed into two volumes, each volume corresponding to one dielectric material. Then, the Kottler's formulas (1.27) are applied to each volume separately.

sources $\mathbf{J}_2$ and $\mathbf{M}_2$ are located inside the inclusion are emitting fields which possibly radiate outside of the inclusion. This problem can be separated into two parts: an inner and an outer problem.

In the inner problem, the Kottler's formulas (1.27) are used considering that the volume Ω corresponds to Ω_2 , the volume of the inclusion. The permittivity and permeability for this inner problem are constant and correspond to ε_2 and μ_2 . Knowing the impressed sources distribution, the fields everywhere inside the inclusion can be expressed as a function of the unknown tangential fields on the surface of the inclusion, *i.e.* of the unknown equivalent currents $\mathbf{J}_{eq2}$ and $\mathbf{M}_{eq2}$.

In the outer problem, the volume considered in (1.27) corresponds to Ω_1 , the volume of the host medium. This time, the permittivity and permeability of the medium correspond to ε_1 and μ_1 . Again, the fields everywhere outside of the inclusion can be expressed as a function of the unknown equivalent currents $\mathbf{J}_{eq1}$ and $\mathbf{M}_{eq1}$.

First, since the tangential fields are continuous at the interface (see (1.21)) and since the normals to the surface in (1.29) are pointing in opposite directions for the inner and the outer problems, the equivalent current distributions in both problems are opposite:

$$\mathbf{J}_{eq} \equiv \mathbf{J}_{eq1} = -\mathbf{J}_{eq2}, \quad (1.30a)$$

$$\mathbf{M}_{eq} \equiv \mathbf{M}_{eq1} = -\mathbf{M}_{eq2}. \quad (1.30b)$$

In the Poggio-Miller-Chu-Harrington-Wu-Tsai (PMCHWT) formulation [42], one finds $\mathbf{J}_{\text{eq}}$ and $\mathbf{M}_{\text{eq}}$ by additionally imposing that the tangential electric and magnetic fields are identical when approaching the interface from the inside (inner problem) or from the outside (outer problem). If we note k_1 and k_2 the wavenumbers in the host medium and in the inclusion ($k_1^2 = \omega^2 \varepsilon_1 \mu_1$ and $k_2^2 = \omega^2 \varepsilon_2 \mu_2$), then the Green's functions $G_1(\mathbf{r}, \mathbf{r}')$ and $G_2(\mathbf{r}, \mathbf{r}')$ in the host medium and in the inclusion read

$$G_1(\mathbf{r}, \mathbf{r}') = \frac{\exp(-jk_1 R)}{4\pi R}, \quad (1.31a)$$

$$G_2(\mathbf{r}, \mathbf{r}') = \frac{\exp(-jk_2 R)}{4\pi R}. \quad (1.31b)$$

As mentioned, the continuity of the tangential fields at point $\mathbf{r}$ is imposed when approaching the surface from the outside for the outer problem and from the inside for the inner problem. Therefore, using $\mathbf{r}_1 = \lim_{\delta r \rightarrow 0^+} (\mathbf{r} + \delta r \hat{\mathbf{n}})$ and $\mathbf{r}_2 = \lim_{\delta r \rightarrow 0^+} (\mathbf{r} - \delta r \hat{\mathbf{n}})$ with $\hat{\mathbf{n}} \equiv \hat{\mathbf{n}}_1 = -\hat{\mathbf{n}}_2$, the Surface Integral Equation (SIE) can be formulated for any position $\mathbf{r} \in \partial\Omega$ as

$$\hat{\mathbf{n}}(\mathbf{r}) \times \left[\mathbf{E}_1^{\text{inc}}(\mathbf{r}_1) - \iint_{\partial\Omega} \left(jk_1 \eta_1 G_1(\mathbf{r}_1, \mathbf{r}') \mathbf{J}_{\text{eq}}(\mathbf{r}') + \mathbf{M}_{\text{eq}}(\mathbf{r}') \right. \right. \quad (1.32a)$$

$$\left. \left. \times \nabla' G_1(\mathbf{r}_1, \mathbf{r}') - \frac{j\eta_1}{k_1} \nabla' \cdot \mathbf{J}_{\text{eq}}(\mathbf{r}') \nabla' G_1(\mathbf{r}_1, \mathbf{r}') \right) dS(\mathbf{r}') \right]$$

$$= \hat{\mathbf{n}}(\mathbf{r}_2) \times \left[\mathbf{E}_2^{\text{inc}}(\mathbf{r}_2) + \iint_{\partial\Omega} \left(jk_2 \eta_2 G_2(\mathbf{r}_2, \mathbf{r}') \mathbf{J}_{\text{eq}}(\mathbf{r}') + \mathbf{M}_{\text{eq}}(\mathbf{r}') \right. \right.$$

$$\left. \left. \times \nabla' G_2(\mathbf{r}_2, \mathbf{r}') - \frac{j\eta_2}{k_2} \nabla' \cdot \mathbf{J}_{\text{eq}}(\mathbf{r}') \nabla' G_2(\mathbf{r}_2, \mathbf{r}') \right) dS(\mathbf{r}') \right],$$

$$\hat{\mathbf{n}}(\mathbf{r}) \times \left[\mathbf{H}_1^{\text{inc}}(\mathbf{r}_1) - \iint_{\partial\Omega} \left(\frac{jk_1}{\eta_1} G_1(\mathbf{r}_1, \mathbf{r}') \mathbf{M}_{\text{eq}}(\mathbf{r}') - \mathbf{J}_{\text{eq}}(\mathbf{r}') \right. \quad (1.32b)$$

$$\left. \left. \times \nabla' G_1(\mathbf{r}_1, \mathbf{r}') - \frac{j}{k_1 \eta_1} \nabla' \cdot \mathbf{M}_{\text{eq}}(\mathbf{r}') \nabla' G_1(\mathbf{r}_1, \mathbf{r}') \right) dS(\mathbf{r}') \right]$$

$$= \hat{\mathbf{n}}(\mathbf{r}) \times \left[\mathbf{H}_2^{\text{inc}}(\mathbf{r}_2) + \iint_{\partial\Omega} \left(\frac{jk_2}{\eta_2} G_2(\mathbf{r}_2, \mathbf{r}') \mathbf{M}_{\text{eq}}(\mathbf{r}') - \mathbf{J}_{\text{eq}}(\mathbf{r}') \right. \right.$$

$$\left. \left. \times \nabla' G_2(\mathbf{r}_2, \mathbf{r}') - \frac{j}{k_2 \eta_2} \nabla' \cdot \mathbf{M}_{\text{eq}}(\mathbf{r}') \nabla' G_2(\mathbf{r}_2, \mathbf{r}') \right) dS(\mathbf{r}') \right],$$

with $\hat{\mathbf{n}}$ the normal to the surface $\partial\Omega$ pointing toward the host medium, $\eta_i = \sqrt{\mu_i/\varepsilon_i}$ and $\mathbf{E}_i^{\text{inc}}$ and $\mathbf{H}_i^{\text{inc}}$ the incident fields due to the impressed

sources located in medium i :

$$\begin{aligned} \mathbf{E}_i^{\text{inc}}(\mathbf{r}_i) = & \iiint_{\Omega_i} \left[-jk_i\eta_i G_i(\mathbf{r}_i, \mathbf{r}') \mathbf{J}_i(\mathbf{r}') \right. \\ & \left. - \mathbf{M}_i(\mathbf{r}') \times \nabla' G_i(\mathbf{r}_i, \mathbf{r}') + \frac{j\eta_i}{k_i} \nabla' \cdot \mathbf{J}_i(\mathbf{r}') \nabla' G_i(\mathbf{r}_i, \mathbf{r}') \right] dV(\mathbf{r}') \end{aligned} \quad (1.33a)$$

$$\begin{aligned} \mathbf{H}_i^{\text{inc}}(\mathbf{r}_i) = & \iiint_{\Omega_i} \left[\frac{-jk_i}{\eta_i} G_i(\mathbf{r}_i, \mathbf{r}') \mathbf{M}_i(\mathbf{r}') \right. \\ & \left. + \mathbf{J}_i(\mathbf{r}') \times \nabla' G_i(\mathbf{r}_i, \mathbf{r}') + \frac{j}{k_i\eta_i} \nabla' \cdot \mathbf{M}_i(\mathbf{r}') \nabla' G_i(\mathbf{r}_i, \mathbf{r}') \right] dV(\mathbf{r}') \end{aligned} \quad (1.33b)$$

Equations of (1.32) can be simplified in two ways. First, it can be noticed that

$$\nabla G = -\nabla' G. \quad (1.34)$$

Distributing the integral in (1.32) and (1.33), the terms involving the divergence of the currents can be simplified. Taking the corresponding term of (1.33a) as an example, one obtains

$$\begin{aligned} & \iiint_{\Omega} \frac{j\eta}{k} \nabla' \cdot \mathbf{J}(\mathbf{r}') \nabla' G(\mathbf{r}, \mathbf{r}') dV(\mathbf{r}') \\ &= - \iiint_{\Omega} \frac{j\eta}{k} \nabla' \cdot \mathbf{J}(\mathbf{r}') \nabla G(\mathbf{r}, \mathbf{r}') dV(\mathbf{r}') \\ &= -\frac{j\eta}{k} \nabla \cdot \left(\iiint_{\Omega} \nabla' \cdot \mathbf{J}(\mathbf{r}') G(\mathbf{r}, \mathbf{r}') dV(\mathbf{r}') \right) \\ &= -\frac{j\eta}{k} \nabla \cdot \left(\iiint_{\Omega} \left(\nabla' \cdot (\mathbf{J}(\mathbf{r}') G(\mathbf{r}, \mathbf{r}')) - \nabla' G(\mathbf{r}, \mathbf{r}') \cdot \mathbf{J}(\mathbf{r}') \right) dV(\mathbf{r}') \right) \\ &= -\frac{j\eta}{k} \nabla \cdot \left(\iiint_{\Omega} \nabla G(\mathbf{r}, \mathbf{r}') \cdot \mathbf{J}(\mathbf{r}') dV(\mathbf{r}') \right) \\ &= -\frac{j\eta}{k} \nabla \cdot \left(\iiint_{\Omega} \left[\nabla \cdot (G(\mathbf{r}, \mathbf{r}') \mathbf{J}(\mathbf{r}')) - G(\mathbf{r}, \mathbf{r}') \nabla \cdot \mathbf{J}(\mathbf{r}') \right] dV(\mathbf{r}') \right) \\ &= -\frac{j\eta}{k} \nabla \nabla \cdot \left(\iiint_{\Omega} G(\mathbf{r}, \mathbf{r}') \mathbf{J}(\mathbf{r}') dV(\mathbf{r}') \right). \end{aligned} \quad (1.35)$$

The second and last steps are obtained considering that $\mathbf{J}(\mathbf{r}')$ is independent from $\mathbf{r}$. The fourth step is obtained considering that

$$\iiint_{\Omega} \nabla' \cdot (\mathbf{J}(\mathbf{r}') G(\mathbf{r}, \mathbf{r}')) dV(\mathbf{r}') = \iint_{\partial\Omega} (\hat{\mathbf{n}} \cdot \mathbf{J}(\mathbf{r}')) G(\mathbf{r}, \mathbf{r}') dS(\mathbf{r}') \quad (1.36)$$

and noticing that $(\hat{\mathbf{n}} \cdot \mathbf{J}) = 0$ everywhere on the surface, as postulated in (1.28).

The second simplification concerns the limit $\lim_{\delta r \rightarrow 0^+}$. Indeed, it can be seen that the only term that does not behave similarly when approaching the surface from inside and outside is the cross product between the currents and the gradient of the Green's function when $\mathbf{r} \rightarrow \mathbf{r}'$. In order to properly treat that limit case, one has to extract the singular zone $\mathbf{r} \rightarrow \mathbf{r}'$ and integrate it separately [55] to obtain:

$$\begin{aligned} \iint_{\partial\Omega} \hat{\mathbf{n}} \times \mathbf{A}(\mathbf{r}') \times \nabla' G(\mathbf{r}, \mathbf{r}') dS(\mathbf{r}') \\ = \iint_{\partial\Omega} \hat{\mathbf{n}} \times \mathbf{A}(\mathbf{r}') \times \nabla' G(\mathbf{r}, \mathbf{r}') dS(\mathbf{r}') \pm \frac{\mathbf{A}(\mathbf{r})}{2} \end{aligned} \quad (1.37)$$

where $\iint$ is a Cauchy principal value integral (*i.e.* an integral from which the contribution of the singular point $\mathbf{r} = \mathbf{r}'$ has been removed) and the $\pm$ sign corresponds to the case where the interface is approached from positive $\hat{\mathbf{n}}$.

Using both simplifications and noticing that the second term of the RHS of (1.37) on both sides of the interface cancel each other, the SIE becomes

$$\hat{\mathbf{n}} \times \left[\mathbf{E}_1^{\text{inc}}(\mathbf{r}) + \mathbf{E}_1^{\text{s,NS}}(\mathbf{r}) \right] = \hat{\mathbf{n}} \times \left[\mathbf{E}_2^{\text{inc}}(\mathbf{r}) - \mathbf{E}_2^{\text{s,NS}}(\mathbf{r}) \right] \quad (1.38a)$$

$$\hat{\mathbf{n}} \times \left[\mathbf{H}_1^{\text{inc}}(\mathbf{r}) + \mathbf{H}_1^{\text{s,NS}}(\mathbf{r}) \right] = \hat{\mathbf{n}} \times \left[\mathbf{H}_2^{\text{inc}}(\mathbf{r}) - \mathbf{H}_2^{\text{s,NS}}(\mathbf{r}) \right] \quad (1.38b)$$

for all $\mathbf{r} \in \partial\Omega$, with

$$\begin{aligned} \mathbf{E}_i^{\text{inc}}(\mathbf{r}) = \frac{-j\eta_i(k_i^2 + \nabla\nabla\cdot)}{k_i} \iiint_{\Omega_i} G_i(\mathbf{r}, \mathbf{r}') \mathbf{J}(\mathbf{r}') dV(\mathbf{r}') \\ - \iiint_{\Omega_i} \nabla G_i(\mathbf{r}, \mathbf{r}') \times \mathbf{M}(\mathbf{r}') dV(\mathbf{r}') \end{aligned} \quad (1.39a)$$

$$\begin{aligned} \mathbf{H}_i^{\text{inc}}(\mathbf{r}) = \frac{-j(k_i^2 + \nabla\nabla\cdot)}{\eta_i k_i} \iiint_{\Omega_i} G_i(\mathbf{r}, \mathbf{r}') \mathbf{M}(\mathbf{r}') dV(\mathbf{r}') \\ + \iiint_{\Omega_i} \nabla G_i(\mathbf{r}, \mathbf{r}') \times \mathbf{J}(\mathbf{r}') dV(\mathbf{r}') \end{aligned} \quad (1.39b)$$

the incident fields and

$$\begin{aligned} \mathbf{E}_i^{\text{s,NS}}(\mathbf{r}) = -\frac{j\eta_i(k_i^2 + \nabla\nabla\cdot)}{k_i} \iint_{\partial\Omega} G_i(\mathbf{r}, \mathbf{r}') \mathbf{J}_{\text{eq}}(\mathbf{r}') dS(\mathbf{r}') \\ - \iint_{\partial\Omega} \nabla G_i(\mathbf{r}, \mathbf{r}') \times \mathbf{M}_{\text{eq}}(\mathbf{r}') dS(\mathbf{r}') \end{aligned} \quad (1.40a)$$

$$\begin{aligned} \mathbf{H}_i^{\text{s,NS}}(\mathbf{r}) = & -\frac{j(k_i^2 + \nabla \nabla \cdot)}{\eta_i k_i} \iint_{\partial\Omega} G_i(\mathbf{r}, \mathbf{r}') \mathbf{M}_{\text{eq}}(\mathbf{r}') dS(\mathbf{r}') \\ & + \iint_{\partial\Omega} \nabla G_i(\mathbf{r}, \mathbf{r}') \times \mathbf{J}_{\text{eq}}(\mathbf{r}') dS(\mathbf{r}') \end{aligned} \quad (1.40b)$$

the fields scattered by the equivalent currents $\mathbf{J}_{\text{eq}}$ and $\mathbf{M}_{\text{eq}}$ in the inner ($i = 2$) or outer ($i = 1$) problem. The “NS” superscript emphasizes the fact that the contribution of the singular point $\mathbf{r}' = \mathbf{r}$ has been removed from the second integral.

1.2 Discretization of the problem

The SIE as formulated in (1.38) corresponds to a continuous problem. Except for a few canonical geometries, an analytical solution can hardly be found and one has to discretize the problem and solve it numerically. The discretization occurs at two different levels. First, the equivalent currents are expanded using a finite set of N Basis Functions (BF) $\{\mathbf{f}_{B_i}(\mathbf{r})\}$. Most of the time, the same basis is used to expand the electric and magnetic currents, leading to

$$\mathbf{J}_{\text{eq}}(\mathbf{r}) \simeq \sum_{k=1}^N x_k \mathbf{f}_{Bk}(\mathbf{r}), \quad (1.41a)$$

$$\mathbf{M}_{\text{eq}}(\mathbf{r}) \simeq \sum_{k=N+1}^{2N} x_k \mathbf{f}_{Bk}(\mathbf{r}), \quad (1.41b)$$

with $\mathbf{f}_{Bk}(\mathbf{r}) = \mathbf{f}_{Bk+N}(\mathbf{r})$. Second, the continuity of the fields is tested on a discrete set of N' Testing Functions (TF) $\{\mathbf{f}_{Tj}(\mathbf{r})\}$. Indeed, if the fields are continuous in every point $\mathbf{r} \in \partial\Omega$, then their weighted average over the surface is also continuous. Again, the electric and magnetic fields are generally tested separately on identical testing functions $\mathbf{f}_{Tj}(\mathbf{r})$. The boundary conditions of (1.38) then read:

$$\begin{aligned} \iint_{\partial\Omega} [\mathbf{E}_1^{\text{s,NS}}(\mathbf{r}) + \mathbf{E}_2^{\text{s,NS}}(\mathbf{r})] \cdot \mathbf{f}_{Tj}(\mathbf{r}) dS(\mathbf{r}) \\ = \iint_{\partial\Omega} [\mathbf{E}_2^{\text{inc}}(\mathbf{r}) - \mathbf{E}_1^{\text{inc}}(\mathbf{r})] \cdot \mathbf{f}_{Tj}(\mathbf{r}) dS(\mathbf{r}), \end{aligned} \quad (1.42a)$$

$$\begin{aligned} \iint_{\partial\Omega} [\mathbf{H}_1^{\text{s,NS}}(\mathbf{r}) + \mathbf{H}_2^{\text{s,NS}}(\mathbf{r})] \cdot \mathbf{f}_{Tj}(\mathbf{r}) dS(\mathbf{r}) \\ = \iint_{\partial\Omega} [\mathbf{H}_2^{\text{inc}}(\mathbf{r}) - \mathbf{H}_1^{\text{inc}}(\mathbf{r})] \cdot \mathbf{f}_{Tj}(\mathbf{r}) dS(\mathbf{r}), \end{aligned} \quad (1.42b)$$

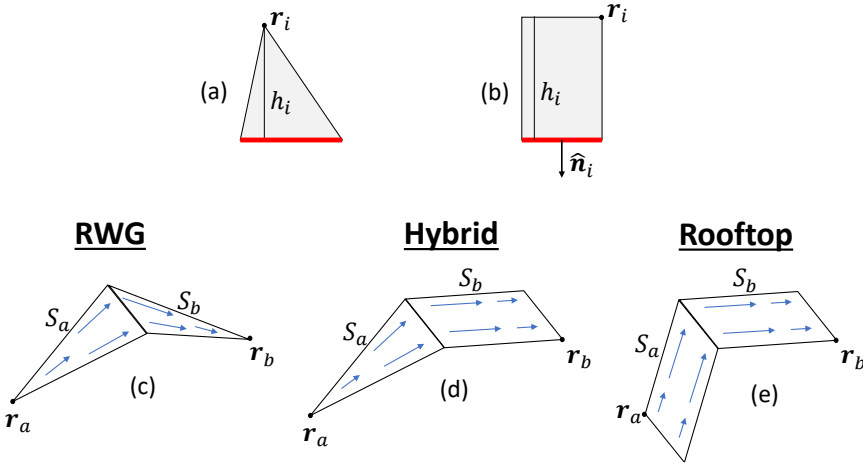


Figure 1.2: The (a) triangles and (b) rectangles used to mesh the surface are paired along the red line to constitute (c) RWG, (d) hybrid or (e) rooftop functions.

for all $j \in [1, N']$. The $2N$ unknowns of the discrete problem corresponds to the unknown coefficients x_k of (1.41). These unknowns can be found solving the $2N'$ equations of (1.42). Generally, the system of equation is chosen to be neither under or overdetermined, leading to $N = N'$.

1.2.1 Choice of the BF

The accuracy of the numerical solution is strongly dependent on the BF and TF used. However, the more evolved the BF and TF are, the more complicated the discretization process (meshing) and the integrals evaluations will be. A good compromise consists in having identical BF and TF (Galerkin testing), dividing the surface into triangles or rectangles and pairing the polygons sharing a common edge. Three kind of BF emerges, as illustrated in Fig. 1.2. If the two polygons are triangles, one obtains a Rao-Wilton-Glisson (RWG) BF [56]. If the two polygons are rectangles, one obtains a rooftop BF. Last, if one of the polygons is a triangle and the other is a rectangle, one obtains an hybrid BF.

To each edge within a closed surface is associated a BF $\mathbf{f}_B$. One of the polygons of the BF, corresponding to S_a in Fig. 1.2, is chosen to be the “positive” part of the function, while the other one, S_b , corresponds to the

“negative” part. The value of the BF on a triangle is

$$\mathbf{f}_B(\mathbf{r}) = \pm \frac{\mathbf{r} - \mathbf{r}_i}{h_i} \quad (1.43)$$

while the value of the BF on a rectangle is given by

$$\mathbf{f}_B(\mathbf{r}) = \pm \frac{(\mathbf{r} - \mathbf{r}_i) \cdot \hat{\mathbf{n}}_i}{h_i} \hat{\mathbf{n}}_i. \quad (1.44)$$

The + sign is chosen if the polygon corresponds to the positive part of the BF and the – sign otherwise; $\mathbf{r}_i$ is one vertex of the polygon S_i that is not on the common edge; h_i is the height of the polygon associated to the common edge, as illustrated in Fig. 1.2(a,b).

The BF defined this way are div-conforming, which means that their divergence is bounded. The divergence of the currents being proportional to the charge density, this property is important to prevent the appearance of charged edges (1D linear charge density), which are not physical and may degrade the solution. Moreover, this property will be used later to simplify the integrals involved in the MoM.

1.2.2 Computation of the impedance matrix

Now that the BF and TF have been defined, one can expand the equations of (1.42) using (1.39) and (1.40), and substitute the approximate expansion of the currents (1.41). Rearranging the expression, one finds that

$$\begin{aligned} b_2^E[j] - b_1^E[j] &= \sum_{k=1}^N \left(Z_1^{EJ}[j, k] + Z_2^{EJ}[j, k] \right) x_k \\ &\quad + \sum_{k=1}^N \left(Z_1^{EM}[j, k] + Z_2^{EM}[j, k] \right) x_{N+k} \end{aligned} \quad (1.45a)$$

$$\begin{aligned} b_2^H[j] - b_1^H[j] &= \sum_{k=1}^N \left(\frac{Z_1^{EJ}[j, k]}{\eta_1^2} + \frac{Z_2^{EJ}[j, k]}{\eta_2^2} \right) x_{N+k} \\ &\quad - \sum_{k=1}^N \left(Z_1^{EM}[j, k] + Z_2^{EM}[j, k] \right) x_k \end{aligned} \quad (1.45b)$$

with

$$b_i^E[j] = \iint_{\partial\Omega} \mathbf{E}_i^{\text{inc}}(\mathbf{r}) \cdot \mathbf{f}_{Tj}(\mathbf{r}) dS(\mathbf{r}) \quad (1.46a)$$

$$b_i^H[j] = \iint_{\partial\Omega} \mathbf{H}_i^{\text{inc}}(\mathbf{r}) \cdot \mathbf{f}_{Tj}(\mathbf{r}) dS(\mathbf{r}) \quad (1.46b)$$

$$Z_i^{EJ}[j, k] = \iint_{\partial\Omega} \mathbf{f}_{Tj}(\mathbf{r}) \cdot \left[\frac{-j\eta_i(k_i^2 + \nabla\nabla\cdot)}{k_i} \times \iint_{\partial\Omega} G_i(\mathbf{r}, \mathbf{r}') \mathbf{f}_{Bk}(\mathbf{r}') dS(\mathbf{r}') \right] dS(\mathbf{r}) \quad (1.46c)$$

$$Z_i^{EM}[j, k] = - \iint_{\partial\Omega} \mathbf{f}_{Tj}(\mathbf{r}) \cdot \left[\iint_{\partial\Omega} \nabla G_i(\mathbf{r}, \mathbf{r}') \times \mathbf{f}_{Bk}(\mathbf{r}') dS(\mathbf{r}') \right] dS(\mathbf{r}). \quad (1.46d)$$

Expressions (1.46c) and (1.46d) are sometimes designated using the terms EFIE and MFIE, respectively, since these integrals were first used to solve the scattering by Perfect Electric Conductors (PEC) objects using the tangential electric field or the normal magnetic field to impose the boundary conditions.

Introducing $\mathbf{b}_i^E$ and $\mathbf{b}_i^H$, which are column vectors whose j^{th} entry correspond to $b_i^E[j]$ and $b_i^H[j]$, respectively, $\mathbf{b}_i$ a column vector whose first N entries correspond to $\mathbf{b}_i^E$ and whose other entries correspond to $\mathbf{b}_i^H$, $\underline{\underline{Z}}^{EJ}$ and $\underline{\underline{Z}}^{EM}$ two matrices whose (j, k) entries correspond to $Z_i^{EJ}[j, k]$ and $Z_i^{EM}[j, k]$, respectively, and $\mathbf{x}$ a column vector whose k^{th} entry corresponds to x_k , (1.45) can be written in matrix form:

$$(\underline{\underline{Z}}_1 + \underline{\underline{Z}}_2) \cdot \mathbf{x} = \mathbf{b}_2 - \mathbf{b}_1 \quad (1.47)$$

with

$$\underline{\underline{Z}}_i = \begin{pmatrix} \underline{\underline{Z}}_i^{EJ} & \underline{\underline{Z}}_i^{EM} \\ -\underline{\underline{Z}}_i^{EM} & \underline{\underline{Z}}_i^{EJ}/\eta_i^2 \end{pmatrix}. \quad (1.48)$$

If the BF and TF used are div-conformal, Equation (1.46c) can be simplified. Indeed, as shown in Appendix A.2, the grad-div operator can be distributed, leading to

$$Z_i^{EJ}[j, k] = \frac{-j\eta_i}{k_i} \iint_{\partial\Omega} \iint_{\partial\Omega} G_i(\mathbf{r}, \mathbf{r}') \times (k_i^2 \mathbf{f}_{Tj}(\mathbf{r}) \cdot \mathbf{f}_{Bk}(\mathbf{r}') - \nabla \cdot \mathbf{f}_{Tj}(\mathbf{r}) \nabla' \cdot \mathbf{f}_{Bk}(\mathbf{r}')) dS(\mathbf{r}') dS(\mathbf{r}). \quad (1.49)$$

In this new expression, one gets rid of the derivatives of the Green's function. The latter being more singular than the Green's function itself, the integral of (1.49) is easier to evaluate numerically.

In order to fill the impedance matrix of (1.48), one needs to evaluate many times the 4D integrals of (1.46d) and (1.49). Most of the time, when the BF and TF are not nearby, these integrals can be evaluated relatively easily using simple Gaussian quadratures [57]. However, when the BF and

TF are nearby, or even overlapping, the integrand becomes singular. Indeed, looking at the value of the Green's function in (1.16), one can see that it is diverging as $1/R$ when the testing point gets close to the source point, and so will do the integrand of (1.49). The gradient of the Green's function is even more singular, diverging as $1/R^2$. Therefore, the evaluation of both (1.49) and (1.46d) requires some care in order to obtain accurate results in a reasonable amount of time. This problem will be tackled in the Section 1.3.

1.2.3 Computation of the losses

Using the MoM, the value of the fields can be found solving a system of equations. From the value of these fields, the power dissipated can be computed. The power dissipated within a region can be estimated through a volume integral of the losses within that region. However, doing so, one great advantage of the MoM, which is the fact that only the surfaces need to be meshed, is mitigated by the fact that the fields need to be estimated inside the lossy zone.

Using the Poynting theorem, the power dissipated within a volume can be computed as the power flux through the surface of that volume. Using this method, the fields only need to be estimated along the surface of the volume. However, in order to obtain the Poynting vector at a given location on the surface, the cross-product between the electric and magnetic fields has to be estimated, which requires some extra calculations.

A last method, which is based on the equivalence principle, provides the power dissipated using only the impedance matrix, which is already available [58]. It is based on the fact that, considering the inner problem within the lossy zone, the electromagnetic fields are null outside of the inclusion. Therefore, all the power dissipated within the inclusion is coming from the equivalent currents on its surface.

The power generated by the equivalent currents on $\partial\Omega$ reads:

$$P = -\frac{1}{2} \iiint_{\Omega} \mathcal{R}\{\mathbf{J}^* \cdot \mathbf{E} + \mathbf{M}^* \cdot \mathbf{H}\} dV \quad (1.50a)$$

$$= -\frac{1}{4} \iint_{\partial\Omega} \mathcal{R}\{\mathbf{J}_{\text{eq}}^* \cdot \mathbf{E} + \mathbf{M}_{\text{eq}}^* \cdot \mathbf{H}\} dS \quad (1.50b)$$

$$= -\frac{1}{8} \iint_{\partial\Omega} (\mathbf{J}_{\text{eq}}^* \cdot \mathbf{E} + \mathbf{E}^* \cdot \mathbf{J}_{\text{eq}} + \mathbf{M}_{\text{eq}}^* \cdot \mathbf{H} + \mathbf{H}^* \cdot \mathbf{M}_{\text{eq}}) dS \quad (1.50c)$$

$$\simeq -\frac{1}{8} \left(\mathbf{x}^* \cdot (2\underline{\underline{Z}}_{\text{in}} \mathbf{x}) + (2\underline{\underline{Z}}_{\text{in}} \mathbf{x})^* \cdot \mathbf{x} \right) \quad (1.50d)$$

$$\simeq -\frac{1}{4} \mathbf{x}^* (\underline{\underline{Z}}_{\text{in}} + \underline{\underline{Z}}_{\text{in}}^*) \mathbf{x} \quad (1.50e)$$

with the factor $1/2$ of (1.50b) that is due to the fact that the fields continuously vary from zero to their actual value across the boundary, and the factor 2 in (1.50d) that is due to the singular term that have been excluded from the computation of the impedance matrix (cf. Equation (1.40)).

1.3 Analytical evaluation of the singular integrals

In the literature, many techniques have been proposed to speed up the evaluation of these integrals. They can mainly be classified into two categories: singularity extraction based techniques [59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76], and singularity cancellation based techniques [77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93].

The singularity extraction techniques rely on the analytical evaluation of the part of the integral that is singular and the numerical computation of the remaining part, which is either an integral of reduced dimensionality or a 4D integral whose integrand is bounded. In [59], the authors propose an analytical formula for the integration of the static kernel of the Green's function over the BF. As suggested in [75], the remaining 2D integral over the TF is sufficiently smooth to be integrated numerically using Gaussian quadrature schemes. In [60], an analytical formula is even proposed for the full 4D integral of the static Green's function over coincident BF and TF. Once the static kernel have been removed from the dynamic Green's function, the integrand of the remaining 4D integral is bounded. However, its derivatives are not, so that its numerical integration may remain challenging. In [76, 61], the convergence of the numerical integral is further accelerated by extracting additional terms analytically.

The analytical integral of the MFIE term over the BF has been proposed in [64, 65] for linear BF, and extended to higher order BF in [62, 63]. However, the remaining integral over the TF includes a logarithmic singularity that has to be handled carefully if the BF and TF share a common point [61, 72]. The technique has even been extended to the super-hypersingular kernel ($1/R^3$) that may arise in some formulation of the EFIE [66, 67]. More recently, techniques in which the two 2D integrals over the BF and TF are decomposed into four 1D integrals whose order can be switched has been proposed, leading to even better results [73, 74, 68, 69, 70, 71]. Three dimensions out of the four are integrated analytically, reducing the 4D singular integral into a set of 1D non-singular integrals that can be evaluated numerically.

The singularity cancellation based techniques are purely numerical techniques. Generally, an irregular sampling of the integrand is used in order to

minimize the number of sampling points required to reach a prescribed accuracy. The problem is formulated as a change of the variables of integration. The new variables are chosen such that the Jacobian of the transformation compensates for the singular behaviour of the integrand, so that the new integrand is smooth and can be integrated using classical quadrature schemes.

An elegant alternative technique has been proposed in [81, 82]. The authors use a non-singular approximate of the Green's function, which corresponds to the exact Green's function that has been filtered in spectral domain. The error introduced when filtering the Green's function is mitigated by the mesh used to discretize the geometry, which naturally acts as a low-pass filter.

In this thesis, we propose an approach to solve analytically the 4D singular integrals that appear in EFIE and MFIE formulations [94, 95, 96]. The proposed method can be used to solve the 4D integral of the static kernel of the Green's function and its gradient, but also the higher order terms [61, 76]. Instead of decomposing the integral over the BF and TF into a sum of 2D or 1D integrals, the initial 4D integral is treated as a whole. The proposed formulation starts by identifying a 4D volume of integration in a 6D space, on which the distance function only varies over three of the six dimensions. By using the divergence theorem, the 4D integral can be reduced to 3D, 2D and then 1D integrals, the latter being solved analytically. Note that the framework of the proposed method is also valid for integral over 3D BF and TF. Therefore the proposed method can be straightforwardly extended to volumetric MoM.

In Section 1.3.1, the different types of integrals that may arise in the EFIE and MFIE for polynomial BF and TF are highlighted. Then, in Section 1.3.2, the 6D geometry in which the integration takes place is described. In Section 1.3.3, the 4D integral taking place in the 6D space is reduced to a sum of classical 3D or 2D integrals taking place in the 3D space. The latter integrals are solved in Section 1.3.4. Section 1.3.5 is dedicated to the treatment of the hypersingular integral that appears in the MFIE. Finally, the technique is validated through representative examples in Section 1.3.6.

This Section is strongly based on the already published work of [96].

1.3.1 Problem definition

Consider the interaction between two flat polygonal BF and TF that are div-conforming. The BF and TF vector fields are polynomial functions of the coordinates, $\mathbf{f}_B(x, y, z)$ and $\mathbf{f}_T(x, y, z)$. Without losing generality, we will chose a right-handed coordinate system such that $\hat{\mathbf{z}}$ corresponds to the normal to the BF ($\hat{\mathbf{z}} = \hat{\mathbf{n}}_B$), $\hat{\mathbf{x}}$ is the direction that is parallel to both the BF and TF ($\hat{\mathbf{x}} = (\hat{\mathbf{n}}_B \times \hat{\mathbf{n}}_T)/|\hat{\mathbf{n}}_B \times \hat{\mathbf{n}}_T|$), with $\hat{\mathbf{n}}_T$ the normal to the TF, and

the $\hat{\mathbf{y}}$ direction is chosen accordingly. If the BF and TF are parallel, then $\hat{\mathbf{x}}$ is any direction parallel to the BF. The impedance matrix entries for a pair of div-conforming BF and TF are given by Equations (1.49) and (1.46d):

$$Z^{EJ} = -\frac{j\eta_0}{4\pi k_0} \int_{S'} \int_S \left(k_0^2 \mathbf{f}_B(\mathbf{r}) \cdot \mathbf{f}_T(\mathbf{r}') - (\nabla \cdot \mathbf{f}_B(\mathbf{r})) (\nabla' \cdot \mathbf{f}_T(\mathbf{r}')) \right) \frac{e^{-jk_0 R}}{R} dS'(\mathbf{r}') dS(\mathbf{r}), \quad (1.51a)$$

$$Z^{EM} = \frac{1}{4\pi} \oint_{S'} \int_S \nabla' \left(\frac{e^{-jk_0 R}}{R} \right) \times \mathbf{f}_B(\mathbf{r}) \cdot \mathbf{f}_T(\mathbf{r}') dS'(\mathbf{r}') dS(\mathbf{r}), \quad (1.51b)$$

with S and S' the surfaces of the BF and TF.

The exponential term in the integrands of (1.51) can be expanded into a Taylor series of order N around the value R_0 [97], leading to

$$\begin{aligned} e^{-jk_0 R} &= e^{-jk_0 R_0} e^{-jk_0(R-R_0)} \\ &\simeq e^{-jk_0 R_0} \sum_{i=0}^N \frac{(-jk_0(R-R_0))^i}{i!} \\ &= e^{-jk_0 R_0} \sum_{i=0}^N K_i^N(k_0, R_0) R^i. \end{aligned} \quad (1.52)$$

with

$$K_i^N(k_0, R_0) = \sum_{\alpha=i}^N \frac{(-jk_0)^\alpha}{\alpha!} \binom{\alpha}{i} (-R_0)^{\alpha-i}. \quad (1.53)$$

Substituting (1.52) into (1.51), using the linearity of the derivative operator and isolating the wavenumber k gives

$$Z^{EJ} = \frac{-j\eta_0 \exp(-jk_0 R_0)}{4\pi k_0} \sum_{i=0}^N K_i^N(k_0, R_0) (k_0^2 A_i - B_i), \quad (1.54a)$$

$$Z^{EM} = \frac{\exp(-jk_0 R_0)}{4\pi} \sum_{i=0}^N K_i^N(k_0, R_0) C_i \quad (1.54b)$$

with the frequency and material independent terms [97]

$$A_i = \int_{S'} \int_S R^{(i-1)} (\mathbf{f}_B \cdot \mathbf{f}_T) dS dS', \quad (1.55a)$$

$$B_i = \int_{S'} \int_S R^{(i-1)} (\nabla \cdot \mathbf{f}_B) (\nabla' \cdot \mathbf{f}_T) dS dS', \quad (1.55b)$$

$$C_i = (i-1) \oint_{S'} \int_S R^{(i-3)} \mathbf{R} \times \mathbf{f}_B \cdot \mathbf{f}_T dS dS'. \quad (1.55c)$$

The $\mathbf{r}$ and $\mathbf{r}'$ dependencies have been omitted for clarity. This formulation is very convenient since each term of (1.55) is independent from frequency and material parameters, so that they can be used for any frequency and materials, as long as the geometry does not change. Moreover, since the Taylor expansion (1.52) is applied to the phase term only, the convergence of the series is very rapid (Taylor expansion of a complex exponential). Last, if R_0 is chosen to correspond to the mean distance between the BF and TF, the convergence of (1.55) is independent from the distance between the BF and TF. An extensive investigation of the number of terms required to reach a prescribed level of accuracy has already been carried out in [97] and is out of the scope of the present paper.

It can be noticed that the three sets of integrals in (1.55) can be reduced to two sets of canonical integrals. As mentioned in the beginning of this Section, the vector fields of the BF and TF can be expressed as polynomial functions of the coordinates, so that the generic shapes of A_i and B_i and of C_i , respectively $\mathcal{A}_i$ and $\mathcal{C}_i$, read:

$$\mathcal{A}_i = \int_{S'} \int_S R^{(i-1)} \mathcal{P}_1(\mathbf{r}, \mathbf{r}') dS dS', \quad (1.56a)$$

$$\mathcal{C}_i = (i-1) \oint_{S'} \int_S R^{(i-3)} (\mathbf{R} \cdot \mathcal{P}_1(\mathbf{r}, \mathbf{r}')) dS dS', \quad (1.56b)$$

with $\mathcal{P}_k(\mathbf{r}, \mathbf{r}')$ and $\mathcal{P}_k(\mathbf{r}, \mathbf{r}')$ corresponding to polynomial scalar and vector functions of the positions $\mathbf{r}$ and $\mathbf{r}'$. The evaluation of the terms of (1.56) may be difficult to handle numerically, since the integrand and/or its higher derivatives are not bounded for even i [76, 61], requiring semi-analytical techniques or advanced quadrature schemes. The rest of this chapter is dedicated to the analytical solution of these integrals.

Most of the time, in the literature, $R = R(\mathbf{r} - \mathbf{r}')$ is seen as a 3D function $R : \mathbb{R}^3 \rightarrow \mathbb{R} : \mathbf{r} \rightarrow |\mathbf{r}|$. Due to this, the two surface integrals of (1.56) are difficult to merge into a single 4D integral since this 4D integral would take place in a 3D space. For this reason, the starting point of this method is to consider that $R = R(\mathbf{r}, \mathbf{r}')$ is a 6D function $R : \mathbb{R}^6 \rightarrow \mathbb{R} : (\mathbf{r}, \mathbf{r}') \rightarrow |\mathbf{r} - \mathbf{r}'|$. The advantage of this formulation is that, now, the $\mathbf{r}$ and $\mathbf{r}'$ vectors can be seen as two orthogonal vectors in the 6D space, $(\mathbf{r}, \mathbf{0})$ and $(\mathbf{0}, \mathbf{r}')$ respectively, such that the two consecutive 2D integrals of (1.56), which both take place in a 3D space, can be merged into a single 4D integral in the 6D space.

Note that the $\mathcal{C}_i$ term is a particular case of the $\mathcal{A}_{i-1}$ term, but with additional properties that will prove to be useful to treat the singular case $R \rightarrow 0$. The method used for both terms being essentially identical, the

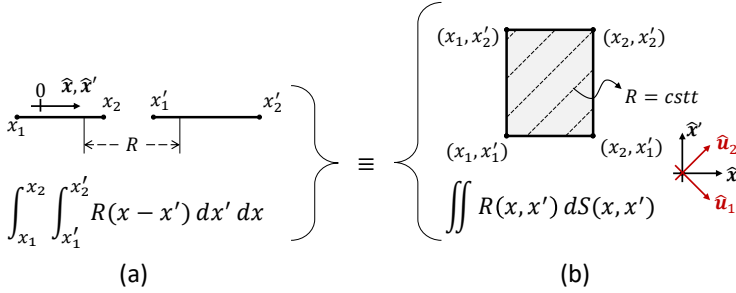


Figure 1.3: The two 1D integrals of (a) are merged into a single 2D integral over the gray surface of (b), which can be solved more easily. First, the divergence theorem can be used. Second, rotating the system of coordinates from $\{x, x'\}$ to $\{u_1, u_2\}$, the R function is independent from the u_2 coordinate.

treatment of the $\mathcal{A}_i$ term will be used as an illustration, while the specificities in the treatment of the $\mathcal{C}_i$ term are provided in Section 1.3.5.

1.3.2 The 6D geometry

Each term of (1.56) corresponds to two consecutive surface integrals (2D) over BF and TF, which lie in the 3D space. Therefore, it can be reformulated in the sense of a 4D integral that takes place within a 6D space, each point $(\mathbf{r}, \mathbf{r}')$ of the 6D space corresponding a pair of points, one on the BF and one on the TF, of coordinates $\mathbf{r}$ and $\mathbf{r}'$, respectively. Then, the 4D volume of integration within this 6D space ($= \Omega_4^6$) corresponds to the combination of the BF with the TF in the 6D space:

$$\Omega_4^6 = \{(\mathbf{r}, \mathbf{r}') | \mathbf{r} \in \text{BF}, \mathbf{r}' \in \text{TF}\} \quad (1.57)$$

To begin with, let us illustrate this manipulation with a 1D example. Consider the integration of the distance function R over a 1D BF and a 1D TF within a 1D space, as illustrated in Fig. 1.3(a). If x denotes the coordinate of the points in the BF, and x' denotes the coordinate of the points in the TF, the distance function becomes $R(x - x') = |x - x'|$. At first glance, the two 1D integrals must be solved sequentially.

Re-writing the problem in two dimensions, one obtains Fig. 1.3(b). Since x and x' are independent, they correspond to two independent directions. In this new 2D space, the two consecutive line integrals (1D) become a single surface (2D) integral. This reformulation has two main advantages. First, the divergence theorem can be applied to the surface of Fig. 1.3(b)

to reduce the 2D integral to a sum of 1D integrals. Second, it can be seen that the R function is very easy to deal with using a change of coordinates. Indeed, using the $\{u_1, u_2\}$ system of coordinates indicated in Fig. 1.3(b), the R function only varies along the $\hat{\mathbf{u}}_1$ direction and is constant along the $\hat{\mathbf{u}}_2$ direction. Similar reasoning will prove to be very useful for the analytical solution of (1.56).

Going back to the original problem, since the whole technique is based on the manipulation of the 4D volume in 6D space, it is worth spending some times to clarify the geometry considered.

First of all, consider the 4D volume itself. Since the integration takes place in a 6D space, the 4D space spanned by the 4D volume is characterized by two normal directions, $\hat{\mathbf{n}}_{v,1}^6$ and $\hat{\mathbf{n}}_{v,2}^6$ (just as a line is in the 3D space). These unit vectors are corresponding to the normals to the BF and TF, respectively $\hat{\mathbf{n}}_B$ and $\hat{\mathbf{n}}_T$. It is important to notice that the scalar product of a normal with the position of any point within the volume is constant. Since the BF and TF are polygonal, the 3D boundary of the 4D volume corresponds to 3D polyhedra, just as the 2D boundary of a 3D polyhedron corresponds to polygons.

Each 3D polyhedron corresponds to the combination of one edge of the BF with the whole TF or one edge of the TF with the whole BF. In order to characterize the 3D space spanned by these volumes, one additional normal direction is required. For volume p , this normal will be noted $\hat{\mathbf{n}}_p^6$. Note that many volumes p are contiguous and therefore share a common surface.

The 2D boundary of one 3D polyhedron corresponds to flat polygons. They are obtained either by convolving one edge of the BF and one edge of the TF, or convolving one vertex of the BF (or TF) with the TF (or BF). The additional normal direction required to describe the 2D space spanned by the 2D surface q will be noted $\hat{\mathbf{n}}_q^6$.

The 1D edges delineating the 2D surfaces are the combination of edges of the BF (or TF) with vertices of the TF (or BF). Their corresponding normals will be noted $\hat{\mathbf{n}}_r^6$.

Last come the vertices of all these geometrical entities. They correspond to the combination of the vertices of the BF with the vertices of the TF, so that the coordinate of the 6D vertex corresponding to the combination of the vertex i of the BF located in $\mathbf{r}_i$ and the vertex j of the TF located in $\mathbf{r}'_j$ is located in $(\mathbf{r}_i, \mathbf{r}'_j)$.

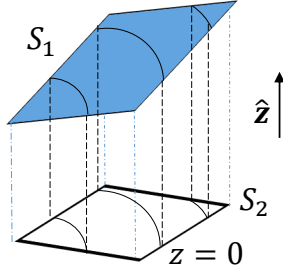


Figure 1.4: The orthogonal projection of the surface of integration S_1 along the $\hat{\mathbf{z}}$ direction does not change the value of the integral (except for the constant Jacobian) as long as the integrand does not depend on z .

Now, we consider a “sum-and-difference” change of coordinates:

$$\begin{aligned} u_1 &= \frac{x - x'}{\sqrt{2}}, & u_4 &= \frac{x + x'}{\sqrt{2}}, \\ u_2 &= \frac{y - y'}{\sqrt{2}}, & u_5 &= \frac{y + y'}{\sqrt{2}}, \\ u_3 &= \frac{z - z'}{\sqrt{2}}, & u_6 &= \frac{z + z'}{\sqrt{2}}. \end{aligned} \quad (1.58)$$

Using this new basis gives $\mathbf{R} = \sqrt{2}(u_1\hat{\mathbf{u}}_1 + u_2\hat{\mathbf{u}}_2 + u_3\hat{\mathbf{u}}_3)$, which is independent from u_4, u_5 and u_6 . This will be fundamental for the analytical evaluation of (1.56). Moreover, it can be seen that, except for BF and TF defined on parallel domains ($\hat{\mathbf{n}}_B = \hat{\mathbf{n}}_T$), neither the $\hat{\mathbf{u}}_5$ nor the $\hat{\mathbf{u}}_6$ direction is contained within the space spanned by the 4D volume of integration. The case of parallel BF and TF will be treated in a dedicated Section.

In order to perform the integral over the 4D volume within the 6D space, three different tools will be repetitively used.

1. *TOOL_1*: If the integrand is modified outside the domain of integration, it does not modify the value of the integral. This can be used to create a new integrand that is independent from one chosen coordinate. For example, consider a $\hat{\mathbf{x}} - \hat{\mathbf{y}} - \hat{\mathbf{z}}$ Cartesian coordinate system. The z coordinate within a non-vertical 2D surface linearly depends on the two other coordinates: $z = k_1x + k_2y + k_3$. Thus, the integral of any function $f(x, y, z)$ within this surface can be reformulated as the integral of $g(x, y) = f(x, y, k_1x + k_2y + k_3)$, with k_1, k_2 and k_3 three constants that depend on the surface.
2. *TOOL_2*: If the integrand is independent from one coordinate u_i , and

if the corresponding direction $\hat{\mathbf{u}}_i$ is not contained within the space spanned by the domain of integration, this domain can be projected into the subspace $u_i = 0$. The new integral will be equal to the previous one within a constant factor, which corresponds to the Jacobian of the transformation. Using this method, the dimensionality of the space in which the integration takes place is reduced. For example, consider the integral of $g(x, y)$ over the surface S_1 represented in Figure 1.4. S_2 is the orthogonal projection of S_1 on the $z = 0$ subspace. The value of the integral of $g(x, y)$ over S_2 is the same as its integral over S_1 within a constant factor corresponding to the Jacobian of the transformation.

3. *TOOL-3*: If a vector field can be found, whose divergence matches the integrand within the domain of integration, applying the divergence theorem reduces the dimensionality of the domain of integration:

$$\begin{aligned} &\text{if } \nabla \cdot \mathbf{G} = f \text{ on } \Omega, \\ &\int_{\Omega} f \, dV = \int_{\Omega} \nabla \cdot \mathbf{G} \, dV = \int_{\partial\Omega} \mathbf{G} \cdot \hat{\mathbf{n}} \, dS, \end{aligned} \quad (1.59)$$

with Ω the domain of integration, $\partial\Omega$ its boundary and $\hat{\mathbf{n}}$ the outward-pointing unit normal. Note that the derivative operator ∇ has to be limited to the space spanned by the domain of integration. For example, if the divergence theorem is applied on a surface in the 3D space, the surface divergence must be considered instead of the volume divergence, and the surface integral can be reformulated as a line (1D) integral.

1.3.3 From 6D to 3D

In this section, the 4D integral within 6D space of Equation (1.56a) is reduced to a sum of 2D or 3D integrals within 3D space.

Formulated in the 6D space, (1.56a) becomes

$$\begin{aligned} \mathcal{A}_i = &\int R^{(i-1)}(u_1, u_2, u_3) \\ &\times \mathcal{P}_2(u_1, u_2, u_3, u_4, u_5, u_6) dV_4^6, \end{aligned} \quad (1.60)$$

with dV_i^j indicating that the integration is performed over a i D volume within the j D space.

First of all, consider the two normals to the 4D volume within the 6D space. Since these normals correspond to the normals to the BF and TF, using (1.58) and considering the specific definitions of the $\hat{\mathbf{x}}$ and $\hat{\mathbf{z}}$ directions

described in Section 1.3.1 gives

$$\hat{\mathbf{n}}_{v,1}^6 = (\hat{\mathbf{n}}_B, \hat{\mathbf{n}}_B)/\sqrt{2} = (0, 0, 1, 0, 0, 1)/\sqrt{2} \quad (1.61a)$$

$$\hat{\mathbf{n}}_{v,2}^6 = (-\hat{\mathbf{n}}_T, \hat{\mathbf{n}}_T)/\sqrt{2} = (0, -a, -b, 0, a, b)/\sqrt{2}, \quad (1.61b)$$

with $a^2 + b^2 = 1$. Note that in the case of parallel BF and TF, $a = 0$. This case will be treated in Section 1.3.3.

The next step consists in the orthogonal projection of the 4D volume into the 5D subspace $u_6 = 0$. First, the orthogonal vectors are combined to obtain:

$$\hat{\mathbf{n}}_{v,1}^5 = \frac{(\hat{\mathbf{n}}_{v,2}^6 \cdot \hat{\mathbf{u}}_6)\hat{\mathbf{n}}_{v,1}^6 - (\hat{\mathbf{n}}_{v,1}^6 \cdot \hat{\mathbf{u}}_6)\hat{\mathbf{n}}_{v,2}^6}{\sqrt{(\hat{\mathbf{n}}_{v,1}^6 \cdot \hat{\mathbf{u}}_6)^2 + (\hat{\mathbf{n}}_{v,2}^6 \cdot \hat{\mathbf{u}}_6)^2}} \quad (1.62a)$$

$$= \frac{b \hat{\mathbf{n}}_{v,1}^6 - \hat{\mathbf{n}}_{v,2}^6}{\sqrt{1 + b^2}},$$

$$\hat{\mathbf{n}}_{v,2}^5 = \frac{(\hat{\mathbf{n}}_{v,1}^6 \cdot \hat{\mathbf{u}}_6)\hat{\mathbf{n}}_{v,1}^6 + (\hat{\mathbf{n}}_{v,2}^6 \cdot \hat{\mathbf{u}}_6)\hat{\mathbf{n}}_{v,2}^6}{\sqrt{(\hat{\mathbf{n}}_{v,1}^6 \cdot \hat{\mathbf{u}}_6)^2 + (\hat{\mathbf{n}}_{v,2}^6 \cdot \hat{\mathbf{u}}_6)^2}} \quad (1.62b)$$

$$= \frac{\hat{\mathbf{n}}_{v,1}^6 + b \hat{\mathbf{n}}_{v,2}^6}{\sqrt{1 + b^2}},$$

so that $\hat{\mathbf{n}}_{v,1}^5 \cdot \hat{\mathbf{u}}_6 = 0$ and $\hat{\mathbf{n}}_{v,1}^5 \cdot \hat{\mathbf{n}}_{v,2}^5 = 0$. In that way, $\hat{\mathbf{n}}_{v,1}^5$ is orthogonal to both the original volume and its projection into the $u_6 = 0$ subspace.

From 6D to 5D

Now, the u_6 dependency of the integrand in (1.60) can be removed using *TOOL-1*. If d_i^j is the distance between the volume of integration and the origin in the $\hat{\mathbf{n}}_i^j$ direction, then

$$\hat{\mathbf{n}}_{v,2}^5 \cdot \mathbf{u} = d_{v,2}^5 \quad \forall \mathbf{u} \in \Omega_v^6, \quad (1.63)$$

with Ω_v^6 the 4D domain of integration lying in the 6D space. Isolating the u_6 term provides

$$u_6 = \frac{d_{v,2}^5 - \sum_{\alpha=1}^5 (\hat{\mathbf{n}}_{v,2}^5 \cdot \hat{\mathbf{u}}_\alpha) u_\alpha}{\hat{\mathbf{n}}_{v,2}^5 \cdot \hat{\mathbf{u}}_6} \quad \forall \mathbf{u} \in \Omega_v^6. \quad (1.64)$$

It can be easily checked that, using the particular basis described in Section 1.3.1, $\hat{\mathbf{n}}_{v,2}^5 \cdot \hat{\mathbf{u}}_6 \neq 0$. Substituting (1.64) into (1.60) gives

$$\begin{aligned} \mathcal{A}_i &= \int R^{(i-1)}(u_1, u_2, u_3) \\ &\quad \times \mathcal{P}_3(u_1, u_2, u_3, u_4, u_5) dV_4^6. \end{aligned} \quad (1.65)$$

Now that the integrand of (1.65) is independent from u_6 , an orthogonal projection of the volume of integration over the $u_6 = 0$ subspace is performed (*TOOL_2*) in order to reduce the dimensionality of the space we are working on. Multiplying the resulting integral by the (constant) Jacobian of the projection provides

$$\mathcal{A}_i = \frac{1}{|\hat{\mathbf{n}}_{v,2}^5 \cdot \hat{\mathbf{u}}_6|} \int R^{(i-1)}(u_1, u_2, u_3) \times \mathcal{P}_3(u_1, u_2, u_3, u_4, u_5) dV_4^5. \quad (1.66)$$

As mentioned previously, since $\hat{\mathbf{n}}_{v,1}^5 \cdot \hat{\mathbf{u}}_6 = 0$, $\hat{\mathbf{n}}_{v,1}^5$ is orthogonal to both the original volume and the projected one. The projected volume being a 4D volume within a 5D space, its orthogonal space is 1D and is therefore entirely spanned by the $\hat{\mathbf{n}}_{v,1}^5$.

From 5D to 4D

This Section is treating the case where the BF and TF are not parallel. The parallel case will be treated in Section 1.3.3. If the BF and TF are not parallel, it means that $a \neq 0$ in (1.61b). Consequently, $\hat{\mathbf{n}}_{v,1}^5 \cdot \hat{\mathbf{u}}_5 \neq 0$, so that the procedure to reduce the dimensionality of the space is identical when going from 6D to 5D and from 5D to 4D.

First, within the volume of integration, the u_5 coordinate can be expressed as a linear combination of the other coordinates (*TOOL_1*):

$$u_5 = \frac{d_{v,1}^5 - \sum_{\alpha=1}^4 (\hat{\mathbf{n}}_{v,1}^5 \cdot \hat{\mathbf{u}}_\alpha) u_\alpha}{\hat{\mathbf{n}}_{v,1}^5 \cdot \hat{\mathbf{u}}_5}. \quad (1.67)$$

Substituting (1.67) into (1.66), the u_5 dependence of the integrand is removed. Putting the $1/|\hat{\mathbf{n}}_{v,2}^5 \cdot \hat{\mathbf{u}}_6|$ factor of (1.66) inside the polynomial $\mathcal{P}_4$ gives:

$$\mathcal{A}_i = \int R^{(i-1)}(u_1, u_2, u_3) \mathcal{P}_4(u_1, u_2, u_3, u_4) dV_4^5. \quad (1.68)$$

Since the integrand of (1.68) no longer depends on u_5 , the 5D space is projected into the 4D subspace $u_5 = 0$ (*TOOL_2*), leading to

$$\mathcal{A}_i = \frac{1}{|\hat{\mathbf{n}}_{v,1}^5 \cdot \hat{\mathbf{u}}_5|} \int R^{(i-1)}(u_1, u_2, u_3) \times \mathcal{P}_4(u_1, u_2, u_3, u_4) dV_4^4. \quad (1.69)$$

It is interesting to consider the behaviour of the method for the case where the BF and TF are close to parallel, without being exactly so. Indeed,

in that case, $\hat{\mathbf{n}}_{v,1}^5 \cdot \hat{\mathbf{u}}_5 \ll 1$. The RHS of (1.67) then corresponds to a nearly canceling difference between large numbers. Therefore, for very small angles (smaller than 1°), one may consider interpolating the value of the integral from its value for parallel BF and TF and for non-parallel BF and TF with a higher angle between them (e.g. $1^\circ, 2^\circ, \dots$). An example using polynomial interpolation of various orders is studied in Section 1.3.6, where the proposed fix is illustrated.

From 4D to 3D

Equation (1.69) is dealing with a 4D volume of integration within a 4D space. The dimensionality of the volume of integration needs to be reduced using the divergence theorem (*TOOL_3*). Looking at (1.69), one can notice that the dependence of the integrand on u_4 is polynomial, so that a vector field whose divergence corresponds to that integrand can be easily found. Introducing $\mathcal{P}_5(u_1, u_2, u_3, u_4)$ such that

$$\mathcal{P}_5(u_1, u_2, u_3, u_4) \triangleq \frac{1}{|\hat{\mathbf{n}}_{v,1}^5 \cdot \hat{\mathbf{u}}_5|} \int_0^{u_4} \mathcal{P}_4(u_1, u_2, u_3, u'_4) du'_4. \quad (1.70)$$

It leads to

$$\nabla \cdot [R^{(i-1)} \mathcal{P}_5 \hat{\mathbf{u}}_4] = \frac{R^{(i-1)} \mathcal{P}_4}{|\hat{\mathbf{n}}_{v,1}^5 \cdot \hat{\mathbf{u}}_5|}. \quad (1.71)$$

Substituting (1.71) into (1.69) and applying the divergence theorem (*TOOL_3*), it can be proven (cf. Appendix A.3) that no special care is required for the possibly singular zone where $R \rightarrow 0$. This zone can be removed from the domain of integration, leading to

$$\begin{aligned} \mathcal{A}_i = \sum_p (\hat{\mathbf{n}}_p^4 \cdot \hat{\mathbf{u}}_4) \oint_{\Omega_p^4} R^{(i-1)}(u_1, u_2, u_3) \\ \times \mathcal{P}_5(u_1, u_2, u_3, u_4) dV_3^4, \end{aligned} \quad (1.72)$$

with Ω_p^6 the p^{th} 3D polyhedron that is part of the boundary of Ω_v^6 , the original volume of integration (cf. Section 1.3.2), Ω_p^4 the projection of Ω_p^6 into the subspace $u_6 = u_5 = 0$, $\hat{\mathbf{n}}_p^4$ the outer normal to $\hat{\mathbf{n}}_p^4$ and $\oint$ denoting the integration in the Cauchy principal value sens. $\hat{\mathbf{n}}_p^4$ can be computed by combining $\hat{\mathbf{n}}_p^6$ with $\hat{\mathbf{n}}_{v,2}^5$ and $\hat{\mathbf{n}}_{v,1}^5$ to remove its u_6 and u_5 components:

$$\begin{aligned} \mathbf{n}_p^4 = \hat{\mathbf{n}}_p^6 - \frac{\hat{\mathbf{n}}_p^6 \cdot \hat{\mathbf{u}}_6}{\hat{\mathbf{n}}_{v,2}^5 \cdot \hat{\mathbf{u}}_6} \hat{\mathbf{n}}_{v,2}^5 \\ - \left(\frac{\hat{\mathbf{n}}_p^6 \cdot \hat{\mathbf{u}}_5}{\hat{\mathbf{n}}_{v,1}^5 \cdot \hat{\mathbf{u}}_5} - \frac{\hat{\mathbf{n}}_p^6 \cdot \hat{\mathbf{u}}_6}{\hat{\mathbf{n}}_{v,1}^5 \cdot \hat{\mathbf{u}}_5} \frac{\hat{\mathbf{n}}_{v,2}^5 \cdot \hat{\mathbf{u}}_5}{\hat{\mathbf{n}}_{v,2}^5 \cdot \hat{\mathbf{u}}_6} \right) \hat{\mathbf{n}}_{v,1}^5 \end{aligned} \quad (1.73)$$

and $\hat{\mathbf{n}}_p^4 = \mathbf{n}_p^4 / |\mathbf{n}_p^4|$.

Using a development similar to the one in Appendix A.3, it can be shown that the value of the integrals of (1.72) are bounded, so that contribution of the terms for which $\hat{\mathbf{n}}_p^4 \cdot \hat{\mathbf{u}}_4 \rightarrow 0$ vanishes. Removing the vanishing terms from the summation, (1.72) becomes

$$\mathcal{A}_i = \sum_{(p|\hat{\mathbf{n}}_p^4 \cdot \hat{\mathbf{u}}_4 \neq 0)} (\hat{\mathbf{n}}_p^4 \cdot \hat{\mathbf{u}}_4) \int_{\Omega_p^4} R^{(i-1)}(u_1, u_2, u_3) \times \mathcal{P}_5(u_1, u_2, u_3, u_4) dV_3^4. \quad (1.74)$$

Now that we are dealing with a 3D volume within a 4D space, we can proceed as we did in Sections 1.3.3 and 1.3.3.

First, the u_4 dependence of the integrand of (1.74) is eliminated (*TOOL-1*) using the fact that, within the volume of integration,

$$u_4 = \frac{d_p^4 - \sum_{\alpha=1}^3 (\hat{\mathbf{n}}_p^4 \cdot \hat{\mathbf{u}}_\alpha) u_\alpha}{\hat{\mathbf{n}}_p^4 \cdot \hat{\mathbf{u}}_4}, \quad (1.75)$$

After, we project the 3D volumes of integration Ω_p^4 into the $u_4 = 0$ subspace (*TOOL-2*), leads to

$$\mathcal{A}_i = \sum_{(p|\hat{\mathbf{n}}_p^4 \cdot \hat{\mathbf{u}}_4 \neq 0)} \frac{(\hat{\mathbf{n}}_p^4 \cdot \hat{\mathbf{u}}_4)}{|\hat{\mathbf{n}}_p^4 \cdot \hat{\mathbf{u}}_4|} \int_{\Omega_p^3} R^{(i-1)}(u_1, u_2, u_3) \times \mathcal{P}_6(u_1, u_2, u_3) dV_3^3. \quad (1.76)$$

Equation (1.76) corresponds to a “classical” volume integral of the $R^{(i-1)}$ function multiplied by a given polynomial. The analytical treatment of that kind of integrals will be tackled in Section 1.3.4.

Parallel BF and TF

In the case where the BF is parallel to the TF, Equation (1.67) in Section 1.3.3 is no longer valid due to the fact that $\hat{\mathbf{n}}_{v,1}^5 \cdot \hat{\mathbf{u}}_5 = 0$. Indeed, in the parallel case, $\hat{\mathbf{n}}_{v,1}^5 = (0, 0, \pm 1, 0, 0)$, so that the u_5 coordinate is independent from the other coordinates within the volume of integration, in (1.66).

However, for the same reason, the $\hat{\mathbf{u}}_5$ direction is entirely contained within the space spanned by this 4D volume of integration. It will be useful to apply the divergence theorem (*TOOL-3*). Introducing $\mathcal{P}_4^\parallel$ such that

$$\mathcal{P}_4^\parallel \triangleq \frac{1}{|\hat{\mathbf{n}}_{v,2}^5 \cdot \hat{\mathbf{u}}_6|} \int_0^{u_5} \mathcal{P}_3 du'_5 \quad (1.77)$$

leads to

$$\nabla \cdot \left[R^{(i-1)} \mathcal{P}_4^\parallel \hat{\mathbf{u}}_5 \right] = \frac{R^{(i-1)} \mathcal{P}_3}{|\hat{\mathbf{n}}_{v,2}^5 \cdot \hat{\mathbf{u}}_6|}. \quad (1.78)$$

Substituting (1.78) into (1.66) and using the divergence theorem gives

$$\begin{aligned} \mathcal{A}_i = & \sum_{(p|\hat{\mathbf{n}}_p^5 \cdot \hat{\mathbf{u}}_5 \neq 0)} (\hat{\mathbf{n}}_p^5 \cdot \hat{\mathbf{u}}_5) \oint_{\Omega_p^5} R^{(i-1)}(u_1, u_2, u_3) \\ & \times \mathcal{P}_4^\parallel(u_1, u_2, u_3, u_4, u_5) dV_3^5, \end{aligned} \quad (1.79)$$

with $\hat{\mathbf{n}}_p^5$ the outer normal of the 3D volume p within the 5D space. No special care is required for the possibly singular zone where $R \rightarrow 0$ (cf. Appendix A.3). Note that the vanishing terms corresponding to $\hat{\mathbf{n}}_p^5 \cdot \hat{\mathbf{u}}_5 = 0$ have been removed from the summation (cf. Section 1.3.3).

Since $\hat{\mathbf{n}}_p^5 \cdot \hat{\mathbf{u}}_5 \neq 0$ for all the remaining terms, u_5 is no longer linearly independent from the other coordinates (*TOOL-1*):

$$u_5 = \frac{d_p^5 - \sum_{\alpha=1}^4 (\hat{\mathbf{n}}_p^5 \cdot \hat{\mathbf{u}}_\alpha) u_\alpha}{\hat{\mathbf{n}}_p^5 \cdot \hat{\mathbf{u}}_5}. \quad (1.80)$$

The substitution of (1.80) into (1.79), followed by the orthogonal projection of the 3D volumes of integration into the 4D subspace $u_5 = 0$ (*TOOL-2*) leads to

$$\begin{aligned} \mathcal{A}_i = & \sum_{(p|\hat{\mathbf{n}}_p^5 \cdot \hat{\mathbf{u}}_5 \neq 0)} \frac{(\hat{\mathbf{n}}_p^5 \cdot \hat{\mathbf{u}}_5)}{|\hat{\mathbf{n}}_p^5 \cdot \hat{\mathbf{u}}_5|} \oint_{\Omega_p^4} R^{(i-1)}(u_1, u_2, u_3) \\ & \times \mathcal{P}_5^\parallel(u_1, u_2, u_3, u_4) dV_3^4, \end{aligned} \quad (1.81)$$

We can iterate to transform (1.81) into a sum of 2D surface integrals taking place in the classical 3D space:

$$\begin{aligned} \mathcal{A}_i = & \sum_{(p|\hat{\mathbf{n}}_p^5 \cdot \hat{\mathbf{u}}_5 \neq 0)} \frac{(\hat{\mathbf{n}}_p^5 \cdot \hat{\mathbf{u}}_5)}{|\hat{\mathbf{n}}_p^5 \cdot \hat{\mathbf{u}}_5|} \sum_{(q|\hat{\mathbf{n}}_q^4 \cdot \hat{\mathbf{u}}_4 \neq 0)}^{\Omega_q^4 \in \partial(\Omega_p^4)} \frac{(\hat{\mathbf{n}}_q^4 \cdot \hat{\mathbf{u}}_4)}{|\hat{\mathbf{n}}_q^4 \cdot \hat{\mathbf{u}}_4|} \\ & \times \oint_{\Omega_q^3} R^{(i-1)}(u_1, u_2, u_3) \mathcal{P}_6^\parallel(u_1, u_2, u_3) dS_2^3, \end{aligned} \quad (1.82)$$

with $\hat{\mathbf{n}}_q^4$ the outward unit vector perpendicular to the surface Ω_q^4 that is part of the boundary of the volume Ω_p^4 .

(1.82) is dealing with the surface integration of the “classical” R function multiplied by a polynomial function of the coordinates, which will be solved in Section 1.3.4.

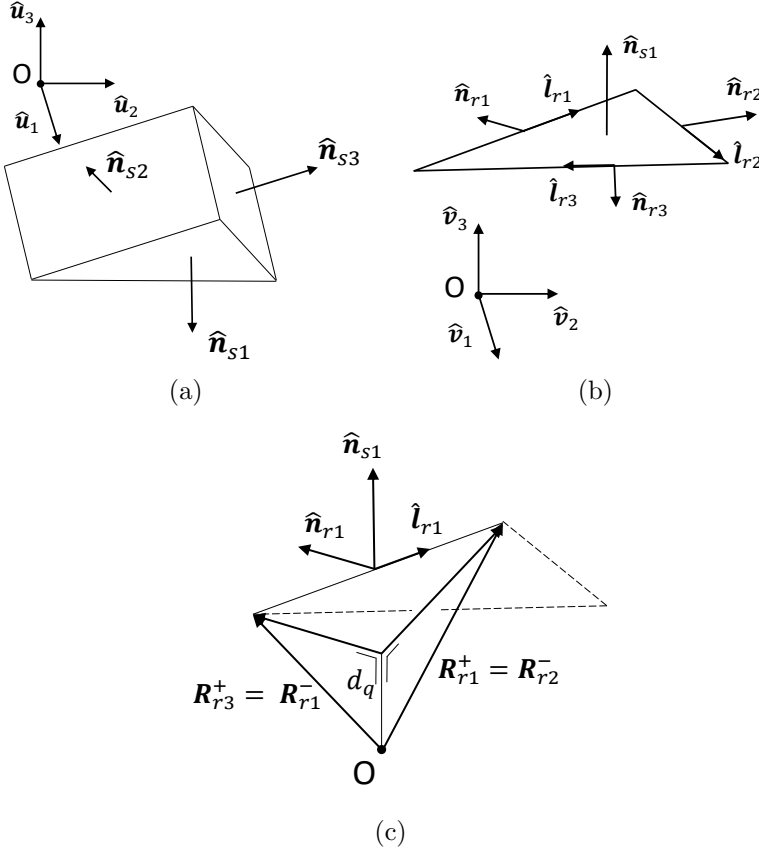


Figure 1.5: Geometry of the (a) 3D, (b) 2D and (c) 1D domains of integration and illustration of the associated quantities.

1.3.4 Estimating the 3D integral

In this section, we solve the 3D and 2D integrals of Equations (1.76) and (1.82). These types of integrals have already been solved by the authors of [62]. The method is summarized here for self-completeness. The geometries described throughout the development are illustrated in Figure 1.5.

We start from (1.76). The polynomial contribution of some coordinate u_α in $\mathcal{P}_6$ can be isolated by rewriting

$$\mathcal{P}_6(u_1, u_2, u_3) = \sum_s P_s(u_\beta, u_\gamma) u_\alpha^s, \quad \alpha \neq \beta \neq \gamma \neq \alpha. \quad (1.83)$$

Each term of (1.83) is treated separately. To reduce the dimensionality

of the integrals of (1.76), the following identities are used:

If $s > 0$:

$$\begin{aligned} \mathcal{P}_s(u_\beta, u_\gamma) u_\alpha^s R^{(\zeta-1)} &= \frac{1}{\zeta+1} \\ &\times \left[\nabla \cdot \left(\mathcal{P}_s(u_\beta, u_\gamma) u_\alpha^{(s-1)} R^{(\zeta+1)} \hat{\mathbf{u}}_\alpha \right) \right. \\ &\quad \left. - (s-1) \mathcal{P}_s(u_\beta, u_\gamma) u_\alpha^{(s-2)} R^{(\zeta+1)} \right], \end{aligned} \quad (1.84a)$$

If $s = 0$ and $P_s(u_\beta, u_\gamma) = cstt$:

$$R^{(\zeta-1)} = \frac{1}{(\zeta+2)} \nabla \cdot (R^\zeta \hat{\mathbf{R}}), \quad (1.84b)$$

Otherwise:

$$\mathcal{P}_s(u_\beta, u_\gamma) R^{(\zeta-1)} = \sum_t \mathcal{P}_t(u_\gamma) u_\beta^t R^{(\zeta-1)}. \quad (1.84c)$$

Substituting these identities recursively into (1.76) and applying the divergence theorem, the volume integral can be expressed as a sum of surface integrals. Note that the $R(\hat{\mathbf{R}} \cdot \hat{\mathbf{n}}_q)$ and $\hat{\mathbf{u}}_\alpha \cdot \hat{\mathbf{n}}_q$ factors are constant on surface q and can therefore be removed from the integral.

Using the development in Appendix A.3, it can be shown that no special treatment is required for the possibly singular zone where $R \rightarrow 0$.

We now have to deal with surface integrals of the type

$$\oint \mathcal{P}_s(u_1, u_2, u_3) R^{(\zeta-1)} dS, \quad \zeta \geq 0. \quad (1.85)$$

First of all, the $\{\hat{\mathbf{u}}_1, \hat{\mathbf{u}}_2, \hat{\mathbf{u}}_3\}$ orthonormal right-handed basis is rotated to match the $\{\hat{\mathbf{v}}_1, \hat{\mathbf{v}}_2, \hat{\mathbf{v}}_3\}$ orthonormal right-handed basis, with $\hat{\mathbf{v}}_1$ and $\hat{\mathbf{v}}_2$ parallel to the surface. In this new basis, the v_3 coordinate is constant along the surface of integration, so that

$$\oint \mathcal{P}_s(u_1, u_2, u_3) R^{(\zeta-1)} dS = \oint \mathcal{P}_s^v(v_1, v_2) R^{(\zeta-1)} dS. \quad (1.86)$$

To reduce the 2D integral of (1.86) into a sum of 1D integrals, the different terms treated separately using (1.84c) and the following identities are recursively used:

If $s > 0$:

$$\mathcal{P}_s^v(v_\beta) v_\alpha^s R^{(\zeta-1)} = \frac{1}{\zeta+1}$$

$$\begin{aligned} & \times \left[\nabla \cdot \left(\mathcal{P}_s^v(v_\beta) v_\alpha^{(s-1)} R^{(\zeta+1)} \hat{\mathbf{v}}_\alpha \right) \right. \\ & \quad \left. - (s-1) \mathcal{P}_s^v(v_\beta) v_\alpha^{(s-2)} R^{(\zeta+1)} \right], \end{aligned} \quad (1.87a)$$

If $s = 0$ and $P_s(v_\beta) = cstt$:

$$R^{(\zeta-1)} = \frac{1}{\zeta+1} \nabla \cdot \left(\frac{R^{(\zeta+1)}}{P_q^2} \mathbf{P}_q \right), \quad (1.87b)$$

Otherwise:

$$\mathcal{P}_s^v(v_\beta) R^{(\zeta-1)} = \sum_w K_w v_\beta^w R^{(\zeta-1)}, \quad (1.87c)$$

with K_w a constant, $\mathbf{P}_q = (v_1 \hat{\mathbf{v}}_1 + v_2 \hat{\mathbf{v}}_2)$, which corresponds to the projection of $\mathbf{R}$ into the plane of the surface q , and $P_q = |\mathbf{P}_q|$. 1D integrals are obtained after application of the divergence theorem. In those integrals, denoting by $\hat{\mathbf{n}}_r$ the outward unit normal to the edge r , the factors $(\mathbf{P}_q \cdot \hat{\mathbf{n}}_r)$ and $\hat{\mathbf{v}}_\alpha \cdot \hat{\mathbf{n}}_r$ are constant along the edge, so that they can be moved outside the integrals.

As explained in [59, 76], a special care is required if the surface contains one point for which $P_q = 0$. Indeed, in that case, the vector field of (1.87b) becomes singular. Following [76], separating the integral into two parts, it can be shown that

$$\begin{aligned} & \int_{\Omega_q^3} \nabla \cdot \left(\frac{R^{(\zeta+1)}}{P_q^2} \mathbf{P}_q \right) dS_2^3 = \\ & \sum_{r|\Omega_r^3 \in \partial\Omega_q^3} \left[(\mathbf{P}_q \cdot \hat{\mathbf{n}}_r) \int_{l_r} \frac{R^{(\zeta+1)}}{P_q^2} dl_1^3 \right. \\ & \quad \left. - d_q^{(\zeta+1)} \left(\tan^{-1} \left(\frac{\hat{\mathbf{l}}_r \cdot \mathbf{R}_r^+}{\hat{\mathbf{n}}_r \cdot \mathbf{R}_r^+} \right) - \tan^{-1} \left(\frac{\hat{\mathbf{l}}_r \cdot \mathbf{R}_r^-}{\hat{\mathbf{n}}_r \cdot \mathbf{R}_r^-} \right) \right) \right], \end{aligned} \quad (1.88)$$

with $d_q = |\hat{\mathbf{n}}_q \cdot \mathbf{R}|$ for $\mathbf{R} \in \Omega_q^3$ the distance between the surface and the origin, Ω_r^3 the projection of edge r into the 3D space, $\mathbf{R}_r^-$ and $\mathbf{R}_r^+$ the position of the beginning and end of Ω_r^3 , respectively, and $\hat{\mathbf{l}}_r = (\mathbf{R}_r^+ - \mathbf{R}_r^-)/|\mathbf{R}_r^+ - \mathbf{R}_r^-|$. The beginning of one edge is chosen to always correspond to the end of another one. The second term of the RHS of (1.88) accounts for the singularity if the point $P_q = 0$ is on the surface, and otherwise vanishes. For more details about the development that leads to (1.88), the reader is referred to Equation (5) of [59] or Equations (39) and (40) of [62]. In this

work, contrarily to [59, 62], Equation (1.88) is used for both the EFIE and MFIE terms when the whole 4D integral is evaluated analytically.

Last comes the 1D integration. Following the same guidelines as for the 3D and 2D integrations, we use the $\{\hat{\mathbf{l}}_r, \hat{\mathbf{n}}_r, \hat{\mathbf{n}}_q\}$ coordinate system, so that the 1D integrals that need to be solved all correspond to

$$\oint l^n R^{(\zeta+1)} dl \quad (1.89)$$

or

$$(\mathbf{P}_q \cdot \hat{\mathbf{n}}_r) \oint \frac{R^{(\zeta+1)}}{P_q^2} dl, \quad (1.90)$$

with $l = \mathbf{R} \cdot \hat{\mathbf{l}}_r$. If $\mathbf{P}_q \cdot \hat{\mathbf{n}}_r = 0$ on an edge, the first and second terms of the right-hand side of (1.88) mutually cancel for that edge, so that this case can be treated by omitting the whole contribution of the edge to (1.88).

We can solve these integrals recursively using the following identities:

$$\int \frac{R^{(\zeta+1)}}{P_q^2} dl = d_q^2 \int \frac{R^{(\zeta-1)}}{P_q^2} dl + \int R^{(\zeta-1)} dl, \quad (1.91a)$$

$$\begin{aligned} \int R^{(\zeta+1)} dl &= (d_q^2 + d_r^2) \int R^{(\zeta-1)} dl \\ &\quad + \int l^2 R^{(\zeta-1)} dl, \end{aligned} \quad (1.91b)$$

$$\begin{aligned} \int l^n R^{(\zeta+1)} dl &= \left[\frac{l^{(n-1)} R^{(\zeta+3)}}{\zeta+3} \right]_{\mathbf{R}^-}^{\mathbf{R}^+} \\ &\quad - \frac{n-1}{\zeta+3} \int l^{(n-2)} R^{(\zeta+3)} dl, \end{aligned} \quad (1.91c)$$

$$\int R^{-2} dl = \left[\frac{1}{\sqrt{d_q^2 + d_r^2}} \tan^{-1} \left(\frac{l}{\sqrt{d_q^2 + d_r^2}} \right) \right]_{\mathbf{R}^-}^{\mathbf{R}^+}, \quad (1.91d)$$

$$\int R^{-1} dl = \left[\ln(R+l) \right]_{\mathbf{R}^-}^{\mathbf{R}^+}, \quad (1.91e)$$

$$\int \frac{R^{-1}}{P_q^2} dl = \left[\frac{1}{d_q d_r} \tan^{-1} \left(\frac{d_q l}{d_r R} \right) \right]_{\mathbf{R}^-}^{\mathbf{R}^+}, \quad (1.91f)$$

$$\int \frac{1}{P_q^2} dl = \left[\frac{1}{d_r} \tan^{-1} \left(\frac{l}{d_r} \right) \right]_{\mathbf{R}^-}^{\mathbf{R}^+}, \quad (1.91g)$$

with $[f(\mathbf{R})]_{\mathbf{R}_1}^{\mathbf{R}_2} = f(\mathbf{R}_2) - f(\mathbf{R}_1)$ and $d_r = |\mathbf{R} \cdot \hat{\mathbf{n}}_r|$. (1.91a) is obtained noticing that $R^2 = P_q^2 + d_q^2$ and that d_q is constant along the edge. (1.91b) is

obtained noticing that d_r is also constant along the edge. The case $d_q \rightarrow 0$ in (1.91f) can be straightforwardly treated considering that $P_q \rightarrow R$ and manipulating (1.91b) to increase the power of R^{-3} .

This last step ends our quest for the 4D integral. It is important to notice that among the large number of terms that need to be computed to solve the original 4D integral, there are many repetitions. Therefore, using an appropriate book-keeping, a significant time saving can be obtained.

1.3.5 Solving the $\mathcal{C}_i$ MFIE term

The solution of the $\mathcal{C}_i$ term, which is necessary when setting up the discretized MFIE, is similar to the solution of the $\mathcal{A}_{i-1}$ term. The only difference lies in the treatment of the singular case $R \rightarrow 0$, which is described in this Section.

To treat the singular case for the $\mathcal{A}_i$ term (cf. Appendix A.3), the domain of integration is first separated into two parts: the singular and the non-singular zones. Since (1.56b) corresponds to a Cauchy integral, only the non-singular zone needs to be treated; more specifically the additional surface S_a that is created when the singular zone is removed from the volume of integration (cf. Figure A.1).

First, since the normal to S_a is orthogonal to the $\hat{\mathbf{u}}_4$ and $\hat{\mathbf{u}}_5$ directions, no additional treatment is required w.r.t. Section 1.3.3. Moreover, since it is well known that (1.56b) vanishes for BF and TF lying in the same plane, contrary to the EFIE case, the case of touching parallel BF and TF does not need to be treated, leading to an integral of the type:

$$\oint R^{(i-3)}(\mathbf{R} \cdot \mathbf{P}_2(u_1, u_2, u_3)) dV_3^3. \quad (1.92)$$

The factor $\mathbf{R} \cdot \mathbf{P}_2$ corresponds to a polynomial that vanishes for $R \rightarrow 0$, i.e. a polynomial whose minimum degree is 1. Therefore, in order to apply the divergence theorem to (1.92), the identity (1.84a) must be used at least once. After using it, it can be seen that the power of the distance term is increased: $R^{(i-3)}$ becomes $R^{(i-1)}$. The resulting 2D integrals thus match the generic shape of Equation (1.85), which has already been treated in Section 1.3.4. Moreover, as explained in Appendix A.3, the contribution of S_a to the 3D volume integral vanishes for a vanishing singular zone.

1.3.6 Numerical validation

In order to validate the method, we first computed the A_0 , B_0 and C_0 terms of (1.55). The reference results were obtained using the methods of [59, 64, 62], which consist of a 2D analytical integration of the singular term over the BF and the 2D numerical integration of the result over the TF.

The numerical integration was performed using the `integral2` function of MATLAB[®] [98, 99]. We computed these terms for half-RWG [56] BF and TF that are close by, sharing a common edge or even interleaved, and for various relative orientations. The geometry considered can be seen in Figure 1.6. The position of the vertices is given by

$$\begin{aligned} \mathbf{p}_1 &= (0, 0, 0), & \mathbf{p}_2 &= (1, 1, 0), \\ \mathbf{p}_3 &= (1, 0, 0), & \mathbf{p}_4 &= \mathbf{p}_1 + \mathbf{t}, \\ \mathbf{p}_5 &= \mathbf{p}_3 + \mathbf{t}, & \mathbf{p}_6 &= (-\cos\theta, 1, \sin\theta) + \mathbf{t}, \end{aligned} \quad (1.93)$$

with $\mathbf{t} = (-0.1, 0, 0)$ when the BF and TF are nearby, $\mathbf{t} = (0, 0, 0)$ when they are touching and $\mathbf{t} = (0.3, 0, -0.2)$ when they are interleaved. The geometry and the results for the three cases can be seen in Fig. 1.6. The error in A_0 , B_0 and C_0 can be seen in Fig. 1.6(b), (c) and (d), respectively. Note that if $\mathbf{t} = (0, 0, 0)$ (common edge), $C_0 = 0$. The results are therefore not displayed for that case in Figure 1.6(d).

The error has been normalized w.r.t. the maximum value obtained for each term. Whatever the geometry considered, the relative error remains below 10^{-7} and is generally smaller than 10^{-10} . It corresponds to the maximum accuracy we could reach for the numerical solution used as a reference.

When the distance between the BF and TF becomes large, some of the analytical integration steps become numerically ill-conditioned, i.e. they involve differences between large values of same order. When the BF and TF are nearly parallel, the non-parallel case becomes ill-conditioned as well. Therefore, we studied both limits, the results for the A_0 term being displayed in Fig. 1.7. Note that a similar behaviour was observed for the A_i and C_i terms ($i \geq 0$) while a much better accuracy was observed for the B_i terms. The latter observation is due to the degree of the polynomial in (1.56), which is 2 for the A_i and C_i terms, and 0 for the B_i term in the case of RWG basis functions.

First, we study the numerical error for increasing distances between the BF and TF. We studied the same configuration as in the previous example (Fig. 1.6(a)) with $\mathbf{t} = (-t, 0, 0)$ and $t = 2, 4, 8, 15$ and 30. As shown in Fig. 1.7(a), the accuracy rapidly drops if the distance between the BF and TF becomes large (t larger than 5 to 10 times the typical size of an edge of the mesh). This is not expected to pose a problem in MoM applications since at such distances classical Gaussian quadratures perform very well (see e.g. [57]). For this reason, the analytical method should be used only for close-range singular interactions, smaller than about 5 times the typical length scale of the mesh.

Second, we studied the evolution of the error for small angles between the BF and TF. To do so, we considered again a geometry similar to the first

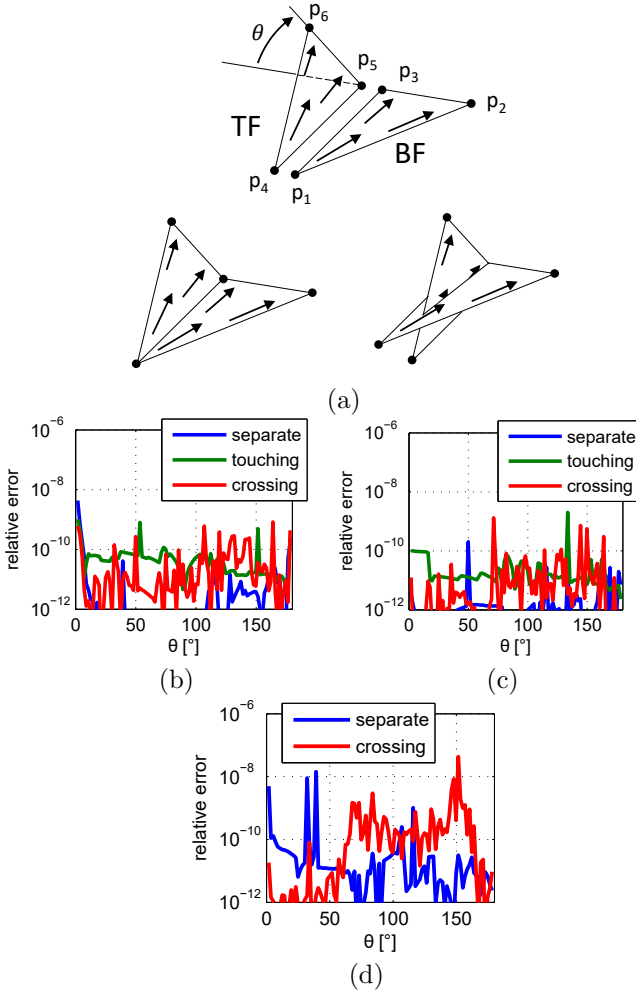


Figure 1.6: Comparison between analytical results and numerical results for the (b) A_0 , (c) B_0 and (d) C_0 terms for the three geometries illustrated in (a).

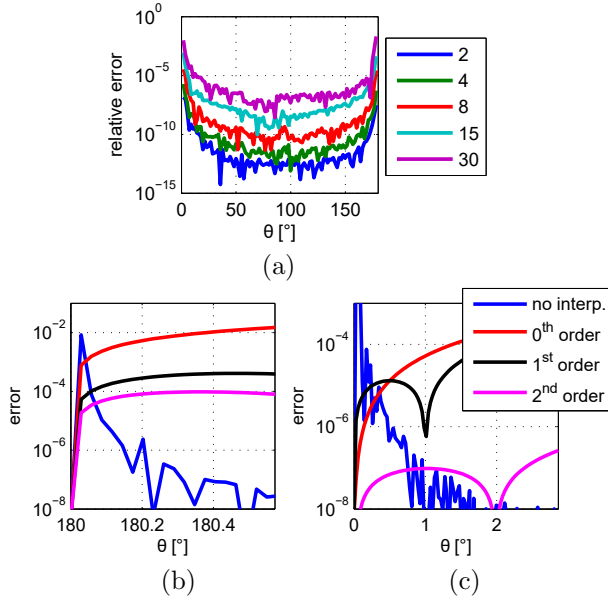


Figure 1.7: Round-off error in the A_0 term for (a) an increasing distance between the BF and TF and (b,c) for nearly parallel BF and TF sharing a common edge. In the latter graphs, the error made using polynomial interpolation techniques is also drawn.

example (Fig. 1.6(a)) with $\mathbf{t} = (0, 0, 0)$. The error for nearly-parallel BF and TF is displayed in blue in Fig. 1.7(b-c). Note that $\theta = 180^\circ$ corresponds to the TF that has been folded back into the BF (identical BF and TF). The other curves correspond to polynomial interpolation of order n of the value obtained for $\theta = 0^\circ, 1^\circ, \dots, n^\circ$ and $\theta = 180^\circ, 181^\circ, \dots, 180 + n^\circ$ (cf. end of Section 1.3.3). An accuracy better than 10^{-4} can be easily achieved using a second order interpolation.

Finally, in order to compare our method with the state of the art for practical geometries, we computed Z^{EJ} and Z^{EM} of (1.51) using the proposed method (in-house C++ code) and the “Direct Evaluation Method” (DEMCEM) of A. Polimeridis [68, 69, 70, 71], whose C++ implementation can be found on the website of the author [100]. Both codes were compiled using the `-O2` optimization flag and run on a single CPU of an Intel i7-3770 chip. The accuracy was checked for varying numbers of points for the 1D numerical integrations in [100] and various orders of the Taylor expansion for the proposed method (N in Equation (1.54)). The comparison was lead for BF and TF sharing a common edge or a common vertex, as illustrated in Fig. 1.8(a).

To obtain a fair comparison, the time required to compute the value of one integral was averaged over 10^4 integrals (100 BF interacting with 100 TF). It is worth noting that the results displayed varied slightly from run to run and may change for different numerical implementations of both methods. However, comparisons have been made as fair as possible, considering that both codes are reasonably optimized and have been compiled and executed on the same computer and the results are averaged over a large number of different interactions.

The times provided for the fully analytical method are actually covering the computation of the two integrals of (1.54), since many factors are reused and therefore both calculations cannot be decoupled efficiently. The results can be seen in Figure 1.8(b-e). The reference solution used to estimate the error corresponds to the results obtained using the code of [100] for 15 points of integration. The first bullet of the DEMCEM results corresponds to one point of integration for each 1D numerical integral, the second one to two points of integration for each 1D numerical integral, etc. Concerning the proposed method, the first bullet corresponds to $N = 0$, the second one to $N = 1$, etc. Relative errors of the order of 10^{-10} are achieved 10 to 40 times faster than with the code of [100].

The convergence of the fully analytical method is not expected to change significantly with respect to the distance between the BF and TF (except for the numerical error that may grow, see Fig. 1.7(a)) since R_0 , the central point of the Taylor expansion of Equation (1.54), is changing accordingly [97]. However, it will strongly vary with the density of the mesh. For BF

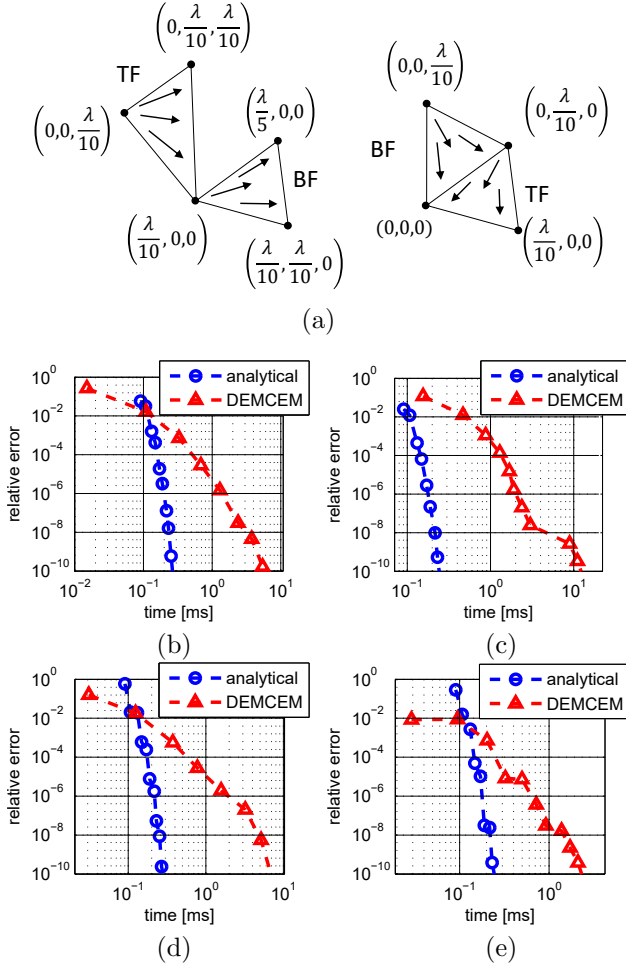


Figure 1.8: Comparison of the proposed method with the method of [100] for the two geometries illustrated in (a). (b) Z^{EJ} and (d) Z^{EM} for BF and TF with a common vertex. (c) Z^{EJ} and Z^{EM} for BF and TF sharing a common edge.

and TF whose characteristic length is $\lambda/10$, the trends shown in Fig. 1.8 are typical and an accuracy of 10^{-10} is achieved with 9 to 11 terms ($N = 8$ to 10).

1.4 Conclusion

The Method of Moments and more particularly its PMCHWT formulation has been derived starting back from Maxwell's equations. It is shown that the simulation of structures using this method requires to routinely evaluate 4D integrals whose integrand and its higher derivatives may not be bounded on the domain of integration.

Evaluating such integrals require some care, since classical Gaussian quadratures fail to provide accurate results in a reasonable amount of time. Based on techniques that were already shown in the literature, we proposed to decompose the phase term into its Taylor expansion and estimate fully analytically the value of each term. To our knowledge, it is the first time that fully analytical solution of the 4D integral is proposed in the literature.

Using the proposed method, results close to machine precision can be obtained in a competitive amount of time. We compared the obtained results with the state-of-the art technique of A. Polimeridis. It is shown that a huge time saving (more than one order of magnitude) can be achieved for high-precision computation. Moreover, once the computation has been done once, the value of the impedance matrix at different frequencies can be obtained in a negligible amount of time.

The technique is numerically ill-posed when the BF and TF are far apart or nearly parallel. A fix was proposed to compensate for the latter. However, this technique, in its present state, should be used only for very short-range interactions between BF and TF. For longer range, since the integrand is not singular, Gaussian quadratures provide excellent results and should be used.

Chapter 2

Numerical modelling of periodic structures

In the previous chapter, the simulation of finite structures was studied. However, in some applications, one is interested in the response of a regular arrays of identical scatterers (*e.g.* with photonic crystals [101], metamaterials [102], metasurfaces [103], large arrays of antennas [104], topological insulators [11], etc.). In that case, using the approximation that the array is infinite, periodic solvers can be used. Using such solvers, the infinite problem can be reduced to a single unit cell considering that a constant phase shift of the fields occurs from one unit cell to the next.

For some applications, it is also important to study phenomena that are located at the interface of semi-infinite periodic arrays [11], or the impact of defects in the periodicity of the structure [48]. In these cases, some limitations on the periodicity appear, preventing the direct use of periodic solvers.

In this Chapter, we will investigate the simulation of periodic or semi-infinite structures. First, the computation of the periodic impedance matrix will be devised for the simulation of structures that are periodic along two dimensions. Then, different methods, based on the post-processing of the periodic impedance matrix, will be presented. First, the interface between two semi-infinite metamaterials is simulated. Then, this method is extended to compute the eigenmodes within a 3D periodic structure. Last the introduction of some defects in the periodicity is tackled. All these methods will be exploited in Chapter 3 to study the absorption by periodic structures.

2.1 Periodic MoM

The non-periodic Method of Moments (MoM) can be extended to the periodic case using a Periodic Green's Function (PGF) [33, 34]. This PGF takes implicitly into account the replicas of the source which have been periodized in order to limit the study of the infinite array to one unit cell. This PGF can be computed in the spatial domain by summing the contribution of the source and every replica. However, this series is slowly convergent and a prohibitive number of terms is required [33]. The periodicity of the PGF implies that its spectrum is discrete along the directions of periodicity. The slowly convergent spatial summation can therefore be replaced by a spectral summation. It converges rapidly (exponentially) provided that the distance between the source and observation points in the direction transverse to the plane of periodicity is large enough. However, if the two points are lying in the same plane, the convergence is slow.

To circumvent this limitation, acceleration methods for the case of coplanar points have been developed. The Ewald method [44, 105] is based on the fact that the PGF can be decomposed into two different series, one that is rapidly converging in the spatial domain (Gaussian convergence), and another one that is rapidly converging in the spectral domain (Gaussian convergence). A splitting parameter has to be optimized, in order to split equally the computational load on the spatial and spectral series [44]. Due to round-off error, the value chosen for given problems may differ from the optimal one [44, 105]. Other methods are based on cylindrical wave decompositions that are accelerated using Shanks or Levin's acceleration techniques [45].

Alternative methods can also be found in the literature, such as [106] which infers the value of the 2D PGF from the value of the 3D PGF, or [107, 108] which simply removes the singular part of the PGF to make it smoother and then extrapolate the value of the remaining function from farther away, where the convergence is still sufficiently good. The reader is referred to [109] for a more comprehensive review about the methods that have been devised for the acceleration of the PGF computation.

Once the PGF has been computed, the impedance matrix of the MoM can be filled by convolving this PGF with basis functions and integrating the resulting fields on testing functions. These integration and convolution generally require the estimate of the value of the PGF for many points. In [110], a regularization of the PGF for layered media has been proposed in order to facilitate its integration along the basis and testing functions. In [34], the regularized periodic Green's function is tabulated to further accelerate its evaluation.

Although many efforts have been spent to accelerate the computation of the PGF, its integration over basis and testing functions is still imple-

mented in a relatively brute-force way. As soon as the phase shift between consecutive unit cells is changed, the PGF has to be recomputed, and the efforts spent to integrate the previous PGF upon the BF and TF can't be exploited.

In this thesis, we propose a method for the filling of the impedance matrix that is based on a plane wave decomposition of the fields (spectral method) [111, 112]. The interaction between domains that are far away in the direction transverse to the plane of periodicity can be computed with an exponentially converging sum. When this distance is not large enough, a Taylor expansion is used to estimate the interaction between the BF and TF from the interaction they would have if they were farther away. The convergence of the Taylor expansion is accelerated by extracting the contribution of the close neighbours.

This method has three advantages. First, using the plane-wave formalism, the integration of the plane wave over the BF and TF becomes separable, so that it scales linearly with the number of BFs and TFs. Moreover, this integration corresponds to a Fourier transform of the BF and TF, which can be obtained in closed-form for RWG and rooftop functions.

The second advantage is that the derivative of the impedance matrix with respect to the position can be obtained from the same kind of spectral summation as the one used to estimate the value of the impedance matrix. Its numerical implementation is therefore easy and its convergence is exponential.

The last advantage is the fact that the singular term that is extracted can be computed once and reused whatever is the phase shift between consecutive unit cells. This proves to be useful if the Array Scanning Method (ASM) [113] is used and the impedance matrix has to be computed for several phase shifts between consecutive unit cells.

The proposed method is particularly well suited for the simulation of 3D metamaterials when one is interested in the response of the structure for many different angles of incidence or when the structure is illuminated by a non-periodic source. As will be shown later, the performance of the method degrades as soon as the size of the unit cells becomes equal to or greater than the wavelength of the source.

This Section is organized as follows. First, a spectral formulation for the computation of the fields emitted by an arbitrary source is derived. Then, the results are exploited to provide a compact formula for the computation of the periodic impedance matrix. Last, a thorough study of the different parameters that are involved in the method and their impact on the accuracy and complexity of the computations is conducted. The parameters chosen for this Thesis are provided.

2.1.1 Spectral formulation of the MoM

Consider an infinite homogeneous medium in which fields are generated by sources consisting of electric and magnetic currents, $\mathbf{J}(\mathbf{r})$ and $\mathbf{M}(\mathbf{r})$, respectively. The value of the fields everywhere has already been computed in the spatial domain in Section 1.1. In this section, we will derive it in the spectral domain. Since the spectrum of the fields generated by periodic sources is discrete, the spectral formulation naturally fits to periodic problems.

To ease the development, the linearity of Maxwell's equations with respect to the sources is exploited in order to treat separately the contribution of the electric and magnetic sources.

Consider an infinite homogeneous medium with permittivity ε and permeability μ . The wavenumber within this medium is denoted as k_0 , $k_0^2 = \omega^2 \varepsilon \mu$. The space is filled with volume electric currents $\mathbf{J}(\mathbf{r}|\mathbf{k})$ that are constant within a phase-factor $\exp(-j\mathbf{k} \cdot \mathbf{r})$ with $\mathbf{k} = (k_x, k_y, k_z)$:

$$\mathbf{J}(\mathbf{r}|\mathbf{k}) = \mathbf{J}_0(\mathbf{k}) \exp(-j\mathbf{k} \cdot \mathbf{r}) \quad (2.1)$$

with $\mathbf{J}_0$ the constant amplitude and orientation of the currents.

The magnetic field generated by these currents can be retrieved from Maxwell's equations (see Appendix A.4):

$$\mathbf{H}(\mathbf{r}|\mathbf{k}) = \frac{j}{k_0^2 - k^2} \mathbf{k} \times \mathbf{J}(\mathbf{r}|\mathbf{k}) \quad (2.2)$$

with $k^2 = \mathbf{k} \cdot \mathbf{k}$. Note that, k^2 does not corresponds to a norm in the usual sense. Indeed, for non-trivial complex $\mathbf{k}$, k may be null or even negative.

The electric field can also be computed (seen Appendix A.4) to give

$$\mathbf{E}(\mathbf{r}|\mathbf{k}) = \frac{j\eta_0}{k_0} \frac{1}{(k_0^2 - k^2)} \left[k_0^2 \mathbf{J}(\mathbf{r}|\mathbf{k}) - (\mathbf{k} \cdot \mathbf{J}(\mathbf{r}|\mathbf{k})) \mathbf{k} \right] \quad (2.3)$$

with η_0 the impedance of the medium, which is such that $k_0/\eta_0 = \omega\varepsilon$. This definition has the advantage of being slightly more general than the usual $\eta_0 = \sqrt{\mu/\varepsilon}$ since it does not require to define the Riemann sheet used for the square root function, as long as the convention is consistent for both k_0 and η_0 .

2D sheet of currents

Now, consider a 2D sheet of currents perpendicular to the $\hat{\mathbf{z}}$ direction whose distribution follows

$$\mathbf{J}(\mathbf{r}|\mathbf{k}_t, z') = \mathbf{J}_0(\mathbf{k}_t, z') \exp(-j\mathbf{k}_t \cdot \mathbf{r}) \delta(z - z') \quad (2.4)$$

with $\mathbf{k}_t = (k_x, k_y, 0)$. Using the identity

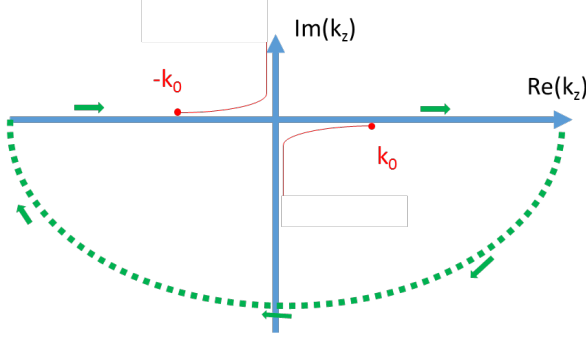


Figure 2.1: Contour deformation used to compute $\int_{-\infty}^{\infty} \mathbf{H}(\mathbf{r}|\mathbf{k}) dk_z$ when $z > z'$. The external part of the contour becomes negligible as it goes to infinity. The value of the infinite integral over the real axis is therefore equal to the value of the residue of the function in the lower pole. The position of the poles depends on $\mathbf{k}_t$. The red lines indicate the possible positions of the poles for real $\mathbf{k}_t$.

$$\delta(z) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(-jk_z z) dk_z \quad (2.5)$$

we obtain

$$\mathbf{J}(\mathbf{r}|\mathbf{k}_t, z') = \frac{\mathbf{J}_0(\mathbf{k}_t, z')}{2\pi} \int_{-\infty}^{\infty} \exp(-j\mathbf{k}_t \cdot \mathbf{r}) \exp(-jk_z(z - z')) dk_z \quad (2.6)$$

Using this formula and noticing that Maxwell's equations are linear with respect to the source, the magnetic field due to the integral of 3D currents will correspond to the integral of the magnetic field induced by each 3D component of the currents, i.e:

$$\mathbf{H}(\mathbf{r}|\mathbf{k}_t, z') = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathbf{H}(\mathbf{r}|\mathbf{k}) \exp(jk_z z') dk_z \quad (2.7a)$$

$$= \frac{j}{2\pi} \exp(-j\mathbf{k}_t \cdot \mathbf{r}) \int_{-\infty}^{\infty} \frac{\mathbf{k} \times \mathbf{J}_0(\mathbf{k}_t, z')}{k_0^2 - k^2} \times \exp(-jk_z(z - z')) dk_z \quad (2.7b)$$

with $\mathbf{k} = \mathbf{k}_t + (0; 0; k_z)$. The value of $\mathbf{H}(\mathbf{r}|\mathbf{k})$ in (2.2) has been computed in a general way and is valid for any complex wave-vector $\mathbf{k}$. The infinite integral can then be computed considering a closed loop in the complex

plane. Indeed, $\mathbf{H}(\mathbf{r}|\mathbf{k})$ is holomorphic over the whole domain, except for two poles on $k_z = \pm\sqrt{k_0^2 - k_t^2}$. It can be easily seen using the identity

$$\begin{aligned} \frac{1}{k_0^2 - k^2} &= \frac{1}{(k_0^2 - k_x^2 - k_y^2) - k_z^2} \\ &= \frac{1}{\left(\sqrt{k_0^2 - k_x^2 - k_y^2} - k_z\right)\left(\sqrt{k_0^2 - k_x^2 - k_y^2} + k_z\right)}. \end{aligned} \quad (2.8)$$

The square root function being a multiple-valued function, we will take $A = \sqrt{B}$ such that $\Im(A) < 0$ or, if $\Im(A) = 0$, such that $\Re(A) > 0$. Moreover, we will consider that the medium considered is (infinitesimally) lossy, so that $\Im(k_0) < 0$.

The contour used to close the loop has to be carefully chosen such that the contribution of the added path asymptotically vanishes (Jordan's Lemma). Looking at the integrand in (2.7b), the exponential term will asymptotically vanish for $\Im(k_z) < 0$ if $z > z'$ and for $\Im(k_z) > 0$ if $z < z'$. The contour used for $z > z'$ is illustrated in Figure 2.1. By virtue of the residue theorem, we obtain

$$\mathbf{H}(\mathbf{r}|\mathbf{k}_t, z') = -\frac{1}{2\gamma} \mathbf{k}^p \times \mathbf{J}_0(\mathbf{k}_t, z') \exp(-j\mathbf{k}^p \cdot (\mathbf{r} - z'\hat{\mathbf{z}})) \quad (2.9)$$

with $\gamma = \sqrt{k_0^2 - k_t^2}$, $\mathbf{k}^p = \mathbf{k}_t + (0; 0; k_z^p)$ and $k_z^p = \pm\gamma$, the plus sign corresponding to $z > z'$ and the minus sign to $z < z'$. The limit case of $z = z'$ won't be treated here since the fields will never be evaluated in the plane of the sources.

An interesting note concerns the use of complex transverse wave-vectors ($\mathbf{k}_t \in \mathbb{C}^2$). Indeed, in that case, the poles can be shifted to the other side of the real axis. In that case, the proper pole has to be accounted for while using the residue theorem, *i.e.* the one inside the contour.

From $\mathbf{H}$ to $\mathbf{E}$

Once the magnetic field is known, we can switch to the electric field using Maxwell's equations, and more particularly

$$\nabla \times \mathbf{H} = j\omega\epsilon\mathbf{E} + \mathbf{J}. \quad (2.10)$$

Since $\mathbf{J} = \mathbf{0}$ for $z \neq z'$, it straightforwardly leads to

$$\mathbf{E}(\mathbf{r}|\mathbf{k}_t, z') = \frac{\eta_0}{2k_0\gamma} (\mathbf{k}^p \times \mathbf{k}^p \times \mathbf{J}_0(\mathbf{k}_t, z')) \exp(-j\mathbf{k}^p \cdot (\mathbf{r} - z'\hat{\mathbf{z}})) \quad (2.11)$$

Fields induced by magnetic currents

The computation of the fields induced by magnetic currents is similar to the computation of the fields induced by electric currents. The fields emitted by a magnetic current distribution of the type

$$\mathbf{M}(\mathbf{r}|\mathbf{k}_t, z') = \mathbf{M}_0(\mathbf{k}_t, z') \exp(-j\mathbf{k}_t \cdot \mathbf{r}) \delta(z - z') \quad (2.12)$$

are corresponding to

$$\mathbf{E}(\mathbf{r}|\mathbf{k}_t, z') = \frac{1}{2\gamma} \mathbf{k}^p \times \mathbf{M}_0(\mathbf{k}_t, z') \exp(-j\mathbf{k}^p \cdot (\mathbf{r} - z'\hat{\mathbf{z}})) \quad (2.13a)$$

$$\mathbf{H}(\mathbf{r}|\mathbf{k}_t, z') = \frac{1}{2\eta_0 k_0 \gamma} (\mathbf{k}^p \times \mathbf{k}^p \times \mathbf{M}_0(\mathbf{k}_t, z')) \exp(-j\mathbf{k}^p \cdot (\mathbf{r} - z'\hat{\mathbf{z}})). \quad (2.13b)$$

Characteristic directions

The problem can be simplified if one considers some specific directions of space that correspond to the usual TE, TM and propagation directions:

$$\hat{\mathbf{e}} = \frac{1}{k_t} (-k_y; k_x; 0), \quad (2.14a)$$

$$\hat{\mathbf{m}} = -\frac{k_z^p}{k_0 k_t} \left(k_x; k_y; -\frac{k_t^2}{k_z^p} \right), \quad (2.14b)$$

$$\hat{\mathbf{k}} = \frac{1}{k_0} (k_x; k_y; k_z^p). \quad (2.14c)$$

It can be checked that $\{\hat{\mathbf{e}}, \hat{\mathbf{m}}, \hat{\mathbf{k}}\}$ forms a right-handed orthonormal basis:

$$\hat{\mathbf{e}} \times \hat{\mathbf{m}} = \hat{\mathbf{k}} \quad (2.15)$$

and

$$\hat{\mathbf{e}} \cdot \hat{\mathbf{e}} = \hat{\mathbf{m}} \cdot \hat{\mathbf{m}} = \hat{\mathbf{k}} \cdot \hat{\mathbf{k}} = 1 \quad (2.16)$$

$$\hat{\mathbf{e}} \cdot \hat{\mathbf{m}} = \hat{\mathbf{e}} \cdot \hat{\mathbf{k}} = \hat{\mathbf{m}} \cdot \hat{\mathbf{k}} = 0 \quad (2.17)$$

Using these directions, Equations (2.9), (2.11) and (2.13) become

$$\begin{aligned} \mathbf{E}(\mathbf{r}|\mathbf{k}_t, z') = & -\frac{k_0}{2\gamma} \left[(\eta_0 J_e(\mathbf{k}_t, z') + M_m(\mathbf{k}_t, z')) \hat{\mathbf{e}} \right. \\ & \left. + (\eta_0 J_m(\mathbf{k}_t, z') - M_e(\mathbf{k}_t, z')) \hat{\mathbf{m}} \right] \exp(-j\mathbf{k}^p \cdot (\mathbf{r} - z'\hat{\mathbf{z}})) \end{aligned} \quad (2.18a)$$

$$\mathbf{H}(\mathbf{r}|\mathbf{k}_t, z') = -\frac{k_0}{2\eta_0 \gamma} \left[(-\eta_0 J_m(\mathbf{k}_t, z') + M_e(\mathbf{k}_t, z')) \hat{\mathbf{e}} \right. \quad (2.18b)$$

$$+ (\eta_0 J_e(\mathbf{k}_t, z') + M_m(\mathbf{k}_t, z')) \hat{\mathbf{m}} \Big] \exp(-j\mathbf{k}^p \cdot (\mathbf{r} - z' \hat{\mathbf{z}}))$$

with $J_e = \mathbf{J}_0 \cdot \hat{\mathbf{e}}$, $J_m = \mathbf{J}_0 \cdot \hat{\mathbf{m}}$, $M_e = \mathbf{M}_0 \cdot \hat{\mathbf{e}}$ and $M_m = \mathbf{M}_0 \cdot \hat{\mathbf{m}}$. It can be noticed that the $\hat{\mathbf{m}}$ and $\hat{\mathbf{k}}$ directions are depending on k_z^p , whose sign changes for sources located above or below the observation plane. In the following, the $+$ and $-$ superscripts will be used to differentiate the directions associated to an observation point located above ($z > z'$) or below ($z < z'$) the sources, respectively.

Contribution of all the currents

Now all the tools and notations have been properly settled, the more complete problem of finding the value of the fields generated by an arbitrary source distribution can be handled. Note that, as mentioned earlier, the hypothesis that no source is lying in the plane where the fields are computed has been made previously and will be maintained hereafter.

Consider the total electric field at a given position $\mathbf{r} = (x, y, h)$ within the plane $z = h$. It is generated by a given electric current distribution $\mathbf{J}(\mathbf{r}')$. For conciseness, magnetic currents are not considered here. However, the extension to magnetic sources is straightforward. Decomposing these currents into successive sheets and applying a Fourier transform to the fields in the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ directions leads to:

$$\mathbf{E}(\mathbf{r}) = \frac{1}{4\pi^2} \iint \int \mathbf{E}(\mathbf{r}|\mathbf{k}_t, z') dz' d\mathbf{k}_t. \quad (2.19)$$

Using (2.18a) and separating the contribution of the sources located above and below the plane leads to

$$\begin{aligned} \mathbf{E}(\mathbf{r}) = & -\frac{k_0 \eta_0}{8\pi^2} \iint \frac{\exp(-j\mathbf{k}^{p,+} \cdot \mathbf{r})}{\gamma} \\ & \times \int_{-\infty}^h \exp(jk_z^{p,+} z') \left[J_{e+}(\mathbf{k}_t, z') \hat{\mathbf{e}}^+ + J_{m+}(\mathbf{k}_t, z') \hat{\mathbf{m}}^+ \right] dz' d\mathbf{k}_t \\ & - \frac{k_0 \eta_0}{8\pi^2} \iint \frac{\exp(-j\mathbf{k}^{p,-} \cdot \mathbf{r})}{\gamma} \\ & \times \int_h^{\infty} \exp(jk_z^{p,-} z') \left[J_{e-}(\mathbf{k}_t, z') \hat{\mathbf{e}}^- + J_{m-}(\mathbf{k}_t, z') \hat{\mathbf{m}}^- \right] dz' d\mathbf{k}_t. \end{aligned} \quad (2.20)$$

Now, consider that the source distribution corresponds to a basis function $\mathbf{f}_B(\mathbf{r}')$ located in a limited zone $z_1 < z' < z_2$. Noticing that the integral over z' corresponds to a Fourier Transform (FT) of the currents along the $\hat{\mathbf{z}}$ direction and that $J_i(\mathbf{k}_t, z')$ is the FT of $J_i(\mathbf{r}')$ along the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ directions,

(2.20) becomes

$$\mathbf{E}(\mathbf{r}) = -\frac{k_0\eta_0}{8\pi^2} \iint \frac{\exp(-j\mathbf{k}^{p,\pm} \cdot \mathbf{r})}{\gamma} \times \left[\tilde{f}_{B,e\pm}(\mathbf{k}^{p,\pm})\hat{\mathbf{e}}^- \pm \tilde{f}_{B,m\pm}(\mathbf{k}^{p,\pm})\hat{\mathbf{m}}^\pm \right] d\mathbf{k}_t \quad (2.21)$$

with $\tilde{f}_{B,j} = \hat{\mathbf{j}} \cdot \tilde{\mathbf{f}}_B$ and $\tilde{\mathbf{f}}_B$ the FT of $\mathbf{f}_B$. The + sign has to be taken if $z > z_2$ and the - sign is taken for $z < z_1$. The case $z_1 \leq z \leq z_2$ has already been excluded due to the initially made hypotheses.

Now consider that these currents are evaluated along a testing function. The corresponding value of the impedance matrix becomes

$$Z^{EJ} = \iiint \mathbf{E}(\mathbf{r}) \cdot \mathbf{f}_T(\mathbf{r}) d\mathbf{r}. \quad (2.22)$$

Substituting the value of the fields and swapping the integration order leads to

$$Z^{EJ} = -\frac{k_0\eta_0}{8\pi^2} \iint \frac{\tilde{f}_{B,e\pm}(\mathbf{k}^{p,\pm})\hat{\mathbf{e}}^- \pm \tilde{f}_{B,m\pm}(\mathbf{k}^{p,\pm})\hat{\mathbf{m}}^\pm}{\gamma} \times \iiint \mathbf{f}_T(\mathbf{r}) \exp(-j\mathbf{k}^{p,\pm} \cdot \mathbf{r}) d\mathbf{r} d\mathbf{k}_t. \quad (2.23)$$

Again, it can be noticed that the last integral corresponds to the FT of the testing function evaluated at the spectral component $-\mathbf{k}^{p,\pm}$, which leads to the final formulation [111, 112]:

$$Z^{EJ} = -\frac{k_0\eta_0}{8\pi^2} \iint \frac{1}{\gamma} \left[\tilde{f}_{B,e\pm}(\mathbf{k}^{p,\pm})\tilde{f}_{T,e\pm}(-\mathbf{k}^{p,\pm}) + \tilde{f}_{B,m\pm}(\mathbf{k}^{p,\pm})\tilde{f}_{T,m\pm}(-\mathbf{k}^{p,\pm}) \right] d\mathbf{k}_t. \quad (2.24)$$

with $\tilde{f}_{T,j} = \hat{\mathbf{j}} \cdot \tilde{\mathbf{f}}_T$ and $\tilde{\mathbf{f}}_T$ the FT of $\mathbf{f}_T$.

Similarly, the electric field generated by magnetic currents can be computed, leading to

$$Z^{EM} = \frac{k_0}{8\pi^2} \iint \frac{1}{\gamma} \left[\tilde{f}_{B,m\pm}(\mathbf{k}^{p,\pm})\tilde{f}_{T,e\pm}(-\mathbf{k}^{p,\pm}) - \tilde{f}_{B,e\pm}(\mathbf{k}^{p,\pm})\tilde{f}_{T,m\pm}(-\mathbf{k}^{p,\pm}) \right] d\mathbf{k}_t. \quad (2.25)$$

2.1.2 Computation of the periodic impedance matrix

The computation of the impedance matrix in the spectral domain requires to evaluate the 2D integral over the transverse wave-vector. However, it

can be proven that if the source repeats itself periodically in the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ directions, its spectrum is discrete and the 2D integral becomes a 2D series.

Consider a BF which is periodic in the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ directions within a phase factor $\exp(-j\mathbf{k}_0 \cdot \mathbf{r})$, with $\mathbf{k}_0 = (k_{x,0}; k_{y,0}; 0)$. The periods in the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ directions are noted d_x and d_y , respectively. In that case, (2.25) becomes [111]

$$\tilde{Z}^{EJ}(\varphi) = \sum_{p=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} \frac{\eta_0 k_0}{2d_x d_y \gamma_{pq}} \left(\tilde{f}_{B,e\pm}(\mathbf{k}_{pq}^{p,\pm}) \tilde{f}_{T,e\pm}(-\mathbf{k}_{pq}^{p,\pm}) \right. \quad (2.26a)$$

$$\left. + \tilde{f}_{B,m\pm}(\mathbf{k}_{pq}^{p,\pm}) \tilde{f}_{T,m\pm}(-\mathbf{k}_{pq}^{p,\pm}) \right),$$

$$\tilde{Z}^{EM}(\varphi) = \sum_{p=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} \frac{k_0}{2d_x d_y \gamma_{pq}} \left(\tilde{f}_{B,e\pm}(\mathbf{k}_{pq}^{p,\pm}) \tilde{f}_{T,m\pm}(-\mathbf{k}_{pq}^{p,\pm}) \right. \quad (2.26b)$$

$$\left. - \tilde{f}_{B,m\pm}(\mathbf{k}_{pq}^{p,\pm}) \tilde{f}_{T,e\pm}(-\mathbf{k}_{pq}^{p,\pm}) \right),$$

with

$$\mathbf{k}_{pq}^{p,\pm} = (k_{x,p}; k_{y,q}; k_{z,pq}^p), \quad (2.27a)$$

$$k_{z,pq}^{p,\pm} = \pm \gamma_{pq}, \quad (2.27b)$$

$$\gamma_{pq} = \sqrt{k_0^2 - k_{x,p}^2 - k_{y,q}^2}, \quad (2.27c)$$

$$k_{x,p} = k_{x,0} + \frac{2\pi}{d_x} p, \quad (2.27d)$$

$$k_{y,q} = k_{y,0} + \frac{2\pi}{d_y} q. \quad (2.27e)$$

with $\tilde{Z}$ the periodic impedance matrix for a given phase-shift between consecutive unit cells and $\varphi = (\varphi_x, \varphi_y)$ the vector containing the phase-shifts $\varphi_x = k_{x,0} d_x$ and $\varphi_y = k_{y,0} d_y$ between consecutive replicas of the BF in the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ directions, respectively. Each harmonic is generally called a *Floquet mode*.

Formulas (2.24) and (2.25) are interesting from a numerical point of view. Indeed, in Chapter 1, the interaction between the BF and TF are computed in the spatial domain. For each pair of BF and TF, a 4D integral has to be evaluated since the integrand is not separable with respect to the $\mathbf{r}$ and $\mathbf{r}'$ coordinates. If the interaction between N BF and N TF is required, N^2 4D integrals are evaluated. In (2.24) and (2.25), it can be noticed that a 2D integral is hidden inside the Fourier transform of the BF and TF. Therefore, one still have to calculate a 4D integral. However, if one can store the FT of the BF and TF after computing them and then reuse it, it can be noticed that only $(2N + N^2)$ 2D integrals have to be

performed. This advantage becomes even more obvious in (2.26), where N^2 2D integrals are transformed into series.

Second, it can be shown that the series in (2.26) are exponentially converging, provided that the BF and TF are separated by a distance $\Delta z \neq 0$ in the $\hat{\mathbf{z}}$ direction. Indeed, expanding the FT in the $\hat{\mathbf{z}}$ direction for the BF and TF leads to

$$\begin{aligned} \tilde{f}_{B,i}(\mathbf{k}_{pq}^p) \tilde{f}_{T,i}(-\mathbf{k}_{pq}^p) &= \int f_{B,i}(z'|\mathbf{k}_{t,pq}) \exp(jk_{z,pq}^p z') dz' \\ &\times \int f_{T,i}(z|\mathbf{k}_{t,pq}) \exp(-jk_{z,pq}^p z) dz \end{aligned} \quad (2.28)$$

with $f_{B,i}(z'|\mathbf{k}_{t,pq})$ (resp. $f_{T,i}(z|\mathbf{k}_{t,pq})$) the FT of $\mathbf{f}_B(\mathbf{r}') \cdot \hat{\mathbf{i}}$ (resp. $\mathbf{f}_T(\mathbf{r}') \cdot \hat{\mathbf{i}}$) in the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ directions and $\mathbf{k}_{t,pq} = (k_{x,p}; k_{y,q}; 0)$, the transverse wave vector of Floquet mode (p, q) . Rearranging the integration order, one obtains that

$$\begin{aligned} \tilde{f}_{B,i}(\mathbf{k}_{pq}^p) \tilde{f}_{T,i}(-\mathbf{k}_{pq}^p) &= \int \int f_{B,i}(z'|\mathbf{k}_{t,pq}) f_{T,i}(z|\mathbf{k}_{t,pq}) \\ &\times \exp(j\gamma|z - z'|) dz dz' \end{aligned} \quad (2.29)$$

Looking at the definition of γ after (2.9), considering that, for the asymptotic case of $k_t \gg k_0$, $\gamma \simeq -jk_t$ and noticing that $|z - z'| > \Delta z$, it finally leads to

$$\begin{aligned} \tilde{f}_{B,i}(\mathbf{k}_{pq}^p) \tilde{f}_{T,i}(-\mathbf{k}_{pq}^p) &\simeq \int \int f_{B,i}(z'|\mathbf{k}_{t,pq}) f_{T,i}(z|\mathbf{k}_{t,pq}) \exp(-k_{t,pq}|z - z'|) dz dz' \end{aligned} \quad (2.30a)$$

$$\leq \int \int f_{B,i}(z'|\mathbf{k}_{t,pq}) f_{T,i}(z|\mathbf{k}_{t,pq}) dz dz' \exp(-k_{t,pq}\Delta z). \quad (2.30b)$$

Since both the BF and TF are bounded and of limited extent, their FT is also bounded so that the double integral over z and z' is bounded. $k_{t,pq}$ evolving linearly with p and q , the convergence is exponential with respect to both indices.

However, if the convergence of the series is rapid provided that the BF and TF are not too close in the $\hat{\mathbf{z}}$ direction, it may be slow if the BF and TF are close, and even diverge or converge to a wrong solution if they are interleaved. Indeed, (2.26) is only valid for non-overlapping BF and TF.

Evaluation of $\tilde{Z}$ for small Δz

To estimate the value of the impedance matrix for BF and TF that are close or even interleaved, a Taylor expansion is used. Consider Δz as a variable.

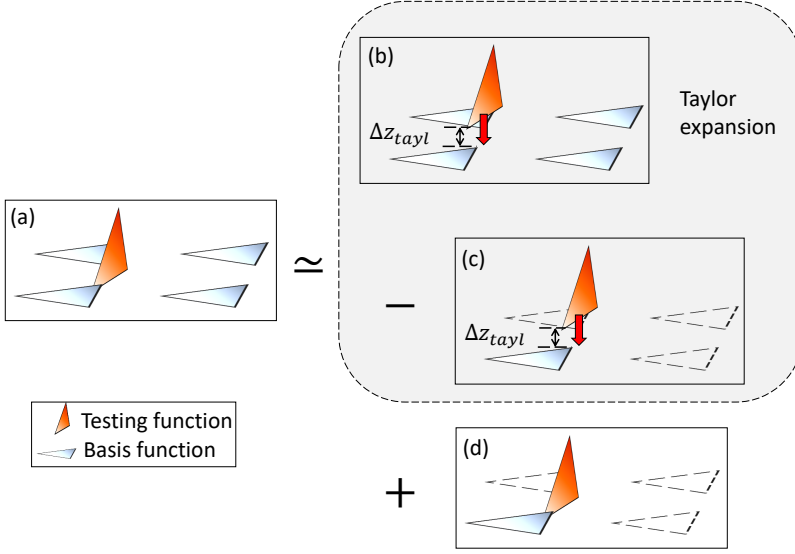


Figure 2.2: Illustration of the procedure applied to compute the periodic impedance matrix in the spectral domain when Δz is small. (a) Actual geometry for which the impedance matrix has to be computed. (b) Taylor expansion of that impedance matrix around $\Delta z = \Delta z_{\text{Tayl}}$ (see Equation (2.31)). (c) Contribution of the close neighbours to the Taylor expansion (cf. second term of the RHS of Equation (2.38c)). (d) Direct contribution of the neighbours to the impedance matrix (cf. first term of the RHS of Equation (2.38c)). The Taylor expansion of both (b) and (c) converges slowly. However, the Taylor expansion of their difference (grey box) converges rapidly.

$\Delta z < 0$ means that there is a layer of width $|\Delta z|$ on which the BF and TF overlap.

The procedure applied to compute the impedance matrix for small Δz can be seen in Figure 2.2. If Δz is too small, the actual value of the impedance matrix is estimated using a Taylor expansion around $\Delta z = \Delta z_{\text{Tayl}}$, with Δz_{Tayl} that is chosen to be big enough so that the spectral series involved in the Taylor expansion converge rapidly (term (b) in Figure 2.2). However, as such, the Taylor expansion itself converges slowly, so that a high order is required. To fasten the convergence of the Taylor expansion, the contribution of the close neighbours to that Taylor expansion is removed (term (c) in Figure 2.2), so that it converges much more rapidly (grey box in Figure 2.2). Finally, the contribution of the neighbours to the impedance

matrix is added directly in the spatial domain (term (d) in Figure 2.2).

To formalize this approach, we introduce two chosen parameters $\Delta z_{\min}$ and Δz_{Tayl} . When $\Delta z < \Delta z_{\min}$, the value of the impedance matrix is estimated using a Taylor expansion of order T around $\Delta z = \Delta z_{\text{Tayl}}$:

$$\tilde{Z}(\Delta z|\varphi) = \tilde{Z}(\Delta z_{\text{Tayl}}|\varphi) + \sum_{t=1}^T \frac{\partial^t \tilde{Z}(\Delta z_{\text{Tayl}}|\varphi)}{\partial \Delta z^t} \frac{(\Delta z - \Delta z_{\text{Tayl}})^t}{t!} \quad (2.31)$$

with $\tilde{Z}$ which may either correspond to $\tilde{Z}^{EJ}$ or $\tilde{Z}^{EM}$. The derivative of the impedance matrix can be evaluated with the exponentially converging series

$$\begin{aligned} \frac{\partial^t \tilde{Z}^{EJ}(\Delta z_{\text{Tayl}}|\varphi)}{\partial \Delta z^t} &= \sum_{p=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} \frac{\eta_0 k_0 (-j\gamma_{pq})^t}{2d_x d_y \gamma_{pq}} \\ &\times \left(\tilde{f}_{B,e\pm}(\mathbf{k}_{pq}^{p,\pm}) \tilde{f}_{T,e\pm}(-\mathbf{k}_{pq}^{p,\pm}) + \tilde{f}_{B,m\pm}(\mathbf{k}_{pq}^{p,\pm}) \tilde{f}_{T,m\pm}(-\mathbf{k}_{pq}^{p,\pm}) \right) \\ &\times \exp(-j\gamma_{pq}(\Delta z_{\text{Tayl}} - \Delta z_{\text{act}})) \end{aligned} \quad (2.32)$$

and

$$\begin{aligned} \frac{\partial^t \tilde{Z}^{EM}(\Delta z_{\text{Tayl}}|\varphi)}{\partial \Delta z^t} &= \sum_{p=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} \frac{k_0 (-j\gamma_{pq})^t}{2d_x d_y \gamma_{pq}} \\ &\times \left(\tilde{f}_{B,e\pm}(\mathbf{k}_{pq}^{p,\pm}) \tilde{f}_{T,m\pm}(-\mathbf{k}_{pq}^{p,\pm}) - \tilde{f}_{B,m\pm}(\mathbf{k}_{pq}^{p,\pm}) \tilde{f}_{T,e\pm}(-\mathbf{k}_{pq}^{p,\pm}) \right) \\ &\times \exp(-j\gamma_{pq}(\Delta z_{\text{Tayl}} - \Delta z_{\text{act}})). \end{aligned} \quad (2.33)$$

Δz_{act} corresponds to the actual distance between the BF and TF for which their FT have been computed.

A brute-force application of the Taylor series requires a huge number of terms in order to converge, or may even converge to a wrong solution if the BF and TF are crossing each other when moving from Δz_{Tayl} to Δz . Actually, the closer the BF gets to the TF, the more rapidly will vary $\tilde{Z}^{EJ}$ and $\tilde{Z}^{EM}$. Thus, the more difficult is the convergence of the Taylor expansion. In order to fasten the convergence, the contribution of the closest occurrences of the periodic BF are removed from the Taylor expansion and computed separately using the 4D spatial integration presented in Chapter 1.

In order to remove the contribution of the neighbouring sources to the derivative of $\tilde{Z}^{EJ}$ and $\tilde{Z}^{EM}$, one has to start back from the interaction between non-periodic BF and TF given in (1.46d) and (1.49):

$$\begin{aligned} Z^{EJ} &= \frac{-j\eta_0}{k_0} \iiint G(\mathbf{r}, \mathbf{r}') \\ &\times (k_0^2 \mathbf{f}_T(\mathbf{r}) \cdot \mathbf{f}_B(\mathbf{r}') - \nabla \cdot \mathbf{f}_T(\mathbf{r}) \nabla' \cdot \mathbf{f}_B(\mathbf{r}')) dS(\mathbf{r}') dS(\mathbf{r}) \end{aligned} \quad (2.34)$$

and

$$Z^{EM} = - \iiint \nabla G(\mathbf{r}, \mathbf{r}') \times \mathbf{f}_B(\mathbf{r}') \cdot \mathbf{f}_T(\mathbf{r}) dS(\mathbf{r}') dS(\mathbf{r}). \quad (2.35)$$

Taking the t^{th} derivative with respect to Δz gives

$$\begin{aligned} \frac{\partial^t Z^{EJ}}{\partial \Delta z^t} &= \frac{-j\eta_0 (\pm 1)^t}{k_0} \iiint \frac{\partial^t G(\mathbf{r}, \mathbf{r}')}{\partial z^t} \\ &\times (k_0^2 \mathbf{f}_T(\mathbf{r}) \cdot \mathbf{f}_B(\mathbf{r}') - \nabla \cdot \mathbf{f}_T(\mathbf{r}) \nabla' \cdot \mathbf{f}_B(\mathbf{r}')) dS(\mathbf{r}') dS(\mathbf{r}) \end{aligned} \quad (2.36)$$

and

$$\begin{aligned} \frac{\partial^t Z^{EM}}{\partial \Delta z^t} &= -(\pm 1)^t \iiint \left[t \frac{\partial^{(t-1)}}{\partial z^{(t-1)}} \left(\frac{1}{R} \frac{\partial G(\mathbf{r}, \mathbf{r}')}{\partial R} \right) \hat{\mathbf{z}} \right. \\ &\quad \left. + \frac{\partial^t}{\partial z^t} \left(\frac{1}{R} \frac{\partial G(\mathbf{r}, \mathbf{r}')}{\partial R} \right) \mathbf{R} \right] \times \mathbf{f}_B(\mathbf{r}') \cdot \mathbf{f}_T(\mathbf{r}) dS(\mathbf{r}') dS(\mathbf{r}), \end{aligned} \quad (2.37)$$

with $R = |\mathbf{r} - \mathbf{r}'|$. The $+$ sign is to be used for TF located above the BF (*i.e.* if Δz increases when z increases), and the $-$ sign otherwise. Equations (2.36) and (2.37) may seem heavy to compute. However, generally, if enough neighbours have been extracted, an order $T = 2 \dots 3$ is sufficient to reach a good accuracy. Moreover, the derivative of the Green's function w.r.t. the $\hat{\mathbf{z}}$ direction can be computed in closed form and therefore can be evaluated rapidly. Last, the integrals of (2.36) and (2.37) have to be performed for $\Delta z = \Delta z_{\text{Tayl}}$. Therefore, the integrand is never singular.

To summarize, the formula used to compute the periodic impedance matrix for $\Delta z < \Delta z_{\text{min}}$ reads

$$\tilde{Z}(\Delta z | \boldsymbol{\varphi}) = \sum_{t=0}^T \frac{\partial^t \tilde{Z}(\Delta z_{\text{Tayl}} | \boldsymbol{\varphi})}{\partial \Delta z^t} \frac{(\Delta z - \Delta z_{\text{Tayl}})^t}{t!} + Z^{\text{corr}}(\Delta z | \boldsymbol{\varphi}) \quad (2.38a)$$

$$Z^{\text{corr}}(\Delta z | \boldsymbol{\varphi}) = \sum_{r,s} Z_{rs}^{\text{corr}}(\Delta z) \exp(-j(r\varphi_x + s\varphi_y)) \quad (2.38b)$$

$$Z_{rs}^{\text{corr}}(\Delta z) = Z_{rs}(\Delta z) - \sum_{t=0}^T \frac{\partial^t Z_{rs}(\Delta z_{\text{Tayl}})}{\partial \Delta z^t} \frac{(\Delta z - \Delta z_{\text{Tayl}})^t}{t!} \quad (2.38c)$$

with Z that may correspond to either Z^{EJ} or Z^{EM} and Z_{rs} the fields induced on the TF by the BF that has been shifted by rd_x in the $\hat{\mathbf{x}}$ direction and sd_y in the $\hat{\mathbf{y}}$ direction.

In (2.38c), the evaluation of Z_{rs}^{corr} is computationally intensive. However, Z_{rs}^{corr} is independent from $\boldsymbol{\varphi}$ and can therefore be computed once and reused for every different phase shift.

Concerning the part that depends on φ and must therefore be recomputed for every new phase shift, it can be decomposed into two parts. The first one is the computation and storage of the FT of the BF and TF. It scales linearly with the number of BFs and TFs and is therefore negligible for impedance matrices of reasonable size. This cost is further reduced if the FT of the BF and TF exists in close form, which is the case for RWG, rooftop and hybrid functions (cf. Appendix A.5). The second step consists in evaluating the exponentially convergent series. However, it can be seen that each term of the series requires very few basic operations, so that (2.38a) is evaluated rapidly. Therefore, the computational load for every additional phase shift after the first one is low.

2.1.3 Fine-tuning of the method

There are a few parameters that can be tuned to optimize the method. In order to provide guidelines in the optimization of these parameters, this section aims at identifying the available parameters and at deriving an estimate of the error and complexity as a function of these parameters.

- **The Taylor order T**

It defines the way the Taylor expansion converges, and therefore the distance Δz_{Taylor} that can be used to reach a prescribed accuracy. However, the higher T , the more terms of the Taylor expansion have to be computed. A higher order also means that higher derivatives of the Green's function are required, which are both characterized by a harder estimation (the expression becomes lengthy) and a harder spatial integration (the function becomes more and more singular for small distance between the BF and TF) of the integrand. In practice, a good compromise generally consists in $T = 2$. $T < 2$ requires to have a low Δz_{Taylor} . For $T > 2$, the time required to precisely estimate (2.36) and (2.37) using Gaussian quadrature becomes prohibitive. In addition, more terms are required in (2.32) and (2.33) for higher T .

- **The Taylor expansion starting distance Δz_{Taylor}**

The higher the distance, the more rapidly converges the spectral series of (2.32) and (2.33). However, the higher the distance, the harder is the convergence of the Taylor expansion, which either requires to increase the order T or the number of neighbouring sources extracted spatially.

- **The minimum distance Δz_{min}**

First, it can be noticed that only $\Delta z_{\text{min}} < \Delta z_{\text{Taylor}}$ makes sense. Indeed, when $\Delta z < \Delta z_{\text{min}}$, (2.31) must be used instead of (2.26), the former being computationally more intensive than the latter for $\Delta z \geq \Delta z_{\text{Taylor}}$.

For a chosen Δz_{Tayl} , the time required to evaluate (2.31) is constant whatever Δz . An optimal choice for Δz_{min} is when the computation of the interaction requires the same time using (2.26) or (2.31). Note that the time required for the latter should include the computational load of the spatial term of (2.38c) distributed over all the phase shifts for which the computations are done.

- **The number of neighbours N_n**

The more neighbours are extracted in the spatial domain, the smoother the extrapolated function becomes and therefore the better the convergence of the Taylor expansion is. For a fixed Taylor order T , a higher N_n implies the possibility to use a higher Δz_{min} , which fasten the computation of the series in frequency domain. It is important to notice that an increase in the number of neighbour extracted only impacts the computation load of (2.38c). The latter does not depend on φ and is thus computed only once.

- **The number of terms N_s of the spectral series**

Having a sufficiently large N_s limits the truncation error in (2.32) and (2.33). On the other hand, the higher is N_s , the more terms are included in the spectral series and therefore the longer it will take to compute the periodic impedance matrix for every phase shift.

The trade-off between the computation time and the accuracy of the method can be optimized using these parameters. There is mainly three different sources of error: θ_s , the error on the truncation of the spectral series in (2.32) and (2.33), θ_t , the error due to the order T Taylor expansion of the impedance matrix in (2.31) and θ_u the spatial integration of the Green's function and its derivatives in (2.36) and (2.37). These three sources of error are relatively independent and can be treated separately. Note that in this work, routines already available in the lab has been used to perform the spatial integration. It was empirically checked that $\theta_u < 10^{-3}$ can be achieved for $T \leq 2$ through simple convergence tests.

Truncation of the spectral series

There are two kinds of spectral series: the plane wave summations of (2.26) and the Taylor expansion of (2.31). To derive a worst case scenario, consider a BF and a TF that are not band-limited, such as point sources. In order to go on, we will consider that enough terms are used such that the behaviour of the sum over discrete k_t can be well approximated by the behaviour of the continuous integration of the function over k_t .

First, we derive the $|\gamma_{\text{max}}|$ that must be considered such that neglecting all the (p, q) terms for which $|\gamma_{pq}| > |\gamma_{\text{max}}|$ leads to an error of the order of

θ_s . The same reasoning as in (2.30) is used.

In (2.31), the amplitude of the terms of the series evolve as $\exp(-j\gamma_{pq}\Delta z)/\gamma_{pq}$ while in (2.32) and (2.33), they evolve as $\gamma_{pq}^{(T-1)} \exp(-j\gamma_{pq}\Delta z)$. It can be noticed that the former expression is a particular case of the latter for $T = 0$. In the continuous integration limit, the truncation error is of the order of

$$\theta_s \sim \frac{\iint \sqrt{k_0^2 - k_x^2 - k_y^2} = \gamma_{\max} \gamma^{(T-1)} \exp(-j\gamma\Delta z) dk_x dk_y}{\int_0^\infty \gamma^{(T-1)} \exp(-j\gamma\Delta z) dk_x dk_y} \quad (2.39)$$

Performing the integration using cylindrical coordinates and taking the asymptotic case of $k_t \gg k_0$ so that $\gamma \simeq -jk_t$ leads to

$$\theta_s \sim \frac{\int_{|\gamma_{\max}|}^\infty k_t^T \exp(-k_t\Delta z) dk_t}{\int_0^\infty k_t^T \exp(-k_t\Delta z) dk_t} \quad (2.40)$$

This simplified expression can be evaluated analytically:

$$\theta_s(T=0) \sim \exp(-|\gamma_{\max}|\Delta z) \quad (2.41a)$$

$$\theta_s(T=1) \sim (|\gamma_{\max}|\Delta z) \exp(-|\gamma_{\max}|\Delta z) \quad (2.41b)$$

$$\theta_s(T=2) \sim \frac{|\gamma_{\max}|^2 \Delta z^2 + 2|\gamma_{\max}|\Delta z + 2}{2} \exp(-|\gamma_{\max}|\Delta z) \quad (2.41c)$$

To link $|\gamma_{\max}|$ to N_s , the number of terms in the spectral series, the approximation of a continuous spectrum is used. The distance in k_x (resp. k_y) between two consecutive terms of the series is $2\pi/d_x$ (resp. $2\pi/d_y$). Therefore, the mean “area” occupied by one term of the series is given by $4\pi^2/(d_x d_y)$. The area over which the terms of the spectral series are kept corresponds to a circle of radius $k_t = |\gamma_{\max}|$ in the $k_x - k_y$ plane (cf. Figure 2.3).

The number of terms N_s included in the spectral series approximately corresponds to the ratio of the area of the circle by the mean area occupied by a term of the series:

$$N_s \simeq \frac{d_x d_y |\gamma_{\max}|^2}{4\pi}. \quad (2.42)$$

It can be noticed that, as expected, the smaller the unit cell of the periodic structure, the more efficient is the plane wave based technique. Substituting (2.42) into (2.41) finally leads to

$$\theta_s(T=0) \sim \exp(-2\sqrt{\pi} K_{\Delta z} \sqrt{N_s}) \quad (2.43a)$$

$$\theta_s(T=1) \sim (2\sqrt{\pi} K_{\Delta z} \sqrt{N_s}) \exp(-2\sqrt{\pi} K_{\Delta z} \sqrt{N_s}) \quad (2.43b)$$

$$\theta_s(T=2) \sim (2\pi K_{\Delta z}^2 N_s + 2\sqrt{\pi} K_{\Delta z} \sqrt{N_s} + 1) \exp(-2\sqrt{\pi} K_{\Delta z} \sqrt{N_s}) \quad (2.43c)$$

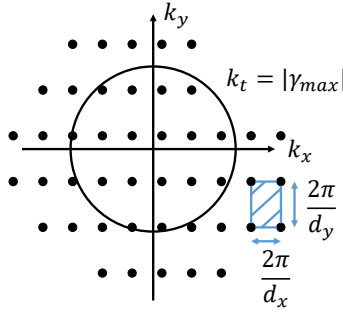


Figure 2.3: Illustration of the $k_x - k_y$ plane for the spectral series. The black dots correspond to terms of the series, while the circle corresponds to the limit of the series. Every term out of that circle is neglected. The mean area occupied by one term of the series has been hatched.

with

$$K_{\Delta z} = \frac{\Delta z}{\sqrt{ab}}. \quad (2.44a)$$

It can be noticed that the convergence of the spectral series only depends on Δz through the adimensional parameter $K_{\Delta z}$. The evolution of the estimate of the error θ_s with the number of terms N_s for $T = 0, 1, 2$ and various values of $K_{\Delta z}$ is presented in Fig. 2.4. For a fixed error, multiplying $K_{\Delta z}$ by a factor of two allows a reduction of the number of terms by a factor of four.

Truncation of the Taylor expansion

As mentioned earlier, the closer is a source to the observation point, the more rapidly the fields will vary. Therefore, the convergence of the Taylor expansion will mainly be limited by the closest replicas of the source that have not been extracted spatially.

For a point source, the error on the fields at a transverse distance x using an order T Taylor expansion along the $\hat{\mathbf{z}}$ direction can be estimated using (2.38c) together with (2.36) and (2.37). We separate two distinct cases: the error made for electric currents, $\theta_t^J(T)$, which is computed using (2.36), and the error made for magnetic currents, $\theta_t^M(T)$, which is computed using (2.37).

The error θ_t is defined as the relative error made when doing the Taylor expansion of order T starting from $\Delta z = \Delta z_{\text{Tayl}}$ to obtain the value of the

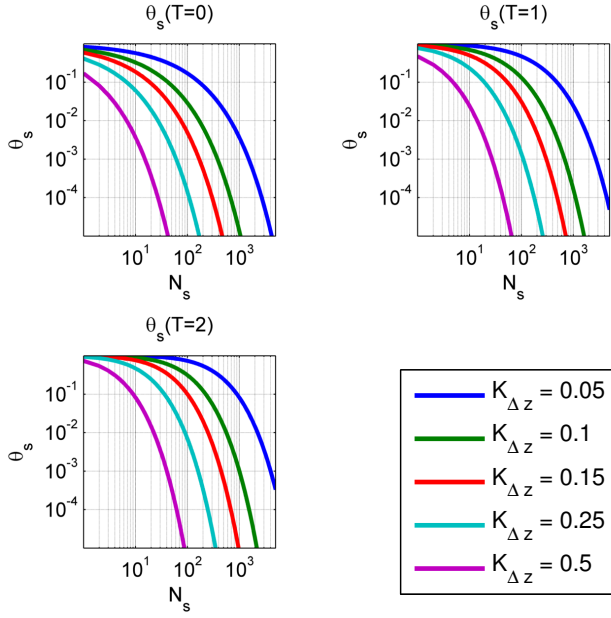


Figure 2.4: Evolution of the estimated error θ_s due to the truncation of the spectral series and its derivative with the number of terms N_s and the distance between the BF and TF in the $\hat{z}$ direction. The curves that are plotted correspond to the theoretical curves of (2.43).

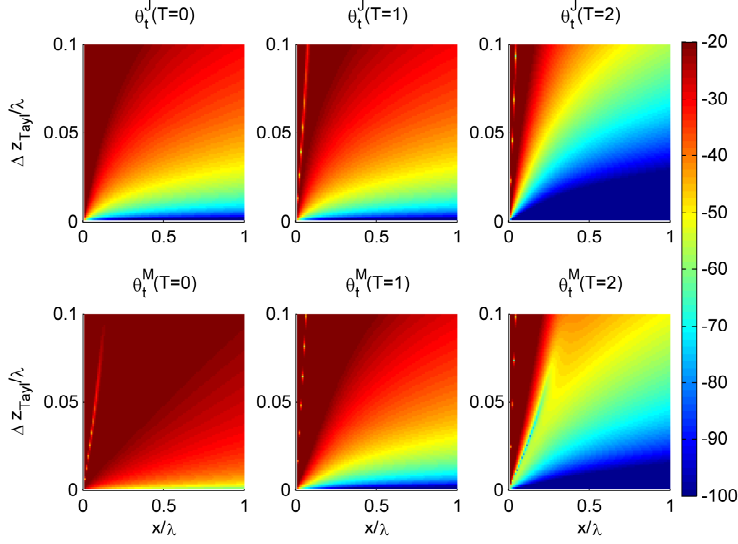


Figure 2.5: Error made when using a Taylor expansion to estimate the value of $Z^{EJ}(\Delta z = 0)$ and $Z^{EM}(\Delta z = 0)$ as a function of the lateral distance x and Δz_{Tayl} for various orders T of the Taylor expansion. The value of the error is provided in dB scale and the distances have been normalized with respect to the normal.

impedance matrix at $\Delta z = 0$ for infinitely small BF and TF:

$$\theta_t = \frac{\left| Z(\Delta z = 0) - \sum_{t=0}^T \frac{\partial^t Z(\Delta z = \Delta z_{\text{Tayl}})}{\partial z^t} \frac{(-\Delta z_{\text{Tayl}})^t}{t!} \right|}{\left| Z(\Delta z = 0) \right|} \quad (2.45)$$

Noticing that $\mathbf{A} \times \mathbf{f}_B \cdot \mathbf{f}_T = (\mathbf{f}_B \times \mathbf{f}_T) \cdot \mathbf{A}$, using Equations (2.34), (2.35), (2.36) and (2.37), the error has been plotted in Fig. 2.5 for $T = 0, 1, 2$ as a function of the lateral distance x between the BF and TF and of Δz_{Tayl} . First, it can be noticed that the error exhibit two different slopes. For small distances, the slope of the error only depends on the ratio between x and Δz_{Tayl} . This convergence is mainly limited by the $1/R$ factor. However, when x becomes significant with respect to the wavelength, an additional error appears due to the phase variation further limiting the convergence. This error is a rough estimate of θ_t . Indeed, on one hand, for overlapping BF and TF, the value of the impedance matrix for $\Delta z < 0$ may be required, leading to a higher error. On the other hand, this error concerns the error

T	Δz_{Tayl}	Δz_{min}	N_n
2	$0.15\sqrt{d_x d_y}$	$0.1\sqrt{d_x d_y}$	25

Table 2.1: Parameters used for the spectral method

made when computing the fields induced on the TF for replicas of the BF that are located relatively far away. The dominant term of the periodic impedance matrix is expected to correspond to the interaction with close neighbours, lowering the final error.

Final parameters used

The targeted accuracy for the periodic impedance matrix is 10^{-3} . First of all, as mentioned previously, $T = 2$ was found as being a good compromise between the complexity of the spatial integration, the convergence of the Taylor expansion and the number of terms required for the spectral series.

For $T = 2$, an error $\theta_t \simeq 10^{-3}$ is achieved for $x/\Delta z_{\text{Tayl}} \simeq 15$ provided that $x < \lambda$. Since the structures simulated in this thesis have a subwavelength periodicity, we chose to extract the 25 closest neighbours and to use $\Delta z_{\text{Tayl}} = 0.15\sqrt{d_x d_y}$. The relatively long computation time required for the terms of (2.38c) were found to remain small with respect to the computation of the periodic impedance matrix if the periodic impedance matrix were computed for a sufficient number of phase shifts (10x10 and more).

Once fixed the Taylor order T and the Δz_{Tayl} , one can find Δz_{min} . In our case, we chose $\Delta z_{\text{min}} = 0.1\sqrt{d_x d_y}$ such that the number of terms required using the Taylor expansion and the spectral series are nearly identical (446 vs. 380 for $\theta_s = 10^{-3}$). The summary of the parameters used can be seen in Table 2.1.

2.1.4 Validation of the method

First, in order to show the potential of the method for the simulation of densely packed structures, the interaction between two planes made of 450 rooftop functions and the interaction between such a plane and a sphere made of 690 RWG functions have been computed using the plane wave summation of (2.26). The wavelength considered is $\lambda = 1 \mu\text{m}$ and the periodicities in the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ directions are $d_x = d_y = 400 \text{ nm}$. The radius of the sphere is $r = 100 \text{ nm}$. The time required as a function of the distance Δz for an error threshold $\theta_s = 10^{-5}$ has been plotted in Fig. 2.6, together with the geometry. The code were run on one core of an i7-3770 processor. It can be seen that, for distances $\Delta z > 0.1d_x$, the time required falls below 10 seconds.

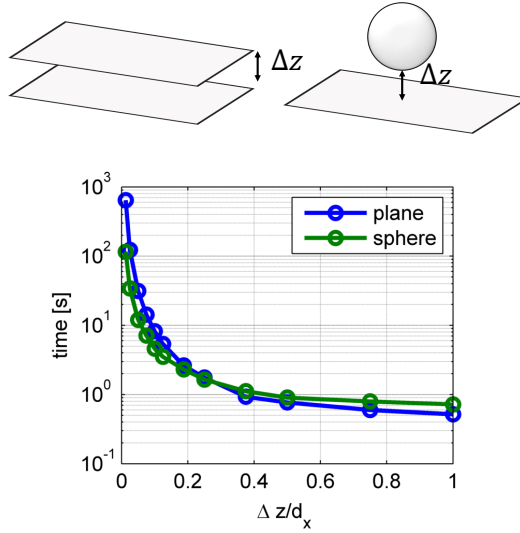


Figure 2.6: Geometries for which the periodic impedance matrix has been computed and time required for their computation as a function of the distance Δz between the two structures.

In order to assess the accuracy of the code, the results of [114] concerning the radiation pattern of a leaky-wave antenna have been reproduced. The antenna is made of an infinite array of rectangular free-standing perfectly conducting metallic patches. The patches are rectangular, and their dimensions in the $\hat{x}$ and $\hat{y}$ directions are 12.5 mm and 1 mm respectively. The array is periodic of periods 13.5 mm and 3mm in the $\hat{x}$ and $\hat{y}$ directions respectively. The array is located 19 mm above a perfectly conducting ground plane. The whole structure is excited at a frequency of 9.5 GHz by a $\hat{x}$ -directed dipole located 9.5 mm above the ground plane and aligned vertically with the center of a patch. The E- and H-planes are defined as the $x - z$ and $y - z$ planes, respectively. The geometry has been illustrated in Fig. 2.7(a).

The radiation pattern of the antenna has been computed along these E- and H-planes, and the results obtained have been compared with the results of [114]. The data was extracted from the graph using the free software “Engauge” and superposed to the solution we obtained. The results can be seen in Fig. 2.7(b). The difference between both curves most probably corresponds to the error in the data extraction. Indeed, the smaller the amplitude, the bigger the error when extracting the data from the graph of [114], due to its polar shape. However, except for that source of errors, a

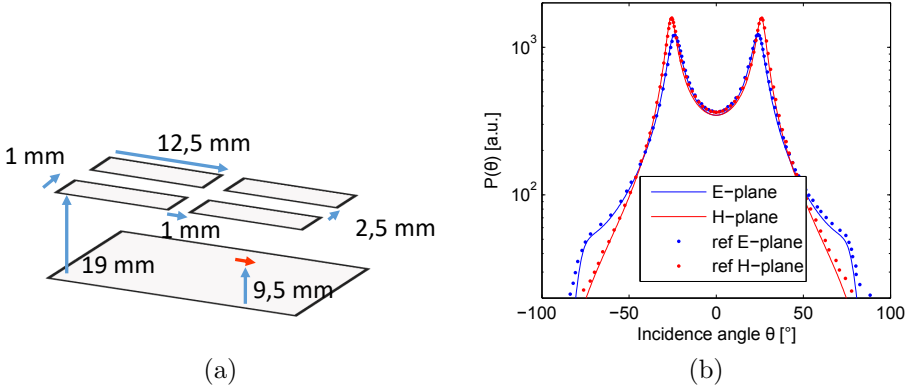


Figure 2.7: (a): Geometry of the leaky wave antenna used to validate the periodic code. (b): Radiation pattern of the leaky wave antenna illustrated in (a). The continuous lines correspond to the results obtained using the spectral method while the dots correspond to the results of [114] that have been extracted using the free software “Engauge”.

very good agreement between the results provided by the presented method and the results of [114] is obtained.

2.2 Simulation of semi-infinite medium

In the previous Section, we derived a method to rapidly compute the periodic impedance matrix for many different phase shifts between consecutive unit cells. However, as mentioned in the beginning of Chapter 1, one great asset of the MoM is its flexibility. At every step of the solution, there is room for physics-based (or purely mathematical) acceleration techniques. Just playing around with the geometry and post-processing the 2D periodic impedance matrices, 3D semi-infinite periodic materials can be simulated. This Section, which is strongly based on [115], will focus on the simulation of such geometries (see Fig. 2.9(a)).

The technique consists in decomposing the metamaterial into 2D-periodic layers of inclusions that are stacked (cf. Fig. 2.9(b) and (c)). The interactions within a given layer are made independent from the other layers through the use of fictitious interfaces [46, 116]. Thus, the coupling between the two interfaces through the layer can be computed without accounting for what is outside of the layer.

Once the behaviour of one layer has been computed, two of these lay-

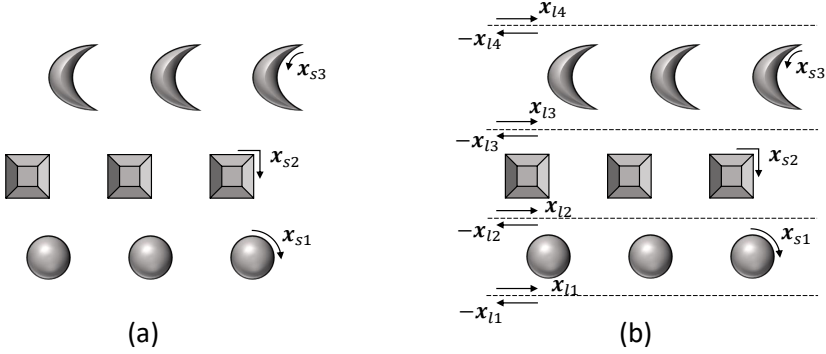


Figure 2.8: Periodic array of scatterers (b) with and (a) without the fictitious interfaces. In (b), the scatterers are only interacting through the equivalent currents on the fictitious interfaces.

ers can be stacked and the coupling between the outer interfaces of this two-layers structure can be computed. Once the two-layers structure has been characterized, two of them can be stacked to study the behaviour of a four-layers structure, etc. If small losses are added, after a few iterations, the coupling between the two outer interfaces of the metamaterial becomes negligible [117]. The number of iterations required to reach a given accuracy increases only linearly for exponentially decreasing losses. Thus, losses can be made arbitrarily small.

This Section can be decomposed into two parts. First, the fictitious interfaces, which were proposed in [46, 116], is briefly summarized for self-completeness. Then, the stacking procedure is described. A detailed convergence study for the stacking procedure can be found in Section 2.3.3.

2.2.1 Decoupling 2D periodic layers through fictitious interfaces

Consider a metamaterial which is 2D periodic along the $\hat{x}$ and $\hat{y}$ directions and which is made of a stack of few scatterers in the $\hat{z}$ directions, as the one presented in Figure 2.8. If the metamaterial is made of L layers of scatterers, noting $\underline{\underline{\hat{Z}}}_{si,sj}$ the impedance matrix describing the interactions between the BF on scatterer j and the TF on scatterer i , the impedance matrix describing the geometry corresponds to

$$\underline{\underline{\tilde{Z}}}_L = \begin{pmatrix} \underline{\underline{\tilde{Z}}}_{s1,s1} & \underline{\underline{\tilde{Z}}}_{s1,s2} & \cdots & \underline{\underline{\tilde{Z}}}_{s1,sL} \\ \underline{\underline{\tilde{Z}}}_{s2,s1} & \underline{\underline{\tilde{Z}}}_{s2,s2} & \cdots & \underline{\underline{\tilde{Z}}}_{s2,sL} \\ \vdots & \vdots & \ddots & \vdots \\ \underline{\underline{\tilde{Z}}}_{sL,s1} & \underline{\underline{\tilde{Z}}}_{sL,s2} & \cdots & \underline{\underline{\tilde{Z}}}_{sL,sL} \end{pmatrix}, \quad (2.46)$$

which is a full matrix whose size corresponds to the sum of the unknowns on each layers:

$$N_{\text{tot}} = \sum_{k=1}^L N_k \quad (2.47)$$

with N_k the number of unknowns on the k^{th} scatterer.

If one wants to fill this impedance matrix and then invert it, the respective complexities are $\mathcal{O}(N_{\text{tot}}^2)$ and $\mathcal{O}(N_{\text{tot}}^3)$. Moreover, if the scatter within one layer is modified, or the distance between two consecutive scatters is modified, an important part of the impedance matrix must be recomputed and the new system of equations need to be solved again starting from scratch.

When filling the impedance matrix, the free space Green's function has been considered so far. However, if the scatterers are deposited on a dielectric substrate or separated by some infinite dielectric layers, the layered Green's function must be used [118]. Computing this layered Green's function requires some extra computations and therefore extra simulation time.

One way to avoid this is to use (possibly fictitious) interfaces between each scatterer [46, 116]. Using the equivalence principle (cf. Chapter 1), the whole problem can be decomposed into sub-problems, each one corresponding to one layer. These sub-problems are related to the neighbouring sub-problems through the equivalent currents on the fictitious interfaces.

This approach has many advantages [116]. First, the impedance matrix of the structure, while becoming larger due to the additional unknowns on the interfaces, also becomes block-diagonal:

$$\underline{\underline{\tilde{Z}}}_L = \begin{pmatrix} \underline{\underline{\tilde{Z}}}_{l1,l1} & \underline{\underline{\tilde{Z}}}_{l1,s1} & \underline{\underline{\tilde{Z}}}_{l1,l2} & 0 & 0 & \cdots \\ \underline{\underline{\tilde{Z}}}_{s1,l1} & \underline{\underline{\tilde{Z}}}_{s1,s1} & \underline{\underline{\tilde{Z}}}_{s1,l2} & 0 & 0 & \cdots \\ \underline{\underline{\tilde{Z}}}_{l2,l1} & \underline{\underline{\tilde{Z}}}_{l2,s1} & \underline{\underline{\tilde{Z}}}_{l2,l2} & \underline{\underline{\tilde{Z}}}_{l2,s2} & \underline{\underline{\tilde{Z}}}_{l2,l3} & \cdots \\ 0 & 0 & \underline{\underline{\tilde{Z}}}_{s2,l2} & \underline{\underline{\tilde{Z}}}_{s2,s2} & \underline{\underline{\tilde{Z}}}_{s2,l3} & \cdots \\ 0 & 0 & \underline{\underline{\tilde{Z}}}_{l3,l2} & \underline{\underline{\tilde{Z}}}_{l3,s2} & \underline{\underline{\tilde{Z}}}_{l3,l3} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \quad (2.48)$$

Since the matrix is block diagonal, its filling and solution times scale linearly with the number of layers L .

A second major advantage is that what is happening inside one layer is decoupled from the outer materials and geometry by the currents on the interfaces. Therefore, if the structure is deposited on a substrate or some dielectric layer is used as a spacer between consecutive scatterers, the Green's function for an homogeneous medium can still be used within each layer provided that interfaces are located in each transition between one medium and another.

A third advantage is that every inclusion is only interacting with the two neighbouring interfaces, so that the unknowns linked to that inclusion can be algebraically removed from the system of equations describing the layer:

$$\begin{pmatrix} \ddots & & & & \\ & \underline{\underline{\tilde{Z}}}_{li,li} & \underline{\underline{\tilde{Z}}}_{li,si} & \underline{\underline{\tilde{Z}}}_{li,l(i+1)} & \\ \cdots & \underline{\underline{\tilde{Z}}}_{si,li} & \underline{\underline{\tilde{Z}}}_{si,si} & \underline{\underline{\tilde{Z}}}_{si,l(i+1)} & \cdots \\ & \underline{\underline{\tilde{Z}}}_{l(i+1),li} & \underline{\underline{\tilde{Z}}}_{l(i+1),si} & \underline{\underline{\tilde{Z}}}_{l(i+1),l(i+1)} & \\ & & \vdots & & \ddots \end{pmatrix} \begin{pmatrix} \vdots \\ x_{li} \\ x_{si} \\ x_{l(i+1)} \\ \vdots \end{pmatrix} = \begin{pmatrix} \vdots \\ b_{li} \\ b_{si} \\ b_{l(i+1)} \\ \vdots \end{pmatrix}$$

becomes

$$\begin{pmatrix} \ddots & & & & \\ & \underline{\underline{\tilde{Z}}}_{li,li} & \underline{\underline{\tilde{Z}}}_{li,l(i+1)} & & \\ \cdots & \underline{\underline{\tilde{Z}}}_{l(i+1),li} & \underline{\underline{\tilde{Z}}}_{l(i+1),l(i+1)} & & \\ & & & & \ddots \end{pmatrix} \begin{pmatrix} \vdots \\ x_{li} \\ x_{l(i+1)} \\ \vdots \end{pmatrix} = \begin{pmatrix} \vdots \\ \mathfrak{b}_{li} \\ \mathfrak{b}_{l(i+1)} \\ \vdots \end{pmatrix} \quad (2.49)$$

with

$$\underline{\underline{\tilde{Z}}}_{lj,lk} = \underline{\underline{\tilde{Z}}}_{lj,lk} - \underline{\underline{\tilde{Z}}}_{lj,si} \underline{\underline{\tilde{Z}}}_{si,si}^{-1} \underline{\underline{\tilde{Z}}}_{si,lk} \quad (2.50a)$$

$$\mathfrak{b}_{lk} = b_{lk} - \underline{\underline{\tilde{Z}}}_{lk,si} \underline{\underline{\tilde{Z}}}_{si,si}^{-1} b_{si}. \quad (2.50b)$$

Last but not least, adding, removing or modifying one layer can be easily done. Only the corresponding bloc of the impedance matrix is modified. It provides a lot of flexibility, which will be exploited in the following sections for the simulation of semi-infinite metamaterials or the computation of the propagating and evanescent eigenmodes inside a 3D infinite metamaterial.

2.2.2 Full-wave simulation of semi-infinite 3D periodic materials

Consider a 3D-periodic semi-infinite metamaterial located in the half-space $z > 0$ and periodic along the $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$ and $\hat{\mathbf{z}}$ directions. The metamaterial can

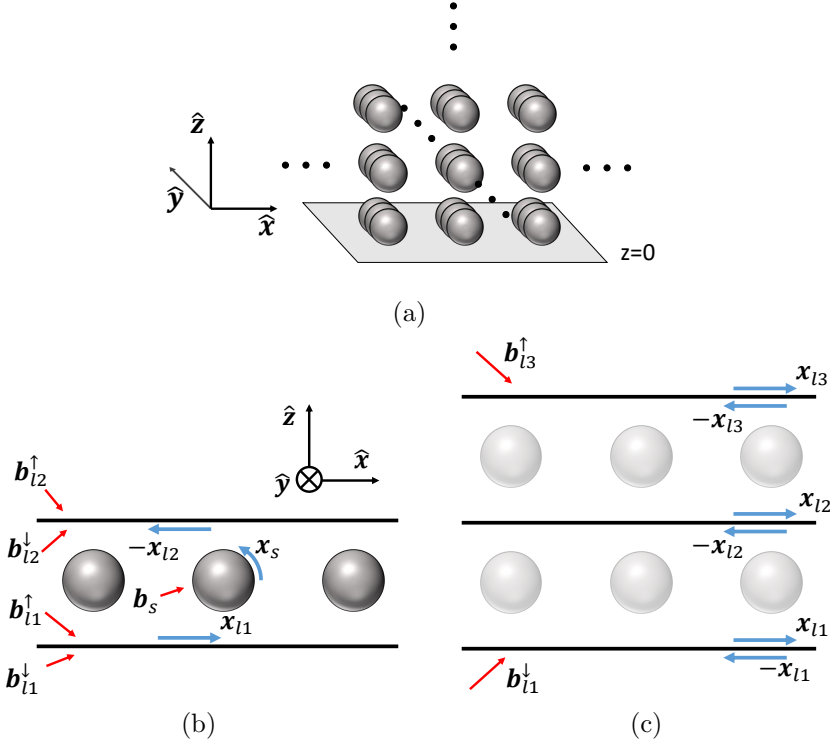


Figure 2.9: (a) Typical semi-infinite metamaterial made of a 3D-periodic array of spheres. (b) One isolated metamaterial layers. (c) Two-layer structure. The sign conventions for the currents x_i are indicated.

be decomposed into layers that lie on the $\hat{x} - \hat{y}$ plane and that are stacked along the $\hat{z}$ direction. Such a structure, consisting of an array of spheres, can be seen in Fig. 2.9(a).

To model the whole metamaterial, we start by modeling the behaviour of one of the layers constituting the metamaterial when excited by any source located outside the layer. The source is “quasi-periodic”, i.e. it shares the same periodicity as the structure, within a linear phase shift. The problem of non-periodic excitation can be rephrased in terms of quasi-periodic excitations using the Array Scanning Method (ASM) [113]. The layered-medium problem will be solved through the use of “interstitial” equivalent currents at each interface between layers [46]. Using the periodic MoM and the PMCHWT formulation [33, 42], the scattering of the excitation by a

single layer can be found solving the following system of equations [119]:

$$\begin{pmatrix} \tilde{\underline{\underline{Z}}}_{l1,l1}^{\uparrow} + \tilde{\underline{\underline{Z}}}_{l1,l1}^{\downarrow} & \tilde{\underline{\underline{Z}}}_{l1,s} & -\tilde{\underline{\underline{Z}}}_{l1,l2} \\ \tilde{\underline{\underline{Z}}}_{s,l1} & \tilde{\underline{\underline{Z}}}_{s,s} & -\tilde{\underline{\underline{Z}}}_{s,l2} \\ -\tilde{\underline{\underline{Z}}}_{l2,l1} & -\tilde{\underline{\underline{Z}}}_{l2,s} & \tilde{\underline{\underline{Z}}}_{l2,l2}^{\uparrow} + \tilde{\underline{\underline{Z}}}_{l2,l2}^{\downarrow} \end{pmatrix} \begin{pmatrix} \mathbf{x}_{l1} \\ \mathbf{x}_s \\ \mathbf{x}_{l2} \end{pmatrix} = \begin{pmatrix} -\mathbf{b}_{l1} \\ -\mathbf{b}_s \\ -\mathbf{b}_{l2} \end{pmatrix}, \quad (2.51)$$

with $\tilde{\underline{\underline{Z}}}_{ij}$ the block of the impedance matrix describing the fields generated on i by equivalent currents on j , $\mathbf{x}_i$ the (unknown) equivalent currents on i and $\mathbf{b}_i$, the fields induced by the source on i . Subscript $l1$, s and $l2$ correspond to the lower plane, the inclusion and the upper plane, respectively. The total excitation on the interfaces is defined as $\mathbf{b}_{li} = \mathbf{b}_{li}^{\uparrow} - \mathbf{b}_{li}^{\downarrow}$. $\tilde{\underline{\underline{Z}}}_{i,i}^{\uparrow}$ and $\tilde{\underline{\underline{Z}}}_{i,i}^{\downarrow}$ correspond to the self-interaction of the interface is computed through the medium located above or below the plane, respectively. The sign conventions are illustrated in Fig. 2.9(b). The source being located outside the layer, $\mathbf{b}_s = \mathbf{0}$. Consequently, $\mathbf{x}_s$ will only depend on $\mathbf{x}_{l1}$ and $\mathbf{x}_{l2}$ and may therefore be algebraically removed from (2.51) [116], leading to

$$\begin{pmatrix} \tilde{\underline{\underline{Z}}}_{l1,l1}^{(0)\uparrow} + \tilde{\underline{\underline{Z}}}_{l1,l1}^{\downarrow} & -\tilde{\underline{\underline{Z}}}_{l1,l2}^{(0)} \\ -\tilde{\underline{\underline{Z}}}_{l2,l1}^{(0)} & \tilde{\underline{\underline{Z}}}_{l2,l2}^{\uparrow} + \tilde{\underline{\underline{Z}}}_{l2,l2}^{(0)\downarrow} \end{pmatrix} \begin{pmatrix} \mathbf{x}_{l1} \\ \mathbf{x}_{l2} \end{pmatrix} = \begin{pmatrix} -\mathbf{b}_{l1} \\ -\mathbf{b}_{l2} \end{pmatrix}, \quad (2.52)$$

with $\tilde{\underline{\underline{Z}}}^{(0)}$ the impedance matrix in which the scatterers are implicitly taken into account. The procedure can be extended to a stack made of two superimposed layers (see Fig. 2.9(c)). As we did with the inclusion in the single-layer structure, we can substitute the unknown equivalent currents $\mathbf{x}_{l2}$ and obtain the impedance matrices describing the interactions of $\mathbf{x}_{l1}$ and $\mathbf{x}_{l3}$ through the two-layers structure. Stacking the layers, to find the interaction of the currents through a 2^{n+1} -layers structure from their interaction through a 2^n -layers structure, one can use

$$\tilde{\underline{\underline{Z}}}_{ii}^{(n+1)\uparrow\downarrow} = \tilde{\underline{\underline{Z}}}_{ii}^{(n)\uparrow\downarrow} - \tilde{\underline{\underline{Z}}}_{ij}^{(n)} (\tilde{\underline{\underline{Z}}}_{jj}^{(n)\downarrow\uparrow} + \tilde{\underline{\underline{Z}}}_{ii}^{(n)\uparrow\downarrow})^{-1} \mathcal{Z}_{ji}^{(n)} \quad (2.53a)$$

$$\tilde{\underline{\underline{Z}}}_{ij}^{(n+1)} = \tilde{\underline{\underline{Z}}}_{ij}^{(n)} (\tilde{\underline{\underline{Z}}}_{jj}^{(n)\downarrow\uparrow} + \tilde{\underline{\underline{Z}}}_{ii}^{(n)\uparrow\downarrow})^{-1} \tilde{\underline{\underline{Z}}}_{ij}^{(n)} \quad (2.53b)$$

with $i, j = l1, l2$, $i \neq j$. After N iterations, the impedance matrices obtained are describing the response of a 2^N -layers structure. Therefore, a 10^9 -layers structure only requires 30 iterations. If losses are introduced, it can be shown that $\lim_{n \rightarrow \infty} \tilde{\underline{\underline{Z}}}_{ij}^{(n)} = 0$ if $i \neq j$ and that convergence is better than exponential. This convergence will be shown in Section 2.3.3. If $\tilde{\underline{\underline{Z}}}_{l1,l1}^{\infty\uparrow}$

is the self-impedance matrix of the lower plane through the semi-infinite metamaterial, we have

$$(\underline{\tilde{Z}}_{l1,l1}^{\infty\uparrow} + \underline{\tilde{Z}}_{l1}^{\downarrow})\mathbf{x}_{l1}^{\infty} = -\mathbf{b}_{l1} \simeq (\underline{\tilde{Z}}_{11}^{(N_0)\uparrow} + \underline{\tilde{Z}}_{11}^{\downarrow})\mathbf{x}_{l1}^{\infty}, \quad (2.54)$$

with N_0 big enough so that the coupling between the two outer interfaces of the 2^{N_0} -layers metamaterial slab becomes negligible and $\mathbf{x}_{li}^{\infty}$ the equivalent currents on the i^{th} interface of the semi-infinite metamaterial. Once $\mathbf{x}_{l1}^{\infty}$ has been computed, the equivalent currents on the scatterers and on the next interfaces can be obtained recursively:

$$\begin{pmatrix} \mathbf{x}_{si}^{\infty} \\ \mathbf{x}_{l(i+1)}^{\infty} \end{pmatrix} = \begin{pmatrix} \underline{\tilde{Z}}_{s,s} & -\underline{\tilde{Z}}_{s,l2} \\ -\underline{\tilde{Z}}_{l2,s} & \underline{\tilde{Z}}_{l2,l2}^{\downarrow} + \underline{\tilde{Z}}_{l1,l1}^{(N_0)\uparrow} \end{pmatrix}^{-1} \begin{pmatrix} -\underline{\tilde{Z}}_{s,1} \\ \underline{\tilde{Z}}_{l2,l1} \end{pmatrix} \mathbf{x}_{li}^{\infty}, \quad (2.55)$$

with $\mathbf{x}_{si}^{\infty}$ the equivalent currents on the inclusions located in the i^{th} layer of the semi-infinite metamaterial. Combining (2.54) and (2.55), the fields near the interface of the semi-infinite metamaterial can be computed. Equation (2.55) looks similar to the T-matrix method. However, unlike the latter, it is numerically stable [119, 120], because it does not entail any back-propagation.

2.2.3 Numerical results

We performed full-wave simulations of one of the structures presented in [37] in order to compare the results obtained using analytical models and numerical techniques. The structure can be seen in Fig. 2.9. The metamaterial consists of a semi-infinite 3D periodic array of silver spheres that are embedded in a dielectric medium whose relative permittivity $\epsilon_r^d = 2.2$. The radius of the spheres is 10 nm. The period of the structure in the $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$ and $\hat{\mathbf{z}}$ directions is 40 nm. The structure is excited by a normally incident plane wave coming from $z < 0$ with a wavelength of 400 nm. At that frequency, the complex relative permittivity of silver is $\epsilon_r^s = -3.46 - 0.049j$.

In order to compare our results with the results of [37], we defined the dipole momentum of a sphere as being proportional to the integral of the equivalent currents on its surface. The comparison of the results of the two methods can be seen on Fig. 2.10 (a) and (b), displaying the norm and the phase of the dipole momentum of the spheres of the 10 first layers, within a normalization factor.

Three layers away from the interface, the evolution of the dipole momentum is monotonous. Looking at the equivalent refractive index of the bulk metamaterial [37], the difference between the single-dipole approximation ($n_{\text{eff}} = 0.476 - 0.036j$) and the full-wave method ($n_{\text{eff}} = 0.5136 - 0.050j$) is

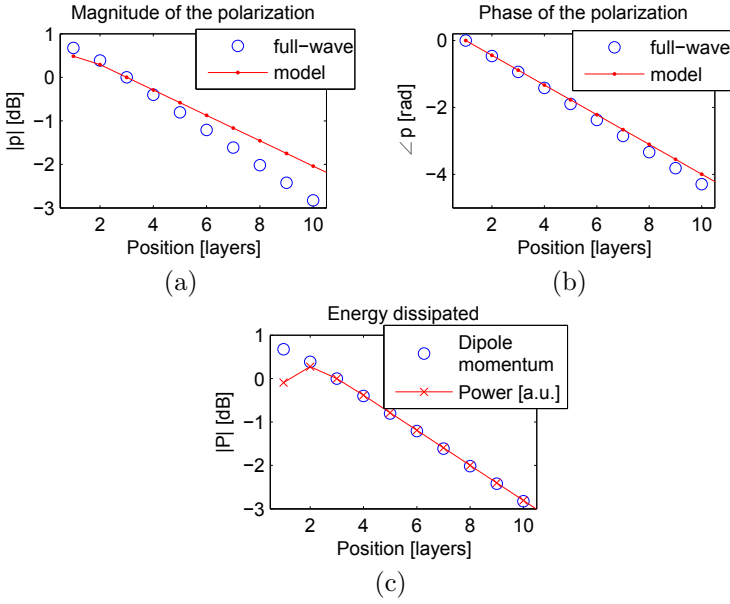


Figure 2.10: Dipole momentum of the spheres vs. depth into the metamaterial obtained numerically (full-wave) and analytically (model) [37]. (a) Magnitude and (b) phase of the dipole momentum of the spheres. (c) Energy dissipated by the spheres vs. square of their dipole momentum.

about 8%. However, the error on the losses is about 28%. It probably comes from the single-dipole approximation made in [37]. We can also compute the total power dissipated by each sphere. According to the single-dipole approximation, these losses are proportional to the square of the dipolar momentum. The results in Fig. 2.10(c) suggest that single-dipole approximation may not provide sufficiently accurate results within the first layers.

2.3 Computation of dispersion diagram in 3D periodic materials

One way to characterize numerically the response of an infinite metamaterial to any excitation at a given frequency is to compute its dispersion diagram and the corresponding Bloch modes of the structure at the frequency of interest. Relevant information can be extracted from this diagram [121], such as the behaviour of the Poynting vector [122], or the presence of photonic band gaps [123]. However, the process can be numerically complex if the problem is not properly tackled [48]. Fast techniques based on plane wave decomposition have been proposed [124, 125]. In [126], a more efficient method based on hybrid plane-wave-integral-equations is proposed in the context of metallic crystals. A method based on root-searching is provided in [127]. Methods of [117, 128] are based on a combination of Transfer (T)-matrix formalism and plane-wave decomposition of the fields, the latter partly compensating for the ill-conditioning of the T-matrix. However, this issue is confirmed in [129], where the authors propose to use the symmetry properties of the eigenvalues and the Rayleigh quotients to relieve the accuracy limitations.

A method to circumvent the issue of T-matrix ill-conditioning has been proposed in [130] for the computation of the dispersion diagrams. However, information about the shape of the modes is then lost.

In this Section, we propose a general method to compute the dispersion diagram and the shape of the corresponding eigenmodes of any 3D periodic metamaterial. Using fictitious interfaces between consecutive layers of the metamaterial, imposing the continuity of the fields across these interfaces and imposing the periodicity of the currents, within a complex transmission coefficient, between consecutive layers, it is possible to determine the eigenmodes inside the structure. In a first instance, the resulting formulation of the problem is non-linear w.r.t. the transmission coefficient of the eigenmodes. To solve this problem, we use the iterative technique described in Section 2.2 and demonstrate how it linearizes the problem such that all the modes —propagative and evanescent— characterized by a given transverse wave-vector can be computed at once with great accuracy without signifi-

cantly increasing the complexity of the method. The material presented in this Section has already been published in [119].

The presented method can be transposed into the Scattering (S-)matrix formalism, and is therefore related to [117, 128]. However, using the iterative technique, the problem can be linearized without resorting to the T-matrix, which is known to be ill-conditioned [120]. Consequently, any field decomposition (i.e. not only plane waves [117, 128]) can be used.

The remainder of this Section is divided as follows. First, the eigenvalue problem is introduced and the non-linear formulation is derived in the context of MoM simulations. The problem is then linearized using the technique described in Section 2.2 and the convergence of the method is discussed. Afterwards, the formulation is extended to a more general formalism based on scattering matrix approach and a comparison with other techniques presented in the literature is established. Finally, numerical results are presented and commented.

2.3.1 Non-Linear Formulation

We first focus on a single layer of metamaterial, as the one illustrated in Fig. 2.11. In order to decouple the layer from the outer medium, equivalent currents are placed on the two interfaces separating it from outer space [46, 116]. Using the equivalent currents, the inside of the layer is isolated from the outer source distribution and the inner and outer problems can be treated separately (cf. Chapter 1). The 3D metamaterial under study is made of an infinite stack of such layers. The system of coordinates is chosen such that the layer is periodic along the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ directions with periods of d_x and d_y respectively, and perpendicular to the $\hat{\mathbf{z}}$ direction.

Using periodic impedance matrices, the equivalent currents on both sides of the layer and on the surface of the inclusions can be found by solving the following system of equations:

$$\begin{pmatrix} \underline{\underline{\tilde{Z}}}_{l1,l1} & \underline{\underline{\tilde{Z}}}_{l1,s} & -\underline{\underline{\tilde{Z}}}_{l1,l2} \\ \underline{\underline{\tilde{Z}}}_{s,l1} & \underline{\underline{\tilde{Z}}}_{s,s} & -\underline{\underline{\tilde{Z}}}_{s,l2} \\ -\underline{\underline{\tilde{Z}}}_{l2,l1} & -\underline{\underline{\tilde{Z}}}_{l2,s} & \underline{\underline{\tilde{Z}}}_{l2,l2} \end{pmatrix} \cdot \begin{pmatrix} \mathbf{x}_{l1} \\ \mathbf{x}_s \\ \mathbf{x}_{l2} \end{pmatrix} = - \begin{pmatrix} \mathbf{b}_{l1} \\ \mathbf{b}_s \\ \mathbf{b}_{l2} \end{pmatrix} \quad (2.56)$$

with $\underline{\underline{\tilde{Z}}}_{pq}$ the periodic impedance matrix describing the influence of basis functions of surface q on testing functions of surface p , $\mathbf{b}_p$ the exciting fields on surface p , where indices $l1$, s and $l2$ stand for the lower interface of the layer, the surface of the inclusions and the upper interface of the layer, respectively. The φ_x and φ_y dependency of the periodic impedance matrices have been omitted for the sake of compactness. The $\underline{\underline{\tilde{Z}}}_{p,p}$ blocs of the impedance matrix are composed of two terms, one for each of the two

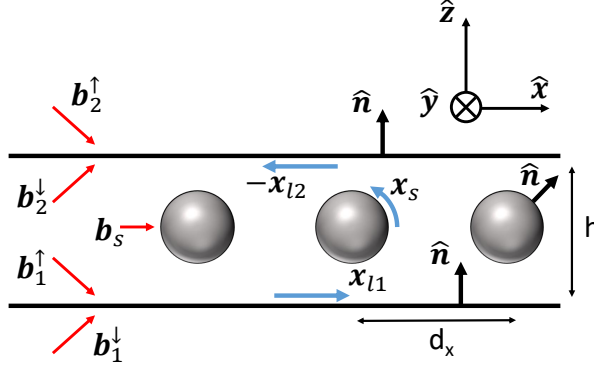


Figure 2.11: One layer of the metamaterial under study. The fields exciting the structure are represented with red arrows, while equivalent currents are represented using blue arrows. The normals to the surfaces are defined as indicated by the $\hat{\mathbf{n}}$ arrows.

media that the surface p is separating. Similarly, the excitation vector on one surface corresponds to the difference between the exciting fields on one side of the surface and the other. Therefore, for $p = l1, l2$, we can explicitly decompose the total excitation into its two contributions: $\mathbf{b}_p = \mathbf{b}_p^\uparrow - \mathbf{b}_p^\downarrow$, $\mathbf{b}_p^\uparrow$ and $\mathbf{b}_p^\downarrow$ being the value of the exciting fields from above and below the surface, respectively.

The excitations $\mathbf{b}_{l1}^\uparrow$, $\mathbf{b}_{l2}^\downarrow$ and $\mathbf{b}_s$ are due to sources located inside the layer, while the other ones are due to sources located outside the layer. The eigenmodes of the structure are solutions of the homogeneous Maxwell's equations and therefore can exist without internal excitation. Since we are only interested in the eigenmodes of the structure, we will not consider sources located inside the layer, thus the internal excitation is set to zero:

$$\mathbf{b}_{l1} = -\mathbf{b}_{l1}^\downarrow \quad \mathbf{b}_{l2} = \mathbf{b}_{l2}^\uparrow \quad \mathbf{b}_s = \mathbf{0} \quad (2.57)$$

The unknowns describing the equivalent currents on the surface of the inclusions can be analytically removed from the system of equations [116] (cf. Section 2.2.1), leading to

$$\begin{pmatrix} \tilde{\underline{\underline{Z}}}_{l1,l1} & -\tilde{\underline{\underline{Z}}}_{l1,l2} \\ -\tilde{\underline{\underline{Z}}}_{l2,l1} & \tilde{\underline{\underline{Z}}}_{l2,l2} \end{pmatrix} \cdot \begin{pmatrix} \mathbf{x}_{l1} \\ \mathbf{x}_{l2} \end{pmatrix} = - \begin{pmatrix} \mathbf{b}_{l1} \\ \mathbf{b}_{l2} \end{pmatrix} \quad (2.58)$$

with

$$\tilde{\underline{\underline{Z}}}_{l1,l1} = \tilde{\underline{\underline{Z}}}_{l1,l1} - \tilde{\underline{\underline{Z}}}_{l1,s} \tilde{\underline{\underline{Z}}}_{s,s}^{-1} \tilde{\underline{\underline{Z}}}_{s,l1} \quad (2.59a)$$

$$\tilde{\underline{\underline{Z}}}_{l1,l2} = \tilde{\underline{\underline{Z}}}_{l1,l2} - \tilde{\underline{\underline{Z}}}_{l1,s} \tilde{\underline{\underline{Z}}}_{s,s}^{-1} \tilde{\underline{\underline{Z}}}_{s,l2} \quad (2.59b)$$

$$\tilde{\underline{\underline{Z}}}_{l2,l1} = \tilde{\underline{\underline{Z}}}_{l2,l1} - \tilde{\underline{\underline{Z}}}_{l2,s} \tilde{\underline{\underline{Z}}}_{s,s}^{-1} \tilde{\underline{\underline{Z}}}_{s,l1} \quad (2.59c)$$

$$\tilde{\underline{\underline{Z}}}_{l2,l2} = \tilde{\underline{\underline{Z}}}_{l2,l2} - \tilde{\underline{\underline{Z}}}_{l2,s} \tilde{\underline{\underline{Z}}}_{s,s}^{-1} \tilde{\underline{\underline{Z}}}_{s,l2} \quad (2.59d)$$

We now consider the full 3D metamaterial and search for its eigenmodes, each of them being characterized by its equivalent currents distribution on the lower interface of the layer and a complex wave vector $\mathbf{k}_{\text{eig}}$, such that the fields and currents have the same periodicity as the structure when multiplied by $\exp(j\mathbf{k}_{\text{eig}} \cdot \mathbf{r})$. Note that $\mathbf{k}_{\text{eig}}$ may be complex. Its real part corresponds to a linear phase shift of the mode from one unit cell to the next and the imaginary part corresponds to a change in its amplitude. The transverse wave-vector components $k_{\text{eig},x} = \mathbf{k}_{\text{eig}} \cdot \hat{\mathbf{x}}$ and $k_{\text{eig},y} = \mathbf{k}_{\text{eig}} \cdot \hat{\mathbf{y}}$ have been set when computing the periodic impedance matrices: $k_{\text{eig},x} = \varphi_x/d_x$, $k_{\text{eig},y} = \varphi_y/d_y$. For such a mode, the relation between the equivalent currents on consecutive planes is given by

$$\mathbf{x}_{q+1} = g \mathbf{x}_q, \quad g = \exp(-jh\mathbf{k}_{\text{eig}} \cdot \hat{\mathbf{z}}) \quad (2.60)$$

with h the thickness of the layer and $\mathbf{x}_q$ the currents distribution on the lower interface of the q^{th} layer. These eigenmodes correspond to the Bloch modes of the structure. The field distribution inside one layer only depends on the currents on the layer interfaces. Hence imposing the tangential fields continuity across one interface only requires to consider two consecutive layers (cf. Figure 2.12). The two layers being identical, translational symmetry can be used:

$$\tilde{\underline{\underline{Z}}}_{(p+1),(q+1)}^{\text{L2}} = \tilde{\underline{\underline{Z}}}_{p,q}, \quad p, q \in \{l1, l2\} \quad (2.61)$$

with $\tilde{\underline{\underline{Z}}}^{\text{L2}}$ the impedance matrices describing the Layer 2 in the absence of Layer 1. Using (2.58), the continuity of the fields is expressed as

$$-\tilde{\underline{\underline{Z}}}_{l2,l1} \mathbf{x}_{l1} + (\tilde{\underline{\underline{Z}}}_{l2,l2} + \tilde{\underline{\underline{Z}}}_{l1,l1} - \tilde{\underline{\underline{Z}}}_{l1,l1}) \mathbf{x}_{l2} - \tilde{\underline{\underline{Z}}}_{l1,l2} \mathbf{x}_{l3} = \mathbf{0} \quad (2.62)$$

The third term in the parenthesis appears due to the fact that the self-interaction of Plane 2 through the homogeneous media above and below the plane is implicitly taken into account twice, since it appears in both $\tilde{\underline{\underline{Z}}}_{l1,l1}$ and $\tilde{\underline{\underline{Z}}}_{l2,l2}$ (see (2.59a) and (2.59d), with $\tilde{\underline{\underline{Z}}}_{l2,l2} = \tilde{\underline{\underline{Z}}}_{l1,l1}$). The repetition of $\tilde{\underline{\underline{Z}}}_{l1,l1}$ must therefore be removed. From (2.62) and using (2.60), the eigenmodes inside the structure satisfy the following equation:

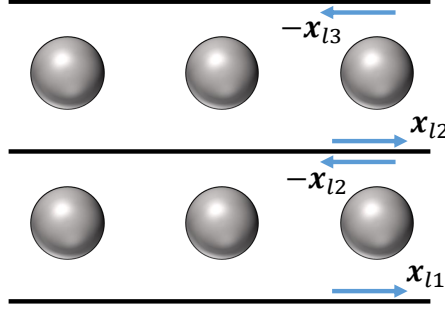


Figure 2.12: Two consecutive layers of the infinite 3D metamaterial. The influence of any source located outside these two layers on interface 2 is screened by the equivalent currents on interfaces 1 and 3.

$$\left(\tilde{\underline{\underline{Y}}}_{l2,l1} + g^2 \tilde{\underline{\underline{Y}}}_{l1,l2} \right) \mathbf{x}_{l2} = g \mathbf{x}_{l2} \quad (2.63)$$

with

$$\tilde{\underline{\underline{Y}}}_{l2,l1} = \left(\tilde{\underline{\underline{Z}}}_{l1,l1} + \tilde{\underline{\underline{Z}}}_{l2,l2} - \tilde{\underline{\underline{Z}}}_{l1,l1} \right)^{-1} \tilde{\underline{\underline{Z}}}_{l2,l1} \quad (2.64a)$$

$$\tilde{\underline{\underline{Y}}}_{l1,l2} = \left(\tilde{\underline{\underline{Z}}}_{l1,l1} + \tilde{\underline{\underline{Z}}}_{l2,l2} - \tilde{\underline{\underline{Z}}}_{l1,l1} \right)^{-1} \tilde{\underline{\underline{Z}}}_{l1,l2} \quad (2.64b)$$

Equation (2.63) does not correspond to a basic eigenvalue equation because the matrix $\left(\tilde{\underline{\underline{Y}}}_{l2,l1} + g^2 \tilde{\underline{\underline{Y}}}_{l1,l2} \right)$, whose eigenvalues are being computed, depends on the eigenvalues themselves, through the g^2 factor. This results in a non-linear formulation of the problem, where the terms $g^2 \tilde{\underline{\underline{Y}}}_{l1,l2}$ and $\tilde{\underline{\underline{Y}}}_{l2,l1}$ describe the influence of $\mathbf{x}_{l3}$ and $\mathbf{x}_{l1}$ on the interface 2, respectively.

The eigenvalue problem of Equation (2.63) can be linearized by doubling the number of unknowns of the system of equations. Starting from (2.63), it can be rearranged to obtain

$$\tilde{\underline{\underline{Y}}}_{l2,l1} \mathbf{x}_{l2} + g \tilde{\underline{\underline{Y}}}_{l1,l2} \mathbf{x}_{l3} = \mathbf{x}_{l3} \quad (2.65)$$

with $\mathbf{x}_{l2}$ and $\mathbf{x}_{l3}$ that are both vectors of unknowns. The system of equations being underdetermined, the periodicity conditions of (2.60) can be added to lead to

$$\begin{pmatrix} 0 & \underline{\underline{I}} \\ -\tilde{\underline{\underline{Y}}}_{l1,l2}^{-1} \tilde{\underline{\underline{Y}}}_{l2,l1} & \tilde{\underline{\underline{Y}}}_{l1,l2}^{-1} \end{pmatrix} \cdot \begin{pmatrix} \mathbf{x}_{l2} \\ \mathbf{x}_{l3} \end{pmatrix} = g \begin{pmatrix} \mathbf{x}_{l2} \\ \mathbf{x}_{l3} \end{pmatrix} \quad (2.66)$$

with $\underline{\underline{I}}$ the identity matrix. However, $\tilde{\underline{\underline{Y}}}_{l1,l2}^{-1} = \tilde{\underline{\underline{Z}}}_{l1,l2}^{-1} \left(\tilde{\underline{\underline{Z}}}_{l1,l1} + \tilde{\underline{\underline{Z}}}_{l2,l2} - \tilde{\underline{\underline{Z}}}_{l1,l1} \right)$ factor appears. Inverting the matrix $\tilde{\underline{\underline{Z}}}_{l1,l2}$ physically means that the fields are being back-propagated, which is numerically unstable. This problem also appears with methods that involve the T-matrix. As will be seen in Section 2.3.5, it dramatically decreases the accuracy of the results. In the next Section, we propose an alternative formulation that is linear and free of back-propagation and is therefore numerically stable.

This method is based on the fact that, due to energy conservation, in the presence of losses, the amplitude of the g factor has to be smaller than unity. Therefore, if the two-layer structure is modified so that the upper layer is actually made of a semi-infinite stack of inclusions, the contribution of $\mathbf{x}_{l3}$ to the fields on layer $l2$ which linearize the problem. To rapidly simulate such a semi-infinite stack of inclusions, the method presented in Section 2.2 is used.

It is interesting to mention that finding the eigenmodes inside a structure corresponds to a linear eigenvalue problem if the Müller formulation [131] is used instead of the PMCHWT. Indeed, currents can be determined considering only one layer and two interfaces, such that no g^2 term appears in the final problem. However, it is proved in Appendix A.6 that finding eigenmodes using Müller formulation also implies back-propagation of the fields and is therefore numerically unstable.

2.3.2 Linear formulation

The straightforward way of solving (2.63) without resorting to back-propagation is to search for the complex eigenvalues in the complex plane and find them one by one. Finding the eigenmodes in this way is inefficient from a numerical point of view and may require a prohibitive time. A second possibility is to compute the eigenmodes using an asymmetrical two-layers structure, the first layer being made of a single array of inclusions, while the second layer is made of a huge number of stacked arrays, as illustrated in Fig. 2.13. If interfaces $l2$ and $l3$ are located sufficiently far away, and if small losses are introduced, the coupling between both interfaces tends to vanish, leading to a linear eigenvalue problem.

For small losses, the number of stacked arrays required for the coupling to vanish may be huge. In order to simulate such a huge number of layers, the technique of Section 2.2 is used. After n iterations, the system of equations relating the value of the currents on interface $l2$ to the value of the currents on interfaces $l1$ and $l3$ reads:

$$-\tilde{\underline{\underline{Z}}}_{l2,l1} \mathbf{x}_{l1} + (\tilde{\underline{\underline{Z}}}_{l2,l2}^{\downarrow} + \tilde{\underline{\underline{Z}}}_{l2,l2}^{(n)\uparrow}) \mathbf{x}_{l2} - \tilde{\underline{\underline{Z}}}_{l1,l2}^{(n)} \mathbf{x}_{l3} = \mathbf{0} \quad (2.67)$$

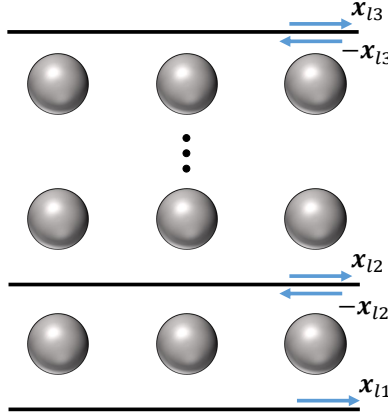


Figure 2.13: Structure considered when computing the eigenmodes of the structure. The number of layers separating interfaces 2 and 3 is equal to 2^n , n being the number of iterations.

Using the periodicity conditions of (2.60) and considering that interface $l3$ is separated from interface $l2$ by stack of $N = 2^n$ arrays of inclusions, the eigenvalue problem to be solved becomes

$$\left(\tilde{Y}_{l2,l1}^{(n)} + g^{2^n+1} \tilde{Y}_{l1,l2}^{(n)} \right) \mathbf{x}_{l2} = g \mathbf{x}_{l2} \quad (2.68)$$

with

$$\tilde{Y}_{l2,l1}^{(n)} = \left(\tilde{Z}_{l2,l2}^\downarrow + \tilde{Z}_{l1,l1}^{(n)\dagger} \right)^{-1} \tilde{Z}_{l2,l1} \quad (2.69a)$$

$$\tilde{Y}_{l1,l2}^{(n)} = \left(\tilde{Z}_{l2,l2}^\downarrow + \tilde{Z}_{l1,l1}^{(n)\dagger} \right)^{-1} \tilde{Z}_{l1,l2}^{(n)} \quad (2.69b)$$

If N is large enough and the structure is lossy, the coupling between interfaces $l3$ and $l2$ vanishes, *i.e.* $\tilde{Z}_{l1,l2}^{(n)} \rightarrow \underline{0}$. Moreover, since the amplitude of the transmission coefficient is smaller than unity due to energy conservation and causality, $g^{N+1} \rightarrow 0$. For these two reasons, (2.68) can be simplified to give

$$\tilde{Y}_{l2,l1}^{(n)} \mathbf{x}_{l2} \simeq g \mathbf{x}_{l2} \quad (2.70)$$

All the eigenmodes and eigenvectors can now be found directly applying an eigenvalue decomposition of the matrix in the left-hand side.

The advantage of this method is that the method is numerically stable and each iteration of the stacking procedure only requires the inversion

of one block of the impedance matrix and few matrix-matrix multiplications (see Equations of (2.53)). Moreover, the number of layers growing exponentially, the convergence is very rapid. Generally, the time needed to retrieve all the eigenmodes starting from (2.56) is negligible compared to that needed to compute the required impedance matrices.

2.3.3 Convergence of the method

The method we presented is based on the hypothesis that the fields excited on one side of a slab of lossy metamaterial will tend to decrease when traveling to the other end of the slab, even considering multiple reflections at the interfaces, provided that the number of layers is large enough. The advantage of the proposed method is that the number of layers grows exponentially with the number of iterations, such that such large numbers can be rapidly obtained.

To estimate the number of iterations required, it is necessary to evaluate the convergence of the method and the influence of losses. In this section, we show that the convergence of the proposed method with respect to the number of iterations and for a given level of losses is doubly exponential, leading to the rapid convergence of the results. Moreover, the number of iterations required for a given level of accuracy increases only linearly for exponentially decreasing losses. The convergence of the method is estimated using a formalism based on eigenmodes. However, the results obtained are also valid for the simulation of a semi-infinite 3D periodic structure as presented in Section 2.2.

Consider a mode α traveling through a slab of metamaterial made of N layers. This mode is characterized by the fields distribution within one layer $(\mathbf{E}_\alpha(\mathbf{r}), \mathbf{H}_\alpha(\mathbf{r}))$ and the transmission coefficient g_α . The fields distribution is normalized, such that

$$\iint_S (|\mathbf{E}_\alpha|^2 + |\eta \mathbf{H}_\alpha|^2) dS = 1 \quad (2.71)$$

with S the surface of the lower interface of the layer limited to one unit cell, η the impedance of the medium just above that surface and $|\mathbf{A}|$ the L2 norm of vector $\mathbf{A}$. Note that this normalization has been chosen arbitrarily, but any other normalization might have been chosen instead. In the following, the direction of propagation of a mode is defined so that it corresponds to the direction of the energy flow associated to that mode at each interface.

Using energy conservation, it is possible to prove that the magnitude of the transmission coefficient $|g_\alpha|$ has to be smaller than unity provided that the metamaterial is lossy: the power due to one mode crossing two consecutive interfaces is constant within a $|g_\alpha^2|$ factor. The difference in the power

entering one layer and the power exiting that same layer corresponds to the dissipations, which are strictly positive for a lossy medium. It provides:

$$|g_\alpha| < 1 \quad (2.72)$$

Moreover if losses are introduced using a non-zero conductivity σ that is small enough, the transmission coefficient can be expressed as a function of σ using first-order Taylor series:

$$|g_\alpha| \simeq 1 - \rho_\alpha \sigma \quad (2.73)$$

with ρ_α a constant that depends on the geometry of the structure and the fields distribution of the mode when there are no losses. A more formal derivation of these results and a physical insight on ρ_α can be found in Appendix A.7.

Now, we consider the error in the fields due to the finiteness of the metamaterial slab represented in Fig. 2.13. Rearranging (2.67), one finds that the exact currents $\mathbf{x}_{l2}$ are given by

$$\mathbf{x}_{l2} = \left(\underline{\tilde{\mathbf{Z}}}_{l1,l1}^{(n)} \right)^{-1} \left(\underline{\tilde{\mathbf{Z}}}_{l2,l1} \mathbf{x}_{l1} + \underline{\tilde{\mathbf{Z}}}_{l1,l2}^{(n)} \mathbf{x}_{l3} \right) \quad (2.74)$$

The solution, that is found combining the periodicity condition of (2.60) with (2.74), corresponds to one of the eigenmodes of the structure. Without any loss of generality, we consider that this mode is the mode α of the structure. This mode is excited by currents $\mathbf{x}_{l1}$ at the lowest interface of the structure and its amplitude is 1 on interface $l2$ (see Fig. 2.13). In the following, each slab consisting of one of the 2D arrays of inclusions that constitute layer 2 is indexed starting from the one just above interface $l2$ (index 0) up to the one just below interface $l3$ (index $2^n - 1$). The power transported by that mode crossing Plane p , between the $(p-1)^{\text{th}}$ and p^{th} arrays of inclusions, is given by

$$P_\alpha^p = \Re \left\{ \iint_{S_p} \frac{\mathbf{E}_\alpha(\mathbf{r}) \times \mathbf{H}_\alpha^*(\mathbf{r})}{2} \cdot \hat{n} \, dS \right\} \quad (2.75)$$

with $\Re\{A\}$ the real part of A , $\hat{n}$ the unit vector normal to Plane p , toward slab p , and S_p the area of that plane limited to one unit-cell. Using Equation (2.60) the total power crossing Plane p can be related to the power crossing Plane 0:

$$\begin{aligned} P_\alpha^p &= |g_\alpha|^{2p} \Re \left\{ \iint_{S_0} \frac{\mathbf{E}_\alpha(\mathbf{r}) \times \mathbf{H}_\alpha^*(\mathbf{r})}{2} \cdot \hat{n} \, dS \right\} \\ &= |g_\alpha|^{2p} P_\alpha^0. \end{aligned} \quad (2.76)$$

Now, we consider what happens in Plane N where currents $\mathbf{x}_{l3}$ are flowing. The amplitude of mode α after propagating from interface $l2$ to interface $l3$ is g_α^N . This mode will be scattered at the interface between the metamaterial and the air (interface $l3$). It means that the energy transported by this mode will be partially transmitted into air and partially reflected back into the metamaterial. The part of the energy that is reflected at the interface will spread over many different propagating and evanescent modes. We consider here the worst case, where all the power transported by mode α would be reflected back into the metamaterial and redirected into a single mode that we will call β . As a worst-case, that mode is chosen as the mode inducing the biggest fields on Plane 2 for a given amplitude of mode α in interface $l3$ (cf. Fig. 2.13). If we define $C_{\beta,\alpha}$ as the scattering coefficient of mode α into mode β , using energy balance in interface $l3$ leads to:

$$|C_{\beta,\alpha}|^2 = \frac{P_\alpha}{P_\beta} = -\frac{\Re\{\iint_{S_0} \mathbf{E}_\alpha(\mathbf{r}) \times \mathbf{H}_\alpha^*(\mathbf{r}) \cdot \hat{n} dS\}}{\Re\{\iint_{S_0} \mathbf{E}_\beta(\mathbf{r}) \times \mathbf{H}_\beta^*(\mathbf{r}) \cdot \hat{n} dS\}} \quad (2.77)$$

Note that using this equation, only the amplitude of $C_{\beta,\alpha}$ can be determined, not its phase. The mode β generated in interface $l3$ will propagate back to interface $l1$, where its amplitude will be reduced by a factor g_β^{N+1} . There, the same worst-case reasoning can be applied, considering that all the energy transported by mode β is reflected back into the metamaterial and entirely contained into a single mode γ . That mode is chosen as the worst possible case, i.e. the mode inducing the biggest fields on interface $l2$ for a given amount of power transported through interface $l1$. This mode γ will propagate until it reaches interface $l3$. There, again, we consider that all the energy transported by mode γ is reflected back into the metamaterial and is entirely contained in the worst possible mode, which we previously defined as β . Iterating the same procedure for an infinite number of reflections at the interfaces, one can find the total amplitudes K_β and K_γ of modes β and γ , respectively, on interface $l2$, for a unit amplitude of mode α on interface $l2$:

$$K_\beta = g_\alpha^N \sum_{q=0}^{\infty} C_{\beta,\alpha} g_\beta^N \left(C_{\gamma,\beta} C_{\beta,\gamma} g_\beta^{N+1} g_\gamma^{N+1} \right)^q \quad (2.78a)$$

$$K_\gamma = g_\alpha^N \sum_{q=0}^{\infty} C_{\beta,\alpha} C_{\gamma,\beta} g_\beta^{N+1} g_\gamma \left(C_{\gamma,\beta} C_{\beta,\gamma} g_\beta^{N+1} g_\gamma^{N+1} \right)^q \quad (2.78b)$$

Using (2.72) and (2.77), one can notice that Equation (2.78) corresponds to a geometrical series whose terms are smaller than unity. It yields

$$K_\beta = g_\alpha^N \frac{C_{\beta,\alpha} g_\beta^N}{1 - \exp(j\varphi) g_\beta^{N+1} g_\gamma^{N+1}} \quad (2.79a)$$

$$K_\gamma = g_\alpha^N \frac{C_{\beta,\alpha} C_{\gamma,\beta} g_\beta^{N+1} g_\gamma}{1 - \exp(j\varphi) g_\beta^{N+1} g_\gamma^{N+1}} \quad (2.79b)$$

with φ the phase of the $C_{\gamma,\beta} C_{\beta,\gamma}$ term, whose magnitude is 1 according to (2.77). Noting that $C_{i,j}$ has to be of finite amplitude and that $|g_i^N|$ can be made arbitrarily small by increasing the number of inclusions in layer 2, we see that if the number of layers grows, (2.79) converges toward $K_\beta = K_\gamma = 0$. Therefore, for a growing number of layers and considering that the medium is lossy, we can see that multiple reflections at the interfaces become negligible and the proposed method converges toward the right solution. This proof can be generalized to the case of multiple propagative modes. The scattering coefficients $C_{i,j}$ then become matrices of finite spectral radius. Using the same reasoning, we can demonstrate that it does not change the convergence of the solution, i.e. $K_\alpha = 1$, $K_\delta = 0$, $\forall \delta \neq \alpha$.

An interesting digression here concerns phenomena such as extraordinary transmission through a layered medium that strongly depends on the number of layers considered [132]. Such phenomena are due to multiple reflections on both interfaces of the metamaterial slab and the air. Mathematically, this is due to the denominator of (2.79) that may vary significantly with the phase of the $\exp(j\varphi) g_\beta^{N+1} g_\gamma^{N+1}$ term. However, in the presence of losses, the amplitude of $\exp(j\varphi) g_\beta^{N+1} g_\gamma^{N+1}$ becomes negligible for $N \gg 1$. Thus, the variation of the fields with the number of layers becomes negligible. Therefore, phenomena like the one described in [132] disappear and the eigenmodes of the structure can be retrieved, provided that the number of layers considered is large enough.

Now that the convergence of the method has been proven, it is interesting to derive an upper bound for the error with respect to the number of iterations. We define the error on the fields for a number N of slabs in layer 2, i.e. the difference between the exact solution and the approximate one, which contains some β and γ modes, as

$$e = \frac{\iint_{S_0} |\mathbf{f}_\alpha - (\mathbf{f}_\alpha + K_\beta \mathbf{f}_\beta + K_\gamma \mathbf{f}_\gamma)| dS}{\iint_{S_0} |\mathbf{f}_\alpha| dS} \quad (2.80)$$

with $\mathbf{f}_i = (\mathbf{E}_i, \eta \mathbf{H}_i)$ the fields on interface $l2$ due to mode i of unit amplitude. In the following, we will consider that the solution has converged if the error e defined by (2.80) is smaller than a predefined threshold $e_0 \ll 1$. Going back to the definition of the modes (2.71), it can be seen that $\iint_{S_0} |\mathbf{f}_i| dS = 1$. We then obtain

$$e \leq |K_\beta| + |K_\gamma| \quad (2.81)$$

As explained previously, the geometrical series in Equation (2.78) are converging toward zero for an increasing number of layers N . Geometrical series are absolutely convergent [133]. We can hence consider that there exists an integer N_0 such that the magnitude of the sums in (2.78) is smaller than $1/2$ for any $N > N_0$. From there, two possibilities:

- The mode α is highly evanescent. In that case, the magnitude of the term g_α^N in Equations (2.78) will decrease much faster than the magnitude of the sums. The convergence may therefore be reached for $N < N_0$.
- The mode α is propagative or slightly evanescent. In that case, the convergence of the solution will require that $N > N_0$.

In the first case, imposing $N = N_0$ is sufficient to ensure convergence. Indeed, the evanescent aspect of the mode leads to natural convergence. In the second case, which treats the dominant modes—in which we are primarily interested—a number of layers $N > N_0$ is required to reach convergence. Substituting (2.78) into (2.81) and considering that the magnitude of the sums of (2.78) is smaller than $1/2$ gives:

$$e < |g_\alpha|^N \quad (2.82)$$

Imposing that the solution is converged and using (2.73), we obtain

$$(1 - \rho_\alpha \sigma)^{2^n} < e_0 \quad (2.83)$$

which can be reformulated as

$$-2^n \ln(1 - \rho_\alpha \sigma) > -\ln(e_0) \quad (2.84)$$

The conductivity being small, the logarithm on the left-hand side can be approximated using first-order Taylor expansion. Taking the logarithm of the resulting expression, we obtain

$$n + \log_2(\rho_\alpha \sigma) > \log_2(-\ln(e_0)) \quad (2.85)$$

After few manipulations, the number of iterations n required for the error to remain below the threshold e_0 reads:

$$n > \log_2(\ln(e_0^{-1})) - \log_2(\rho_\alpha \sigma) \quad (2.86)$$

Equation (2.86) illustrates an exponential convergence with respect to the losses introduced in the material and doubly exponential convergence with respect to the error threshold.

It is interesting to notice that the shape and constitutive parameters of the inclusions are only impacting the convergence through the factor ρ_α (see (2.73) and Appendix A.7). Indeed, the solutions to Maxwell's equations will change depending on the geometry and constitutive parameters of the inclusions. So will do the dissipations associated to these solutions.

So far, losses have been introduced via a small conductivity σ . Another possibility to introduce losses is to numerically decrease the amplitude of the transmission coefficient g by an arbitrary factor $(1 - \gamma)$. In that case, the losses, which have no physical origin, are independent of the geometry and constitutive parameters of the inclusions. The number of iterations required to reach a given level of accuracy becomes

$$n > \log_2 (\ln(e_0^{-1})) - \log_2 (\gamma) \quad (2.87)$$

which is independent of the structure considered.

Note that the accuracy of the method can be tested a posteriori by substituting the obtained results into the non-linear formulation (2.63).

2.3.4 Comparison with T-matrix based methods

The proposed method has been presented using the MoM formalism as a support. However, the only information that is needed is the way in which the fields propagate through one layer. In this section, we extend the method to the more versatile Scattering-matrix (S-matrix) formalism [120].

The S-matrix of a structure is the matrix that relates the fields incident on the structure to those scattered by the structure. That matrix is generally well conditioned [120]. The Transfer-matrix (T-matrix) of the layer is the matrix that relates the total fields (incident and scattered) on one side of the layer to the total fields on the other side of the layer. Since it has to handle back-propagation, the T-matrix is numerically ill-conditioned [120]. Such as the MoM impedance matrix, S- and T-matrices are different ways to represent the response of a structure to incident fields.

Methods that use the information of S- and T-matrices to determine the eigenmodes of a structure have already been demonstrated in the literature [117, 128, 129]. The response of one layer of the structure studied to incident electromagnetic fields is computed through the computation of the S-matrix associated to that layer. To determine the eigenmodes of the structure from the information stored in the S-matrix, the latter is used to compute the T-matrix of a layer. All the eigenmodes and their corresponding eigenvalues can be computed at once using an eigenvalue decomposition of that T-matrix. However, as shown in [129], the computation of the T-matrix is numerically ill-conditioned and therefore prone to numerical noise. The maximum precision that can be achieved is therefore limited.

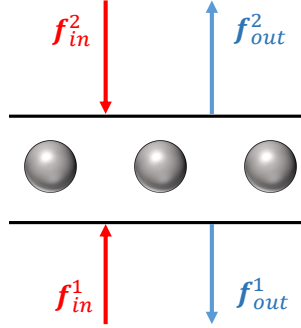


Figure 2.14: Scheme of the S-matrix formalism used. The relation between the incoming fields that excite the layer (in red) and the fields scattered by the layer (in blue) is characterized by the scattering matrix $\underline{\underline{S}}^{(0)}$.

Although the method is still relatively robust using plane-wave decomposition of the fields [117], we found it to be unstable when the decomposition of the fields were done using equivalent currents. We encountered a strong dependence of the results on the mesh used to express the currents distribution and to test the fields using the Müller formulation of the MoM [33]. Results obtained for the linear problem with a double number of unknowns (cf. Section 2.3.1) were found to be more stable, but still prone to numerical error propagation, as will be shown in Section 2.3.5.

As shown for MoM impedance matrix formalism, this limitation can be circumvented by linearizing the eigenvalue problem associated to the S-matrix without using the equivalent T-matrix.

We first consider one layer of the metamaterial. The field scattered by the layer can be related to the fields incident on that layer using the S-matrix $\underline{\underline{S}}^{(0)}$:

$$\begin{pmatrix} \underline{\underline{S}}_{11}^{(0)} & \underline{\underline{S}}_{12}^{(0)} \\ \underline{\underline{S}}_{21}^{(0)} & \underline{\underline{S}}_{22}^{(0)} \end{pmatrix} \begin{pmatrix} \mathbf{f}_{in}^1 \\ \mathbf{f}_{in}^2 \end{pmatrix} = \begin{pmatrix} \mathbf{f}_{out}^1 \\ \mathbf{f}_{out}^2 \end{pmatrix} \quad (2.88)$$

with $\mathbf{f}_{in}^i$ and $\mathbf{f}_{out}^i$ the fields incident on and radiated from the layer, respectively, as illustrated in Figure 2.14. The eigenmodes of the metamaterial can then be found using

$$\mathbf{f}_{out}^1 = g^{-1} \mathbf{f}_{in}^2 \quad (2.89a)$$

$$\mathbf{f}_{out}^2 = g \mathbf{f}_{in}^1 \quad (2.89b)$$

Substituting these conditions into Equation (2.88), one can obtain the non-linear formulation of the problem equivalent to (2.63). A linear formulation can be found using an iterative procedure similar to that described in Section 2.3.2.

Now, add a second layer on top of the first one. The total scattering matrix can be computed for the structure made of two layers:

$$\begin{pmatrix} \underline{\underline{S}}_{11}^{(1)} & \underline{\underline{S}}_{12}^{(1)} \\ \underline{\underline{S}}_{21}^{(1)} & \underline{\underline{S}}_{22}^{(1)} \end{pmatrix} \begin{pmatrix} \mathbf{f}_{in}^1 \\ \mathbf{f}_{in}^2 \end{pmatrix} = \begin{pmatrix} \mathbf{f}_{out}^1 \\ \mathbf{f}_{out}^2 \end{pmatrix} \quad (2.90)$$

with

$$\underline{\underline{S}}_{11}^{(i+1)} = \underline{\underline{S}}_{11}^{(i)} + \underline{\underline{S}}_{12}^{(i)} \underline{\underline{A}}_{11}^{(i)} \underline{\underline{S}}_{21}^{(i)} \quad (2.91a)$$

$$\underline{\underline{S}}_{12}^{(i+1)} = \underline{\underline{S}}_{12}^{(i)} \underline{\underline{A}}_{12}^{(i)} \underline{\underline{S}}_{12}^{(i)} \quad (2.91b)$$

$$\underline{\underline{S}}_{21}^{(i+1)} = \underline{\underline{S}}_{21}^{(i)} \underline{\underline{A}}_{21}^{(i)} \underline{\underline{S}}_{21}^{(i)} \quad (2.91c)$$

$$\underline{\underline{S}}_{22}^{(i+1)} = \underline{\underline{S}}_{22}^{(i)} + \underline{\underline{S}}_{21}^{(i)} \underline{\underline{A}}_{22}^{(i)} \underline{\underline{S}}_{12}^{(i)} \quad (2.91d)$$

and

$$\begin{pmatrix} \underline{\underline{A}}_{11}^{(i)} & \underline{\underline{A}}_{12}^{(i)} \\ \underline{\underline{A}}_{21}^{(i)} & \underline{\underline{A}}_{22}^{(i)} \end{pmatrix} = \begin{pmatrix} -\underline{\underline{S}}_{22}^{(i)} & \underline{\underline{I}} \\ \underline{\underline{I}} & -\underline{\underline{S}}_{11}^{(i)} \end{pmatrix}^{-1} \quad (2.92)$$

$\underline{\underline{I}}$ standing for the identity matrix. Note that $\mathbf{f}_{in}^i$ ($\mathbf{f}_{out}^i$) still represents the fields incident on (scattered by) the device, which now consists of a stack of two layers. Iterating the procedure n times, the obtained scattering matrix describes the scattering of incident fields by a metamaterial made of 2^n consecutive layers. If the number of layers considered is large enough and some losses are added to the structure, the spectral radius of matrices $\underline{\underline{S}}_{12}^{(n)}$ and $\underline{\underline{S}}_{21}^{(n)}$ will tend to vanish. It is worth noting that the operation of adding layers using this method is numerically stable, as demonstrated in [120].

Once enough layers have been added, we can consider the structure illustrated in Figure 2.13. As $\mathbf{f}_{in}^2$ has now a negligible impact on resulting $\mathbf{f}_{out}^1$, all the quantities are now only depending on $\mathbf{f}_{in}^1$. Simplifying the formula accordingly, one can find the eigenmodes by solving

$$\left(\underline{\underline{I}} - \underline{\underline{S}}_{22}^{(0)} \underline{\underline{S}}_{11}^{(n)} \right)^{-1} \underline{\underline{S}}_{21}^{(0)} \mathbf{f}_{in}^1 \simeq g \mathbf{f}_{in}^1 \quad (2.93)$$

Once solved, the total fields distribution associated to the mode can be found knowing that:

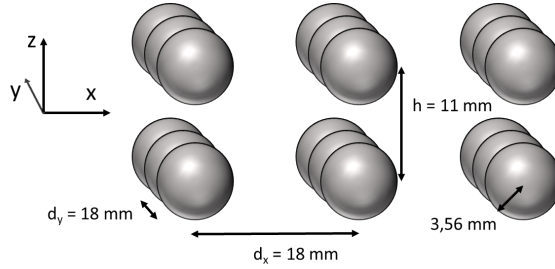


Figure 2.15: Structure from [134] used to test our method.

$$\mathbf{f}_{out}^1 = \underline{\underline{S}}_{11}^{(n)} \mathbf{f}_{in}^1 \quad (2.94)$$

As mentioned previously, the operation of doubling the number of layers considered is numerically stable. The inversion of matrix $\left(\underline{\underline{I}} - \underline{\underline{S}}_{22}^{(0)} \underline{\underline{S}}_{11}^{(n)}\right)$ in (2.93) is numerically stable if the eigenvalues of $\underline{\underline{S}}_{22}^{(0)} \underline{\underline{S}}_{11}^{(n)}$ are different from unity. For a given eigenvector $\mathbf{x}$, $\underline{\underline{S}}_{11}^{(n)} \mathbf{x}$ corresponds to the fields reflected by the 2^n layers situated above. Multiplying the results by $\underline{\underline{S}}_{22}^{(0)}$ provides the fields re-reflected by the layer below. In the case of lossy layers, or in the case where some energy leaks into the free space when the fields are scattered on the top or bottom interface, $\underline{\underline{S}}_{22}^{(0)} \underline{\underline{S}}_{11}^{(n)} \mathbf{x}$ cannot reproduce $\mathbf{x}$, which in turn ensures the stability of the inversion in (2.93).

The convergence of the method demonstrated in Section 2.3.3 still holds for the S-matrix formalism, ensuring that accurate results without significant numerical error spreading can always be obtained with a doubly exponential convergence rate.

2.3.5 Numerical results

To test the efficiency of the method, we considered an array of spheres, for which quasi-analytical solutions are known [134]. We simulated one of the structures studied in [134] (cf. Fig. 2.15), which corresponds to a lattice of dielectric spheres of relative permittivity $\varepsilon_r = 40$, relative permeability $\mu_r = 1$ and whose radius is 3.56 mm. Inside one layer, the spheres are arranged in a square lattice along the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ directions with a periodicity of $d_x = d_y = 18$ mm. The periodicity along the $\hat{\mathbf{z}}$ direction, which corresponds to the thickness of the layers constituting the metamaterial, is $h = 11$ mm. The spheres are located in vacuum.

The eigenmodes inside the structure have been studied for several frequencies, with no phase shift between consecutive unit-cells in $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ di-

rections inside a layer ($\varphi_x = \varphi_y = 0$). The frequency is expressed in terms of its normalized wave-vector $k_0 h$, with $k_0 = 2\pi/\lambda_0$ and λ_0 the wavelength in free space. The phase and amplitude of the transmission coefficient g corresponding to the main propagative mode can be seen in Figure 2.16. It can be seen on graph 2.16(b) that the transmission coefficient of evanescent modes inside the band-gap is smaller than unity.

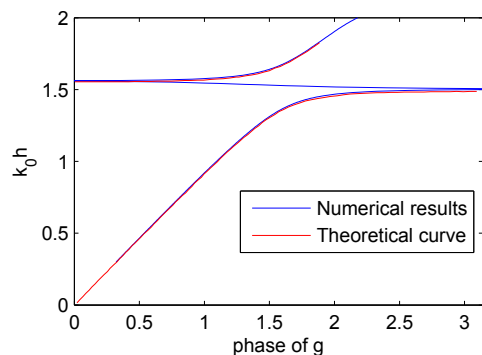
To obtain these results, we used the linearized formulation. Losses were artificially introduced by multiplying the $\underline{\tilde{Z}}_{12}$ and $\underline{\tilde{Z}}_{21}$ matrices by a factor $(1 - 10^{-4})$. The precision with which the impedance matrices have been computed being of the same order of magnitude as the loss factor, multiplication by that factor does not introduce a significant change in the accuracy of the final results. Introducing losses in that way prevents the degradation of the results near resonances, where small losses can induce huge changes in the modal distribution.

The results obtained using the linearized formulation were tested by substituting them into the parabolic formulation (2.63) and testing the continuity of the fields at the interface between two layers. First, using the linearized formulation, the two following quantities have been computed: (i) $\mathbf{x}_{lin}$, the equivalent currents on the interface between two consecutive layers corresponding to one mode, and (ii) g_{lin} , the corresponding transmission coefficient. Then, we replaced $\mathbf{x}_{l1}$ and $\mathbf{x}_{l3}$ in (2.62) by $\mathbf{x}_{lin}/g_{lin}$ and $\mathbf{x}_{lin} g_{lin}$, respectively. Then, $\mathbf{x}_{l2}$ has been computed and compared with $\mathbf{x}_{lin}$; the error e is defined as

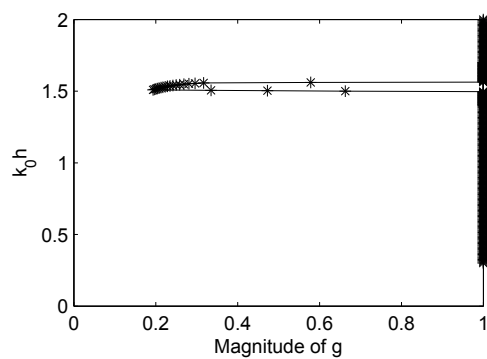
$$e = \frac{|\mathbf{x}_{lin} - \mathbf{x}_{l2}|}{|\mathbf{x}_{lin}|} \quad (2.95)$$

First, using the loss factors introduced for linearization into the parabolic formulation, machine precision is achieved for all frequencies after 30 iterations. Second, the error has been checked using the non-modified impedance matrix for the parabolic formulation. The maximum error was found to be $e = 10^{-4}$, which corresponds to the error introduced by the loss factor.

The convergence of the method has also been tested when introducing a varying amount of conduction losses inside the metamaterial. This has been implemented adding a complex component ε'' to the permittivities of the air and of the dielectric. The loss tangent $\tan(\delta) = \varepsilon''/\varepsilon$ has been made identical for air and dielectric, the frequency has arbitrarily been chosen to be such that $k_0 h = 1$. Results are shown in Figure 2.17. On the top graph, we can see the doubly exponential convergence of the method for a fixed amount of losses (cf. Equation (2.86)). On the second graph, the number of iterations required to reach an error e smaller than a predefined threshold $e_0 = 10^{-10}$ is shown. The predicted exponential convergence with respect to the losses is clearly visible.



(a)



(b)

Figure 2.16: Phase (a) and magnitude (b) of the transmission coefficient corresponding to the main propagative mode inside the structure. (a) Red: analytical results from [134], blue: numerical results.

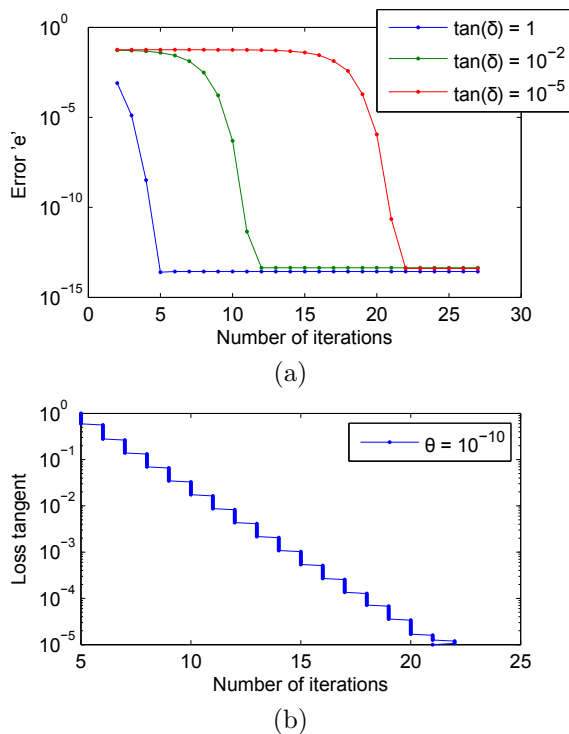


Figure 2.17: Convergence of the method. (a) Evolution of the error with the number of iterations for different amount of losses. (b) Relation between the losses and the number of iterations required to reach an error e smaller than a threshold $e_0 = 10^{-10}$.

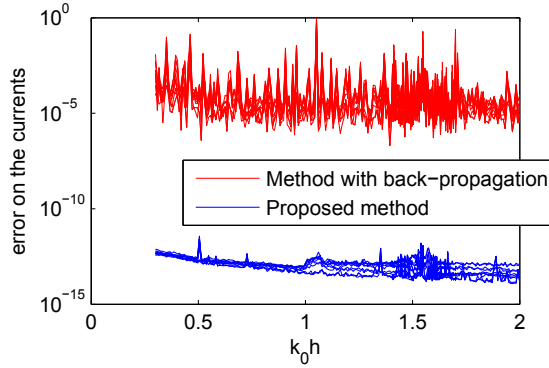


Figure 2.18: Numerical error introduced when computing the first ten eigenmodes of the structure using two different linear methods. Red curves: linear formulation that has to handle back-propagation (cf. Section 2.3.1). Blue curves: proposed method.

We also compared the accuracy of the results that can be achieved using the proposed method with the accuracy achieved by linear methods handling back-propagation. Using the same set of matrices as the one used to provide the results displayed on Fig. 2.16, we computed the eigenmodes of the structure using the proposed formulation and the one based on doubling the number of unknowns, which is provided at the end of Section 2.3.1 (Equation (2.66)). The numerical error introduced by both techniques for the first ten eigenmodes was computed using (2.95) and is shown in Fig. 2.18. The error is only originating from the numerical round-off error.

First, we can notice that numerical error is limited when we use the method we presented (blue curves), due to the fact that every step of the method is well-conditioned. The increase in the error for small wave vectors $k_0 h$ is probably due to the “low frequency breakdown” that is related to the MoM simulation technique rather than on the method used to determine eigenmodes.

Second, as explained in [129], methods that have to handle back-propagation are ill-conditioned. Therefore, the numerical noise tends to grow during the computation of the modes (red curves).

As we can see, the accuracy of the proposed method is between five and ten orders of magnitude better than the accuracy provided by techniques handling back-propagation.

We also compared the accuracy of the proposed method using S-matrix formalism with the accuracy that can be achieved when using the associated T-matrix. The S-matrix of the layer has been obtained from the MoM

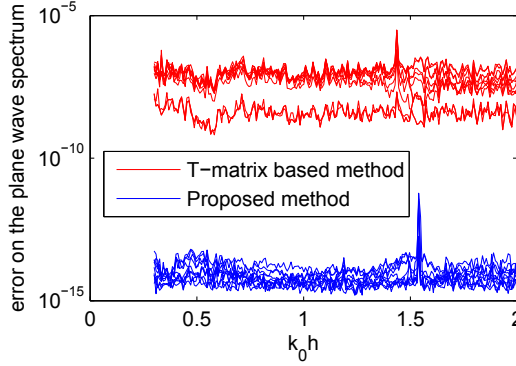


Figure 2.19: Numerical error for the computation of the first ten eigenmodes using the S-matrix of the structure. Red curves: eigenvalue decomposition of the T-matrix. Blue curves: iterative method.

simulation results. One layer of metamaterial has been excited by several propagative and evanescent plane waves, so that the total number of degrees of freedom is preserved, i.e. we used as many plane waves as we used basis functions to describe the currents on the interface between consecutive layers.

The error has been computed as follows. First, the eigenmodes and their associated eigenvectors have been computed using the methods presented in Section 2.3.4. The eigenfields associated to these eigenvectors can be decomposed into fields incident on the layer $\mathbf{f}_{in}^1$ and $\mathbf{f}_{in}^2 = g\mathbf{f}_{out}^1$, and fields scattered by the layer $\mathbf{f}_{out}^1$ and $\mathbf{f}_{out}^2 = g\mathbf{f}_{in}^1$. The incident fields were multiplied by the S-matrix of one layer, and the resulting vector were compared with the expected scattered fields from Equations (2.89).

The results can be seen in Fig. 2.19. The numerical error has been computed for the first ten eigenmodes of the structure. The red curves represent the error obtained when the T-matrix of the layer is computed from its S-matrix, while the blue curves represent the error obtained using the iterative method presented in Section 2.3.4.

First, we can notice, as mentioned previously, that using a plane wave decomposition of the fields tends to improve the accuracy reached due to natural filtering of the ill-conditioned modes. Indeed, the error of the red curves in Fig. 2.19 is much lower than the error in Fig. 2.18. Moreover, the lower red curves of Fig. 2.19 are corresponding to the less evanescent eigenmodes of the structure. They are characterized by a lower contribution of the highly evanescent plane waves, which explain the better filtering, thus the lower numerical noise.

Second, we can see that the error obtained when stacking the layers remains close to the machine precision. This is a direct consequence of the fact that all the matrix operations involved in computing the eigenmodes of the structure are well-conditioned.

Finally, the time for filling the impedance matrix for a fixed frequency ranged between 1h55' and 2h40', while the time spent to compute all the eigenmodes and eigenvalues after 30 iterations for one frequency took less than 20 seconds, which is negligible with respect to matrix filling time.

2.4 Surface Fictitious Source Superposition Method

Up to now, this Chapter has focused on the numerical simulation of periodic metamaterials. However, the presented methods fail as soon as a defect in the periodicity of the structure appears. Such a defect may be due to the unavoidable variability in the fabrication process or be introduced on purpose for a given application (e.g. defective waveguides in photonic crystals [101], absorbing surfaces [49], study of the impact of defects in metamaterials response [135]).

The Array Scanning Method (ASM) [113], which provides the response of a periodic structure to a non-periodic source, is limited to non-interacting sources, i.e. sources that do not depend on the scattered field. An extension of that technique to scattering defects in otherwise perfectly periodic gratings has been devised more recently: the Fictitious Source Superposition (FSS) method [136]. The method is based on one key idea : if a defect is introduced in the periodicity, the fields scattered as well as the boundary conditions are locally changed. Starting from the infinite-array solution, additional fictitious sources are strategically placed inside the defective zone. A corrective field is emitted depending on the local field density to adapt the periodic solution to the new boundary conditions. The determination of the fields emitted by the fictitious sources depends on the formulation of the problem, which generally depends on the geometry of the structure simulated. Different formulations can be seen on [136, 137, 138] where the structure is only made of cylindrical inclusions, or [47], where more complex shapes are considered. Several limitations and technical issues are limiting its applicability to general problems, such as the position of the fictitious sources, the choice of the basis functions used to describe the fields emitted or the possible combination with a full-wave 3D solver.

In this Section, we combine the FSS method with the Method of Moment (MoM) to provide a versatile, 3D and general way to compute the fields scattered by periodic structures in presence of defects in their period-

icity. The formulation is made general with respect to the shape, position and constitutive parameters of the inclusions. This work has already been presented in [139].

The Section is organized as follows. First, the basics of the method are presented. Then, a general formulation of the technique is developed based on MoM. Last, this general formulation is illustrated through a practical implementation using the impedance matrices.

2.4.1 The FSS method

We begin with the presentation of the structure simulated and remind rapidly the formulation of the ASM. Then, the FSS method is presented using different formulations, depending on the type of defect (material added or removed).

We consider a structure periodic along 2 directions inside the 3D space. The periods are d_x and d_y along the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ directions respectively. Note that $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ do not have to be orthogonal. The adaptation to 3D or 1D periodicities is straightforward. The structure is excited by quasi-periodic sources, whose periodicity coincides with the periodicity of the structure according to a linear phase-shift $\boldsymbol{\varphi} = (\varphi_x, \varphi_y)$ between consecutive unit cells in the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ directions respectively. Using a periodic solver, we can focus on the resulting fields within one unit cell, the fields in the other unit cells being identical according to a phase-factor. We then obtain:

$$\tilde{\mathbf{f}}^I(\mathbf{r}|\boldsymbol{\varphi}) = \iiint_{\text{RUC}} \tilde{\underline{\underline{G}}}_{out}(\mathbf{r}, \mathbf{r}'|\boldsymbol{\varphi}) \cdot \tilde{\mathbf{J}}_I(\mathbf{r}'|\boldsymbol{\varphi}) d\mathbf{r}' \quad (2.96)$$

with $\tilde{\mathbf{f}}^I(\mathbf{r}|\boldsymbol{\varphi})$ the value of the fields in position $\mathbf{r}$ for sources with a phase-shift $\boldsymbol{\varphi}$ between consecutive cells, $\tilde{\underline{\underline{G}}}_{out}(\mathbf{r}, \mathbf{r}'|\boldsymbol{\varphi})$ the periodic dyadic Green's function providing the fields in position $\mathbf{r}$ when the structure is excited by a periodic source positioned in $\mathbf{r}'$ and $\tilde{\mathbf{J}}_I(\mathbf{r}', \boldsymbol{\varphi})$ the source distribution. The integration is carried out over the volume of one unit-cell, which we will designate as the reference unit cell (RUC). Both $\mathbf{r}$ and $\mathbf{r}'$ lie within the reference unit cell. Note that $\tilde{\mathbf{f}}^I$ (resp. $\tilde{\mathbf{J}}_I$) is a vector, as it contains both electric and magnetic fields (resp. currents) in the 3 directions of space.

The ASM [113] exploits the linearity of the Maxwell's equations with respect to the excitation to decompose the response to any general (non-periodic) source distribution into quasi-periodic problems, corresponding to the different Bloch modes of the structure (i.e. functions that have the same periodicity as the structure within a linear phase shift):

$$\mathbf{f}^I(\mathbf{r}) = \frac{1}{(2\pi)^2} \iint_0^{2\pi} \tilde{\mathbf{f}}^I(\mathbf{r}|\boldsymbol{\varphi}) d\boldsymbol{\varphi} \quad (2.97)$$

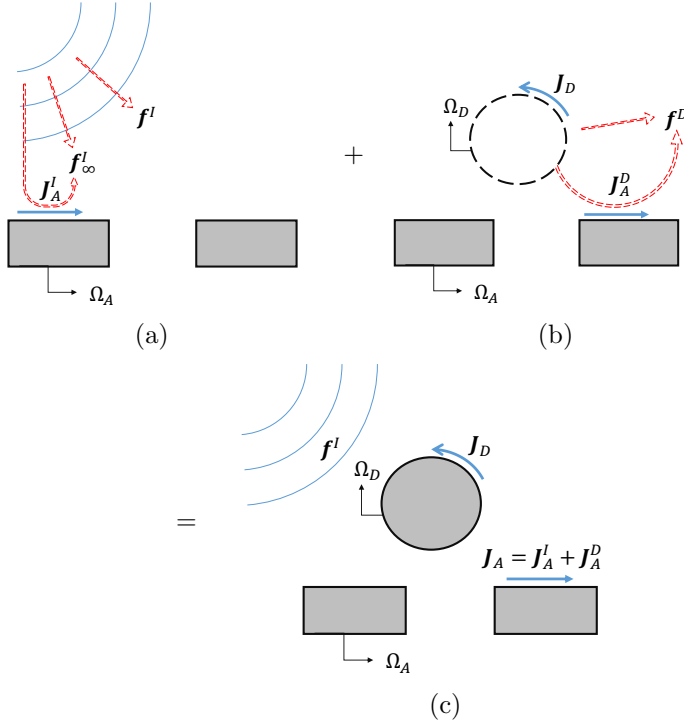


Figure 2.20: General scheme of the FSS method. The rectangles represent the periodic array and the sphere the defect in the periodicity (additional scatterer). **(a) Infinite array solution:** the fields distribution everywhere (f_∞^I) is the combination of the initial incoming field (f^I) and the field scattered by the periodic array, corresponding to the field emitted by the equivalent currents J_A^I on the surface of the periodic structure (Ω_A). **(b) Determination of the modes:** the fields due to a fictitious sources distribution (J_D) on the surface of the defect (Ω_D) is the combination of the fields directly emitted by the fictitious sources and the fields scattered by the periodic array (corresponding to the fields emitted by J_A^D). **(c) The problem solved:** the fictitious sources distribution (J_D) is chosen to satisfy the boundary conditions on the surface of the defect. The equivalent currents on the surface of the infinite array (J_A) are the combination of the currents due to the primary excitation and the currents due to the fictitious sources on the surface of the defect.

$$= \frac{1}{(2\pi)^2} \int_0^{2\pi} \iint_{\text{RUC}} \tilde{G}_{out}(\mathbf{r}, \mathbf{r}'|\varphi) \cdot \tilde{\mathbf{J}}_I(\mathbf{r}'|\varphi) d\mathbf{r}' d\varphi \quad (2.98)$$

with

$$\tilde{\mathbf{J}}(\mathbf{r}'|\varphi) = \sum_p \sum_q \mathbf{J}(\mathbf{r}' + pd_x \hat{\mathbf{x}} + qd_y \hat{\mathbf{y}}) \exp(-j(p\varphi_x + q\varphi_y)). \quad (2.99)$$

and RUC indicating that the integral is carried over the reference unit cell.

A major hypothesis needed to use the ASM is the fact that the sources do not interact with the local fields, *i.e.* the value of the sources does not depend on the local value of the fields. If one wants to study the behaviour of a defect in the periodicity, the formulation has to be adapted: the defect will interact with the local fields to produce new fields. Then, the different Bloch modes cannot be treated independently. Consequently, the FSS method is used (cf. Figure 2.20).

A fictitious source is embedded within the defect. Generally, the fields emitted by that source are described using a multipole expansion [136, 137, 138, 47]. First, new constraints (*i.e.* radiation or boundary conditions) are determined to describe the defect. Then, the response of the periodic structure to the different modes that can be emitted by the fictitious source is computed (cf. Figure 2.20(b)). The combination of the fields emitted by the fictitious source and scattered by the structure corresponds to a solution of Maxwell's equations that satisfies the boundary conditions on the surface of the periodic structure. To compute the response of the defective array to any excitation, the solution is first computed for the non-defective array (cf. Figure 2.20(a)) and then adapted using a set of modes computed previously in order to satisfy the additional constraints (cf. Figure 2.20(c)).

In [137], some inclusions of the infinite array are removed using the additional constraint of zero-field scattered by these inclusions: the fields emitted by the fictitious sources are chosen to perfectly compensate for the fields scattered in the infinite array problem by the inclusions we want to make disappear. The formulation has been adapted in [138], where change of local constitutive parameters or of the radius of some inclusions is also considered. However, the method is only formulated for 2D photonic crystals made of cylindrical inclusions and uses multipole expansion of the fields.

In [47], the method is generalized to any fields decomposition and an explicit link with the ASM is made. An extension using transfer matrices is suggested to generalize the technique to inclusions of any shape.

Our formulation differs from the previous ones in the fact that the fictitious source is not situated inside the defect but is made of surface currents on its boundary. For that reason, we will refer to it as the Surface Fictitious

Source Superposition (SFSS) method. In the case of additional scatterer, the additional constraint corresponds to the boundary conditions along that surface, while the constraint for object disappearance is the cancellation of the total surface currents on the boundary of the inclusion we want to remove.

2.4.2 Conventions and notations

Before proceeding with the derivation of the SFSS formulation, it is worth spending some time on the conventions that will be used. Consider the geometry illustrated in Figure 2.20: a periodic array (A) of blocs on top of which one single scatterer (D) is located. The structure is illuminated by some incident fields $\mathbf{f}^I$. The goal of this Section is to solve this scattering problem that involves both a periodic structure and a non-periodic sphere, *i.e.* find the equivalent currents that appear on the blocs ($\mathbf{J}_A$) and on the sphere ($\mathbf{J}_D$).

First, we consider a simplified problem without the sphere. In this problem, the infinite array of blocs is illuminated by the primary excitation $\mathbf{f}^I$. This problem can be solved and equivalent currents $\mathbf{J}_A^I$ on the array (A) due to the primary excitation (I) can be found. In this simplified problem, the total fields (incident + scattered) in any position correspond to the infinite array solution and are therefore noted $\mathbf{f}_\infty^I$.

Then, the non-periodic scatterer can be introduced. Using the equivalence principle, we consider the outer problem (cf. Chapter 1) as illustrated in Figure 2.20(b). The fields emitted by equivalent currents $\mathbf{J}_D$ on the sphere are computed in order to impose the boundary conditions. As for the primary excitation, in order to find the total fields, one has to find the equivalent currents $\mathbf{J}_A^D$ induced on the periodic array (A) by equivalent currents on the sphere (D). The total fields emitted by equivalent currents on the sphere taking into account the scattering by the periodic array are noted $\mathbf{f}^D$.

Imposing the boundary conditions on the surface of the sphere, the equivalent currents $\mathbf{J}_D$ on the sphere and the total equivalent currents on the blocs $\mathbf{J}_A = \mathbf{J}_A^I + \mathbf{J}_A^D$ can be determined.

2.4.3 The SFSS-MoM formulation

In a first instance, consider an isolated scatterer (A) excited by an incoming field $\mathbf{f}^I(\mathbf{r})$, the boundary conditions are satisfied if the tangential electric

and magnetic fields are continuous across the surface of the scatterer:

$$-\hat{\mathbf{n}}(\mathbf{r}) \times \mathbf{f}^I(\mathbf{r}) = \hat{\mathbf{n}}(\mathbf{r}) \times \int_{\Omega_A} \left(\underline{\underline{G}}_{in}(\mathbf{r}, \mathbf{r}') + \underline{\underline{G}}_{out}(\mathbf{r}, \mathbf{r}') \right) \cdot \mathbf{J}_A^I(\mathbf{r}') d\mathbf{r}' \quad \forall \mathbf{r} \in \Omega_A \quad (2.100)$$

with Ω_A the surface of the scatterer A , $\mathbf{J}_A^I(\mathbf{r}')$ the (unknown) equivalent current density on point $\mathbf{r}'$ of the surface of A due to the incident field (I), and $\underline{\underline{G}}_{in}(\mathbf{r}, \mathbf{r}')$ and $\underline{\underline{G}}_{out}(\mathbf{r}, \mathbf{r}')$ the dyadic Green's functions describing the fields induced on point $\mathbf{r}$ by currents on point $\mathbf{r}'$ through the medium respectively inside and outside the scatterer (cf. Chapter 1).

Now, consider that the scatterer A is repeated periodically, forming an infinite array. To treat infinite arrays of scatterers, the ASM is used. The excitation $\mathbf{f}^I(\mathbf{r})$ is decomposed into Bloch modes using formula (2.99). Then, for each Bloch mode, the boundary conditions are satisfied using formula (2.100) and substituting the dyadic periodic Green's function $\underline{\underline{G}}(\mathbf{r}, \mathbf{r}'|\varphi)$ to the non-periodic one.

The final current distribution on the infinite array of scatterers is the sum of the contributions of all the Bloch modes:

$$\mathbf{J}_A^I(\mathbf{r}) = \frac{1}{(2\pi)^2} \iint_0^{2\pi} \tilde{\mathbf{J}}_A^I(\mathbf{r}|\varphi) d\varphi \quad (2.101)$$

with $\tilde{\mathbf{J}}_A^I(\mathbf{r}|\varphi)$ the infinite array solution obtained for phase shift φ between consecutive unit cells. The integration is performed over the first Brillouin zone. $\tilde{\mathbf{J}}_A^I$ corresponds to the infinite-array solution that will be adapted using the fictitious sources. The next step consists of determining a set of fields distribution that can be emitted by the fictitious currents on the surface of the defect and that satisfies the boundary conditions on the surface of the array.

Considering a current distribution $\mathbf{J}_D(\mathbf{r})$ on the surface of the defect, the corresponding fields that satisfies the boundary conditions on the surface of the infinite array are:

$$\begin{aligned} \mathbf{f}_{out}^D(\mathbf{r}) &= \int_{\Omega_D} \underline{\underline{G}}_{out}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{J}_D(\mathbf{r}') d\mathbf{r}' \\ &\quad + \int_{\Omega_A} \underline{\underline{G}}_{out}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{J}_A^D(\mathbf{r}') d\mathbf{r}' \end{aligned} \quad (2.102)$$

$$\mathbf{f}_{in}^D(\mathbf{r}) = - \int_{\Omega_D} \underline{\underline{G}}_{in}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{J}_D(\mathbf{r}') d\mathbf{r}' \quad (2.103)$$

with $\mathbf{J}_A^D(\mathbf{r}')$ the currents induced on the periodic structure by $\mathbf{J}_D(\mathbf{r}')$, which designates the currents density on the surface of the defect. Equation (2.102)

describes the fields outside the defect and Equation (2.103) describes the fields inside the defect due to the fictitious currents on its surface. Interestingly, due to the linearity of Maxwell's equations with respect to the current distribution, $\mathbf{J}_A^D(\mathbf{r})$ is a linear function of $\mathbf{J}_D(\mathbf{r}')$

$$\mathbf{J}_A^D(\mathbf{r}) = \int_{\Omega_D} \underline{\underline{\mathcal{L}}}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{J}_D(\mathbf{r}') d\mathbf{r}'. \quad (2.104)$$

Therefore, if one can determine $\underline{\underline{\mathcal{L}}}$, $\mathbf{f}_{out}^D(\mathbf{r})$ and $\mathbf{f}_{in}^D(\mathbf{r})$ are just depending on the equivalent currents on the surface of the defect. Additional information concerning the determination of $\underline{\underline{\mathcal{L}}}(\mathbf{r}, \mathbf{r}')$ will be provided later, in Section 2.4.3. For now, it will simply be treated as a black box.

Last, new constraints will be applied to Maxwell's equations. As mentioned previously, those constraints depend on the type of defect. If the defect consists of an additional scatterer, new boundary conditions have to be satisfied. However, if the defect consists of the removal of an inclusion, then no-scattering conditions will be applied. For more complex defects (holes or outgrowths on an inclusion), a mixed formulation has to be used, no-radiation conditions being applied on one part of the surface while new boundary conditions being applied on the rest of the surface.

Note that physically, the $\underline{\underline{\mathcal{L}}}(\mathbf{r}, \mathbf{r}')$ operator provides the equivalent surface currents that appear on each scatterer of the periodic array (at position $\mathbf{r}$) when the array is excited by a delta-like impressed current located at position $\mathbf{r}'$. Therefore, in order to compute the value of $\underline{\underline{\mathcal{L}}}(\mathbf{r}, \mathbf{r}')$, one has to solve a full scattering problem for each possible $\mathbf{r}'$.

Additional scatterer

In the case of an additional scatterer, new boundary conditions are applied on the surface of the defect. First, we start from the field distribution corresponding to the infinite-array solution (i.e. without the defect):

$$\mathbf{f}_\infty^I(\mathbf{r}) = \mathbf{f}^I(\mathbf{r}) + \int_{\Omega_A} \underline{\underline{G}}_{out}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{J}_A^I(\mathbf{r}') d\mathbf{r}' \quad (2.105)$$

$$\mathbf{f}_\infty^I(\mathbf{r}) = - \int_{\Omega_A} \underline{\underline{G}}_{in}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{J}_A^I(\mathbf{r}') d\mathbf{r}' \quad (2.106)$$

with $\mathbf{f}_\infty^I(\mathbf{r})$, the fields everywhere respectively outside and inside the periodic structure. The new boundary conditions are

$$\hat{\mathbf{n}}(\mathbf{r}) \times \left(\mathbf{f}_\infty^I(\mathbf{r}) + \mathbf{f}_{out}^D(\mathbf{r}) \right) = \hat{\mathbf{n}}(\mathbf{r}) \times \mathbf{f}_{in}^D(\mathbf{r}), \quad \forall \mathbf{r} \in \Omega_D \quad (2.107)$$

with Ω_D the surface of the defect. Injecting formulas (2.102), (2.103) and (2.104), we obtain

$$\begin{aligned} -\hat{\mathbf{n}}(\mathbf{r}) \times \mathbf{f}_\infty^I(\mathbf{r}) &= \hat{\mathbf{n}}(\mathbf{r}) \times \int_{\Omega_D} \left[\underline{\underline{G}}_{in}(\mathbf{r}, \mathbf{r}') + \underline{\underline{G}}_{out}(\mathbf{r}, \mathbf{r}') \right. \\ &\quad \left. + \int_{\Omega_A} \underline{\underline{G}}_{out}(\mathbf{r}, \mathbf{r}'') \cdot \underline{\underline{\mathcal{L}}}(\mathbf{r}'', \mathbf{r}') d\mathbf{r}'' \right] \cdot \mathbf{J}_D(\mathbf{r}') d\mathbf{r}' \end{aligned} \quad (2.108)$$

with $\mathbf{f}_\infty^I(\mathbf{r})$ that has to be replaced by equation (2.106) or (2.105) if the defect is embedded or not within the periodic structure.

The most computationally intensive part of that formulation concerns the third term of the sum, which requires to compute the response of an infinite structure to any current distribution on the surface of the defect via the term $\underline{\underline{\mathcal{L}}}(\mathbf{r}'', \mathbf{r}')$. That issue will be addressed in Section 2.4.3.

Missing element

In the case of a defect consisting of a missing element within the array, the new constraint is the cancellation of the fields scattered by the missing element. In the MoM formulation, the scattered fields are proportional to the equivalent currents on the surface of the structure. Therefore, locally, fictitious sources have to perfectly compensate for the currents in the infinite array solution as well as for the new currents they induce. Note that in this case, the inclusion virtually does not exist. No boundary condition have to be satisfied on its surface anymore. The currents on the scatterer are given by:

$$\mathbf{J}_D(\mathbf{r}) = -[\mathbf{J}_A^I(\mathbf{r}) + \mathbf{J}_A^D(\mathbf{r})]. \quad (2.109)$$

Injecting Equation (2.104), we obtain

$$-\mathbf{J}_A^I(\mathbf{r}) = \int_{\Omega_D} [\underline{\underline{\mathcal{I}}} \delta(\mathbf{r} - \mathbf{r}') + \underline{\underline{\mathcal{L}}}(\mathbf{r}, \mathbf{r}')] \cdot \mathbf{J}_D(\mathbf{r}') d\mathbf{r}' \quad \forall \mathbf{r} \in \Omega_D \quad (2.110)$$

with $\delta(\mathbf{r} - \mathbf{r}')$ the 2D Dirac's function and $\underline{\underline{\mathcal{I}}}$ the unitary matrix.

Decomposition of $\underline{\underline{\mathcal{L}}}$

Using the formulation presented previously, both kinds of defects require to use of $\underline{\underline{\mathcal{L}}}$, an operator providing the response of the infinite array to any current distribution on the surface of the defect. The computation of that operator is the most computationally intensive part of the SFSS method and deserves some more comments. First, we will provide the equation that one has to solve to compute $\underline{\underline{\mathcal{L}}}$. Then, we will present a technique based on the ASM to decompose the infinite problem into a finite set of finite problems.

As mentioned in Section 2.4.3, the fields induced by a fictitious source distribution on the surface of the defect have to satisfy the boundary conditions on the surface of the periodic structure. The latter read:

$$\begin{aligned} \hat{\mathbf{n}}(\mathbf{r}) \times & \left(\int_{\Omega_D} \underline{\underline{G}}_{out}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{J}_D(\mathbf{r}') d\mathbf{r}' \right. \\ & \left. + \int_{\Omega_A} \underline{\underline{G}}_{out}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{J}_A^D(\mathbf{r}') d\mathbf{r}' \right) \\ & = -\hat{\mathbf{n}}(\mathbf{r}) \times \int_{\Omega_A} \underline{\underline{G}}_{in}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{J}_A^D(\mathbf{r}') d\mathbf{r}', \quad \forall \mathbf{r} \in \Omega_A. \end{aligned} \quad (2.111)$$

The main issue comes from the infinite surface Ω_A . However, the ASM can be used to reduce the problem to the reference unit cell using a periodic solver:

$$\begin{aligned} \tilde{\mathbf{J}}_D(\mathbf{r}|\varphi) = \\ \sum_p \sum_q \mathbf{J}_D(\mathbf{r} + p d_x \hat{\mathbf{x}} + q d_y \hat{\mathbf{y}}) \exp(-j(p\varphi_x + q\varphi_y)) \end{aligned} \quad (2.112)$$

such that

$$\mathbf{J}_D(\mathbf{r}) = \frac{1}{(2\pi)^2} \iint_0^{2\pi} \tilde{\mathbf{J}}_D(\mathbf{r}|\varphi) d\varphi \quad (2.113)$$

with the integration performed over the first Brillouin zone of the periodic structure. Each of the Bloch components of the fictitious currents has to satisfy the boundary conditions separately:

$$\begin{aligned} \hat{\mathbf{n}}(\mathbf{r}) \times & \int_{\Omega_D} \tilde{\underline{\underline{G}}}_{out}(\mathbf{r}, \mathbf{r}'|\varphi) \cdot \tilde{\mathbf{J}}_D(\mathbf{r}'|\varphi) d\mathbf{r}' \\ & + \hat{\mathbf{n}}(\mathbf{r}) \times \int_{\Omega_A^{RUC}} \tilde{\underline{\underline{G}}}_{out}(\mathbf{r}, \mathbf{r}'|\varphi) \cdot \tilde{\mathbf{J}}_A^D(\mathbf{r}'|\varphi) d\mathbf{r}' \\ & = -\hat{\mathbf{n}}(\mathbf{r}) \times \int_{\Omega_A^{RUC}} \tilde{\underline{\underline{G}}}_{in}(\mathbf{r}, \mathbf{r}'|\varphi) \cdot \tilde{\mathbf{J}}_A^D(\mathbf{r}'|\varphi) d\mathbf{r}' \\ & \forall \mathbf{r} \in \Omega_A^{RUC}, \quad \forall \varphi_x, \varphi_y \in [0; 2\pi[\end{aligned} \quad (2.114)$$

with Ω_A^{RUC} the surface of the periodic structure within the reference unit cell. The total equivalent currents on the periodic structure are made of the superposition of all these modes:

$$\mathbf{J}_A^D(\mathbf{r}) = \frac{1}{(2\pi)^2} \iint_0^{2\pi} \tilde{\mathbf{J}}_A^D(\mathbf{r}|\varphi) d\varphi \quad (2.115)$$

with

$$\tilde{\mathbf{J}}_A^D(\mathbf{r}|\varphi) = \int_{\Omega_D} \tilde{\underline{\underline{L}}} \cdot \tilde{\mathbf{J}}_D(\mathbf{r}'|\varphi)(\mathbf{r}, \mathbf{r}'|\varphi) d\mathbf{r}'. \quad (2.116)$$

The simulation of the infinite structure has been traded off with the evaluation of the integral of simpler problems over the first Brillouin zone. The most straightforward way to evaluate the integral is to use a Riemann sum:

$$\frac{1}{(2\pi)^2} \iint_0^{2\pi} \tilde{\mathbf{J}}_A^D(\mathbf{r}|\boldsymbol{\varphi}) d\boldsymbol{\varphi} \simeq \frac{1}{MN} \sum_{m=0}^{M-1} \sum_{n=0}^{N-1} \tilde{\mathbf{J}}_A^D(\mathbf{r}|\boldsymbol{\varphi}_{mn}), \quad (2.117)$$

$$\boldsymbol{\varphi}_{mn} = (\varphi_{x,0} + \frac{m2\pi}{M}, \varphi_{y,0} + \frac{n2\pi}{N}). \quad (2.118)$$

Interestingly, the error using that discretization corresponds to the repetition of the currents $\tilde{\mathbf{J}}_A^D$ every M and N unit-cells with a phase shift of $M\varphi_{x,0}$ and $N\varphi_{y,0}$ in the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ directions respectively. The finer the sampling, the farther away the replicas of the actual currents on the surface of the defect. The precision reached using a given sampling can therefore be roughly estimated.

Practical example

The different infinite-array problems described in the previous Section can be solved using any full-wave solver (including solvers that require to mesh the volume) as we remained general from the point of view of the discretization. In this Section, we will illustrate what we established previously at the expense of generality.

Consider the following discretized problem for which the defect is outside the periodic structure. The currents on the surface of the defect are expressed using a finite set of basis functions:

$$\tilde{\mathbf{J}}_D(\mathbf{r}|\boldsymbol{\varphi}) \simeq \sum_i x_{D,i}(\boldsymbol{\varphi}) \tilde{\mathbf{J}}_{D,i}(\mathbf{r}). \quad (2.119)$$

The currents on the infinite array can be discretized the same way:

$$\tilde{\mathbf{J}}_A(\mathbf{r}|\boldsymbol{\varphi}) \simeq \sum_j x_{A,j}(\boldsymbol{\varphi}) \tilde{\mathbf{J}}_{A,j}(\mathbf{r}). \quad (2.120)$$

Using that discretization, the $\tilde{\mathcal{L}}$ operator can be represented as a matrix such that

$$\mathbf{x}_A = \underline{\underline{\tilde{\mathcal{L}}}} \mathbf{x}_D \quad (2.121)$$

with $\mathbf{x}_A$ (resp. $\mathbf{x}_D$), a vector whose j^{th} entry contains the coefficient $x_{A,j}$ (resp. $x_{D,j}$). The currents on the surface of the infinite array induced by

normalized currents on the basis function i of the defect are given solving:

$$\begin{aligned} \sum_j x_{A,j}^{D_i}(\varphi) \int_{\Omega_A^{RUC}} \left[\tilde{\underline{G}}_{in}(\mathbf{r}, \mathbf{r}'|\varphi) + \tilde{\underline{G}}_{out}(\mathbf{r}, \mathbf{r}'|\varphi) \right] \cdot \tilde{\mathbf{J}}_{A,j}(\mathbf{r}') d\mathbf{r}' \\ = - \int_{\Omega_D} \tilde{\underline{G}}_{out}(\mathbf{r}, \mathbf{r}'|\varphi) \cdot \tilde{\mathbf{J}}_{D,i}(\mathbf{r}') d\mathbf{r}' \quad \forall \mathbf{r} \in \Omega_A^{RUC} \end{aligned} \quad (2.122)$$

with $x_{A,j}^{D_i}(\varphi)$, the (unknown) coefficients of the decomposition of $\tilde{\mathbf{J}}_A^{D_i}$ on basis functions $\{\tilde{\mathbf{J}}_{A,j}\}$, $\tilde{\mathbf{J}}_A^{D_i}$ being the currents induced on the surface of the array due to normalized currents on basis function i of the defect. The set of basis functions being finite, the test of the boundary conditions must be performed over a finite set of testing functions, which will be called $w_{A,k}$.

$$\begin{aligned} \sum_j x_{A,j}^{D_i}(\varphi) \int_{\Omega_A^{RUC}} w_{A,k}(\mathbf{r}) \int_{\Omega_A^{RUC}} \left[\tilde{\underline{G}}_{in}(\mathbf{r}, \mathbf{r}'|\varphi) + \tilde{\underline{G}}_{out}(\mathbf{r}, \mathbf{r}'|\varphi) \right] \\ \cdot \tilde{\mathbf{J}}_{A,j}(\mathbf{r}') d\mathbf{r}' d\mathbf{r} = -x_{D,i}(\varphi) \int_{\Omega_A^{RUC}} w_{A,k}(\mathbf{r}) \\ \times \int_{\Omega_{D_i}} \tilde{\underline{G}}_{out}(\mathbf{r}, \mathbf{r}'|\varphi) \cdot \tilde{\mathbf{J}}_{D,i}(\mathbf{r}') d\mathbf{r}' d\mathbf{r} \quad \forall k. \end{aligned} \quad (2.123)$$

Then, one can obtain entry (j, i) of $\tilde{\mathcal{L}}$, which corresponds to $x_{A,j}^{D_i}(\varphi)$, solving

$$\sum_j Z_{k,j}^{(1)}(\varphi) x_{A,j}^{D_i}(\varphi) = -Z_{k,i}^{(2)}(\varphi) \quad \forall k \quad (2.124)$$

with

$$\begin{aligned} Z_{k,j}^{(1)} = \int_{\Omega_A^{RUC}} w_{A,k}(\mathbf{r}) \int_{\Omega_A^{RUC}} \left[\tilde{\underline{G}}_{in}(\mathbf{r}, \mathbf{r}'|\varphi) + \tilde{\underline{G}}_{out}(\mathbf{r}, \mathbf{r}'|\varphi) \right] \\ \cdot \tilde{\mathbf{J}}_{A,j}(\mathbf{r}') d\mathbf{r}' d\mathbf{r} \end{aligned} \quad (2.125)$$

and

$$Z_{k,i}^{(2)} = \int_{\Omega_A^{RUC}} w_{A,k}(\mathbf{r}) \int_{\Omega_{D_i}} \tilde{\underline{G}}_{out}(\mathbf{r}, \mathbf{r}'|\varphi) \cdot \tilde{\mathbf{J}}_{D,i}(\mathbf{r}') d\mathbf{r}' d\mathbf{r}. \quad (2.126)$$

Synthetic Green's Function

The problem of computing the response of the infinite array can also be related to the problem of computing a Synthetic Green's Function (SGF) [140]. Let's consider a delta-source situated on point $\mathbf{r}'$ and oriented along

the direction $\hat{\mathbf{a}}_s$. The fields induced by this source in presence of the infinite array ($\mathbf{f}_\infty^\delta$) are the sum of two contributions : the fields directly emitted by the source and the fields scattered by the infinite array:

$$\mathbf{f}_\infty^\delta(\mathbf{r}) = \underline{\underline{G}}_{out}(\mathbf{r}, \mathbf{r}') \cdot \hat{\mathbf{a}}_s + \int_{\Omega_A} \underline{\underline{G}}_{out}(\mathbf{r}, \mathbf{r}'') \cdot \mathbf{J}_A^\delta(\mathbf{r}'') d\mathbf{r}'' \quad (2.127)$$

with $\mathbf{J}_A^\delta$ the currents induced on the surface of the infinite array due to the delta-source. Using Equation (2.104), one can obtain:

$$\mathbf{f}_\infty^\delta(\mathbf{r}) = \left[\underline{\underline{G}}_{out}(\mathbf{r}, \mathbf{r}') + \int_{\Omega_A} \underline{\underline{G}}_{out}(\mathbf{r}, \mathbf{r}'') \cdot \underline{\underline{\mathcal{L}}}(\mathbf{r}'', \mathbf{r}') d\mathbf{r}'' \right] \cdot \hat{\mathbf{a}}_s \quad (2.128a)$$

$$\equiv \underline{\underline{\mathcal{G}}}_{out}(\mathbf{r}, \mathbf{r}') \cdot \hat{\mathbf{a}}_s \quad (2.128b)$$

with $\underline{\underline{\mathcal{G}}}_{out}(\mathbf{r}, \mathbf{r}')$, the SGF of the periodic array. Using the ASM, the infinite-array problem can be decomposed into quasi-periodic problems:

$$\tilde{\mathbf{f}}_\infty^\delta(\mathbf{r}|\varphi) = \left[\tilde{\underline{\underline{G}}}_{out}(\mathbf{r}, \mathbf{r}'|\varphi) \right. \quad (2.129a)$$

$$\left. + \int_{\Omega_{RUC}} \tilde{\underline{\underline{G}}}_{out}(\mathbf{r}, \mathbf{r}''|\varphi) \cdot \tilde{\underline{\underline{\mathcal{L}}}}(\mathbf{r}'', \mathbf{r}'|\varphi) d\mathbf{r}'' \right] \cdot \hat{\mathbf{a}}_s$$

$$\equiv \tilde{\underline{\underline{\mathcal{G}}}}_{out}(\mathbf{r}, \mathbf{r}'|\varphi) \cdot \hat{\mathbf{a}}_s. \quad (2.129b)$$

Using the SGF, the boundary conditions on the surface of the defect become

$$\begin{aligned} \hat{\mathbf{n}}(\mathbf{r}) \times \int_{\Omega_D} [\tilde{\underline{\underline{G}}}_{in}(\mathbf{r}, \mathbf{r}'|\varphi) + \tilde{\underline{\underline{G}}}_{out}(\mathbf{r}, \mathbf{r}'|\varphi)] \cdot \tilde{\mathbf{J}}_D(\mathbf{r}'|\varphi) d\mathbf{r}' \\ = -\hat{\mathbf{n}}(\mathbf{r}) \times \tilde{\mathbf{f}}_\infty^I(\mathbf{r}|\varphi) \quad \forall \mathbf{r} \in \Omega_D. \end{aligned} \quad (2.130)$$

Note that if the system is excited by currents distribution $\mathbf{J}_I(\mathbf{r}')$, the corresponding excitation reads:

$$\tilde{\mathbf{f}}_\infty^I(\mathbf{r}|\varphi) = \iiint \tilde{\underline{\underline{G}}}_{out}(\mathbf{r}, \mathbf{r}'|\varphi) \cdot \tilde{\mathbf{J}}_I(\mathbf{r}'|\varphi) d\mathbf{r}'. \quad (2.131)$$

Using the concept of SGF, the boundary conditions can be solved classically. Only the Green's function used has to be adapted. That new Green's function can be computed using any full-wave solver.

2.4.4 Implementation

In this section, we present a discretized version of the SFSS-MoM formulation that can be solved numerically using only MoM impedance matrices.

First, the surfaces of the infinite array and of the defect are discretized using two meshes corresponding to the basis and testing functions. The basis functions will be used as equivalent current sources while boundary conditions will be satisfied on testing functions. Using matrix notations, the tangential fields discontinuity induced on the testing functions of a surface i by the basis functions of surface j can be written:

$$\mathbf{f}_i^j = \underline{\underline{Z}}_{ij} \cdot \mathbf{x}_j \quad (2.132)$$

with $\mathbf{f}_i^j$ a vector containing the coefficients of the tangential fields discontinuity integrated over the testing functions of i , $\mathbf{x}_j$ a vector containing the coefficients multiplying the currents on each basis function of j and $\underline{\underline{Z}}_{ij}$ the impedance matrix. More information about the computation of the entries of $\underline{\underline{Z}}_{ij}$ can be found in Chapter 1, Section 1.2. Depending on the geometry, $\underline{\underline{Z}}_{ij}$ can contain two terms corresponding to the interactions by the inside and the outside if $i = j$ (cf. G_{in} and G_{out} in Section 2.4.3). The periodic structure under quasi-periodic excitation can be treated similarly using the periodic impedance matrix (see Section 2.1.2):

$$\tilde{\mathbf{f}}_i^j(\varphi) = \tilde{\underline{\underline{Z}}}_{ij}(\varphi) \cdot \tilde{\mathbf{x}}_j(\varphi). \quad (2.133)$$

The solution of a scattering problem consists in finding the unknown equivalent currents coefficients $\mathbf{x}_i$ to satisfy the boundary conditions, which read

$$-\mathbf{f}_i^I = \underline{\underline{Z}}_{ii} \cdot \mathbf{x}_i \quad (2.134)$$

with $\mathbf{f}_i^I$ the coefficients of the tangential fields discontinuity induced on testing functions of the surface of i due to the incoming excitation. Inverting the impedance matrix, one obtains the currents:

$$\mathbf{x}_i = -\underline{\underline{Z}}_{ii}^{-1} \cdot \mathbf{f}_i^I. \quad (2.135)$$

Considering the case of the scattering by a defective infinite array, we first compute the infinite array solution. The case of a non-periodic excitation is considered for the sake of generality. The excitation is decomposed into its different Bloch modes using Equation (2.99):

$$\tilde{\mathbf{f}}_A^I(\varphi) = \sum_p \sum_q \mathbf{f}_A^I(p, q) \exp(-j(p\varphi_x + q\varphi_y)) \quad (2.136)$$

with $\mathbf{f}_A^I(p, q)$ the coefficients of the tangential fields discontinuity induced by the excitation on the testing functions of the periodic array contained in unit-cell (p, q) .

For each phase shift φ the equivalent currents on the periodic structure are found using boundary conditions

$$\tilde{\mathbf{x}}_A^I(\varphi) = -\underline{\underline{\tilde{Z}}}_{AA}^{-1}(\varphi) \cdot \tilde{\mathbf{f}}_A^I(\varphi). \quad (2.137)$$

Last, the currents on the periodic array are found after combining all the modes:

$$\mathbf{x}_A^I(p, q) = \frac{1}{(2\pi)^2} \iint_0^{2\pi} \tilde{\mathbf{x}}_A^I(p, q|\varphi) d\varphi \quad (2.138a)$$

$$\simeq \frac{1}{MN} \sum_{m=0}^{M-1} \sum_{n=0}^{N-1} \tilde{\mathbf{x}}_A^I(\varphi_{mn}) \exp(j(p\varphi_{x,m} + q\varphi_{y,n})) \quad (2.138b)$$

with $\mathbf{x}_A^I(p, q)$ the coefficients associated to the currents on basis function in the unit cell (p, q) of the infinite array. When the indices are not indicated, $p = 0$ and $q = 0$ are assumed. To ease the notation, in the following, we will consider that the defect is entirely contained within the reference unit cell. The generalization to any defect only involves one additional phase term. The tangential fields discontinuity on the surface of the defect due to the infinite array solution ($\mathbf{f}_{D,\infty}^I$) becomes:

$$\mathbf{f}_{D,\infty}^I \simeq \mathbf{f}_D^I - \frac{1}{MN} \sum_{m=0}^{M-1} \sum_{n=0}^{N-1} \underline{\underline{\tilde{Z}}}_{DA}(\varphi_{mn}) \cdot \underline{\underline{\tilde{Z}}}_{AA}^{-1}(\varphi_{mn}) \cdot \tilde{\mathbf{f}}_A^I(\varphi_{mn}) \quad (2.139)$$

with $\mathbf{f}_D^I$, the fields discontinuity on the surface of the defect due to the excitation.

Now that we have computed the infinite array solution, we need to compute the set of modes that satisfy the boundary conditions on the surface of the periodic structure when fictitious sources are placed on the surface of the defect. The method is similar to the infinite array simulation except for the excitation, which now consists of the fields produced by the fictitious sources:

$$\tilde{\mathbf{f}}_A^D(\varphi) = \underline{\underline{\tilde{Z}}}_{AD}(\varphi) \cdot \tilde{\mathbf{x}}_D(\varphi). \quad (2.140)$$

If we consider that the defect is not periodic, the double summation in equation (2.99) is reduced to one term.

$$\tilde{\mathbf{x}}_D(\varphi) = \mathbf{x}. \quad (2.141)$$

Additional scatterer

The tangential fields discontinuity induced at the surface of the defect by the fictitious sources is the sum of two contributions, one coming directly

from the fields emitted by the fictitious source, the other coming from the scattering by the infinite structure. It can be written as:

$$\mathbf{f}_D^D \simeq \left[\underline{\underline{Z}}_{DD} - \frac{1}{MN} \right. \quad (2.142a)$$

$$\times \sum_{m,n} \tilde{\underline{\underline{Z}}}_{DA}(\varphi_{mn}) \cdot \tilde{\underline{\underline{Z}}}_{AA}^{-1}(\varphi_{mn}) \cdot \tilde{\underline{\underline{Z}}}_{AD}(\varphi_{mn}) \left. \right] \cdot \mathbf{x}_D$$

$$\equiv \underline{\underline{Z}}_{DD} \cdot \mathbf{x}_D \quad (2.142b)$$

with $\sum_{m,n}$ being a compact representation for the double summation over the discrete set of Bloch modes. Combining this equation with Equation (2.139), we can apply the boundary conditions for the defect. The equivalent currents on the surface of the defect and on the surface of the infinite array due to the excitation become:

$$\mathbf{x}_D = -\underline{\underline{Z}}_{DD}^{-1} \cdot \tilde{\mathbf{f}}_{D,\infty}^I \quad (2.143a)$$

$$\mathbf{x}_A(p, q) = -\frac{1}{MN} \sum_{m,n} \tilde{\underline{\underline{Z}}}_{AA}^{-1}(\varphi_{mn})$$

$$\cdot \left[\tilde{\mathbf{f}}_A^I(\varphi_{mn}) + \tilde{\underline{\underline{Z}}}_{AD}(\varphi_{mn}) \cdot \mathbf{x}_D \right]$$

$$\times \exp(j(p\varphi_{x,m} + q\varphi_{y,n})). \quad (2.143b)$$

These formulas are used in Chapter 3, Section 3.4.1, to study the absorption taking place in a periodic structure when a scattering layer with a different periodicity is added on top.

Missing element

In the case of a missing element, the new constraint consists in the cancellation of the fields scattered by the element (cf. Section 2.4.3), which means that the total equivalent currents on the the surface of the defect have to vanish:

$$\mathbf{x}_A = -\mathbf{x}_D. \quad (2.144)$$

Injecting the results presented previously and denoting the unitary matrix by $\underline{\underline{I}}$, one obtains:

$$\mathbf{x}_D = \left[\underline{\underline{I}} - \frac{1}{MN} \sum_{m,n} \tilde{\underline{\underline{Z}}}_{AA}^{-1}(\varphi_{mn}) \cdot \tilde{\underline{\underline{Z}}}_{AD}(\varphi_{mn}) \right]^{-1}$$

$$\cdot \left[\frac{1}{MN} \sum_{m,n} \tilde{\underline{\underline{Z}}}_{AA}^{-1}(\varphi_{mn}) \cdot \tilde{\mathbf{f}}_A^I(\varphi_{mn}) \right], \quad (2.145)$$

$$\begin{aligned}
\mathbf{x}_A(p, q) = & -\frac{1}{MN} \sum_{m,n} \tilde{\underline{\underline{Z}}}_{AA}^{-1}(\boldsymbol{\varphi}_{mn}) \\
& \cdot \left[\tilde{\mathbf{f}}_A^I(\boldsymbol{\varphi}_{mn}) + \tilde{\underline{\underline{Z}}}_{AD}(\boldsymbol{\varphi}_{mn}) \cdot \mathbf{x}_D \right] \\
& \times \exp(j(p\varphi_{x,m} + q\varphi_{y,n})).
\end{aligned} \tag{2.146}$$

These formulas are used in Chapter 3, Section 3.2.5, to study a periodic structure when half of the scatterers are removed (two scatterers every four unit cells).

2.5 Conclusion

In this Chapter, we tackled the simulation of periodic structures. First, a plane wave based formalism for the computation of the 2D periodic impedance matrix has been presented. This formulation has been optimized for the rapid simulation of densely packed structures provided that the periodic problem has to be solved for many different phase shifts. It is therefore well suited for the simulation of metamaterials and metasurfaces to obtain the response of the structure for many different phase shifts between consecutive unit cells at a given frequency.

Once the simulation of 2D perfectly periodic structures has been made possible, we presented a stacking procedure that can be used to rapidly simulate 3D periodic semi-infinite structures. The stacking procedure can be seen as a post-processing of the impedance matrix through an iterative process. The convergence of the method is better than exponential with respect to the number of iterations, so that accurate results can be obtained in a negligible amount of additional time. Using this technique, surface-bounded phenomena can be studied.

Exploiting the simulation of 3D periodic semi-infinite metamaterials, the eigenmodes of a structure can be computed solving a linear eigenvalue problem. We showed that, contrarily to techniques already available in the literature, the presented technique is both linear and numerically well conditioned, since it does not entail any back-propagation.

Last, we proposed a technique to introduce some defects in the periodicity, such as a missing element or a non-periodic scatterer. In that way, the impact of defects on a periodic structure can be studied.

All these techniques can be seen as a very handful toolbox for the study of bulk and surface properties of periodic structures. Some of them will be used in the next chapter for the characterization of periodic absorbers.

Chapter 3

Characterization of periodic absorbers

There are many applications in which the absorption of electromagnetic fields must be carefully controlled. For example, considering photovoltaic technology, a better absorption of the fields leads to a better efficiency [141]. In [142], a precise control of the absorbing properties of a structure was used to cool down below the ambient temperature a radiative sample exposed to sunlight. For medical applications, the Specific Absorption Rate must be precisely controlled in order either to limit it and avoid a temperature rise inside the body of the patient (see e.g. [143]), or to the contrary, maximize it at a given location within the body (e.g. a tumor) in order to weaken or damage this region [144, 145, 146]. Last, imaging systems working in the infrared and visible spectrum are generally based on bolometers, so that a precise control of the absorbing capabilities of the detectors (selectivity and amplitude of the absorption) can lead to important improvements in the image resolution. For all the applications of this non-exhaustive list, a complete and efficient characterization of the absorption capabilities of a given structure is essential.

Characterizing the way in which a structure can scatter incident fields is facilitated by the fact that Maxwell's equations are linear with respect to the source terms. However, when it comes to absorption, the power dissipated is a quadratic quantity of the fields, such that the superposition principle can no longer be applied to the incident fields. The characterization of absorption may therefore become more complicated and physical insight into the phenomena through which absorption takes place may be partially or totally lost.

In many papers (see e.g. [14, 15, 16]), the quality of a periodic absorber

is assessed by showing its plane wave absorption versus angle of incidence. However, as soon as sources are located in the near field or the periodicity of the absorber becomes too large, this information is not sufficient to fully describe the absorption capabilities of the structure. Moreover, even for far-field excitations and a periodicity smaller than half the wavelength, the absorber may be sensitive to a given polarization of the fields (e.g. circular [147] vs. linear [148]) which cannot be known a-priori.

Another problem in the characterization of an absorbing structure arises at high frequencies (typically, terahertz and above): incident radiation is generally thermal in origin and so is only expected to be partially spatially coherent and in a partial state of polarization on reaching the structure. This non-deterministic behaviour needs be accounted for to provide reliable predictions.

In [30], the authors developed a formalism to efficiently treat the absorption of partially coherent fields. Based on this formalism, they built the Energy Absorption Interferometry (EAI), an experimental technique that allows to fully and efficiently characterize the way a structure can absorb energy [29, 149]. The technique consists of illuminating the sample using two sources whose positions, orientations and relative phase can be controlled. For fixed positions and orientations, the total power absorbed by the sample exhibits fringes when the relative phase is varied, highlighting the correlation between the sources. By measuring and storing the correlation function for various positions and orientations, one can find all the information required to fully characterize the absorption capabilities of the structure.

One of the key points of this formalism is the fact that lossy structures are absorbing energy through independent and orthogonal absorption modes. Any structure can be completely characterized through the shape and amplitude of its natural absorption modes, leading to a compact and intuitive formulation. Among the benefits of the proposed formalism are an easy treatment of partially spatially coherent incident fields, such as those originating from thermal sources, or the possibility to retrieve the absorption modes of a structure from experiments [149], provided that the power dissipated by the structure can be measured e.g. through an increase of its temperature.

In [31, 150], the EAI formalism has been extended to the study of periodic structures with near-field and far-field excitations. It was shown that, imposing the quasi-periodicity of the fields (i.e. periodicity of the fields within a linear phase-shift), the study of the structure can be restrained to a single unit cell (Bloch modes). The Bloch modes characterized by different phase shifts are orthogonal to each other.

This Chapter aims at providing a full derivation of the EAI formalism

and to illustrate it through practical examples. First, the concept of partial spatial coherence and the tools available to treat partially spatially coherent fields are presented and illustrated. Then, the EAI formalism is derived in the general case of non-periodic structures and then specialized to the case of 2D periodic structure. It is shown how the natural absorption modes of a structure can be obtained as the solution of an eigenvalue problem. The limitations of more simple ways of characterizing an absorbing structure—such as the plane wave absorption vs. angle of incidence—are illustrated through a practical example.

In a second part of the Chapter, the EAI formalism is used to characterize two plasmonic absorbers and identify the phenomena through which the absorption takes place. It is shown that, with the knowledge of its absorption mechanisms, the absorption of the incident fields by a periodic structure can be enhanced by one order of magnitude by adding a properly engineered scattering layer.

3.1 Theory of spatial coherence

The concept of partial spatial coherence, while widely used in the community working in optical frequencies, is far less widespread among the electrical engineers. It is mainly due to the fact that, when it comes to antennas, the zone responsible for the emission of the fields corresponds to the feed of the antenna, which is much smaller than the wavelength of operation. As explained in [151], a small emitting volume produces highly correlated fields. In the limit of a discrete port, the fields emitted are fully coherent. Note that, in this Thesis, only spatial coherence will be treated. Indeed, in the limit of infinite measurement time, there is no coupling in the power absorbed by a structure for incident fields whose frequencies differ [30].

A good way to understand a concept is to first set up a problem for which the targeted concept appears as a solution. Consider two antennas A and B located at two different (and known) positions $\mathbf{r}_a$ and $\mathbf{r}_b$ (cf. Figures 3.1(a) and (b)). In one case, the distance between the antennas is comparable to the distance each antenna and the observation point. In the second case, the distance between the antennas is much smaller than the distance from each antenna to the observation point. In both cases, the two antennas are emitting two uncorrelated signals at a fixed frequency. These signals randomly fluctuate over time. The fluctuations happen slowly enough to neglect their impact on the frequency of the emitted signals. The amplitude and phase of the signal emitted by each antenna at time $t_1, t_2, \dots, t_N$ is not known. The fluctuations are rapid enough so that there is no correlation in the signals emitted at different times.

The problem is the following. From the value of the fields at a given

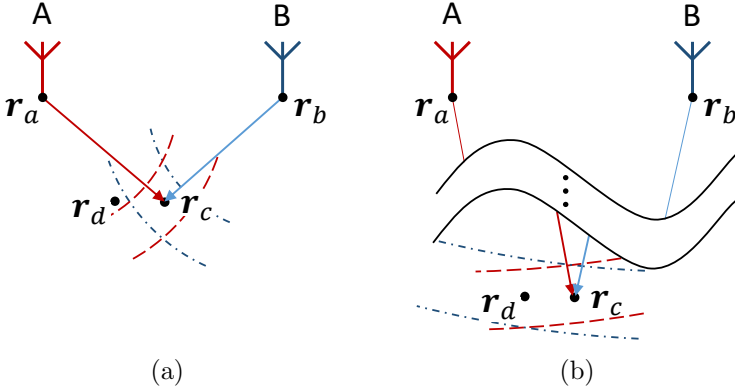


Figure 3.1: Illustration of the concept of spatial coherence. The field are measured in point $\mathbf{r}_c$. From this measure, the fields in $\mathbf{r}_d$ have to be estimated. (a) Poor spatial coherence: the value of the fields in $\mathbf{r}_d$ strongly depend on the relative contribution of antennas A and B in the fields in $\mathbf{r}_c$. Therefore, no information can be retrieved. (b) High spatial coherence: the value of the fields in $\mathbf{r}_d$ is correlated to the fields in $\mathbf{r}_c$ in a very similar way whatever the relative contribution of antennas A and B. A good guess on the fields is possible.

position $\mathbf{r}_c$ at time t_n ($n \in [1, N]$), is it possible to infer the value at a different position $\mathbf{r}_d$? Intuitively, one would say that the evolution of the signals coming from antenna A and antenna B behave in a much similar manner in case (b) of Figure 3.1 than in case (a). Therefore, the value of the fields in position $\mathbf{r}_d$ is much more predictable in case (b) than in case (a): the spatial coherence of the fields is higher in case (b) than in case (a). It illustrates the fact that the spatial coherence of fields increases as these fields propagate away from the sources [151].

This rather qualitative reasoning can be extended to continuous source distribution and quantified using the cross spectral density dyadic $\underline{\underline{W}}(\mathbf{r}, \mathbf{r}')$, defined as [151]

$$\underline{\underline{W}}(\mathbf{r}, \mathbf{r}') = \langle \mathbf{E}_i^*(\mathbf{r}) \mathbf{E}_i(\mathbf{r}') \rangle, \quad (3.1)$$

which describes the state of spatial coherence of the incident fields. Note that the angle bracket denote an ensemble average. In our previous example, it would correspond to the average of the results for many different tests made at times t_n , $n = 1, \dots, N$. Note that $\underline{\underline{W}} = (\mathbf{a}\mathbf{b})$ corresponds to the dyadic product of $\mathbf{a}$ and $\mathbf{b}$ ($W_{ij} = a_i b_j$).

It can be proven that the behaviour of the $\underline{\underline{W}}$ function is governed by the wave equations with respect to the coordinates $\mathbf{r}$ and $\mathbf{r}'$. Therefore,

knowing the value of that function on a reference plane is sufficient to know the value of that function everywhere in space. However, propagating that function through an optical system or within the absorbing structure can be computationally intensive [152]. An elegant way of easing the problem is to decompose the stochastic fields into a sum of non-stochastic (*i.e.* fully deterministic) modes, whose relative amplitudes are completely uncorrelated [152, 153]. Each of these modes can then be treated using classical coherent-field solvers. The corresponding expansion of $\underline{\underline{W}}$ reads

$$\underline{\underline{W}}(\mathbf{r}, \mathbf{r}') = \sum_p \lambda_p \mathbf{E}_p^*(\mathbf{r}) \mathbf{E}_p(\mathbf{r}'), \quad (3.2)$$

with

$$\mathbf{E}_i(\mathbf{r}) = \sum_p a_p \mathbf{E}_p(\mathbf{r}) \quad (3.3)$$

$$\langle a_p^* a_q \rangle = \lambda_p \delta_{pq}, \quad (3.4)$$

where δ_{pq} is the Kronecker delta. The propagation of the correlation function then corresponds to the independent propagation of each mode. The modes and their coefficients can be found solving the eigenvalue equation [153]

$$\iint_S \underline{\underline{W}}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{E}_p^*(\mathbf{r}') d\mathbf{r}' = \lambda_p \mathbf{E}_p(\mathbf{r}). \quad (3.5)$$

In the two-antennas example, the solution of (3.5) would give two modes of given amplitude, one mode corresponding to a given linear combination of the fields emitted by each port (*i.e.* fixed relative amplitude and phase shift).

This concept can be transferred to the spectral domain noticing that the relation between the spatial and the spectral domains is linear. In this Chapter, we will only consider incident fields such that an orthonormal coordinate system $\hat{\mathbf{x}} - \hat{\mathbf{y}} - \hat{\mathbf{z}}$ can be found, the fields coming from $z > 0$. In that case, as seen in Chapter 2, Equation (2.20), the incident fields can be described using a plane wave expansion:

$$\tilde{E}_{i,\text{TE}}(\mathbf{k}_t) = \iint_{-\infty}^{\infty} \mathbf{E}_i(x, y) \cdot \hat{\mathbf{e}}^-(\mathbf{k}_t) \exp(j\mathbf{k}_t \cdot \mathbf{r}) d\mathbf{r} \quad (3.6a)$$

$$\tilde{E}_{i,\text{TM}}(\mathbf{k}_t) = \iint_{-\infty}^{\infty} \mathbf{E}_i(x, y) \cdot \hat{\mathbf{m}}^-(\mathbf{k}_t) \exp(j\mathbf{k}_t \cdot \mathbf{r}) d\mathbf{r} \quad (3.6b)$$

with $\tilde{E}_{i,\text{TE}}$ and $\tilde{E}_{i,\text{TM}}$ the amplitude of the TE and TM waves on the plane $z = 0$.

Applying a Fourier transform to (3.1) and (3.2) with respect to both $\mathbf{r}$ and $\mathbf{r}'$ coordinates and using the orthogonality of the Fourier kernel over the infinite plane, it can be shown that

$$\underline{\underline{\tilde{W}}}(\mathbf{k}_t, \mathbf{k}'_t) = \sum_p \lambda_p \underline{\underline{\tilde{W}}}_p(\mathbf{k}_t, \mathbf{k}'_t) \quad (3.7)$$

$$\underline{\underline{\tilde{W}}}_p(\mathbf{k}_t, \mathbf{k}'_t) = \tilde{\mathbf{E}}_p^*(\mathbf{k}_t) \tilde{\mathbf{E}}_p(\mathbf{k}'_t) \quad (3.8)$$

with

$$\underline{\underline{\tilde{W}}}(\mathbf{k}_t, \mathbf{k}'_t) = \begin{pmatrix} \langle \tilde{E}_{i, \text{TE}}^*(\mathbf{k}_t) \tilde{E}_{i, \text{TE}}(\mathbf{k}'_t) \rangle & \langle \tilde{E}_{i, \text{TE}}^*(\mathbf{k}_t) \tilde{E}_{i, \text{TM}}(\mathbf{k}'_t) \rangle \\ \langle \tilde{E}_{i, \text{TM}}^*(\mathbf{k}_t) \tilde{E}_{i, \text{TE}}(\mathbf{k}'_t) \rangle & \langle \tilde{E}_{i, \text{TM}}^*(\mathbf{k}_t) \tilde{E}_{i, \text{TM}}(\mathbf{k}'_t) \rangle \end{pmatrix}. \quad (3.9)$$

Note that the phase factor of the Fourier transform of $E(\mathbf{r})$ with respect to $\mathbf{r}$ in both (3.1) and (3.2) is $\exp(-j\mathbf{k}_t \cdot \mathbf{r})$ instead of $\exp(j\mathbf{k}_t \cdot \mathbf{r})$ due to the complex conjugation.

The modal decomposition of 3.7 can be used to compute the power dissipated by a structure submitted to partially coherent modes. The fields corresponding to one mode are fully coherent. Thus, the power dissipated by the structure for one mode can be computed using classical techniques. Once the power dissipated by each mode separately has been computed, the total power dissipated will correspond to the sum of the powers dissipated by each mode since they add up incoherently.

This technique is very useful to characterize some fixed incident fields and compute the way they would be absorbed by different structures. In this chapter, we will show that a similar modal decomposition can be done for an absorbing structure. Since there is no coupling between different absorption modes, projecting the correlation function $\underline{\underline{\tilde{W}}}$ directly into these modes provides the total power absorbed by the structure. In that way, it is possible to characterize the some fixed structure can absorb different partially coherent incident fields.

3.2 Power absorption in periodic structures

In the previous section, partially coherent fields were characterized and decomposed into an incoherent sum of fully coherent modes. The modes obtained from the characterization of the fields are much easier to manipulate than the original correlation function, which is a quadratic function of the fields. A similar modal decomposition can be applied to the power dissipation in lossy structures, the power being a quadratic quantity of the fields. This modal decomposition is the subject of this section.

3.2.1 Absorption by non-periodic structures

First consider the general case of a finite lossy structure. The structure is characterized by a given distribution of real permittivity (ε), permeability (μ) and resistivity (ρ). The resistivity accounts for all the loss mechanisms, including dielectric losses. For clarity, magnetic losses are not considered hereafter. However, the extension of the proposed method to such losses is straightforward. We will assume that the incident fields are temporally stationary, as is this generally the case for fields of thermal origin. For a stationary field, the cross-correlation function vanishes over time [154], which is equivalent to saying that the different frequency components of the field are fully incoherent. As a result, the total power absorbed is simply the sum of the power absorbed at each of the different frequencies present, which we may consider separately. An $\exp(j\omega t)$ time dependence of the fields and currents will be implicitly assumed hereafter, with ω the angular frequency for which the structure is characterized.

Let $\mathbf{E}_i(x, y)$ denote the incident electric field over the reference plane $z = 0$ located above the structure. The basis formed using the x , y and z axes is orthonormal and right-handed. For later convenience, we decompose the incident field into vector components resulting from Transverse-Electric (TE) and Transverse-Magnetic (TM) field modes:

$$\tilde{\mathbf{E}}_i(\mathbf{k}_t) = \begin{pmatrix} \tilde{E}_{i,\text{TE}}(\mathbf{k}_t) \\ \tilde{E}_{i,\text{TM}}(\mathbf{k}_t) \end{pmatrix}, \quad (3.10)$$

with $\tilde{E}_{i,\text{TE}}(\mathbf{k}_t)$ or $\tilde{E}_{i,\text{TM}}(\mathbf{k}_t)$ the amplitude of the plane wave whose real transverse wave-vector is $\mathbf{k}_t = (k_x, k_y, 0)$ and whose electric or magnetic fields are transverse to the plane $z = 0$, respectively. The polarization vectors of these plane waves, as defined in Chapter 2, Equation (2.14), are

$$\hat{\mathbf{e}}^-(\mathbf{k}_t) = \frac{1}{k_t} (-k_y \hat{\mathbf{x}} + k_x \hat{\mathbf{y}}) \quad (3.11a)$$

$$\hat{\mathbf{m}}^-(\mathbf{k}_t) = \frac{\gamma}{k_t k_0} (k_x \hat{\mathbf{x}} + k_y \hat{\mathbf{y}} + k_t^2 / \gamma \hat{\mathbf{z}}), \quad (3.11b)$$

with $\mathbf{k} = (k_x, k_y, k_z)$, the wave vector of the plane wave, $k_t = |\mathbf{k}_t|$ is the magnitude of the transverse wave-vector, $k_0 = \omega \sqrt{\varepsilon_0 \mu_0}$ the free-space wave number, $k_z = -\gamma$ since the incident fields are coming from $z > 0$ and $\gamma = \sqrt{(k_0^2 - k_t^2)}$. As a reminder, the square root function were defined such that $\arg(\gamma) \in]-\pi, 0]$. ε_0 and μ_0 are the free space permittivity and permeability respectively.

The transformation from the spatial to the spectral representations takes the form

$$\tilde{E}_{i,\text{TE}}(\mathbf{k}_t) = \iint_{-\infty}^{\infty} \mathbf{E}_i(x, y) \cdot \hat{\mathbf{e}}^-(\mathbf{k}_t) \exp(j\mathbf{k}_t \cdot \mathbf{r}) d\mathbf{r} \quad (3.12a)$$

$$\tilde{E}_{i,\text{TM}}(\mathbf{k}_t) = \iint_{-\infty}^{\infty} \mathbf{E}_i(x, y) \cdot \hat{\mathbf{m}}^-(\mathbf{k}_t) \exp(j\mathbf{k}_t \cdot \mathbf{r}) d\mathbf{r}, \quad (3.12b)$$

with $\mathbf{r} = (x, y, z)$ the position where the incident fields are estimated and E^* the complex conjugate of E . The integration is carried out over the reference plane $z = 0$. The dot product used throughout this paper is defined by $\mathbf{a} \cdot \mathbf{b} = \sum a_i b_i$. In the rest of this paper, integration from $-\infty$ to ∞ should be assumed unless other limits are stated. The reverse operation, which consists of computing the spatial incident fields distribution in the plane $z = 0$ using their plane wave spectrum, is given by

$$\begin{aligned} \mathbf{E}_i(x, y) = & \frac{1}{4\pi^2} \iint \left(\tilde{E}_{i,\text{TE}}(\mathbf{k}_t) \hat{\mathbf{e}}^-(\mathbf{k}_t) \right. \\ & \left. + \tilde{E}_{i,\text{TM}}(\mathbf{k}_t) \hat{\mathbf{m}}^-(\mathbf{k}_t) \right) \exp(-j\mathbf{k}_t \cdot \mathbf{r}) d\mathbf{k}_t. \end{aligned} \quad (3.13)$$

The incident fields are partially coherent, which means that the total fields within the structure correspond to stochastic functions [154]. The mean power density dissipated over time at point $\mathbf{r}$ can be computed using

$$P(\mathbf{r}) = \frac{1}{2} \rho(\mathbf{r}) \langle |\mathbf{K}(\mathbf{r})|^2 \rangle, \quad (3.14)$$

where angle brackets denote an ensemble averaging, which in this case is equivalent to a time-averaging due to the stationarity of the stochastic fields. The vector $\mathbf{K}(\mathbf{r})$ corresponds to the current density in $\mathbf{r}$. The currents being a linear function of the incident fields, they can be decomposed according to the contribution of each incident plane wave:

$$\mathbf{K}(\mathbf{r}) = \frac{1}{4\pi^2} \iint \tilde{\underline{\underline{K}}}^o(\mathbf{r}|\mathbf{k}_t) \cdot \tilde{\mathbf{E}}_i(\mathbf{k}_t) d\mathbf{k}_t, \quad (3.15)$$

with $\tilde{\underline{\underline{K}}}^o(\mathbf{r}|\mathbf{k}_t)$ a tensor describing the currents induced in $\mathbf{r}$ by incident plane waves of transverse wave-vector $\mathbf{k}_t$ and both possible polarizations. If one is interested in the total power absorbed by the structure, substituting (3.15) into (3.14) and integrating over the whole structure, we obtain:

$$\begin{aligned} P = & \frac{1}{32\pi^4} \iiint_{\Omega} \rho(\mathbf{r}) \left\langle \left(\iint \tilde{\underline{\underline{K}}}^o(\mathbf{r}|\mathbf{k}_t) \cdot \tilde{\mathbf{E}}_i(\mathbf{k}_t) d\mathbf{k}_t \right)^* \right. \\ & \left. \cdot \left(\iint \tilde{\underline{\underline{K}}}^o(\mathbf{r}|\mathbf{k}'_t) \cdot \tilde{\mathbf{E}}_i(\mathbf{k}'_t) d\mathbf{k}'_t \right) \right\rangle d\mathbf{r}, \end{aligned} \quad (3.16)$$

with $\iiint_{\Omega}$ the integration over the structure. Rearranging the integration and averaging orders and using the double-dot product

$$\underline{\underline{A}} : \underline{\underline{B}} = \sum_{i,j} A_{i,j} B_{i,j}, \quad (3.17)$$

one can show that

$$\mathbf{a}^* \cdot \underline{\underline{A}} \cdot \mathbf{b} = (\mathbf{a}^* \mathbf{b}) : \underline{\underline{A}}, \quad (3.18)$$

leading to:

$$P = \frac{1}{16\pi^4} \iiint \langle \tilde{\mathbf{E}}_i^*(\mathbf{k}_t) \tilde{\mathbf{E}}_i(\mathbf{k}'_t) \rangle : \underline{\underline{P}}_o(\mathbf{k}_t, \mathbf{k}'_t) d\mathbf{k}_t d\mathbf{k}'_t, \quad (3.19)$$

with

$$\underline{\underline{P}}_o(\mathbf{k}_t, \mathbf{k}'_t) = \frac{1}{2} \iiint_{\Omega} \rho(\mathbf{r}) \tilde{\underline{\underline{K}}}^{o\dagger}(\mathbf{r}|\mathbf{k}_t) \cdot \tilde{\underline{\underline{K}}}^o(\mathbf{r}|\mathbf{k}'_t) d\mathbf{r} \quad (3.20)$$

the cross-spectral power density function, where $\underline{\underline{A}}^T$ and $\underline{\underline{A}}^\dagger$ are used to denote the transpose and Hermitian transpose of dyadic $\underline{\underline{A}}$ respectively. Equation (3.20) is the extension of (6) in [31]. The dyadic notation arises from the treatment of the polarization of the incident fields.

In Equation (3.19), two different contributions can be highlighted: the ensemble average of the incident fields, which is independent of the structure, and $\underline{\underline{P}}_o(\mathbf{k}_t, \mathbf{k}'_t)$, which only depends on the structure. Both factors can be treated separately because the excitation is decoupled from the structure properties and geometry. It is worth noting that if we are only interested in the power absorbed in a given region of the structure (e.g. detectors), then the domain of integration of Equation (3.20) can be limited to that region.

In the case of partially coherent incident fields, one can compute the power dissipated using the modal decomposition of Equation 3.7:

$$P = \frac{1}{16\pi^4} \sum_p \lambda_p \iiint \tilde{\underline{\underline{W}}}_p(\mathbf{k}_t, \mathbf{k}'_t) : \underline{\underline{P}}_o(\mathbf{k}_t, \mathbf{k}'_t) d\mathbf{k}_t d\mathbf{k}'_t. \quad (3.21)$$

3.2.2 Absorption by periodic structures

The computation of the total power absorbed by a structure using formula (3.19) requires the evaluation of several integrals. The first one is a volume integral over the structure. The two others are 2D integrals over the plane wave spectrum of the incident light. In case the structure studied is periodic, these expressions can be simplified. Only the case of 2D periodicity of period d_x and d_y along the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ directions will be considered hereafter. The extension to any other type of periodicity is straightforward.

In this Thesis, the term *quasiperiodic* refers to fields that are periodic within a linear phase shift. Using the Floquet theorem, it can be shown that the currents $\tilde{\underline{\underline{K}}}^o(\mathbf{r}|\mathbf{k}_t)$ induced on a periodic structure by a quasiperiodic excitation share the same quasiperiodicity as the excitation. This means that the product $\rho(\mathbf{r}) \tilde{\underline{\underline{K}}}^{o\dagger}(\mathbf{r}|\mathbf{k}_t) \cdot \tilde{\underline{\underline{K}}}^o(\mathbf{r}|\mathbf{k}'_t) \exp(j(\mathbf{k}'_t - \mathbf{k}_t) \cdot \mathbf{r})$, which appears in

Equation (3.20), is periodic with periods d_x and d_y in the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ directions, respectively, and can be decomposed into a Fourier series

$$\begin{aligned} \underline{\underline{P_o}}(\mathbf{k}_t, \mathbf{k}'_t) &= \frac{1}{2} \iiint_{\Omega} \exp(-j(\mathbf{k}'_t - \mathbf{k}_t) \cdot \mathbf{r}) \\ &\times \sum_{m,n=-\infty}^{\infty} \underline{\underline{Q_{mn}}}(z|\mathbf{k}_t, \mathbf{k}'_t) \exp(-j2\mathbf{k}_t^{mn} \cdot \mathbf{r}) d\mathbf{r} \end{aligned} \quad (3.22)$$

with

$$\begin{aligned} \underline{\underline{Q_{mn}}}(z|\mathbf{k}_t, \mathbf{k}'_t) &= \frac{1}{d_x d_y} \int_{0,0}^{d_x, d_y} \rho(\mathbf{r}) \underline{\underline{\tilde{K}}}^{o\dagger}(\mathbf{r}|\mathbf{k}_t) \cdot \underline{\underline{\tilde{K}}}^o(\mathbf{r}|\mathbf{k}'_t) \\ &\times \exp(j(\mathbf{k}'_t - \mathbf{k}_t) \cdot \mathbf{r}) \exp(j2\mathbf{k}_t^{mn} \cdot \mathbf{r}) dy dx, \end{aligned} \quad (3.23)$$

$$\mathbf{k}_t^{mn} = \left(m \frac{\pi}{d_x}, \quad n \frac{\pi}{d_y}, \quad 0 \right) \quad m, n \in \mathbb{Z}. \quad (3.24)$$

These expressions can be used in Equation (3.21). Changing the order of summation and integration and noticing that $\iint \exp(j\mathbf{k}) d\mathbf{k} = (2\pi)^2 \delta(\mathbf{k})$, the mean power dissipated in each unit cell (3.21) can be expressed as

$$\begin{aligned} P &= \frac{1}{4\pi^2} \sum_p \lambda_p \sum_{m,n} \iint \underline{\underline{\tilde{W}_p}}(\mathbf{k}_t - \mathbf{k}_t^{mn}, \mathbf{k}_t + \mathbf{k}_t^{mn}) \\ &\quad : \underline{\underline{\mathcal{H}_{mn}}}(\mathbf{k}_t) d\mathbf{k}_t, \end{aligned} \quad (3.25)$$

$$\begin{aligned} \underline{\underline{\mathcal{H}_{mn}}}(\mathbf{k}_t) &= \frac{1}{2} \\ &\times \iiint_{\Omega_0} \rho(\mathbf{r}) \underline{\underline{\tilde{K}}}^{o\dagger}(\mathbf{r}|\mathbf{k}_t - \mathbf{k}_t^{mn}) \cdot \underline{\underline{\tilde{K}}}^o(\mathbf{r}|\mathbf{k}_t + \mathbf{k}_t^{mn}) d\mathbf{r}, \end{aligned} \quad (3.26)$$

with Ω_0 the intersection of the volume Ω with the volume of one unit cell of the structure.

As mentioned in [31] for the 2D case, both $\underline{\underline{\tilde{W}_p}}(\mathbf{k}_t - \mathbf{k}_t^{mn}, \mathbf{k}_t + \mathbf{k}_t^{mn})$ and $\underline{\underline{\mathcal{H}_{mn}}}(\mathbf{k}_t)$ tend to vanish for large spatial frequencies or large m, n indices. Therefore the summation and the spectral integration can be truncated. The upper values to consider depend on the distance that the fields have to travel before reaching the structure, and the depth of penetration of the fields inside the structure. Thus, they depend on the geometry of the structure studied.

$\mathbf{k}_t^{mn}$ takes discrete values, so $\underline{\underline{P_o}}(\mathbf{k}_t, \mathbf{k}'_t)$ is also discrete with respect to the difference of spatial frequencies. As underlined in Equation (3.63), a Fourier relation links $\underline{\underline{P_o}}$ to the data collected by the EAI, which is invariant w.r.t.

a shift by an integer number of cells. Therefore, $\underline{\underline{C}}^\Delta(\mathbf{r}^+, \mathbf{r}^-)$ is periodic with respect to $\mathbf{r}^+$. Consequently, to fully characterize a periodic structure, one of the two sources only has to scan one unit-cell, while the other one still has to scan the whole structure, decreasing the total amount of data needed.

A final observation concerns the computation of the power absorbed by an infinite periodic structure excited by a non-periodic source. The non-periodic source can always be decomposed into a sum (or integral) of quasiperiodic sources [155], each quasiperiodic component being periodic within a different phase factor. Then, the total power absorbed by the structure corresponds to the sum of the powers absorbed by the structure for each quasiperiodic component of the source taken separately. Indeed, the interference between different quasiperiodic components of the source will vanish when summing the power dissipated by each unit cell of the infinite structure. However, if one is interested in the power dissipated within one unit cell, the local interference between the different quasiperiodic components of the source does not vanish anymore. Thus, equation (3.21) must be used instead of Equation (3.25). Adapting the phase of the correlation between the different quasiperiodic components of the source, it is possible to compute the power dissipated in any unit-cell (see (3.20)).

Evolution of H_{mn} with height

In most practical cases, the source of the incident fields (e.g: thermal source or optical system) is not touching the absorbing structure. The incident fields then have to propagate to reach the structure. Consider an incident field $\tilde{\mathbf{E}}_i(h|\mathbf{k}_t)$ in $z = h > 0$. In $z = h' < h$, the fields will change according to the factor

$$\tilde{\mathbf{E}}_i(h'|\mathbf{k}_t) = \tilde{\mathbf{E}}_i(h|\mathbf{k}_t) \exp(-j\gamma(h-h')). \quad (3.27)$$

Using Equation (3.19), the dissipated power becomes

$$P = \frac{1}{32\pi^4} \iiint \iiint \left\langle \tilde{\mathbf{E}}_i^*(\mathbf{k}_t) \tilde{\mathbf{E}}_i(\mathbf{k}'_t) \right\rangle \times \exp(-j(\gamma + \gamma')h) : \underline{\underline{P}}_o(\mathbf{k}_t, \mathbf{k}'_t) d\mathbf{k}_t d\mathbf{k}'_t, \quad (3.28)$$

where

$$\gamma' = \sqrt{k_0^2 - k_t'^2}. \quad (3.29)$$

We can then introduce the notation $\underline{\underline{P}}(z|\mathbf{k}_t, \mathbf{k}'_t)$, which corresponds to the cross-correlation function for absorption if the fields are emitted in $z > 0$

$$\underline{\underline{P}}(z|\mathbf{k}_t, \mathbf{k}'_t) = \exp(-j(\gamma + \gamma')z) \underline{\underline{P}}_o(\mathbf{k}_t, \mathbf{k}'_t). \quad (3.30)$$

Similarly, for the periodic case, it leads to

$$\underline{\underline{\mathcal{H}}}_{mn}(z|\mathbf{k}_t + \mathbf{k}_t^{mn}) = \exp(-j(\gamma + \gamma^{mn})z) \underline{\underline{\mathcal{H}}}_{mn}(\mathbf{k}_t + \mathbf{k}_t^{mn}) \quad (3.31)$$

with

$$\gamma^{mn} = \sqrt{k_0^2 - |\mathbf{k}_t + 2\mathbf{k}_t^{mn}|^2}. \quad (3.32)$$

The main consequence of Equations (3.30) and (3.31) is that the amplitude of the correlation function decreases exponentially with respect to the distance between the sources and the structure in the evanescent part of the spectrum. It means that, for a predefined accuracy, the farther the sources, the smaller the domain on which the $\underline{\underline{P}}$ and $\underline{\underline{\mathcal{H}}}_{mn}$ functions need to be actually tabulated.

Moreover, if we consider that $k_t \gg k_0$, we have

$$\gamma = \sqrt{k_0^2 - k_t^2} \simeq \sqrt{-k_t^2} = -jk_t. \quad (3.33)$$

Therefore, for high (m, n) indices,

$$\begin{aligned} & \left| \underline{\underline{\mathcal{H}}}_{mn}(z|\mathbf{k}_t + \mathbf{k}_t^{mn}) \right| \\ &= \left| \exp(-j(\gamma + \gamma^{mn})z) \underline{\underline{\mathcal{H}}}_{mn}(\mathbf{k}_t + \mathbf{k}_t^{mn}) \right| \\ &\simeq \left| \exp(-j\gamma z) \exp(-|2\mathbf{k}_t^{mn} + \mathbf{k}_t|z) \underline{\underline{\mathcal{H}}}_{mn}(\mathbf{k}_t + \mathbf{k}_t^{mn}) \right| \\ &\leq \left| \exp(-(2k_t^{mn} - 2k_0)z) \underline{\underline{\mathcal{H}}}_{mn}(\mathbf{k}_t + \mathbf{k}_t^{mn}) \right| \end{aligned} \quad (3.34)$$

This means that once a certain distance between the sources and the structure is exceeded, the high order correlation functions then decrease exponentially with respect to $\sqrt{m^2 + n^2}$. Consequently, the further the sources are from the absorbing device, the smaller the number of correlations functions required to characterize the absorber's behaviour, and the smaller the domain over which these functions must be tabulated. Since the results from EAI and the correlation function are related by a Fourier transform, it also means that the further the sources are from the structure, the coarser the spatial sampling of the data can be.

3.2.3 Natural absorption modes of a structure

As suggested in [29] and implemented in [156] for a 2D geometry, this mathematical framework can be used to compute the modes through which a structure can absorb power. The total power dissipated by the structure corresponds to the sum of the powers dissipated by each of these modes separately.

Equation (3.19) can be restated within the theory of the linear operators of Hilbert spaces. We consider the functional space made of all the possible

incident field distributions and define the scalar product between two fields distributions $\tilde{\mathbf{E}}_p(\mathbf{k}_t)$ and $\tilde{\mathbf{E}}_q(\mathbf{k}_t)$ as follows:

$$[\mathbf{E}_p|\mathbf{E}_q] = \iint \mathbf{E}_p^\dagger(\mathbf{k}_t) \cdot \mathbf{E}_q(\mathbf{k}_t) d\mathbf{k}_t. \quad (3.35)$$

An unconventional ‘bra-ket’ notation has been used to avoid confusion with $\langle \mathbf{E}_p | \mathbf{E}_q \rangle$, which corresponds to the ensemble average of the fields. For any physical fields distribution, this scalar product is sesquilinear, positive-definite and exhibits a conjugate symmetry (i.e. $[\tilde{\mathbf{E}}_p|\tilde{\mathbf{E}}_q] = [\tilde{\mathbf{E}}_q|\tilde{\mathbf{E}}_p]^*$). In the framework of this Hilbert space, we can define the operator $\hat{P}$ such that

$$[\hat{P}\tilde{\mathbf{E}}] = \frac{1}{16\pi^4} \iint \underline{P}_o(\mathbf{k}_t, \mathbf{k}'_t) \cdot \tilde{\mathbf{E}}(\mathbf{k}'_t) d\mathbf{k}'_t. \quad (3.36)$$

Equation (3.19) then reads

$$P = \langle [\tilde{\mathbf{E}}_i|\hat{P}\tilde{\mathbf{E}}_i] \rangle. \quad (3.37)$$

Equation (3.37) can be extended to the case of partially coherent fields using the modal decomposition of the fields (3.7):

$$P = \sum_p \lambda_p [\tilde{\mathbf{E}}_p|\hat{P}\tilde{\mathbf{E}}_p] \quad (3.38)$$

Another possibility is to compute the natural absorption modes of the structure. Using the definition of $\underline{P}_o$ in (3.20), it can be shown that the operator $\hat{P}$ is Hermitian, so that its eigenvalues Λ_α are real and the corresponding eigenvectors $\mathcal{E}_\alpha(\mathbf{k}_t)$ are orthogonal. From a physical point of view, one of the main consequences is that the power dissipated by any incident field $\tilde{\mathbf{E}}_i(\mathbf{k}_t)$ is

$$P = \sum_\alpha \Lambda_\alpha \left| [\mathcal{E}_\alpha|\tilde{\mathbf{E}}_i] \right|^2, \quad (3.39)$$

with $|a|$ the magnitude of a . Therefore, the power is always real-valued, as required by physical law. Moreover, from a mathematical point of view, it means that a simple orthogonal projection of the incident fields on the different modes is required to obtain the total power absorbed. Therefore, once all the modes with a non-negligible eigenvalue are known, the exact projection of the incident fields into these modes does not require any knowledge about the other modes. This is convenient in the sense that only the incident fields are required, and not the total fields (incident and reflected), as it is generally the case with mode-matching techniques (see e.g. [157] or [158]). In the latter case, since the total field is required, the knowledge about all the modes is required to obtain exact results.

Last, for finite structures, it can be shown that the $\hat{P}$ operator is Hilbert-Schmidt and therefore compact. It means that the number of modes whose contribution to absorption is not negligible is finite. Moreover, in the case of structures that are small with respect to the wavelength of operation, this number is generally small.

From a numerical point of view, the $\hat{P}$ operator has to be discretized to compute these modes through an eigenvector decomposition. It can also be proven that, in the case of a periodic structure, each absorption mode is only composed of Floquet modes characterized by a common phase shift between consecutive unit cells. Therefore, the absorption modes of a periodic structure for a given phase shift can be computed by simulating just one unit cell with a periodic solver and the appropriate periodic boundary conditions. This results in a naturally discretized $\hat{P}$ operator, such that the numerical solution of the problem is straightforward.

As mentioned previously, only the modes whose contribution to absorption is non-negligible need to be kept, resulting in a significant reduction in the amount of data that must be stored. The data required to fully characterize the absorption by non-periodic structures reduces from a 4D function to a compact set of 2D functions corresponding to the absorption modes $\mathcal{E}_\alpha(\mathbf{k}_t)$ for $\alpha = 1, 2, \dots$ and $\mathbf{k}_t \in \mathbb{R}^2$. For periodic structures, a discrete set of discrete functions has to be stored for each possible phase shift between consecutive unit cells. That data can be reorganized into a discrete set of 2D functions, where each function is defined over the first Brillouin zone. Generally, both sets for periodic and non-periodic structures are small if the structure or its unit cell are not large with respect to the wavelength of the incident fields.

Absorption in a structure through its natural modes

Once the natural absorption modes of a structure have been computed, as mentioned previously, the power absorbed by a structure excited by partially coherent fields can be computed without resorting to the modal decomposition of the fields proposed in Section 3.1.

Expanding Equation (3.39), the total absorbed power for any coherent excitation becomes

$$P = \sum_{\alpha} \Lambda_{\alpha} \iint \mathcal{E}_{\alpha}^{\dagger}(\mathbf{k}_t) \cdot \tilde{\mathbf{E}}_i(\mathbf{k}_t) d\mathbf{k}_t \iint \tilde{\mathbf{E}}_i^{\dagger}(\mathbf{k}'_t) \cdot \mathcal{E}_{\alpha}(\mathbf{k}'_t) d\mathbf{k}'_t. \quad (3.40)$$

Rearranging this expression and noticing that a partially coherent excitation can be rephrased as a sum of coherent excitations that are orthogonal to each other, it can be shown that the total power absorbed by a structure

when it is illuminated by partially coherent fields is

$$P = \sum_{\alpha} \Lambda_{\alpha} \iiint \mathcal{E}_{\alpha}^{\dagger}(\mathbf{k}_t) \cdot \underline{\tilde{W}}(\mathbf{k}_t, \mathbf{k}'_t) \cdot \mathcal{E}_{\alpha}(\mathbf{k}'_t) d\mathbf{k}_t d\mathbf{k}'_t. \quad (3.41)$$

In compact notation, this becomes

$$P = \sum_{\alpha} \Lambda_{\alpha} [\mathcal{E}_{\alpha} | \hat{W} \mathcal{E}_{\alpha}]. \quad (3.42)$$

Notice the resemblance between (3.42) and (3.38). Modes $\mathcal{E}_{\alpha}$ and $\tilde{\mathbf{E}}_p$ are obtained using an eigenvalue decomposition of the operators $\hat{P}$ and $\hat{W}$, respectively. One can see that, provided that this eigenvalue decomposition has been performed for at least one of the two operators, the partially coherent nature of the fields can be handled using either (3.21) or (3.41). If one wants to study the way in which given partially coherent fields can be absorbed by any structure, the eigenvalue decomposition of the incident fields, which is independent from the structure, can be performed once and the power absorbed by each structure computed using (3.21), while if one is interested in the way a given structure can absorb any partially coherent incident fields, it is more interesting to compute the absorption modes of the structure, which are independent from the incident fields, and apply (3.41) to compute the power absorbed for each excitation.

3.2.4 Application of EAI formalism to a lossy periodic structure

To illustrate the formalism presented so far, we computed the $\underline{\mathcal{H}}_{mn}$ functions for a periodic structure mimicking the typical design of room-temperature bolometers [159]. The structure consists of a squared lattice of gold nanospheres used as an absorbing layer deposited on a suspended membrane made of silicon nitride (Si_3N_4). The membrane is 200 nm thick and the radius of the spheres is 100 nm. The spacing between two consecutive spheres is 200 nm. We positioned the spheres 5 nm above the surface of the layer to avoid some numerical issues. However, this distance being smaller than $1/100^{\text{th}}$ of the wavelength, it has a negligible impact on the final results. The free-space wavelength of the incident fields is 750 nm, which corresponds to a maximum of absorption for a 100 nm free-standing single golden sphere [160]. Plasmonic effects of gold at that frequency are taken into account by using a negative value for the real part of the permittivity, while losses mechanisms are taken into account adding a negative imaginary part to the permittivity. At this wavelength, the complex relative permittivity of gold

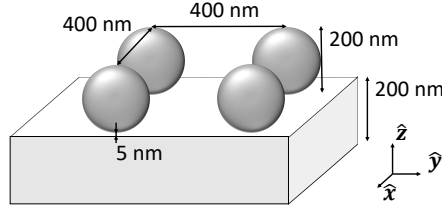


Figure 3.2: Structure used for the simulations: an infinite array of golden nanospheres deposited on a suspended membrane.

is $\varepsilon_r = -21.2 - j1.56$ [161] and the permittivity of the suspended membrane is $\varepsilon_r = 4$. The structure can be seen in Figure 3.2. The $z = 0$ plane coincides with the top of the spheres.

First, we computed $\underline{\mathcal{H}}_{mn}(\mathbf{k}_t)$ using (3.26). The results can be seen in Figure 3.3 for different m, n and different entries of the matrix. The first two graphs having purely real values, their phase is not displayed. The log-magnitude of the field is shown for better readability.

First we consider Fig. 3.3(a). Two circles centered on $k_x = k_y = 0$ are visible. The inner one corresponds to the limit of the visibility angle. Inside that circle, modes are propagative in free space while outside, modes are evanescent. The $\underline{\mathcal{H}}_{00}(\mathbf{k}_t)$ function has to vanish when approaching this circle from the inside, as the power carried by the incident plane wave is vanishing for grazing incidence. The second circle corresponds to a leaky surface mode of the structure (see for example [162] and references therein). Most of the other noticeable inhomogeneities correspond to the replicas of these circles into other Brillouin zones [163].

Looking at Fig. 3.3(b), we can observe similar circles. Interestingly, the wave vector of the surface leaky wave is slightly different for TM or TE excitations ($1.5k_0$ vs. $1.7k_0$, respectively), corresponding to the fact that there exist two different surface leaky waves. The central square is due to the excitation of this TM leaky wave through its harmonics, while the others inhomogeneities in the visible region are due to the excitation of the TE leaky wave.

The graph (c) in Fig. 3.3 clearly exhibits the features associated with the visibility limit and the two leaky surface waves. In addition, some straight lines for which the coupling between TE and TM modes vanishes appear due to the symmetries of the structure. Finally, in graph (e), we can see that the circles are centered on $k_y = \pm 0.9375k_0$. The reciprocal lattice vectors for a periodicity of 400 nm corresponding to $2 \times 0.9375k_0$, it is coherent with the expected results.

We also computed the natural absorption modes of the structure and

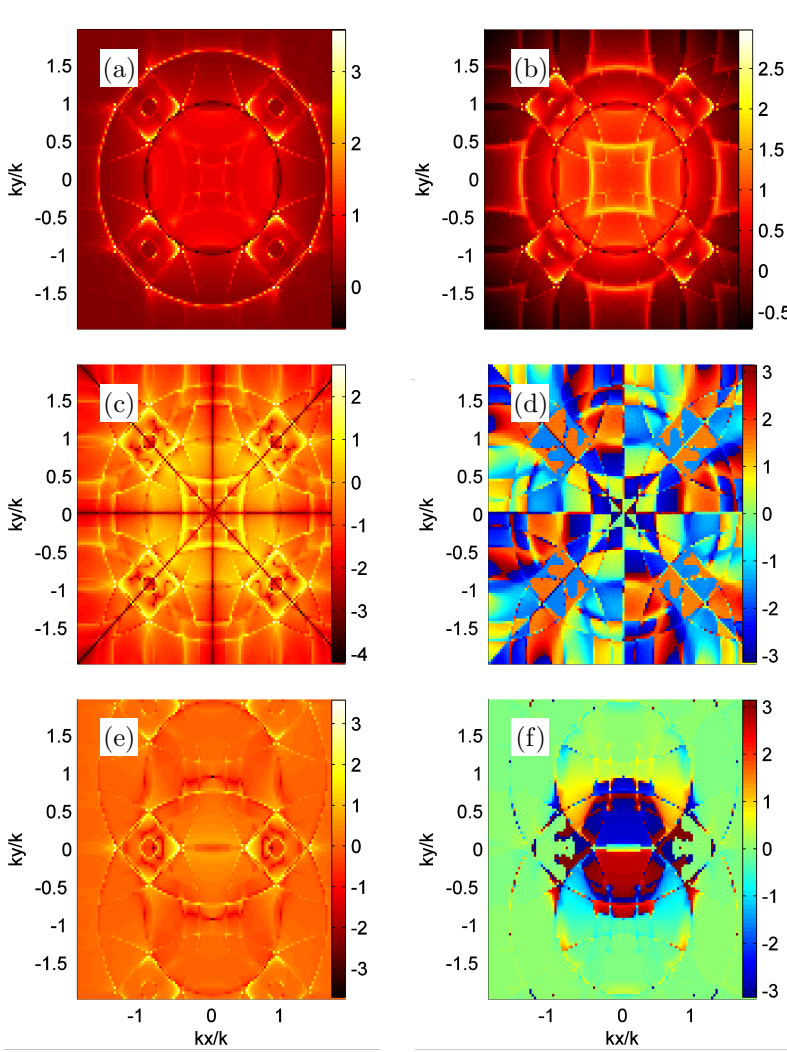


Figure 3.3: Amplitude ($\log_{10}(|\underline{\mathcal{H}}_{mn}|)$) and phase of the $\underline{\mathcal{H}}_{mn}$ functions. (a) to (d): $\underline{\mathcal{H}}_{00}$ function. (a,b): Norm of entry (a) (1,1) and (b) (2,2) corresponding to the absorption of TE and TM waves, respectively. (c,d): Norm and phase of the entry (1,2) corresponding to the coupling between TE and TM waves. (e,f): Norm and phase of the entry (1,1) of $\underline{\mathcal{H}}_{01}$, which corresponds to the coupling between TE waves of transverse wave-vectors $\mathbf{k}_t \pm \mathbf{k}_t^{01}$.

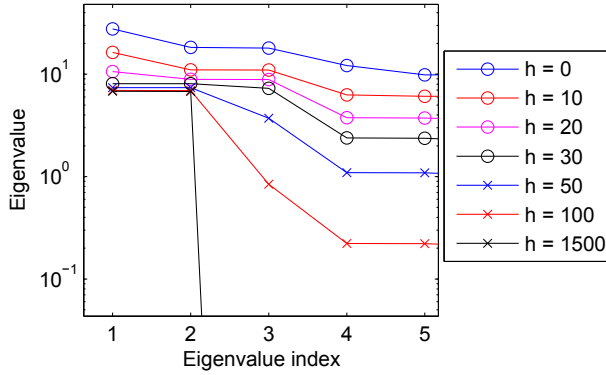


Figure 3.4: Eigenvalues associated to the absorption modes of the structure. The eigenmodes have been computed for different distances between the sources and the structure. The distance is in nm.

their corresponding eigenvalues for periodic excitations with no phase shift between consecutive unit cells. The eigenvalues were computed for different distances between the reference plane and the absorbing structure. The results can be seen in Figure 3.4. We observe that the closer the sources are to the structure, the higher is the number of different modes through which the structure can absorb energy. It is consistent if we consider that evanescent modes can transport energy if there is some reflection on the surface of the structure, but that the amplitude of these modes will decrease over the distance separating the reference plane and the structure. Further, we see that, as the distance of the sources from the observer increases, the far-field solution is eventually recovered. Note that such an increase in the absorption by a structure when going from far-field to near-field is a well-established phenomenon (see *e.g.* [10, 164] and references therein).

As a final illustration of the technique, we consider the following example. The structure simulated here above is illuminated by an incident plane wave which is partially polarized into TE mode. This plane wave is split into two parts of equal amplitudes and one of the two beams goes through a TE polarizer. The incident fields are not perfectly single-frequency and are therefore characterized by a finite coherence length, which is supposed to be much larger than the typical dimensions of one unit-cell of the structure under study. The two beams follow paths with different lengths before reaching the structure, so that the amplitude of the two waves is not perfectly coherent. The non-polarized wave reaching the structure is characterized by a

transverse wave vector $\mathbf{k}_t^{(1)} = (-\pi/d_x, 0, 0)$ and the polarized beam is characterized by the transverse wave vector $\mathbf{k}_t^{(2)} = (\pi/d_x, 0, 0)$. These two wave vectors correspond to an identical phase shift between consecutive unit cells, so that the power absorbed due to one mode depends on the amplitude of the other mode. We want to compute the way in which this excitation can be absorbed by the structure.

First, the fields exciting the structure can be characterized using the spectral cross-correlation function $\underline{\underline{W}}(\mathbf{k}_t, \mathbf{k}_t')$. The excitation consisting of only two plane waves, we have

$$\underline{\underline{W}}(\mathbf{k}_t^{(1)}, \mathbf{k}_t^{(1)}) = \begin{pmatrix} 0.5 + A & 0 \\ 0 & 0.5 - A \end{pmatrix} \quad (3.43a)$$

$$\underline{\underline{W}}(\mathbf{k}_t^{(1)}, \mathbf{k}_t^{(2)}) = \begin{pmatrix} B(0.5 + A) & 0 \\ 0 & 0 \end{pmatrix} \quad (3.43b)$$

$$\underline{\underline{W}}(\mathbf{k}_t^{(2)}, \mathbf{k}_t^{(2)}) = \begin{pmatrix} 0.5 + A & 0 \\ 0 & 0 \end{pmatrix}, \quad (3.43c)$$

with A a real factor that describes the degree of polarization of the incident wave and B a complex factor that depends on the coherence length of the excitation and the path difference of the two beams. $A = 0.5$ corresponds to a perfectly polarized TE wave while $A = 0$ corresponds to a perfectly unpolarized wave. If the two beams travel over the same distance, they arrive in phase and $B = 1$. But if the lengths the two beams travel are different, B becomes complex and its amplitude tends to decrease, until the difference between paths is much bigger than the coherence length, in which case $|B| \rightarrow 0$. Using (3.9), it can be shown that $\underline{\underline{W}}(\mathbf{k}_t^{(2)}, \mathbf{k}_t^{(1)}) = \underline{\underline{W}}(\mathbf{k}_t^{(1)}, \mathbf{k}_t^{(2)})^\dagger$.

We can decompose this correlation matrix into a sum of properly weighted perfectly coherent modes (cf. Equation (3.2)), which provides

$$\begin{aligned} \tilde{\mathbf{E}}_1(\mathbf{k}_t^{(1)}) &= \begin{pmatrix} 0 \\ 1 \end{pmatrix} & \tilde{\mathbf{E}}_1(\mathbf{k}_t^{(2)}) &= \begin{pmatrix} 0 \\ 0 \end{pmatrix} \\ \lambda_1 &= 0.5 - A \end{aligned} \quad (3.44a)$$

$$\begin{aligned} \tilde{\mathbf{E}}_2(\mathbf{k}_t^{(1)}) &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} & \tilde{\mathbf{E}}_2(\mathbf{k}_t^{(2)}) &= \frac{1}{\sqrt{2}} \begin{pmatrix} B/|B| \\ 0 \end{pmatrix} \\ \lambda_2 &= (1 + |B|)(0.5 + A) \end{aligned} \quad (3.44b)$$

$$\begin{aligned} \tilde{\mathbf{E}}_3(\mathbf{k}_t^{(1)}) &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} & \tilde{\mathbf{E}}_3(\mathbf{k}_t^{(2)}) &= \frac{1}{\sqrt{2}} \begin{pmatrix} -B/|B| \\ 0 \end{pmatrix} \end{aligned}$$

$$\lambda_3 = (1 - |B|)(0.5 + A) \quad (3.44c)$$

From a physical point of view, we can see that the partially coherent excitation can be decomposed into

1. a TM plane wave of transverse wave vector $\mathbf{k}_t^{(1)}$,
2. two TE plane waves of equal amplitude and transverse vectors $\mathbf{k}_t^{(1)}$ and $\mathbf{k}_t^{(2)}$,
3. two TE plane waves of opposite amplitude and transverse vectors $\mathbf{k}_t^{(1)}$ and $\mathbf{k}_t^{(2)}$.

The amplitude of each of these modes depends on the degree of coherence of the incident fields. The total power dissipated inside the structure corresponds to the sum of the powers absorbed by each of these modes separately.

Alternatively, the natural modes of absorption of the structure can be determined using the data computed previously (see Fig. 3.3). Since we are dealing with a far-field excitation, only four terms have to be taken into account in Equation (3.39), whose associated fields distribution are a linear combination of the four propagating Floquet modes associated to the π phase shift between consecutive unit cells.

In matrix form, the eigenmodes and the associated eigenvalues are

$$\begin{aligned} \boldsymbol{\varepsilon}_1(\mathbf{k}_t^{(1)}) &= \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \end{pmatrix} & \boldsymbol{\varepsilon}_1(\mathbf{k}_t^{(2)}) &= \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ -1 \end{pmatrix} \\ \Lambda_1 &= 5.75 \end{aligned} \quad (3.45a)$$

$$\begin{aligned} \boldsymbol{\varepsilon}_2(\mathbf{k}_t^{(1)}) &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} & \boldsymbol{\varepsilon}_2(\mathbf{k}_t^{(2)}) &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ \Lambda_2 &= 3.58 \end{aligned} \quad (3.45b)$$

$$\begin{aligned} \boldsymbol{\varepsilon}_3(\mathbf{k}_t^{(1)}) &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} & \boldsymbol{\varepsilon}_3(\mathbf{k}_t^{(2)}) &= \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 0 \end{pmatrix} \\ \Lambda_3 &= 2.74 \end{aligned} \quad (3.45c)$$

$$\begin{aligned} \boldsymbol{\varepsilon}_4(\mathbf{k}_t^{(1)}) &= \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \end{pmatrix} & \boldsymbol{\varepsilon}_4(\mathbf{k}_t^{(2)}) &= \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ \Lambda_4 &= 2.06. \end{aligned} \quad (3.45d)$$

Applying Equation (3.41), we can see that the total power dissipated by each unit cell of the structure (in arbitrary units) is

$$\begin{aligned}
 P = & 3.905(0.5 - A) \\
 & + (1 + |B|)(0.5 + A) \\
 & \times \left(0.895|1 + B/|B||^2 + 0.685|1 - B/|B||^2 \right) \\
 & + (1 - |B|)(0.5 + A) \\
 & \times \left(0.895|1 - B/|B||^2 + 0.685|1 + B/|B||^2 \right).
 \end{aligned} \tag{3.46}$$

As we can see, provided that the absorbing modes of the structure are known, a closed form expression of the power absorbed by the structure when it is illuminated by any partially coherent fields can be easily derived.

3.2.5 From EAI formalism to plane wave absorption

Often in the literature, the efficiency of periodic absorbing metasurfaces is assessed by showing the reflection coefficient of incident plane waves on the surface (see e.g. [14, 15, 16]). One could argue that the latter approach is much simpler and therefore preferable. However, this description proves to provide reliable results only for far field excitation of the metasurface, since the periodicity of the latter is smaller than half a wavelength and the coupling between the two polarizations considered is negligible. That simplified approach fails as soon as one of the three hypotheses (far field, subwavelength periodicity and negligible cross-polarization) is broken, as shown in this section.

This phenomenon can be explained starting from Equation (3.34):

$$|\tilde{\mathcal{H}}_{mn}(\mathbf{k}_t|h=h_0)| \leq |\tilde{\mathcal{H}}_{mn}(\mathbf{k}_t|h=0^+)| \exp(2(k_0 - k_t^{mn})h_0). \tag{3.47}$$

For a periodicity smaller than half the wavelength ($a, b < \lambda/2$), the term $k_0 - k_t^{mn} < 0$ for any pair $(m, n) \neq (0, 0)$. It means that, as soon as the source is in the far-field ($h_0 \rightarrow \infty$), the coupling between the incident plane waves vanishes and the $\underline{P}_0$ operator becomes diagonal. In that case, the absorption modes of the structure, which correspond to the eigenvectors of $\underline{P}_0$, become the different plane waves themselves and the absorption capabilities of the structure are fully described through the way in which each plane wave can be absorbed independently from the others (provided that the coupling between the two polarizations is negligible).

However, if the periodicity of the structure is bigger than $\lambda/2$ or if the absorption capabilities of the structure are studied for near-field excitation, the $\underline{P}_0$ operator is no longer diagonal and the formalism described previously must be used to characterize the absorbing structure.

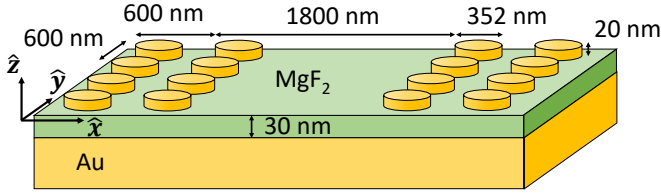


Figure 3.5: Modified version of the absorber of [14]. It is made of a periodic arrangement of gold patches deposited on a MgF_2 spacer and backed with a gold ground plane. The periodicities along the $\hat{x}$ and $\hat{y}$ directions are 2400 and 600 nm respectively.

This statement is illustrated using the structure in Figure 3.5, which consists in a slightly modified version of the absorber described in [14]. The original structure is made of gold patches whose periodicities are 600 nm in the $\hat{x}$ and $\hat{y}$ directions. These patches are deposited on a dielectric spacer made of MgF_2 whose relative permittivity is 1.9. The whole layer is backed by an infinite ground plane made of gold. To compute the relative permittivity of the gold, we used the same model as in the original paper, i.e. a Drude model with parameters that have been modified in order to take into account the poor quality of the deposited gold layers [14]. The free space wavelength of the excitation is chosen to be 1550 nm, which gives a relative permittivity of $-124.639 - 12.6455j$. In the original paper [14], this absorber exhibits a nearly perfect absorption of propagating incident plane waves over a wide range of angles of incidence. The absorption is due to the resonant mode that takes place in the dielectric spacer under each patch.

In order to decrease the absorption to approximately 50%, we removed two patches every four unit-cells. The structure studied can be seen in Fig. 3.5. The periodicity in the $\hat{x}$ direction of the modified structure is greater than one half of the wavelength. For any fixed phase shift between consecutive unit cells, at least 6 different Floquet modes can propagate in the air (three TE and three TM plane waves), leading to a possible coupling in the absorption between them.

The normalized absorption of an incident plane-wave as a function of its transverse wave vector $\mathbf{k}_t = (0, k_x)$ has been plotted in Fig. 3.6(a) and (b). For most of the angles of incidence, the structure absorbs between 40% and 70% of the incident power. In Fig. 3.6(c) and (d), the first six absorption modes associated to the incident plane waves are shown. Due to the symmetries of the structure and the excitation, it can be shown that the

coupling between TE and TM modes vanishes. For ease of interpretation, TE and TM modes have been drawn in separate figures (plot (c) and (d), respectively). Plots (c) and (d) clearly indicate that using a proper combination of propagative incident plane waves, the power absorbed can rise to more than 90% or drop below 5%.

Let's illustrate this with an example. Imagine that the structure is illuminated by a plane wave whose intensity is I_1 . The power absorbed by the structure by unit area I_{tot} will lie somewhere between $0.4I_1$ and $0.7I_1$. In order to increase the total power absorbed, the structure is illuminate by two other plane waves with intensities of the same order of magnitude I_2 and I_3 . Looking at plots (a) and (b), one would expect the total dissipation by the structure to be $I_{tot} \simeq 0.5(I_1 + I_2 + I_3)$. However, if the combination of waves corresponds to the non-dissipative mode, the total power intensity absorbed by the structure I_{tot} will drop to few percent of the total incident power, so that $I_{tot} = 0.05(I_1 + I_2 + I_3) < 0.4I_1$. The incident power has increased, but the total absorption by the structure has decreased. Indeed, using the proper combination of plane waves, the fields can be focused into the places where there is no golden patch, leading to a low absorption.

In this case, Since the unit cell is bigger than half a wavelength, the EAI formalism is required to fully characterize the absorbing structure, even for far-field excitations. Note that even for unit cells smaller than half a wavelength, the EAI formalism may be required if the symmetries of the structure and/or the excitation is broken, so that cross-polarization coupling may happen.

3.3 Experimental characterization of an absorber

All the derivations and results obtained so far where considering a plane wave decomposition of the incident fields. That kind of decomposition is very handy from a numerical and analytical points of view. However, when it comes to the experimental characterization of an absorbing structure, the production of single propagative or evanescent plane way is a tricky task. Therefore, it would be beneficial to extend the EAI formalism to any kind of exciting sources and describe some way to retrieve the absorption modes of a structure from experiments.

The Energy Absorption Interferometry (EAI) is an experimental technique used to characterize the way a structure can absorb electromagnetic fields [29]. The Structure Under Test (SUT) is illuminated with two sources whose positions and relative phases can be controlled. Recording the powers absorbed for different positions and phase difference between sources, it

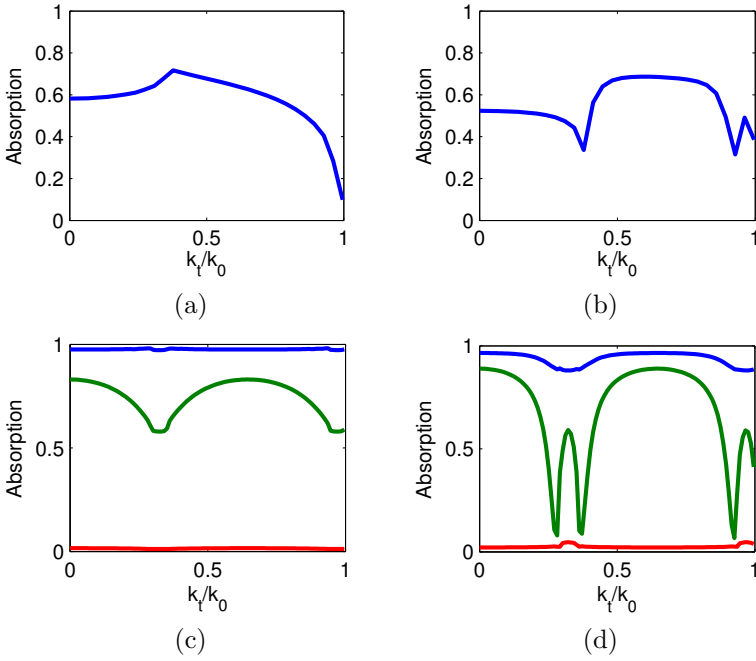


Figure 3.6: Far-field characterization of the structure illustrated in Fig. 3.5. (a),(b): Plane wave absorption of the structure. (c),(d): Three first natural absorption modes of the structure for different phase-shifts between consecutive unit cells.

is possible to predict the power absorbed by the structure when illuminated by any incident fields.

EAI can be implemented experimentally in many different ways, and over a wide range of wavelengths [165], depending on the way the SUT is illuminated (e.g: near-field probes, far field radiators) and the way the power absorbed by the sample is recorded. The power absorption can be measured directly when the SUT corresponds to photovoltaics and electromagnetic detectors, while, for other types of structures, the absorption can be recorded through the local temperature rise using bolometric calorimeters. A first demonstration has been reported at submillimeter-wavelengths [149].

Consider two horizontal point sources corresponding to oscillating currents $\mathbf{J}_1(\mathbf{r})$ and $\mathbf{J}_2(\mathbf{r})$ such that

$$\mathbf{J}_1(\mathbf{r}) = \mathbf{p}_1 \delta(\mathbf{r}_1) \quad (3.48a)$$

$$\mathbf{J}_2(\mathbf{r}) = \mathbf{p}_2 \delta(\mathbf{r}_2), \quad (3.48b)$$

where δ is the Dirac delta function in 3D and $\mathbf{p} = (p_x; p_y; 0)$ where p_i is the component of the current density in the direction i . The positions of the two sources, $\mathbf{r}_1$ and $\mathbf{r}_2$ respectively, both lie in the plane $z = h > 0$. The relative phase, positions and orientations of the sources can be controlled. The SUT is located in the half-space $z < 0$. This experimental arrangement is illustrated in Figure 3.7.

We can define the matrix $\underline{\underline{S}}(\mathbf{k}_t|\mathbf{r})$ that provides the fields generated on the $z = 0$ plane by a point source located at $\mathbf{r}$:

$$\tilde{\mathbf{E}}_i(\mathbf{k}_t) \equiv \underline{\underline{S}}(\mathbf{k}_t|\mathbf{r}) \cdot \mathbf{p}. \quad (3.49)$$

As a translation of the source in the spatial domain induces a linear phase slope in the angular spectrum domain, (3.49) simplifies to

$$\tilde{\mathbf{E}}_i(\mathbf{k}_t) = \exp(j\mathbf{k}_t \cdot \mathbf{r}) \underline{\underline{S}}_o(\mathbf{k}_t) \cdot \mathbf{p}. \quad (3.50)$$

$\underline{\underline{S}}_o(\mathbf{k}_t)$ is the plane-wave decomposition of the fields over $z = 0$ produced by a source located at $\mathbf{r} = (0, 0, h)$. The different dyadic components are given by

$$S_{o,11} = \frac{\eta k_y k_0}{2\gamma k_t} \exp(-j\gamma h) \quad (3.51)$$

$$S_{o,12} = -\frac{\eta k_x k_0}{2\gamma k_t} \exp(-j\gamma h) \quad (3.52)$$

$$S_{o,21} = -\frac{\eta k_x}{2k_t} \exp(-j\gamma h) \quad (3.53)$$

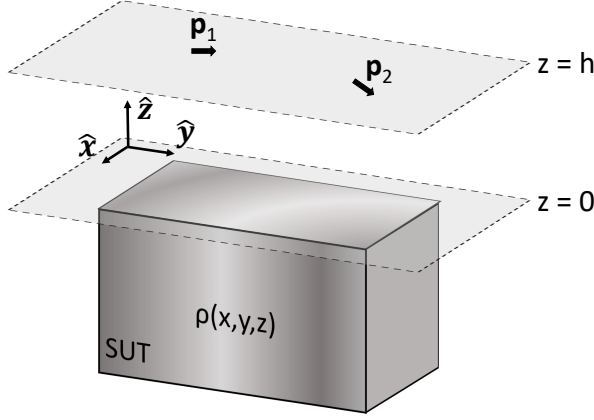


Figure 3.7: Setup of the EAI. The two sources $\mathbf{p}_1$ and $\mathbf{p}_2$ are located in the $z = h$ plane. The power absorbed by the structure located in the half-space $z < 0$ is recorded for each positions, orientations and relative phases of the two source.

$$S_{o,22} = -\frac{\eta k_y}{2k_t} \exp(-j\gamma h), \quad (3.54)$$

with $\eta = \sqrt{\mu_0/\varepsilon_0}$ the free space impedance. Substituting (3.50) into (3.15), the currents induced in the structure by a point source $\mathbf{p}_1$ in $\mathbf{r}_1$ become

$$\begin{aligned} \mathbf{K}(\mathbf{r}) &\equiv \underline{\underline{K}}^p(\mathbf{r}|\mathbf{r}_1) \cdot \mathbf{p}_1 \\ &= \frac{1}{4\pi^2} \iint \exp(j\mathbf{k}_t \cdot \mathbf{r}_1) \tilde{\underline{\underline{K}}}^0(\mathbf{r}|\mathbf{k}_t) \cdot \underline{\underline{S}}_o(\mathbf{k}_t) \cdot \mathbf{p}_1 d\mathbf{k}_t. \end{aligned} \quad (3.55)$$

If the system is excited by two different point sources $\mathbf{p}_1$ and $\mathbf{p}_2$ located at positions $\mathbf{r}_1$ and $\mathbf{r}_2$ respectively, whose relative phase shift is ϕ , starting from Equation (3.14) and using (3.55), the total power absorbed is

$$\begin{aligned} P &= \frac{1}{2} \iiint_{\Omega} \rho(\mathbf{r}) \left(\underline{\underline{K}}^p(\mathbf{r}|\mathbf{r}_1) \cdot \mathbf{p}_1 + \underline{\underline{K}}^p(\mathbf{r}|\mathbf{r}_2) \cdot \mathbf{p}_2 e^{j\phi} \right) \\ &\quad \cdot \left(\underline{\underline{K}}^p(\mathbf{r}|\mathbf{r}_1) \cdot \mathbf{p}_1 + \underline{\underline{K}}^p(\mathbf{r}|\mathbf{r}_2) \cdot \mathbf{p}_2 e^{j\phi} \right) d\mathbf{r}. \end{aligned} \quad (3.56)$$

Distributing the product, separating the integrals and using the same compact notation as in Equation (3.19), the total power absorbed reads:

$$P = \frac{1}{2} (\alpha_{11} + \alpha_{22} + 2\alpha_{12} \cos(\phi - \beta_{12})), \quad (3.57)$$

with

$$\alpha_{pq} e^{j\beta_{pq}} = \iiint_{\Omega} \left(\rho(\mathbf{r}) \underline{\underline{K}}^{p\dagger}(\mathbf{r}|\mathbf{r}_p) \cdot \underline{\underline{K}}^p(\mathbf{r}|\mathbf{r}_q) \right) d\mathbf{r} : \left(\mathbf{p}_p^* \mathbf{p}_q \right) \quad (3.58)$$

and $\beta_{pp} = 0$. The correlation function between the point sources thus corresponds to

$$\underline{\underline{C}}(\mathbf{r}_1, \mathbf{r}_2) = \iiint_{\Omega} \left(\rho(\mathbf{r}) \underline{\underline{K}}^{p\dagger}(\mathbf{r}|\mathbf{r}_1) \cdot \underline{\underline{K}}^p(\mathbf{r}|\mathbf{r}_2) \right) d\mathbf{r}. \quad (3.59)$$

Using EAI experiments, the magnitude and phase of $\underline{\underline{C}}(\mathbf{r}_1, \mathbf{r}_2)$ can be obtained varying the relative phase of the sources and measuring the oscillating pattern in the absorption.

The $\underline{\underline{C}}$ function provides relevant information about the typical coherence length within the structure. If the coupling between two sources is non-negligible, it means that the power absorbed by the structure will strongly depend on the relative phase of the sources. To the opposite, if the correlation between the two sources is negligible ($\underline{\underline{C}}(\mathbf{r}, \mathbf{r}') \rightarrow \underline{\underline{0}}$), it means that the powers absorbed from each source will add incoherently and will therefore be insensitive to their relative phase.

Relation between EAI and spectral correlation

In this section, we will provide a link between the data that can be gathered using EAI, which corresponds to the spatial correlation function $\underline{\underline{C}}(\mathbf{r}_1, \mathbf{r}_2)$, and the cross-spectral power density function $\underline{\underline{P}}_o(\mathbf{k}_t, \mathbf{k}'_t)$ as defined in (3.20). Starting from the definition of the correlation function given in (3.59), we can use (3.55) to obtain

$$\begin{aligned} \underline{\underline{C}}(\mathbf{r}_1, \mathbf{r}_2) = & \frac{1}{(2\pi)^4} \iiint \iiint \exp(-j\mathbf{k}_t \cdot \mathbf{r}_1) \underline{\underline{S}}_o^\dagger(\mathbf{k}_t) \\ & \cdot \left[\iiint_{\Omega} \rho(\mathbf{r}) \underline{\underline{K}}^{\circ\dagger}(\mathbf{r}|\mathbf{k}_t) \cdot \underline{\underline{K}}^o(\mathbf{r}|\mathbf{k}'_t) d\mathbf{r} \right] \\ & \cdot \underline{\underline{S}}_o(\mathbf{k}'_t) \exp(j\mathbf{k}'_t \cdot \mathbf{r}_2) d\mathbf{k}'_t d\mathbf{k}_t. \end{aligned} \quad (3.60)$$

This expression can be simplified using (3.20) and the change of variables

$$\begin{aligned} \mathbf{r}^+ &= \frac{\mathbf{r}_2 + \mathbf{r}_1}{2} & \mathbf{r}^- &= \mathbf{r}_1 - \mathbf{r}_2 \\ \mathbf{k}_t^+ &= \frac{\mathbf{k}_t + \mathbf{k}'_t}{2} & \mathbf{k}_t^- &= \mathbf{k}_t - \mathbf{k}'_t, \end{aligned} \quad (3.61)$$

to yield

$$\begin{aligned} \underline{\underline{C}}(\mathbf{r}_1, \mathbf{r}_2) = & \frac{1}{8\pi^4} \iiint \iiint \underline{\underline{S}}_o^\dagger(\mathbf{k}_t) \cdot \underline{\underline{P}}_o(\mathbf{k}_t, \mathbf{k}'_t) \cdot \underline{\underline{S}}_o(\mathbf{k}'_t) \\ & \times \exp(-j\mathbf{k}_t^- \cdot \mathbf{r}^+) \exp(-j\mathbf{k}_t^+ \cdot \mathbf{r}^-) d\mathbf{k}_t^+ d\mathbf{k}_t^-. \end{aligned} \quad (3.62)$$

As in [31], we can notice that Equation (3.62) corresponds to a double inverse Fourier transform. Therefore, using the relation between a function and its Fourier transform, we finally obtain

$$\underline{\underline{P_o}}(\mathbf{k}_t, \mathbf{k}'_t) = \frac{1}{2} (\underline{\underline{S_o}}^{-1}(\mathbf{k}_t))^\dagger \cdot \left[\iiint \iiint \underline{\underline{C}}^\Delta(\mathbf{r}^+, \mathbf{r}^-) e^{j(\mathbf{k}_t^- \cdot \mathbf{r}^+ + \mathbf{k}_t^+ \cdot \mathbf{r}^-)} d\mathbf{r}^+ d\mathbf{r}^- \right] \cdot \underline{\underline{S_o}}^{-1}(\mathbf{k}'_t), \quad (3.63)$$

with

$$\underline{\underline{C}}^\Delta(\mathbf{r}^+, \mathbf{r}^-) = \underline{\underline{C}}\left(\mathbf{r}^+ + \frac{\mathbf{r}^-}{2}, \mathbf{r}^+ - \frac{\mathbf{r}^-}{2}\right). \quad (3.64)$$

To summarize the results, if the spatial spectrum of the sources is known (through the matrix $\underline{\underline{S_o}}$), one has to apply a Fourier transform on the measurements to obtain the cross correlation function in the spectral domain.

Generalization to a discrete number of sources

One interesting aspect of the formalism developed here above is that $\underline{\underline{P_0}}$ can be obtained from experiments using the Energy Absorption Interferometry (EAI). “Experiments” can be real experimental setup in a lab [149] or numerical experiments using a commercial or in-house software. However, generally, the number of experiments available is finite. Moreover, sometimes, the number of degrees through which a structure can be excited is limited. For example, it happens when the absorbing structure is placed at the end of an optical system that has a limited number of channels.

Consider a chosen set of sources $\{\hat{\mu}_i\}$ used to characterize a structure. Each element is characterized by its orientation, its position and its radiation pattern. The spectral response of source i is given by $\mathbf{S}_i(\mathbf{k}_t)$ such that, the source i excited with an amplitude μ_i excite the structure with incident fields:

$$\tilde{\mathbf{E}}_{\text{inc}}(\mathbf{k}_t) = \mathbf{S}_i(\mathbf{k}_t) \mu_i \quad (3.65)$$

Generalizing (3.65) to any linear combination of the elementary sources $\hat{\mu}_i$, one obtains

$$\tilde{\mathbf{E}}_{\text{inc}}(\mathbf{k}_t) = \underline{\underline{S}}(\mathbf{k}_t) \cdot \boldsymbol{\mu} \quad (3.66)$$

with $\underline{\underline{S}}$ a matrix whose n^{th} column corresponds to the the spectral content of $\hat{\mu}_n$ and $\boldsymbol{\mu}$ a vector containing the amplitudes of the elementary sources.

Substituting (3.66) into (2.53) and noticing that $(\mathbf{a}\mathbf{b}) : \underline{\underline{c}} = \mathbf{a}^T \cdot \underline{\underline{c}} \cdot \mathbf{b}$ gives

$$P_{\text{tot}} = \boldsymbol{\mu}^\dagger \cdot \underline{\underline{P_\mu}} \cdot \boldsymbol{\mu} \quad (3.67)$$

with

$$\underline{\underline{P}}_\mu = \frac{1}{16\pi^4} \iiint \underline{\underline{S}}^\dagger(\mathbf{k}_t) \cdot \underline{\underline{P}}_0(\mathbf{k}_t, \mathbf{k}'_t) \cdot \underline{\underline{S}}(\mathbf{k}'_t) d\mathbf{k}_t d\mathbf{k}'_t. \quad (3.68)$$

It can be seen that the modes $\mathcal{E}_\mu$, which are corresponding to the limited set of sources, will be different from the modes $\mathcal{E}_a$, which are obtained for a continuous spectrum of sources. Indeed, (3.68) does not correspond to a change of basis. Therefore, the shape and value of the modes are modified. The new modes will fit into the new space of possible excitations. This property can be very useful to study the absorption capabilities of the structure when the possible excitations are constrained in some way (e.g. limited number of antennas, limited aperture, limited number of available channels through an optical system). Moreover, these modes can adapt to the available degrees of freedom, regardless of the correlation that may exist in the excitation produced by these degrees of freedom. For example, two exciting antennas placed close together will produce nearly similar fields, but will be interpreted as two independent degrees of freedom by the new modes. This may result in an improvement in the conditioning of the absorption-based inverse problems [146, 145] when the fields emitted by different possible excitations are strongly correlated.

The change in the intensity and shape of the modes is due to the fact that, when considering a discrete number of sources, the “structure” that is characterized corresponds to the system made of the structure combined with the sources, which can be seen as a bigger structure that includes these sources. For example, considering a non-zero height h at which the sources are located, an air layer is added to the structure. This air layer will act as a low-pass filter, decreasing the relevance of very large wavenumbers. Thus, the response of the structure with the air layer will be different from the response of the structure without the air. Since the structure has changed, so do the modes. Extending this reasoning to the case of discrete sources, it can be shown that the discreteness of the sources is acting as a filtering of the possible excitations, so that the absorption modes of the structure excited by this limited set of sources are different from the absorption modes of the structure excited by arbitrary fields.

However, if the spectral content of the sources used to perform the experiments is known and if a sufficient number of different sources is used, their influence can be removed by inverting (3.68) to obtain the intrinsic response of the structure. More information about this procedure can be found in [31].

3.4 Characterization and design of two periodic absorbers

As explained earlier, the EAI formalism can provide a good insight into the absorption mechanisms that are taking place inside the structure. In this sections, this statement is illustrated through a practical example. First, two different plasmonic absorbers are studied using the different quantities involved in the EAI formalism. Surface modes are identified and their relevant characteristics (wave vector, extinction length, etc.) are determined from numerical “experiments”. Using the previously acquired knowledge, a scattering layer with a controlled periodicity is used to improve the absorption by one order of magnitude.

Identification of the absorption mechanisms in two plasmonic structures.

In order to identify the absorption mechanisms that can be exploited to improve absorption, we studied two different kinds of plasmonic absorbers using the EAI for an excitation whose free space wavelength is 488 nm. The first one consists of a silver slab, which is known to support plasmonic surface waves at the frequency studied. The wave vector associated with that surface wave is slightly evanescent in free space [166] and can propagate over long distances due to the relatively good conductivity of silver at this frequency. The second absorber corresponds to the structure described in [167], but arranged in a square lattice (the original structure is hexagonal). It is made of parallel free-standing silver rods whose dimensions can be seen in Figure 3.8. As explained in [167], these rods exhibit very localized resonance when they are excited in the near-field. For that reason, they were primarily used for imaging purposes. However, since the response of the structure is very local, each wire is expected to support its own independent absorption mode, so that the number of modes available per unit area is expected to be very high [168]. Moreover, these absorption modes are expected to be localized, since they are based on the individual resonance of the rods rather than collective oscillations within the array.

Both structures are characterized for sources located 10 nm away and whose free-space wavelength is 488 nm. The frequency has been chosen to match that of [167] so that the wire medium exhibits a resonant behaviour. At this frequency, the relative permittivity of silver is $\varepsilon_r = -9.121 - 0.304j$ [169].

First, we computed the $\underline{C}$ function for both absorbers (cf. Section 3.3). The results can be seen in Figs. 3.9 and 3.10 for sources located 10 and 25 nm above the surface.

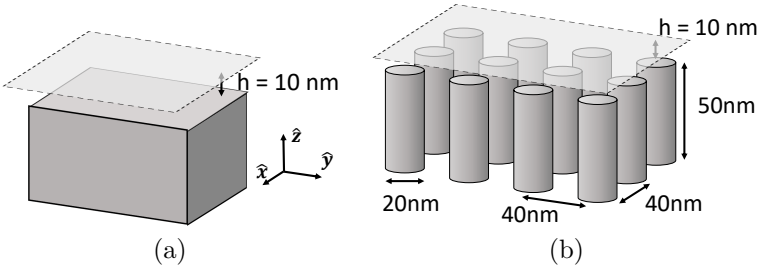


Figure 3.8: The two absorbers studied for near-field sources ($h = 10$ nm). (a) The silver slab. (b) The wire medium described in [167]. The gray plane is the reference plane from which the exciting field is emitted (plane wave or dipole).

First, we analyse Fig. 3.9. In the top graphs, a sharp high spot corresponding to the free-space singularity can be seen for sources that are close together. On top of it, we can notice a very long-range absorbing mechanism that corresponds to the surface plasmon of the interface. The observed wavelength of the oscillations in the correlation function is 460 nm, which is slightly shorter than the free-space wavelength of the excitation. It is in excellent agreement with the theory [166] which predicts that the transverse wave vector of surface plasmons at that frequency is $(1.06 - 2.2 \cdot 10^{-3}j)k_0$, corresponding to a wavelength of 460.5 nm. Since the shape of this mode can be matched with slightly evanescent incident waves, this absorption mechanism is still limited to the near-field, but not the very near-field. Due to the small losses in silver at this frequency (cf. small imaginary part of the wavenumber of the plasmon), this phenomenon is intrinsically long-range. Any mechanism aiming at an improvement of the absorption should therefore be thought on large scales due to the large coherence length within the structure.

Looking at the phase, the $\underline{C}$ function being real is a direct consequence of the translational symmetry of the interface.

Now, looking at the results for the wire medium in Fig. 3.10, we can first see that the response is much more localized. Indeed, the coupling between two sources vanishes very rapidly. It is due to the fact that the dipoles tend to excite very localized resonant modes along the wires [167]. This behaviour clearly appears for sources located 10 nm and 25 nm away from the surface. However, in the first case, in addition to the general pattern, variations within unit-cells can be distinguished, while the response in the second case is much smoother. It is due to the exponential term in (3.47). Indeed, in the first case, it is equal to 0.27, while in the second case it drops

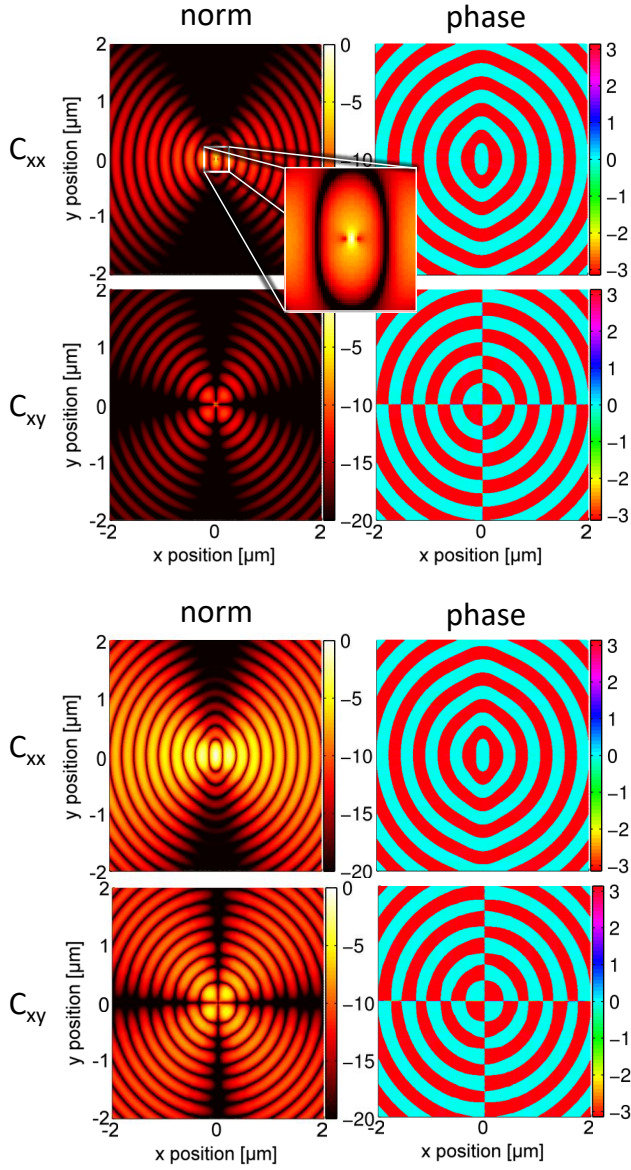


Figure 3.9: $\underline{\underline{C}}(\mathbf{r}, \mathbf{r}')$ of the silver-air interface as a function of $\mathbf{r}'$ for sources located 10 nm (top) and 25 nm (bottom) above the surface and $\mathbf{r} \cdot \hat{\mathbf{x}} = \mathbf{r} \cdot \hat{\mathbf{y}} = 0$. Each experiment (top and bottom) has been normalized separately according to the maximum value of $\underline{\underline{C}}$. The magnitude is provided in dB scale.

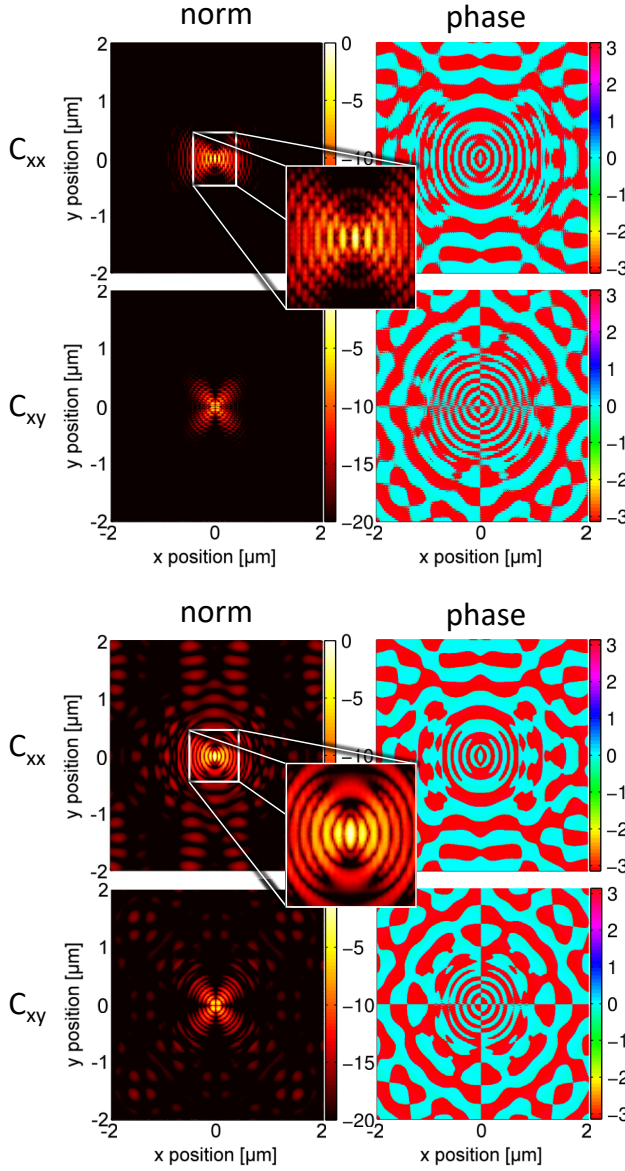


Figure 3.10: $\underline{\underline{C}}(\mathbf{r}, \mathbf{r}')$ of the wire medium [167] as a function of $\mathbf{r}'$ for sources located 10 nm (top) and 25 nm (bottom) above the surface and $\mathbf{r}$ shifted 20 nm away from the center of one rod in the $\hat{\mathbf{x}}$ direction. Each experiment (top and bottom) has been normalized separately according to the maximum value of $\underline{\underline{C}}$. The magnitude is provided in dB scale.

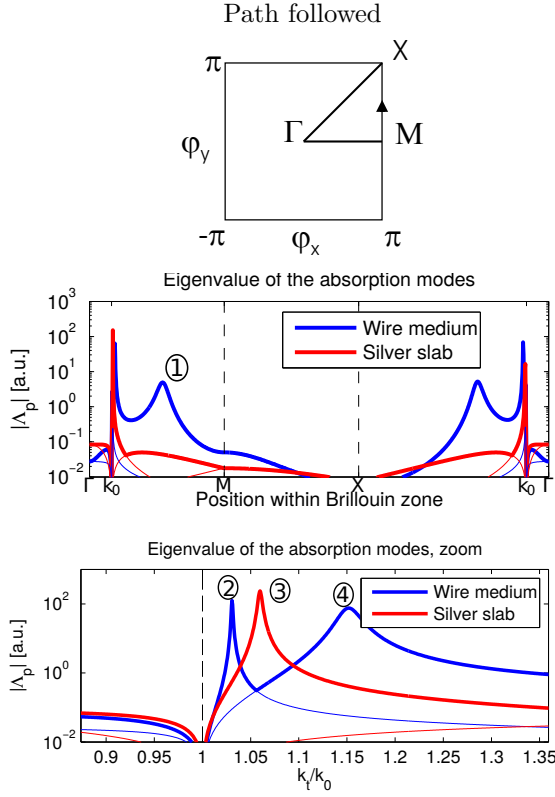


Figure 3.11: Evolution of the amplitude of the absorption modes Λ_a within the first Brillouin zone. The curve corresponding to the maximum value of Λ_a for each phase-shift is thicker than the others for better readability.

down to 0.038. Therefore, as explained previously, the microstructure is still clearly visible in the first case while in the second case, the structure is essentially seen as being homogeneous by the incident fields.

Last, we can see some minor ripples appearing in bottom graphs. These ripples have a longer wavelength than the hot spot in the center of the figure and correspond to some long range surface wave that are also excited by the sources, but whose contribution to the absorption is less important. The geometrical pattern exhibited by this long-range mode is unusual for classical surface modes. It is due to simulation artifacts. Indeed, in order to simulate the presence of two sources in front of a periodic structure the Array Scanning Method has been used, with 250×250 phase shifts [113]. It means that the surface was not excited by dipoles, but rather by arrays of dipoles whose periodicity is $10 \mu\text{m}$. Since the second mode is a long-range mode, as will be shown later in Table 3.1, interferences due to the spurious replicas of the sources are appearing, leading to the strange pattern that can be seen in the bottom graphs of Figure 3.10. However, increasing the number of phase-shifts considered in the ASM, which corresponds to an increase of the periodicity of the sources, or adding losses in the air in order to reduce the propagation length of the mode, the typical length of the oscillation due to this long-range surface mode is preserved while the geometrical pattern exhibited converges toward a more classical shape of long-range surface mode.

In order to further investigate about these modes, the eigenvalues Λ_a of (3.39) have been plotted for various phase shifts between consecutive unit cells. The phase shifts have been chosen along a path in the first Brillouin zone of the lattice, which can be seen in Fig. 3.11, together with the results. The peaks that can be seen correspond to eigenmodes of the structure with associated transverse wave vector and attenuation constant [170]. These modes correspond to poles in the complex plane for the fields excitation. Since the total power absorbed is a quadratic quantity of the fields, the peaks correspond to Lorentzian curves whose position and thickness provides information about the complex wavenumber of the modes.

First, for the wire medium, we can see a large but moderately high bump for transverse wave-vectors that are around $3k_0$ (peak 1). This bump correspond to the main near-field absorption mechanism of the wire medium. Its large width is the signature of a localized mode (high attenuation constant), while its position correspond to the wavelength of the oscillations that can be seen in Fig. 3.10. Zooming around the visibility limits, we can see one high and narrow peak for the silver slab (peak 3), and two slightly smaller narrow peaks for the wire medium (peaks 2 and 4). The former corresponds to the surface plasmon of the silver slab, while the latters correspond to the long-range absorption mechanisms that can be seen in the bottom graphs

mode index	wave number
1	$3.315 - 0.269j$
2	$1.031 - 8.66 \cdot 10^{-4}j$
3	$1.060 - 0.0023j$
4	$1.152 - 0.014j$

Table 3.1: Wave number of the surface modes corresponding to the peaks in Fig. 3.11.

of Figure 3.10.

The presence of two surface modes whose transverse wave-number is that close, with one mode that is more lossy than the other, is typical for thin-films supporting surface waves [171, 172]. Each interface between the wire medium and the air is supporting a surface mode with an associated penetration depth of the field that is bigger than the actual thickness of the layer. Since the fields of the two surface modes are overlapping, an hybridization of the modes occurs. On one hand, the symmetric coupling of the two surface waves corresponds to a mode for which the field inside the wire medium is increased (constructive interferences within the wire medium). Therefore, the corresponding modes will be characterized by a higher transverse wavenumber and higher losses (peak 4). On the other hand, the antisymmetric coupling of the surface waves corresponds to a mode for which the fields inside the wire medium are low (destructive interferences within the wire medium), resulting in a lower transverse wavenumber and lower losses (peak 2).

A quantitative analysis of these modes can be performed considering that each peak correspond to a Lorentzian. By determining the position and width of the Lorentzian, the wave number associated to the modes can be found and are displayed in Table 3.1. Comparing the wave number obtained in that way with the theoretical wave number of the surface plasmon of the silver slab [166], it can be seen that the agreement is very good ($1.06 - 0.0023j$ vs. $1.06 - 0.0022j$).

3.4.1 Absorption improvement using a scattering layer

Knowing the response of the silver slab and the wire medium to external excitations, one can try to optimize the absorption of the structure for propagative wavelength, i.e. wavelength whose transverse wavenumber is smaller than k_0 . To do so, a scattering layer made of a periodic grating is added on top of the absorber in order to couple propagative plane waves to the evanescent surface waves.

First, one has to chose between the surface slab and the wire medium.

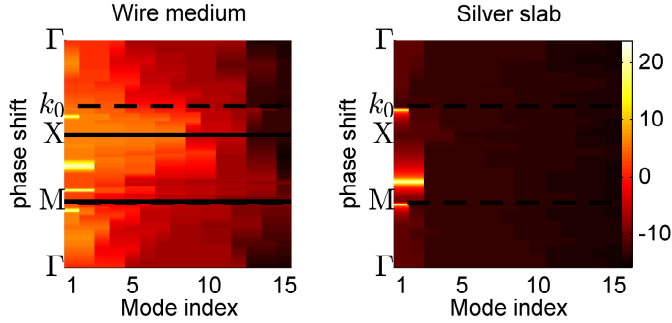


Figure 3.12: Magnitude of the eigenvalue Λ_a of the first 15 eigenmodes for the wire medium and the silver slab. The magnitude is in dB scale.

Roughly speaking, the grating on top the surface will randomly scatter the incident fields wave into each of the available modes, both upward (in the air) and backward (in the silver slab or the wire medium). If the periodicity of the grating is small enough (smaller than $\lambda/2$), only two of these modes are propagative in the air, providing only two degrees of freedom for the system to evacuate the incident energy without dissipating it. Therefore, a higher number of available lossy modes in the wire medium or the silver slab should provide a higher absorption of the incident fields [168, 49].

In order to quantitatively compare the potential absorption that the wire medium and the silver slab can provide, the eigenvalue of the 15 highest absorbing modes within a $240 \times 240 \text{ nm}^2$ unit cell are plotted for the wire medium and the silver slab for a given path within the first Brillouin zone. The path considered is the same as in the previous example (see Fig. 3.11), but with the Brillouin zone which has been reduced due to the expansion of the unit cell. The results can be seen in Fig. 3.12.

It can be clearly seen that the silver slab has a great potential to selectively absorb the fields coming from particular incidence angles, while the wire medium is potentially much more efficient for non-selective absorption. For that reason, the latter will be used as a substrate for the improved absorber.

Next comes the question of the periodicity of the grating. The grating will correspond to silver trenches aligned with the $\hat{y}$ direction and deposited 5 nm above the top of the wires. The trenches are 40 nm wide and 20 nm thick. In order to simplify the problem, the trench is replicated every n wires, n being an integer. The geometry is drawn in Fig. 3.13 for $n = 3$.

Increasing the periodicity of the unit cell using a grating will introduce spectral folding, so that absorption modes of the wire medium that cannot

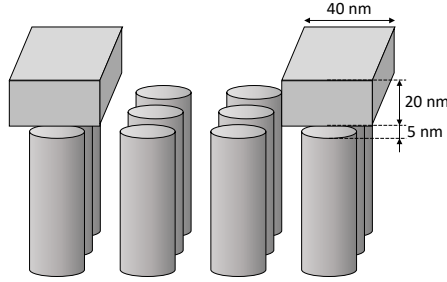
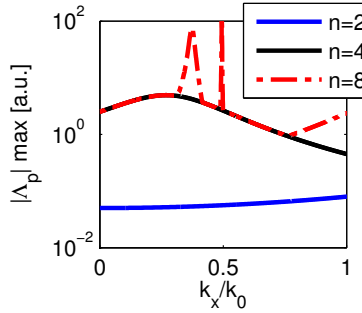


Figure 3.13: Geometry of the improved absorber.

Figure 3.14: Maximum absorption mode to which propagating plane wave can couple if the period of the scatterer is n times that of the underlying absorber in the $\hat{x}$ direction.

couple with propagating plane waves can be folded back into the visible zone and therefore be coupled to the incident waves through the periodic grating. In figure 3.14, the maximum value Λ_a with which incident waves of transverse wave vector $\mathbf{k}_t = (k_x, 0)$ can couple for a periodicity of the grating $n = 2, 4$ and 8 has been drawn. It can be seen that for $n = 4$, the localized mode (peak 1) has been folded back into the visible zone, while for $n = 8$ sharp peaks corresponding to the spectral folding of the long-range surface modes of the wire medium (peaks 2 and 4 in Fig. 3.11(c)) are also visible.

A full wave study of the plane wave absorption with the periodic grating of periodicity $n = 2, 4$ and 8 has also been performed and its results are displayed in Fig 3.15. First of all, it can be noticed that an unexpected increase in the absorption is happening for TE waves near grazing incidence for $n = 2$. Since half of the power is absorbed within the grating, it corresponds to some hybrid absorption mode that appears due to the cou-

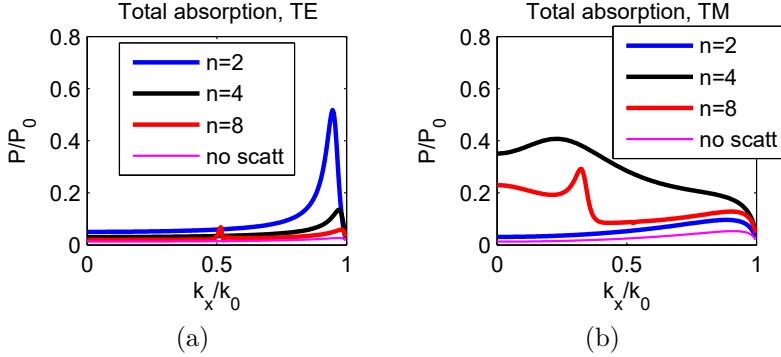


Figure 3.15: Normalized absorption of incident TE (a) and TM (b) plane waves by the improved absorber for varying incidence angles and periodicities of the grating.

pling between the wire medium and the grating. This behaviour cannot be predicted from the sole study of the wire medium. A small glitch around $k_x \simeq 0.5 k_0$ can also be noticed for $n = 8$. It corresponds to the coupling between the grating and mode 2 of the wire medium. This effect is much more visible for TM incident waves: looking at the absorption of the TM waves, a strong similarity between the graph 3.14 and the graph 3.15(b) is noticeable. Indeed, for TM waves, most of the absorption is taking place within the wire medium. It means that the grating is scattering the incident fields into the absorption modes of the wire medium. The latter dissipates a non-negligible part of the incident energy. It can be noticed that the dissipation in the case $n = 8$ is lower than in the case $n = 4$. It is probably due to the fact that the scattering cross section of the grating decreases as the trenches are placed farther away. Increasing the covering by the scatterer without modifying the periodicity would probably solve the issue.

3.5 Conclusion

In this section, the characterization of the absorption capabilities of a structure is discussed. It is complicated by the fact that the dissipations within a lossy material is a quadratic quantity of the fields. This characterization is further complicated by the fact that the incident fields may be only partially spatially coherent.

A formalism proposed in [30] was presented here. The idea is to compute the eigenvectors of the dissipation operator. Since this operator is Hermitian, these eigenvectors form an orthonormal basis of the fields that

diagonalize the operator. It means that the total power absorbed by the structure is the sum of the powers absorbed through each mode separately. Projecting the incident fields into this basis, the absorption problem becomes linear with respect to the intensity of each mode, which facilitates the characterization of one structure. One key point of this formalism is that the information required to compute these natural absorption modes can be obtained experimentally provided that one is capable to measure the power dissipated within the structure [149].

It was shown theoretically and numerically that using this approach to characterize periodic structures is essential to provide reliable results when sources are located in the near-field region of the structure, when the periodicity of the structure is bigger than half the wavelength or when the coupling in the absorption between the two possible polarization of the incident fields is not negligible.

The formalism has been applied to two different plasmonic structures in order to identify the absorption mechanisms through which they absorb power. Using this information, it is shown that, simply adding a properly designed scattering layer on top of the structure, absorption within that structure can be enhanced by one order of magnitude.

Chapter 4

The wire medium

In the field of metamaterials, the Wire Medium (WM) has been subject to intense research due to its unique dispersive and anisotropic properties. The WM has been proved to present a hyperbolic dispersion curve [173] for sufficiently conducting wires. Metamaterials with exotic dispersion curves at optical frequency can be realized using plasmonic materials such as silver and gold [174, 175, 167]. The possible exploitations of this property appear in several fields: waveguiding structures [8], subwavelength imaging [167], magnetic field enhancement [4] and improved absorption [176].

In Chapters 1 and 2, we discussed about numerical methods for the full-wave simulation of finite and infinite periodic structures. These techniques can be used to study the WM. However, if full-wave solvers generally provide accurate results, these results are just numbers. Building an intuitive understanding of the phenomena dominating the scattering process may be difficult and require a lot of experience. In order to build an intuitive understanding, simplified models are preferred.

These models are used to derive approximate solutions that provide a meaningful insight. The solutions are relying on hypotheses that may be only valid for a limited range of input parameters. For that reason, it is essential to clearly understand the hypotheses that are made and their implications when building up such models.

In Chapter 3, the absorption capabilities of the WM in the optical part of the spectrum have been highlighted numerically using the EAI. In this chapter, we consider the behaviour of a metallic WM at lower frequencies. Metal at low frequency can be well approximated by a Perfect Electrical Conductor (PEC). First, some models that were already developed in the literature are presented, and their main results are highlighted. These models are generally difficult to manipulate, and it is hard to remove or adapt one of their constitutive hypotheses in order to extend their range of validity.

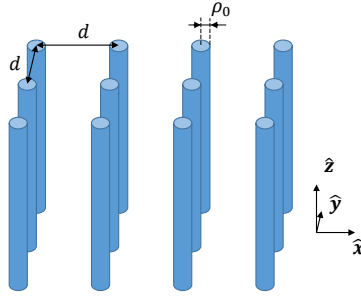


Figure 4.1: Scheme of the wire medium (WM). The periodic PEC structure is embedded in a dielectric of permittivity ε_h .

To circumvent this limit, in a second time, we develop our own model. A special attention is paid to the clear statement of the hypotheses and their consequences. The proposed model is easier to manipulate: hypotheses can be removed at the expense of simplicity in order to extend the validity of the results obtained.

Last, a scalar product is proposed for which the propagating and evanescent modes inside a WM made of PEC wires are naturally orthogonal. This scalar product is also valid for lossless 2D periodic structures that are invariant along the third dimension.

This chapter corresponds to a lead that has been followed in the beginning of the PhD but has not been further investigated due to the lack of time. In order to be exploitable for energy absorption purposes, lossy and plasmonic materials should have been included in the model.

4.1 Definition of the problem

Before describing the existing models, it is useful to set the conventions that will be used throughout this Chapter.

In the following, unless specifically mentioned, we will consider an infinite 2D periodic array of PEC vertical wires embedded in a dielectric medium of permittivity ε_h . The structure is invariant along the $\hat{\mathbf{z}}$ direction and periodic in the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ directions. The position of the center of the wires is $(x_{m,n}, y_{m,n}) = (md, nd)$ with m, n two integers and d the size of the unit cell. ρ_0 is the radius of the wires. A schematic representation can be seen in Figure 4.1.

The main goal of the modeling is to determine the eigenmodes of the structure. Therefore, many different wave-vectors will be considered. $\mathbf{q} =$

(q_x, q_y, q_z) is the homogenized wave-vector, i.e. the vector describing the phase shift observed between consecutive unit-cells. $\mathbf{k} = (k_x, k_y, k_z)$ is the wave-vector of waves in free-space. $\mathbf{q}_t = (q_x, q_y, 0)$ (resp. k_t) is the transverse part of the wave vector $\mathbf{q}$ (resp. $\mathbf{k}_t$). In this Chapter, only real $\mathbf{q}_t$ will be considered.

The corresponding scalar values can be derived: $q = \mathbf{q} \cdot \mathbf{q}$, $k = \mathbf{k} \cdot \mathbf{k}$, $q_t = \mathbf{q}_t \cdot \mathbf{q}_t$ and $k_t = \mathbf{k}_t \cdot \mathbf{k}_t$. k_h is the wave vector in the host medium in which the wires are embedded: $k_h = \omega^2 \varepsilon_h \mu_0$ with ω the angular frequency of the fields and μ_0 the magnetic permeability of free space.

A last note concerns the denomination that will be used for the propagative eigenmodes. TE modes are the modes whose electric field is perpendicular to the direction of the wires (i.e. $\hat{\mathbf{z}}$). TM mode will then correspond to the modes whose magnetic field is perpendicular to the wires. Last, TEM modes are special modes for which both electric and magnetic fields are perpendicular to the wires, whatever is the value of the transverse wave-vector.

4.2 Existing models

As mentioned in the introduction, several models for a WM made of PEC wires have already been proposed in the literature, based on several hypotheses. In this section, these models are described. A special emphasis is put on the hypotheses that are made in these models.

4.2.1 The WM to mimic plasma

Historically, the wire medium has first been used to study electromagnetic waves propagation inside a plasma. The idea was to obtain easily a plasma-like behaviour (free electrons) for tunable frequencies [177].

The formula used to describe the equivalent permittivity of the medium when electromagnetic waves propagate through a plasma is:

$$\varepsilon(\omega) = \left(1 - \frac{\omega_p^2}{\omega(\omega + i\gamma)}\right) \varepsilon_0 \quad (4.1)$$

with ε and ε_0 , the effective permittivities inside the plasma and in free space, ω the angular frequency of the wave considered, ω_p the plasma frequency, i.e. the frequency for which the oscillation of the plasma charges becomes resonant, and γ a damping parameter due to dissipations. One of the interesting features is that this permittivity can become negative.

The resonant frequency can be estimated using a simple harmonic oscillator model :

$$\omega_p^2 = \frac{ne^2}{\varepsilon_0 m_{\text{eff}}}, \quad (4.2)$$

with n , the electron concentration, e the electron's charge, ε_0 the free space permittivity and m_{eff} the effective mass of the electrons inside the plasma.

The idea using a wire medium was to mimic a plasma whose characteristics can be easily controlled. Indeed, if the periodicity of the medium is small with respect to the wavelength, the medium will be perceived as homogeneous by the electromagnetic waves. Moreover, the good conductivity of metals at microwave frequencies provide a motion-free behaviour for the electrons parallel to the wires axis. Therefore, tuning the filling ratio of metal, the resonant frequency can be controlled and negative permittivity on the direction of the wires can be achieved for the frequency of interest.

First formula for the plasma frequency

In 1996, Pendry *et al.* proposed a formula to compute the equivalent plasma frequency for the wire medium [178]. They showed that two effects have to be taken into account due to the discrete nature of the medium : the decrease of the number of carriers and the increase of the effective mass due to self-inductance.

For the new effective number of carriers, the formula is straightforward:

$$n_{\text{eff}} = n \frac{\pi \rho_0^2}{d^2}, \quad (4.3)$$

with n_{eff} the effective carrier concentration, n the carrier concentration in the bulk metal, ρ_0 the radius of the wires and d the size of the unit-cell.

For the change in the effective mass, a quasi-static model is considered. The mutual inductance of the wires is approximated and the new formula for the effective mass is :

$$m_{\text{eff}} = \frac{\mu_0 \rho_0^2 e^2 n}{2} \ln(d/\rho_0). \quad (4.4)$$

Second formula for the plasma frequency

In 2002, a new model is developed by Belov, Tretyakov and Viitanen, based on modal analysis [175]. The periodic array of vertical wires is again considered. But this time, to each wire is associated a polarizability coefficient, determined using PEC boundary conditions.

Since the medium is periodic, the different Floquet modes are treated separately. Consider a phase shift between consecutive cells φ_x (resp. φ_y) in the $\hat{\mathbf{x}}$ (resp. $\hat{\mathbf{y}}$) direction. For any field/current f , we can write the relation

$$f(x + ma, y + na) = f(x, y) \exp(-j(m\varphi_x + n\varphi_y)). \quad (4.5)$$

Hypothesis 1: *The current on the wire is approximated by a current directed along the $\hat{\mathbf{z}}$ direction flowing along the center of the wire.*

Using Hypothesis 1 and the invariance of the structure along the $\hat{\mathbf{z}}$ direction, we can describe the fields induced by currents along a wire using the 2D Green's function :

$$G(r, z) = \frac{j}{4} H_0^{(2)} \left(\sqrt{k_h^2 - q_z^2} r \right) \exp(-jq_z z), \quad (4.6)$$

with $H_0^{(2)}$ the zero order Hankel function of the second kind, $r = \sqrt{x^2 + y^2}$ the distance to the wire and k_h the wave-vector inside the host medium. We know that the currents on the wires will be such that they ensure the PEC boundary conditions, i.e. the electric field that is tangential to the surface of the wires is null.

Hypothesis 2: *Since the wires are thin, currents transverse to their axis will have a negligible impact. Therefore, the zero-electric field boundary condition is not applied in the $\hat{\mathbf{x}} - \hat{\mathbf{y}}$ plane.*

Hypothesis 3: *The wires are thin enough to consider that the fields do not vary significantly over their section.*

Using Hypotheses 2 and 3, combined with the Green's function of (4.6), we obtain that boundary conditions are ensured for currents on the wire such that, for each wire:

$$E_z^{(inc)} + E_z^{(r)} = 0 \quad (4.7)$$

with $E_z^{(inc)}$ the incoming field, and $E_z^{(r)}$ the field produced by the currents on the wire considered,

$$E_z^{(r)} = \frac{j\eta_h(k_h^2 - q_z^2)}{k_h} G(r, z) I_z. \quad (4.8)$$

η_h is the impedance of the host medium, and I_z the intensity of the currents flowing along the wire.

We can implicitly ensure these boundary conditions using a polarizability of the wire, that provide a relation between the local electric field and the resulting current:

$$\alpha \equiv \frac{I_z}{E_z^{inc}}. \quad (4.9)$$

If we consider that the local field is due to currents of the same amplitude but different phase on the other wires of the array (see Equation (4.5)), the propagative eigenmodes inside the structure can be determined. If one consider a very dense array ($a \ll \lambda$) of very thin wires ($\rho_0 \ll a$), we can approximate the resulting expression using first order Taylor expansion.

Hypothesis 4: *First-order Taylor expansion.*

It leads to the final result of [175]:

$$q^2 = k_h^2 - k_p^2, \quad (4.10)$$

with k_p the plasma frequency

$$k_p^2 = \frac{2\pi}{d^2} \frac{1}{\ln \frac{d}{2\pi\rho_0} + 0.5275}. \quad (4.11)$$

Third formula for the plasma frequency

Later in 2002, Belov *et al.*, proposed another formula for the plasma frequency, which is based on quasi-static approximation [179]. Let's consider two parallel planes that are perpendicular to the wires and separated by a distance h that is small with respect to the variation of the phase along the $\hat{\mathbf{z}}$ direction (q_z). The phase shift between consecutive wires is null: $\mathbf{q}_t = \mathbf{0}$.

Hypothesis 1: *The external electric field is parallel to the wires*

Hypothesis 2: *Quasi-static case : all the dimensions are much smaller than the wavelength in the host medium : $d, h \ll \frac{2\pi}{k_h}$*

The two planes can be considered as the two plates of a capacitor. The voltage between both is given by

$$U = E_z d. \quad (4.12)$$

Due to this voltage, a current will flow through the wires. Since they are made of a PEC, only inductive effects will limit the current :

$$U = j\omega I L d \quad (4.13)$$

with L , the total inductance, including mutual coupling between the wires. Last, the displacement vector $\mathbf{D}$ can be written as

$$\mathbf{D} = \varepsilon_h \mathbf{E} + \mathbf{P}, \quad (4.14)$$

with $\mathbf{P}$ the polarization, given by

$$\mathbf{P} = \frac{\mathbf{J}}{j\omega}. \quad (4.15)$$

Combining these 4 last equations leads to

$$\mathbf{D} = \left(\varepsilon_h \underline{\underline{I}} - \frac{\hat{\mathbf{z}}\hat{\mathbf{z}}}{\omega^2 d^2 L} \right) \cdot \mathbf{E}. \quad (4.16)$$

The second step is to find an approximated expression for the inductance, which depends on the magnetic field distribution. One can observe two important features :

- If the wires are sufficiently thin, most of the inductance will be due to the high magnetic field that is concentrated near the surface and decreases as $1/r$.
- Due to symmetry, the magnetic field at equal distance between two consecutive wires is null.

The magnetic field can be approximated using a simple expression that includes these two salient features.

The magnetic field in the $\hat{\mathbf{y}}$ direction is well approximated by $H_y = \frac{I}{2\pi} \left(\frac{1}{x} \frac{1}{a-x} \right)$ for $x = [\rho_0; a - \rho_0]$.

Hypothesis 3:

Using all these approximations, the third formula to compute the plasma frequency can be found:

$$\omega_p^2 = \frac{2\pi}{\varepsilon_h \mu_h d^2} \frac{1}{\ln \left(\frac{d^2}{4\rho_0(d - \rho_0)} \right)}. \quad (4.17)$$

Conclusion

It can be observed that for small radius ($\rho_0 < 0.1d$), the results provided by the two last formulas are very close to each other. Moreover, they are confirmed by full-wave simulations.

However, none of them holds for wider wires for two reasons. The first one is that the variation of the fields along the section is neglected, and the second one is that currents in the $\hat{\mathbf{x}} - \hat{\mathbf{y}}$ plane are not considered. However, they lead to compact analytical expression.

4.2.2 Deviation according to plasma based model

In 2002, a deeper analysis of the wire medium has been made by Shvets in [180]. Starting from Maxwell's equation, a more formal approach is considered in order to compute the fields everywhere. He reaches the conclusion that the wire medium differs from plasma in two ways :

- The well-known fact that the medium is anisotropic (but its permittivity can still be expressed using a diagonal tensor $\underline{\underline{\varepsilon}}$).
- The fact that the permittivity in the direction parallel to the wires does not correspond to the classical local law $\varepsilon_{zz} \propto (1 - \omega_p^2/\omega^2)$ but depends on the wave-vector $\mathbf{q}$ of the mode considered.

This deviation was estimated showing the physical limits of the local model (i.e. $\varepsilon_{zz} \perp \mathbf{q}$) in [173].

Lets assume that the wire medium can be homogenized using a diagonal permittivity tensor given by the formula

$$\underline{\underline{\varepsilon}} = \begin{pmatrix} \varepsilon_t & 0 & 0 \\ 0 & \varepsilon_t & 0 \\ 0 & 0 & \varepsilon_{zz} \end{pmatrix}. \quad (4.18)$$

On one hand, the following identity has to be satisfied for all propagating modes described by the wave-vector $\mathbf{q}$ [181] :

$$\varepsilon_{\parallel}(q_x^2 + q_y^2) = \varepsilon_{zz}(k_h^2 - q_z^2). \quad (4.19)$$

On the other hand, the electric field along the $\hat{\mathbf{z}}$ direction has also to satisfy the Helmholtz equation

$$[\partial_x^2 + \partial_y^2 + (k_h^2 - q_z^2)] E_z = 0 \quad (4.20)$$

with the boundary condition of zero-field on the wires. From that formula, it is clear that the resulting transverse wave-vector $\mathbf{q}$ does not depend on the host wave-vector k_h^2 but rather on $K = k_h^2 - q_z^2$:

$$k_h = \sqrt{K^2(q_x, q_y, q_z = 0) + q_z^2}. \quad (4.21)$$

Substituting that expression in (4.19), we can see that the formula

$$\varepsilon_z(k_h) = \varepsilon_h \left(1 - \frac{k_p^2}{k_h^2} \right) \quad (4.22)$$

that is used for plasma is incompatible with (4.19) and (4.21) combined. Therefore, the formula has to take into account the spatial dispersion of the permittivity, even in the large wavelength limit. It can be noticed that the three equations can become compatible if the formula of the permittivity is changed to take into account the non-local behaviour :

$$\varepsilon_z(k_h, q_z) = \varepsilon_h \left(1 - \frac{k_p^2}{(k_h^2 - q_z^2)} \right). \quad (4.23)$$

4.2.3 Consequence of spatial dispersion : TE, TM and TEM modes

Determination of the modes

Using this new expression for the effective permittivity, one can determine the propagative modes inside the medium [102]. As a result, postulating that the periodicity is small with respect to the wavelength of operation, one can observe that 3 different modes can propagate through the medium for a given transverse wave-vector $\mathbf{q}_t$. These modes are summarized hereunder [182] :

Dispersion

$$\text{TE mode : } k_h^2 = q^2$$

$$\text{TM mode : } k_h^2 = k_p^2 + q^2$$

$$\text{TEM mode : } k_h = q_z$$

Electric field

$$\text{TE mode : } \mathbf{E} \propto \frac{\mathbf{q}_t \times \hat{\mathbf{z}}}{|\mathbf{q}_t \times \hat{\mathbf{z}}|} \exp(-j\mathbf{q} \cdot \mathbf{r})$$

$$\text{TM mode : } \mathbf{E} \propto \left(\frac{\mathbf{k}_{ht}}{k_h} + \frac{k_h^2 - q^2}{k_h^2 \varepsilon_{zz} - q^2} \frac{q_z}{k_h} \hat{\mathbf{z}} \right) \exp(-j\mathbf{q} \cdot \mathbf{r})$$

$$\text{TEM mode : } \mathbf{E} \propto \frac{\mathbf{q}_t}{q_t} \exp(-j\mathbf{q} \cdot \mathbf{r})$$

It is important to notice that the fields mentioned above come from the homogenization of the medium and therefore correspond to the averaging of the actual field distribution within one unit-cell. For more precision concerning the averaging procedure, one can look at reference [183].

Reflection/transmission of a plane wave

It is known for many decades that if a medium supports more than two modes, the traditional boundary conditions consisting on the continuity of the tangential electric and magnetic fields are no more sufficient to solve the problem of the transmission/reflection of a plane wave impinging on the medium. Additional boundary conditions (ABC) are needed to eliminate the remaining degrees of freedom.

Unfortunately, there is no universal ABC. It is generally specific to the structure studied and comes from physical considerations. A rapid summary of the different solutions proposed can be seen in [182]. However, the most popular one has been found by Silveirinha and is based on the fact that the currents have to vanish at the wire ends.

Indeed, in [183], the following exact relation is derived from the Maxwell's equations and the corresponding boundary conditions:

$$\underbrace{\omega \varepsilon_h \mathbf{E}_{av}}_1 = - \underbrace{(\mathbf{q}_t + j \partial_z \hat{\mathbf{z}}) \times \mathbf{H}_{av}}_2 + \underbrace{\frac{j}{a^2} \int_{\partial A} \mathbf{J}_c(\mathbf{r}) \exp(j\mathbf{q}_t \cdot \mathbf{r}) dl}_3 \quad (4.24)$$

with the subscript av indicating that the value is averaged over the unit cell in the $\hat{\mathbf{x}} - \hat{\mathbf{y}}$ plane and ∂A the boundary of the metallic parts in the unit-cell.

If one considers that the current has to vanish at the end of the wires, the third term of the equality vanishes on both sides of the interface. In addition, the transverse wave vector being continuous over the interface, the $\hat{\mathbf{z}}$ component of the second term is also continuous across the interface. Therefore, the displacement field component perpendicular to the interface has also to be continuous.

That ABC combined to the two classical boundary conditions leads to the compact notation [182] :

- $H_t^{up} = H_t^{down},$
- $\frac{1}{\varepsilon^{up}} \partial_z H_t^{up} = \frac{1}{\varepsilon^{down}} \partial_z H_t^{down},$
- $\partial_z^2 H_t^{up} - \partial_z^2 H_t^{down} = - \left[(k_h^{up})^2 - (k_h^{down})^2 \right] H_t.$

Using these boundary conditions, a linear system of equations can be set-up to determine the transmission and reflection coefficients at interfaces between the wire medium and air, and a finite slab of metamaterial can be considered.

Note that the ABC is necessary because of the averaging of the fields over unit-cells. Indeed, because the homogenized fields are a discrete function of the space, information taking into account the subcell structure is lost and one needs additional information to determine the transmission and reflection coefficients. Such ABC could probably be avoided using Transmission Line equivalence if that equivalence is based on a model that takes into account the sub-cell structure.

4.3 Building a model for the WM

The models previously described provide a good insight on the phenomena happening inside the wire medium. In the case of a subwavelength periodicity, up to three modes can propagate within the wire medium.

The first mode is the TEM mode, which has a fixed longitudinal wave number $q_z = k_h$ whatever the transverse wave number of the mode. It is therefore propagative for any phase-shift between consecutive unit cells.

The second mode is the TE mode. Since the electric fields is transverse to the wires and the section of the wires is electrically small, this mode poorly interact with the wires. For that reason, its dispersion relation is that the homogeneous host medium: $\mathbf{q} \cdot \mathbf{q} = k_h^2$. This mode is propagative as long as $\mathbf{q}_t \cdot \mathbf{q}_t < k_h^2$

Last comes the TM mode. This mode is only propagative for frequencies higher than the plasma frequency of the wire medium. This plasma

frequency can be determined using approximate models that are valid only for very thin wires and small periodicities. If this assumption is broken, there is no straightforward way to extend these models in order to extend the range of validity of their results. Moreover, if one wants to improve the estimation of the plasma frequency of the WM, these models cannot be easily improved and full-wave simulations must be used.

In this Section, we will build a modular model for the propagative modes in the wire medium and the estimation of the plasma frequency. A special emphasis is brought to the hypotheses made throughout the development and their impact on the physics of the problem.

4.3.1 Establishing Helmholtz equations

To compute the eigenmodes inside the WM, we start back from the Maxwell's equations inside a dielectric material:

Hypothesis 1: *The material considered is magnetically isotropic and the relation between the electric and the displacement fields can be described using a tensor : $\mathbf{D} = \underline{\underline{\varepsilon}} \cdot \mathbf{E}$.*

Within such a dielectric material, electric and magnetic fields are determined by the following equations:

$$\Delta \mathbf{E} - \mu \underline{\underline{\varepsilon}} \partial_t^2 \mathbf{E} = \mu \partial_t \mathbf{J} + \underline{\underline{\varepsilon}}^{-1} \nabla \rho, \quad (4.25)$$

$$\Delta \mathbf{H} - \mu \underline{\underline{\varepsilon}} \partial_t^2 \mathbf{H} = -\nabla \times \mathbf{J}, \quad (4.26)$$

with $\Delta = \nabla^2$, μ the permeability of the medium, ∂_t the derivative with respect to the time, $\mathbf{J}$ the current density and ρ the charge density. Note that $\mathbf{J}$ and ρ are the general current and charge terms, including impressed source components. Since we are interested in finding the eigenmodes at a given frequency, a phasor notation is used (an implicit $\exp(j\omega t)$ time dependency is considered).

Hypothesis 2: *To decouple Helmholtz equations for the three directions of the space, $\underline{\underline{\varepsilon}}$ is made diagonal. Its diagonal entries will be denoted ε_x , ε_y and ε_z .*

Note that we are just talking about the permittivity of a dielectric material, not about the equivalent permittivity of the wire medium. Using these two hypotheses, and focusing on the electric field equation, we obtain (for the $\hat{\mathbf{z}}$ direction):

$$[\partial_x^2 + \partial_y^2 + \partial_z^2 + k_{h,z}^2] E_z(x, y, z) = j\mu\omega J_z + \frac{\partial_z \rho}{\varepsilon_z} \quad (4.27)$$

with $k_{h,z}^2 = \omega^2 \mu \varepsilon_z$. Using the charge conservation, we can develop the right-hand side of the equation to obtain :

$$\begin{aligned} & [\partial_x^2 + \partial_y^2 + \partial_z^2 + k_{h,z}^2] E_z(x, y, z) \\ &= j\mu\omega J_z + \frac{j}{\omega\varepsilon_z} \partial_z (\partial_x J_x + \partial_y J_y + \partial_z J_z). \end{aligned} \quad (4.28)$$

We can see that the Helmholtz equations for the 3 directions of space are not totally independent, in the sense that the $\hat{\mathbf{z}}$ component of the electric field still depends on the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ components of the current density. However, we will use that equation as a starting point.

4.3.2 Application to wire medium

Now, we will apply equation (4.28) to the particular case of the wire medium. It is not necessary, but to ease the notations and since most of the dielectric materials used can be considered as isotropic, we will make the following hypothesis

Hypothesis 3: *The permittivity of the dielectric host medium can be described by a scalar quantity ε_h (i.e. it is isotropic).*

The constitutive parameters of the wires differ from the properties of the dielectric matrix. Therefore, we will replace their presence by equivalent currents. In order to simplify the equation, we will make another hypothesis which will only hold for thin wires.

Hypothesis 4 : *The equivalent currents describing the reaction of the wires are only flowing in the $\hat{\mathbf{z}}$ direction. $J_x(x, y, z) = J_y(x, y, z) = 0$.*

Before solving the equation, we will do a last hypothesis. We are only interested in the eigenmodes within the structure, which is invariant along the $\hat{\mathbf{z}}$ direction. Therefore, an $\exp(-jq_z z)$ dependency for the fields and the currents along the $\hat{\mathbf{z}}$ direction is considered. Note that q_z can be complex (or negative).

$$\begin{aligned} \mathbf{J}(x, y, z) &= \mathbf{J}(x, y, 0) \exp(-jq_z z), \\ \textbf{Hypothesis 5:} \quad \mathbf{E}(x, y, z) &= \mathbf{E}(x, y, 0) \exp(-jq_z z), \\ \mathbf{H}(x, y, z) &= \mathbf{H}(x, y, 0) \exp(-jq_z z). \end{aligned} \quad (4.29)$$

The actual hypothesis lies in the fact that we consider that all the possible fields distribution can be described using a set of functions satisfying Hypothesis 5. With that last hypothesis, we can simplify the Helmholtz equations and solve them. If we use the relations $\mu\omega = k_h\eta_h$ and $\varepsilon_h\omega = k_h/\eta_h$, with η_h the impedance of the dielectric host matrix, for the electric field in the $\hat{\mathbf{z}}$ direction, we finally find :

$$[\partial_x^2 + \partial_y^2 + (k_h^2 - q_z^2)] E_z(x, y, 0) = j\eta_h \left(k_h - \frac{q_z^2}{k_h} \right) J_z(x, y, 0). \quad (4.30)$$

Using these same hypotheses, we can write the equation describing the electric field along the $\hat{\mathbf{x}}$ direction :

$$[\partial_x^2 + \partial_y^2 + (k_h^2 - q_z^2)] E_x(x, y, 0) = \frac{\eta_h q_z}{k_h} \partial_x J_z. \quad (4.31)$$

Note that due to the mathematical symmetry between $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ directions, the explicit treatment of the electric field along the $\hat{\mathbf{y}}$ direction will not be done here. However, it has to be treated in a similar way as the $\hat{\mathbf{x}}$ -directed field.

4.3.3 Solution of the Helmholtz equations

These equations are solved in three steps:

1. The fields and the currents are decomposed into their Fourier components. The structure being periodic, the spectrum is discrete. Moreover, using the orthogonality of the Fourier components, each of them can be treated separately. Doing so, a relation between the currents and the fields is obtained.

2. Some particular cases of the equations need to be treated separately. These are analysed and linked to the TE and TEM modes of the WM.
3. Finally, the equation is solved and boundary conditions are applied. This solution correspond to the TM mode, and the plasma frequency can be extracted from its dispersion curve.

Decomposition into Fourier series

The structure being periodic, it can be proven that all the modes propagating inside the structure can be decomposed into Floquet modes. Let us consider the Floquet modes with phase shifts q_x and q_y in the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ directions respectively.

The fields and the current distributions are quasi-periodic in the $\hat{\mathbf{x}} - \hat{\mathbf{y}}$ plane : $f(x + md_x, y + nd_y, z) = f(x, y, z) \exp(-j(mq_x d_x + nq_y d_y))$, with m and n , two integers and f that can represent the electric field, the magnetic field or the current distributions, and d_x and d_y the dimensions of the unit-cell in the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ directions respectively.

Hypothesis 6 :

We then have:

$$\begin{aligned}
 E_z(x, y, 0) &= \sum_{m,n=-\infty}^{\infty} \left(\tilde{E}_{z,mn} \exp \left[-j (k_{x,m}x + k_{y,n}y) \right] \right), \\
 J_z(x, y, 0) &= \sum_{m,n=-\infty}^{\infty} \left(\tilde{J}_{z,mn} \exp \left[-j (k_{x,m}x + k_{y,n}y) \right] \right),
 \end{aligned} \tag{4.32}$$

with

$$\begin{aligned}
 k_{x,m} &= \frac{2\pi m}{d_x} + q_x, \\
 k_{y,n} &= \frac{2\pi n}{d_y} + q_y.
 \end{aligned} \tag{4.33}$$

Substituting (4.32) into (4.30) and applying

$$\iint \frac{\dots}{ab} \exp [j (k_{x,m_0}x + k_{y,n_0}y)] dx dy \tag{4.34}$$

on both side of the equality, with the integration that is carried over one unit-cell, we obtain:

$$\tilde{E}_{z,mn} \underbrace{[k_h^2 - q_z^2 - k_{x,m}^2 - k_{y,n}^2]}_{\text{"1"}} = \underbrace{j\eta_h \left(k_h - \frac{q_z^2}{k_h} \right)}_{\text{"2"}} \tilde{J}_{z,mn} \quad (4.35)$$

which holds $\forall m, n \in \mathbb{Z}$

In a similar way, for the $\hat{\mathbf{x}}$ direction, we obtain:

$$\tilde{E}_{x,mn} [k_h^2 - q_z^2 - k_{x,m}^2 - k_{y,n}^2] = -\frac{j\eta_h q_z k_{x,m}}{k_h} \tilde{J}_{z,mn} \quad (4.36)$$

Particular cases

Three particular cases can be highlighted

Case 1 : "1" = 0 and "2" $\neq$ 0

Case 2 : "1" $\neq$ 0 and "2" = 0

Case 3 : "1" = "2" = 0

Case 1

The first particular case happens iif

$$\{(m_0, n_0) \mid [k_h^2 - q_z^2 - k_{x,m_0}^2 - k_{y,n_0}^2] = 0\} \neq \emptyset. \quad (4.37)$$

For that particular spatial frequencies, the current has to vanish and the amplitude of the fields is undetermined.

$$\tilde{J}_{z,m_0 n_0} = 0. \quad (4.38)$$

However, if we consider that the wires are PEC, the $\hat{\mathbf{z}}$ -directed electric field vanishes in the middle of the wires, so that the following condition has to hold true:

$$\sum_{(m_0, n_0)} \tilde{E}_{z,m_0 n_0} = 0. \quad (4.39)$$

Hypothesis 7 : *The dimensions of the unit cell are smaller than the half-wavelength in the host dielectric: $d_x, d_y < \lambda_h/2$.*

Hypothesis 8 : q_z is real.

Introducing the above hypotheses, one can observe that there can only be one pair of (m_0, n_0) that satisfies condition (4.37). Therefore, we obtain that the electric field along the $\hat{\mathbf{z}}$ direction is zero.

However, if we look at the electric field in the $\hat{\mathbf{x}}$ direction, we do not have any boundary condition. Therefore, $\tilde{E}_x^{(s_0, t_0)}$ can be whatever we want.

Physically, it corresponds to the TE mode (see Section 4.2.3).

First, look at the condition on the currents to be null. If

$$[k_h^2 - q_z^2 - k_{x, m_0}^2 - k_{y, n_0}^2] = 0, \quad (4.40)$$

it means that the mode considered corresponds to the propagation of a plane wave inside the dielectric medium. Which means that the fields generated by the currents on each wire will add up in phase and therefore diverge. It corresponds to the wood anomaly. This result is therefore relevant from a physical point of view.

Second, look at the second condition, which says that $\sum_{(m_0, n_0)} \tilde{E}_{z, m_0 n_0} = 0$. If Hypothesis 7 is broken and the unit cell is big enough, we can consider two plane-waves that would interfere such that the electric field along the $\hat{\mathbf{z}}$ direction cancels periodically. Therefore, the boundary conditions would be ensured without the need for any current along the wires and a propagating TM mode would exist. However, if the unit cell is smaller than half of the wavelength, there cannot exist two propagating waves ($q_z \in \mathbb{R}$) that interfere the right way and therefore no propagating TM mode can exist. Note that if we do not make Hypothesis 8, q_z^2 can be smaller than zero. Thus there can be a combination of evanescent TM modes inside the medium that does not interact with the wires.

Last, the value of the electric field in the $\hat{\mathbf{x}}$ direction is not constrained. It is a direct result of the hypothesis we made that the wires are thin and therefore currents transverse to $\hat{\mathbf{z}}$ can be neglected. Because these currents are neglected, TE waves do not interact with the wires and propagate as if they were not existing (dispersion relation corresponding to plane waves in the dielectric).

Case 2

This case corresponds to the condition

$$q_z^2 = k_h^2. \quad (4.41)$$

Substituting this term in the equations (4.30) and (4.31), we obtain that:

$$\tilde{E}_{z,mn} [k_{x,m}^2 + k_{y,n}^2] = 0 \quad (4.42)$$

It means that, independently of the currents, the electric field along the $\hat{\mathbf{z}}$ direction is null. Note that the special case of $[k_{x,m}^2 + k_{y,n}^2] = 0$ corresponds to the next point and is therefore not treated here.

If we look at the electric field along the $\hat{\mathbf{x}}$ direction, we have

$$\tilde{E}_x^{(s,t)} = -\frac{q_z}{|q_z|} \left[\frac{j\eta_h k_{x,m}}{k_{x,m}^2 + k_{y,n}^2} \right] \tilde{J}_{z,mn}. \quad (4.43)$$

It corresponds to the TEM mode.

We can analyse that result from a physical point of view. Since $\mathbf{q}_t \neq \mathbf{0}$, we have $k > k_h$. We then observe the propagation of non-radiative currents along the wires. Moreover, if we have a given field distribution on one end of the wires, a point-to-point translation of it is achieved. It corresponds to the canalization regime [184].

Case 3

In this case, we consider the intersection between case 1 and case 2, i.e:

$$\begin{aligned} q_z^2 &= k_h^2, \\ \{(m_0, n_0) | [k_{x,m_0}^2 + k_{y,n_0}^2] = 0\} &\neq \emptyset. \end{aligned} \quad (4.44)$$

Without loss of generality, the last condition can be re-written

$$q_x = q_y = 0. \quad (4.45)$$

To see what happens to the TE and TEM modes for that peculiar conditions, we will approach them using the limit $\lim_{q_x \rightarrow 0}$.

For the TE mode, no special behaviour can be observed and therefore we obtain the same results as in case 1.

For the TEM mode, we obtain that

$$\tilde{E}_{x,00} = \lim_{q_x \rightarrow 0} -\frac{q_z}{|q_z|} \left[\frac{j\eta_h}{q_x} \right] \tilde{J}_{z,00}, \quad (4.46)$$

which leads to $\tilde{J}_{z,00} = 0$. The average current flowing through one unit cell has to be null. It corresponds to a degenerated mode for which there is no energy transfer via the currents along the wires.

Solving the equation

Now that all the peculiar cases have been treated, we can solve the Helmholtz equations. For a given current distribution, the spatial frequencies of the electric field along the $\hat{\mathbf{x}}$ and $\hat{\mathbf{z}}$ directions are given by :

$$\begin{aligned}\tilde{E}_{x,mn} &= -j \frac{\eta_h}{k_h} \frac{q_z k_{x,m}}{k_h^2 - q_z^2 - k_{x,m}^2 - k_{y,n}^2} \tilde{J}_{z,mn}, \\ \tilde{E}_{z,mn} &= j \eta_h \left(k_h - \frac{q_z^2}{k_h} \right) \frac{1}{k_h^2 - q_z^2 - k_{x,m}^2 - k_{y,n}^2} \tilde{J}_{z,mn}.\end{aligned}\tag{4.47}$$

Now, we have to chose the boundary conditions used to take into account the presence of the PEC wires.

Hypothesis 9 : *The wires are thin enough to neglect the field variation on their cross-section.*

Using Hypothesis 9, we can simply impose $E_z(0, 0, z) = 0$ to enforce the PEC wire condition. We then obtain:

$$\sum_{m,n=-\infty}^{\infty} \tilde{E}_{z,mn} = 0.\tag{4.48}$$

Substituting the results shown above, we obtain

$$\sum_{m,n=-\infty}^{\infty} \left[\frac{K^2}{K^2 - k_{t,mn}^2} \tilde{J}_{z,mn} \right] = 0\tag{4.49}$$

with

$$\begin{aligned}K^2 &= k_h^2 - q_z^2, \\ k_{t,mn}^2 &= k_{x,m}^2 + k_{y,n}^2.\end{aligned}\tag{4.50}$$

That mode corresponds to the TM mode. To find the dispersion relation of this mode, we can impose $\mathbf{q}_t$ and then look after the q_z for which the infinite series tends to zero.

In the next section, we will determine the conditions under which that mode can exist and compute its dispersion relation for different shapes of the currents : Gaussian currents, circular currents, Dirac- δ like currents.

But some preliminary observations can be made. We can distinguish two terms:

$$\frac{K^2}{K^2 - k_{t,mn}^2}$$

If we refer to Hypothesis 7 ($d_x, d_y < \lambda/2$) and 8 (q_z real), we can see that at most one term of the sum will be positive. Therefore, if the Fourier transform of the currents only contains positive coefficients, the absolute value of the positive term has to be equal to the infinite sum of the other terms of the sum.

$$\tilde{J}_{z,mn}$$

This term depends only on the hypotheses made about the shape of the currents along the wires.

4.3.4 Analysis of TM mode for different current distributions

δ -like currents

The formula for the currents within the first unit cell is given by the formula

$$J_z(x, y) = \delta(x, y), \quad (4.51)$$

with $\delta(x, y)$ the Dirac's delta. The Fourier transform of the current distribution is then the constant function:

$$\tilde{J}_z(k_x, k_y) = 1. \quad (4.52)$$

Therefore, the condition of existence for the TM mode becomes:

$$\sum_{(m,n)} -\frac{K^2}{K^2 - k_{t,mn}^2} = 0. \quad (4.53)$$

Analysing that sum and using Hypotheses 7 and 8, we can see that only one term of the sum can be positive. If we isolate that term, we obtain

$$\sum_{(m,n) \neq (0,0)} -\frac{K^2}{K^2 - k_{t,mn}^2} = \frac{K^2}{K^2 - q_x^2 - q_y^2}. \quad (4.54)$$

The left sum diverges to ∞ (2D sum of $1/r^2$ function). Therefore, a necessary condition for a solution to exist is that the right term has to tend to ∞ , which can be re-written:

$$K^2 - q_x^2 - q_y^2 = k_h^2 - q^2 = 0. \quad (4.55)$$

It corresponds to the spatial dispersion of the TM mode inside the dielectric host without the wires. Therefore, if the wires are made infinitely thin, they do not have any impact on the TM mode. That conclusion is confirmed both by the existing models (e.g: [179]) and the physics of the problem.

Note that strictly speaking, we did not prove that a propagating mode were existing in the mathematical sense, but we proved that if it exists, it has to be described by the dispersion relation provided above.

Other currents

More relevant current distributions have also been investigated numerically and will be presented in this section. To exploit the axial symmetry of these currents, radial coordinates are introduced:

$$\begin{aligned} r &= \sqrt{x^2 + y^2}, \\ k_t &= \sqrt{k_x^2 + k_y^2}. \end{aligned} \tag{4.56}$$

Disc-like currents One possible shape is the disc-like current distribution, which corresponds to uniform currents on the section of the wire, and no current outside. This current distribution is particularly useful for penetrable wires, when their radius is small with respect to the skin depth. For the disc-like currents, the formula is given by :

$$J_z(x, y) = J \operatorname{circ}\left(\frac{r}{\rho_0}\right), \tag{4.57}$$

$$\tilde{J}_z(k_x, k_y) = 2\pi J \rho_0 \frac{J_1(k_t \rho_0)}{k_t},$$

with $\operatorname{circ}(r) = 1$ if $r < 1$ and vanishes otherwise, and $J_\alpha(x)$ the Bessel function of the first kind. A proper extraction of the $k_t = 0$ term leads to

$$\tilde{J}_z(0, 0) = 2\pi \rho_0^2 J \frac{J_0(0)}{2} = \pi \rho_0^2. \tag{4.58}$$

Circular currents Another realistic hypothesis is to consider that the currents are constant, but confined on the surface of the wires. That approximation is useful when the radius of the wires is large with respect to the skin depth (e.g: PEC wires). The formula for a circular current distribution is given by:

$$J_z(x, y) = J \delta(r - \rho_0), \quad (4.59)$$

$$\tilde{J}_z(k_x, k_y) = 2\pi\rho_0 J J_0(k_t\rho_0).$$

It can be noticed that the spectrum of the currents is decreasing slowly when k_t increases. A very large number of terms in (4.49) is thus needed to ensure accurate results. The convergence of this series can be accelerated by modifying the condition used to impose vanishing fields inside the wires.

Improving the convergence of the double summation

The electric field vanishes inside the wires. Previously, this condition was imposed in a weak sense by imposing that the electric field vanishes at a given position that corresponds to the center of the wires. In the spatial domain, it is a condition that is easy to include in a model, since the fields only have to be evaluated in one point. However, in the spectral domain, a point has an infinite spectrum. For that reason, even high frequencies of the fields must be considered in order to impose vanishing fields.

Another possibility is to impose that the electric field vanishes *on average* over the section of the wire. Since the zone that is being tested is wider in the spatial domain, only a limited part of the spectrum actively contributes to the averaged condition on the fields, speeding up the convergence of the series that has to be evaluated.

If the actual electric field distribution along the $\hat{\mathbf{z}}$ direction is denoted $E_z(x, y)$, we know that this function has to be null inside the wire section, i.e. $E_z(r < \rho_0) = 0$. Using the function $f(x, y)$ such that $f(x, y)(1 - \text{circ}(r/\rho_0)) = 0$, we can write:

$$E_z(x, y)f(x, y) = 0. \quad (4.60)$$

In the Fourier domain, this condition reads:

$$FT \{E_z f\}(k_x, k_y) = \tilde{E}_z(k_x, k_y) \otimes \tilde{f}(k_x, k_y) = 0, \quad (4.61)$$

with $\otimes$ the convolution operator. For a discrete spectrum, (4.61) becomes

$$\forall p, q \in \mathbb{Z}, \sum_{m,n} \tilde{E}_{z,mn} \tilde{f}(k_{x,(q-m)}, k_{y,(r-n)}) = 0. \quad (4.62)$$

The first testing procedure used to derive 4.49 consisted in considering $f(x, y) = \delta(x, y)$. However, different functions can be used to introduce

some spatial filtering in the testing procedure. Considering the simple choice of $f(r) = \text{circ}(r/\rho_0)$ leads to

$$\forall p, q \in \mathbb{Z}, \quad \sum_{m,n} \tilde{E}_{z,mn} \frac{J_1(\rho_0 k_{t,(p-m)(q-n)})}{k_{t,(p-m)(q-n)}} = 0. \quad (4.63)$$

If we use (4.47), we can express the field distribution using the current distribution:

$$\forall p, q \in \mathbb{Z}, \quad \sum_{m,n} \frac{K^2}{K^2 - k_{t,mn}^2} \tilde{J}_{z,mn} \frac{J_1(\rho_0 k_{t,(p-m)(q-n)})}{k_{t,(p-m)(q-n)}} = 0. \quad (4.64)$$

For example, considering circular currents on the surface of PEC wires, substituting the FT of the currents (see (4.59)), one obtains

$$\forall p, q \in \mathbb{Z}, \quad \sum_{m,n} \frac{K^2}{K^2 - k_{t,mn}^2} \tilde{J}_0(k_{t,mn}) \frac{J_1(\rho_0 k_{t,(p-m)(q-n)})}{k_{t,(p-m)(q-n)}} = 0. \quad (4.65)$$

Theoretical convergence of the sums

If we consider that the sum is performed over 2 dimensions and that the terms of the sum only depend on k_t , we can get rid of one of the two infinite sums using

$$\sum_m \sum_n f(k_{t,mn}) \sim \sum_m 2\pi k_{t,m0} f(k_{t,m0}). \quad (4.66)$$

That assumption is true when the impact of the discrete nature of the sampling becomes negligible, which is true for large values of k_t . The terms of the remaining series oscillating around zero, we can, as a first approximation, consider that the error is of the same order of magnitude as the last term added.

For large arguments, the envelope of Bessel's functions decreases as $1/\sqrt{k_t}$. Considering that the value of $k_{t,m0}$ linearly depends of m , which is true for large values of m , we obtain the following asymptotic convergences :

Disk-like currents: $e(x_{\max}) \propto \left(\frac{1}{x_{\max}}\right)^{5/2},$

Circular currents: $e(x_{\max}) \propto \left(\frac{1}{x_{\max}}\right)^{3/2},$

Circular currents with modified BC : $e(x_{\max}) \propto \left(\frac{1}{x_{\max}}\right)^3,$

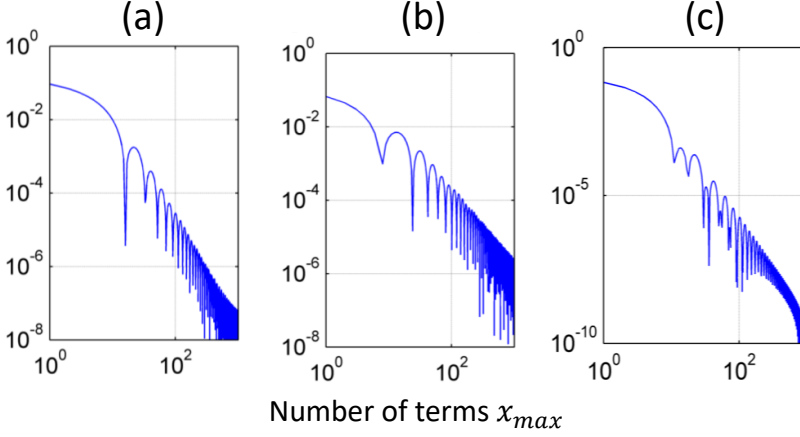


Figure 4.2: Convergence of the sum for (a) the disc-like currents, (b) the circular currents and (c) the circular currents with the averaged boundary conditions. The reference solution is computed using $x_{\max} = 1000$.

with $e(x_{\max})$ the error made when the terms of indices (m, n) such that $|m| > x_{\max}$ or $|n| > x_{\max}$ are truncated.

The convergence of the sum has been tested for the two different current distributions and for the circular current distribution with the modified boundary conditions. The results can be seen in Figure 4.2 for $\rho_0/a = 1/40$ and $K = 0$. Note that the definition of $x_{\max}$ implies that the number of elements involved in the double summation is equal to $(2x_{\max} + 1)^2$.

Propagation of TM mode We define the plasma frequency ω_p as the minimum angular frequency at which TM mode can propagate through the wire medium and the corresponding plasma wave-vector $k_p^2 = \omega_p^2 \varepsilon_h \mu_h$. It corresponds to the value of K for which (4.64) vanishes for $k_{t,00} = 0$. The results obtained are compared with the prediction of [179]. For different radius and different size of the unit-cell, the results can be seen in Figure 4.3.

It can be seen that the circular current distribution provides results that are very similar with the model of [179].

4.3.5 Including losses in the host matrix

Interestingly, introducing losses within the host matrix does not change the results significantly. The modes remain identical. The only difference is that now, q_z is complex to compensate for the imaginary part of k_h .

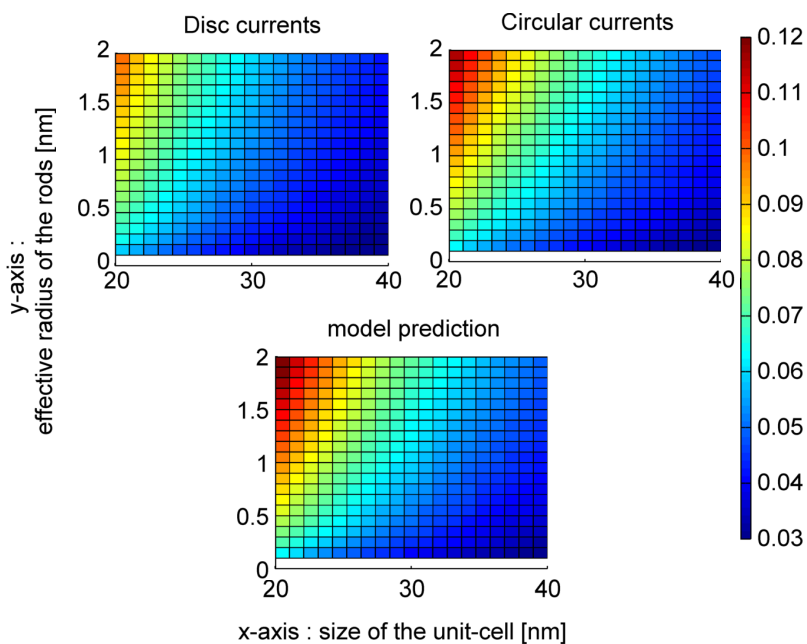


Figure 4.3: Predicted plasma wave-vector k_p using the different currents and the model developed in [179]. The x-axis indicates the size of the unit-cell considered and the y-axis indicate the effective radius of the wires. The wave-vector is expressed in nm^{-1}

Indeed, we can restart from equation (4.35):

$$\tilde{E}_{z,mn} \underbrace{[k_h^2 - q_z^2 - k_{x,m}^2 - k_{y,n}^2]}_{\text{"1"}} = \underbrace{j\eta_h \left(k_h - \frac{q_z^2}{k_h} \right)}_{\text{"2"}} \tilde{J}_{z,mn}. \quad (4.67)$$

For TEM mode, the term "2" has to be null. The condition of $q_z^2 = k_h^2$ is not changed. Therefore, we obtain $q_z = \pm k_h$ (+ for upward modes, - for downward modes).

For TE mode, there is still no interactions with wires, and therefore the plane wave is now propagating in a lossy dielectric without any particular behavior.

Last, for TM mode, we obtain :

$$\sum_{m,n} \frac{k_h^2 - q_z^2}{k_h^2 - q_z^2 - k_{x,m}^2 - k_{y,n}^2} \tilde{J}_{z,mn} = 0 \quad (4.68)$$

It can be seen that, if a solution q'_z can be found for the lossless case ($k_h \in \mathbb{R}$), then the solution to the lossy case is given by

$$q_z = \sqrt{(q'_z)^2 - (k'_h)^2 - 2jk_h k'_h} \quad (4.69)$$

with k'_h the imaginary part that has been added to k_h to account for the losses.

4.3.6 Improving the current distribution

Up to now, only some fixed current distribution has been considered. However, Equation (4.64) has to be true for all p, q . Therefore, one can introduce some degrees of freedom in the currents. One possibility is to add some variations to the currents J_z within the wires. Another possibility is to introduce some currents in the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ directions. However, in order to provide reliable results, the latter method probably requires to impose some additional conditions on the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ directed electric field inside the wires.

4.4 Orthogonality properties in the WM

Now that the modes within the WM can be computed, the next step would be to solve the scattering problem at the interface between the WM and the air. This problem can be solved using mode-matching techniques [158]. The idea is to express the incident fields as a linear combination of the reflected modes in the air and the transmitted modes in the WM. In order to find

the coefficients associated to each mode, one has to solve a linear system of equations.

This system of equations can be solved by inverting the matrix that describes it: the basis made of the different modes is orthogonalized and, once done, the incident fields are projected into this orthogonal basis. This orthogonalization can be done in two different ways. The first one consists in computing all the modes inside structure and then assembling them to create some groups of modes that are orthogonal to each others. The second possibility is to find a scalar product such that, due to the physics of the problem, different modes are automatically orthogonal. Such scalar products have been proposed in [185] for closed waveguides. The advantage of this method is that only the mode on which the fields are projected is required to obtained virtually exact results.

Another possible application of such orthogonality is that, since they are based on the physics, they can provide a good insight on the precision with which a mode has been computed. Indeed, if the eigenmodes are computed using approximate techniques, they will only partially comply with the laws of physics and therefore the orthogonality property will only be partially respected. Therefore, the deviation in this orthogonality is a good indicator of the deviation of the computed mode with respect to the physics, *i.e.* to the exact mode.

In this section we propose such a scalar product for 2D periodic lossless structures that are invariant along the third dimension (like the wire medium). The scalar product is first properly stated, and then the orthogonality of different modes with respect to that scalar product is shown. The proof can be seen as an extension of the proof of [185] to open periodic structures made of different dielectrics.

Consider a lossless structure consisting of a dielectric host and periodic inclusions made of different materials. The cross-section of the structure is periodic in directions $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ and invariant over $\hat{\mathbf{z}}$. $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ are chosen to be perpendicular to $\hat{\mathbf{z}}$ without any loss of generality. Every material constituting the layer is isotropic, homogeneous and non-lossy. An example of such a structure made of two different materials can be seen on Figure 4.4(a).

The homogeneous Maxwell's equations can be solved inside the structure to obtain the eigenmodes of the metamaterial. Using the Floquet theorem, it can be proven that solutions can be decomposed into quasi-periodic modes, *i.e.* modes that are periodic within a linear phase factor $\exp(-j\mathbf{q}_t \cdot \mathbf{r})$ with $\mathbf{r}$ the position. Each eigenmode i is then characterized by its normalized electric and magnetic fields distributions $\mathbf{E}_i(x, y)$ and $\mathbf{H}_i(x, y)$, its transverse wave-vector $\mathbf{q}_t$ and its longitudinal wave-vector $q_{i,z}$. The z -dependence of the fields is given by $\exp(-jq_{i,z}z)$. For two different modes i and j with

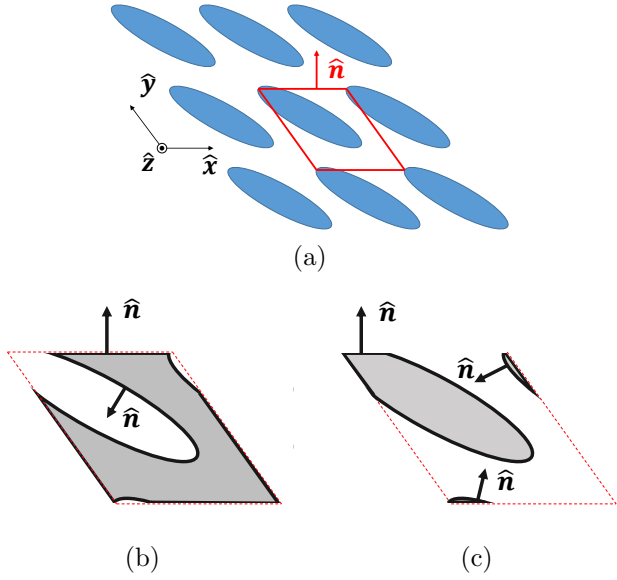


Figure 4.4: (a): Schematic representation of the cross-section of the periodic material. The blue parts correspond to the inclusions while the white part corresponds to the host medium. A unit-cell is bounded by the red line. (b) and (c): The total surface integral is divided into two parts which correspond to the host medium and the dielectric inclusions. Vector $\hat{n}$ is the normal to the contour of the surface of integration.

$q_{i,z}^2 \neq q_{j,z}^{*2}$, it can be proven that

$$\iint (\varepsilon \mathbf{E}_i \cdot \mathbf{E}_j^* - \mu \mathbf{H}_i \cdot \mathbf{H}_j^*) dS = 0 \quad (4.70)$$

with A^* the conjugate of A , ε and μ the local permittivity and permeability, while the integration is performed over one unit-cell.

The special case of $k_{i,z} = k_{j,z}$ with $i \neq j$ can be treated separately: the two modes φ_i and φ_j correspond to the mathematical expression of the two degrees of freedom of a degenerated physical mode. Therefore, they can be orthogonalized using the classical Gram-Schmidt algorithm without any loss of generality.

Note that this orthogonality property has not been used in this Thesis and is therefore seen as a curiosity than a real tool.

4.4.1 Proof of orthogonality

The following proof can be seen as generalization of the one developed in [185] for closed waveguides. Considering that the modes correspond to solutions of the homogeneous Maxwell's equations, they are ruled by the following equations:

$$\nabla_t^2 \mathbf{E}_i = (q_{i,z}^2 - k_0^2) \mathbf{E}_i \quad (4.71a)$$

$$\nabla_t^2 \mathbf{H}_i = (q_{i,z}^2 - k_0^2) \mathbf{H}_i \quad (4.71b)$$

$$\nabla_t^2 \mathbf{E}_j = (q_{j,z}^2 - k_0^2) \mathbf{E}_j \quad (4.71c)$$

$$\nabla_t^2 \mathbf{H}_j = (q_{j,z}^2 - k_0^2) \mathbf{H}_j \quad (4.71d)$$

with $k_0^2 = \omega^2 \varepsilon \mu$ that depends on the local constitutive parameters and therefore depends on the position within the unit cell. These equations can be combined as follows:

$$\varepsilon \mathbf{E}_j^* \cdot \nabla_t^2 \mathbf{E}_i - \varepsilon \mathbf{E}_i \cdot \nabla_t^2 \mathbf{E}_j^* + \mu \mathbf{H}_i \cdot \nabla_t^2 \mathbf{H}_j^* - \mu \mathbf{H}_j^* \cdot \nabla_t^2 \mathbf{H}_i \quad (4.72)$$

Integrating the resulting equation over one unit-cell provides:

$$\begin{aligned} (q_{j,z}^2 - q_{i,z}^2) \iint_S (\varepsilon \mathbf{E}_i \cdot \mathbf{E}_j^* - \mu \mathbf{H}_i \cdot \mathbf{H}_j^*) dS \\ = \iint_S (\varepsilon \mathbf{E}_j^* \cdot \nabla_t^2 \mathbf{E}_i - \varepsilon \mathbf{E}_i \cdot \nabla_t^2 \mathbf{E}_j^* \\ - \mu \mathbf{H}_j^* \cdot \nabla_t^2 \mathbf{H}_i + \mu \mathbf{H}_i \cdot \nabla_t^2 \mathbf{H}_j^*) dS \end{aligned} \quad (4.73)$$

If we can demonstrate that the right-hand side of (4.73) vanishes, it will prove that modes of different q_z^{*2} are orthogonal using the scalar product of (4.70).

The integration can be done separately for different media. Considering the structure of Figure 4.4(a), a first integral is carried out over the host medium, while a second integral is carried out over the inclusions (cf. shaded areas in Figure 4.4(b) and (c)). Using Green's second identity [185], the right-hand side of (4.73) becomes:

$$\oint_{\partial S} \left(\varepsilon \mathbf{E}_j^* \cdot \partial_n \mathbf{E}_i - \varepsilon \mathbf{E}_i \cdot \partial_n \mathbf{E}_j^* - \mu \mathbf{H}_j^* \cdot \partial_n \mathbf{H}_i + \mu \mathbf{H}_i \cdot \partial_n \mathbf{H}_j^* \right) dl \quad (4.74)$$

with ∂S the contour of surface S and ∂_n the derivative with respect to the direction perpendicular to the contour in the plane of the cross-section.

The line integral can also be decomposed into two parts. One part runs along the boundaries of the unit-cell. The second part runs along the interface between the two different media.

Modes i and j being characterized by the same transverse wave vector $\mathbf{q}_t$, it can be easily proven that the different terms in (4.74) has the same absolute value on both sides of the unit-cell, but have opposite signs due to the change in the normal direction.

For the integral on the interface between different media, we can locally replace the basis $\{\hat{\mathbf{x}}, \hat{\mathbf{y}}, \hat{\mathbf{z}}\}$ of the space with $\{\hat{\mathbf{p}}, \hat{\mathbf{n}}, \hat{\mathbf{z}}\}$ to match it with the interface. $\hat{\mathbf{n}}$ is the normal to the interface and $\hat{\mathbf{p}}$ is defined such that $\hat{\mathbf{p}} = \hat{\mathbf{n}} \times \hat{\mathbf{z}}$, and is therefore tangent to the surface contour on the cross-sectional plane. If we express the local electric field using that basis, we obtain

$$\mathbf{E}_i \cdot \partial_n \mathbf{E}_j^* = E_{i,p} \partial_n E_{j,p}^* + E_{i,n} \partial_n E_{j,n}^* + E_{i,z} \partial_n E_{j,z}^* \quad (4.75)$$

Using Maxwell's equations, the fields can be developed to obtain

$$\begin{aligned} \varepsilon \mathbf{E}_i \cdot \partial_n \mathbf{E}_j^* = & \varepsilon E_{i,p} (\partial_p E_{j,n}^* - j\omega B_{j,z}^*) + \varepsilon E_{i,n} (-\partial_p E_{j,p}^* - \partial_z E_{j,z}^*) \\ & + \varepsilon E_{i,z} (j\omega B_{j,p}^* + \partial_z E_{j,n}^*) \end{aligned} \quad (4.76)$$

The same procedure can be applied to the 3 other terms of Equation (4.74). Performing the integration on the two sides of the interface, using the continuity of the fields across an interface and considering that the normal to the contour is pointing in the opposite direction for each side of the interface, one can find that the right-hand side of Equation (4.73) is equal to zero. It is only possible for a lossless structure, since in that case $\varepsilon^* = \varepsilon$ and $\mu^* = \mu$. It leads to

$$(q_{i,z}^2 - q_{j,z}^{*2}) \iint_S \left(\varepsilon \mathbf{E}_i \cdot \mathbf{E}_j^* - \mu \mathbf{H}_i \cdot \mathbf{H}_j^* \right) dS = 0 \quad (4.77)$$

Therefore, as long as there is no loss and if $q_{i,z}^2 \neq q_{j,z}^{*2}$, we obtain that

$$\iint_S \left(\varepsilon \mathbf{E}_i \cdot \mathbf{E}_j^* - \mu \mathbf{H}_i \cdot \mathbf{H}_j^* \right) dS = 0 \quad (4.78)$$

4.5 Conclusion

The peculiar properties of wire medium made of conducting wires have been investigated for many years. In this section, we first reminded different models proposed in the literature to describe the behaviour of the wire medium. These models show that, at sufficiently high frequency, three modes can coexist inside the structure despite its subwavelength periodicity: the TE, TM and TEM modes.

The TE mode poorly interact with the wires and therefore depends only on the host medium in which the wires are embedded. The TM mode is strongly interacting with the wires. To that mode, a threshold frequency can be associated, under which the TM mode is evanescent. This threshold frequency is called the plasma frequency due to the fact that the WM was originally used to mimic plasma. Last, the TEM mode is a mode that is trapped by the wires and propagates along them.

Since the models of the literature are based on hypotheses that cannot be easily removed, we developed another model that can be easily adapted to provide more accurate results. Using this model, the TE, TM and TEM modes are re-obtained. Moreover, the plasma frequency provided by our model is close to that found in the literature.

Last we showed that the modes inside a lossless wire medium are orthogonal to each others using a specific scalar product and presented the proof.

Chapter 5

Conclusion and prospects

As highlighted in the introduction, in the metamaterials community, little attention has been given to the concept of spatial coherence. It is due to the fact that, at low frequencies, man-made sources are generally used, such as antennas. The fields emitted by these sources are fully coherent, so that this concept is not relevant.

However, at infrared and optical frequencies, the fields are generally originating from thermal sources, so that the fields incident on a given structure will only be partially coherent. Characterizing a metamaterial at such frequencies needs to deal with this partial coherence in order to provide accurate results. A proper treatment of the coherence is particularly crucial in absorption problems, for which the power absorbed by a structure is a quadratic quantity of the incident fields.

In the introduction, we highlighted the two main objectives of this thesis, namely the efficient simulation and the characterization of the absorption capabilities of metamaterials, taking into account the spatial coherence of the fields. Through this manuscript, we presented the solutions we found to answer to these objectives.

5.1 Simulation of non-periodic structures

In Chapter 1, the PMCHWT formulation of the Method of Moments was re-derived, starting from Maxwell's equations. This method can be used to compute the response of non-periodic structures to incident electromagnetic fields. First, the surface of the structure is discretized into basis and testing functions. The basis functions are used to expand the unknown equivalent currents on the surface of the structure, while the testing functions are used to impose the continuity of the tangential fields across the interface.

In order to find the equivalent currents on the surface of the sphere, one needs to fill the impedance matrix and to invert it. In order to fill the impedance matrix, the interactions between the basis functions and the testing functions is computed. This interaction corresponds to the convolution of the Green's function with the currents on the basis functions, and then the integration of the resulting function into the testing function. Since the Green's function is singular at the origin, the resulting 4D integral may be time consuming and inaccurate if it is not properly tackled.

To solve this issue, a fully analytical solution of the integral has been proposed. It is based on the observation that the 4D integral is taking place in a 6D space, each point in this 6D space corresponding to a pair of positions in the classical 3D space: one for the source point, and one for the observation point. Using this definition, it can be seen that the Green's function is invariant along three of the six directions of space. Applying recursively the divergence theorem and orthogonal projections, one can find the value of the integral in a fully analytical way.

This technique is not stable for large distance between the basis and testing functions, due to the fact that the analytical evaluation of an integral corresponds to a difference between numbers. The larger the distance, the larger the numbers but the smaller their difference. Since the divergence theorem is applied four consecutive times, the numerical error grows rapidly. It is not a fundamental problem since for distant interactions, the Green's function is not singular and traditional integration techniques based on Gaussian quadratures show great performances.

Some prospective work is foreseen. First, as mentioned, the method becomes unstable for large distances between the basis and testing functions. This ill-conditioning is actually appearing in many other techniques proposed in the literature. However, through a reformulation of the different terms, it is possible to manipulate the final expression to obtain a more stable result. Finding a solution to that problem could be interesting from both a theoretical and numerical point of view.

Another future work is to provide the code that implement the proposed method in open-source form. Indeed, using an efficient book-keeping strategy, the method can be very rapid. However, the implementation of such an algorithm can be long and painful. Providing some code for public use or even benchmarking, as already done by A. Polimeridis, could therefore ease the use of the method by other researchers.

5.2 Periodic Method of Moments

After dealing with non-periodic structures, the simulations were extended to 2D periodic arrays of scatterers. Using the Bloch theorem, the simulation

of the infinite structure can be reduced to an infinite number of simulations over one unit cell of the structure: one simulation for every possible phase shift between consecutive unit cells (first Brillouin zone of the structure).

The Method of Moments can handle such periodic simulations using a periodic Green's function instead of the classical one, and convolving this periodic Green's function with the basis functions and testing functions. In the literature, most of the efforts have been spent on devising methods to rapidly compute this periodic Green's function, while few efforts have been spent on its integration.

We showed an alternative solution based on the plane-wave expansion of the fields. Using this formulation, there is no need to evaluate the periodic Green's function, so that the integration step can be avoided too. We showed that, provided that the distance between the basis and testing functions is large enough, an extremely rapid evaluation of the periodic impedance matrix is possible. For basis functions and testing functions that are close, a estimation procedure based on the Taylor expansion of the impedance matrix is proposed. This method has the advantage that the computationally intensive part of the procedure is independent from the phase shift between consecutive unit cells and is therefore done once and for all.

An estimate of the convergence of the proposed method is presented and it is shown that the method is particularly well suited for densely packed arrays of 3D inclusions, provided that the simulations are conducted for many phase shifts between consecutive unit cells. This description perfectly fits with the objectives of Thesis (characterization of metamaterials).

We also proposed a post-processing method that can be applied to the impedance matrix to simulate a semi-infinite 3D periodic structure. This method is based on the use of fictitious interfaces. Characterizing the response of one layer through its interfaces, it is possible to stack two of these layers to obtain the response of a 2-layers structure. These 2-layers structures can then be stacked to obtain the response of a 4-layers structure and so on. Using this iterative procedure the number of layers grows exponentially. It is shown that the convergence is better than exponential with respect to the number of iterations, so that machine precision can be reached in a negligible amount of time. To our best knowledge, it is the first time that full-wave simulation of semi-infinite metamaterials is conducted. This method can be very useful for the study of surface-related phenomena.

Using the impedance matrix of the semi-infinite 3D periodic structure, the modes within a metamaterials can be found by solving an eigenvalue problem. The proposed method differs from other linear methods proposed in the literature in the sense that it does not entail any back-propagation and is therefore numerically stable. The convergence of the proposed method is

derived and assessed numerically.

Last, we presented a method to simulate defects in otherwise perfectly periodic structures. This method is based on the fictitious sources superposition method [47]. Introducing a defect in the otherwise perfectly periodic structure, this defect will scatter the fields. For that reason, it can be modelled as an equivalent source whose value depends on the local value of the fields. Noticing that this problem is quite similar to the basic principle of the Method of Moments, where equivalent currents are to be found, a MoM based formulation of the method was proposed.

The work in this thesis can still be improved in many ways. First, the computation of the impedance matrix for basis and testing functions that are close is still quite time consuming. The acceleration of this step could be investigated. One lead that can be investigated is the use of traditional techniques based on the periodic Green's function for close interactions and the plane-wave expansion for more distant interactions.

The last method presented for the simulation of defects implies an integration of the infinite array solutions of the MoM over the first Brillouin zone. For now, this integration is approximated using a Riemann sum. However, a better quadrature can surely be devised, especially introducing some contour deformation into the complex plane for the transverse phase shifts.

5.3 Characterization of periodic absorbers

Being able to compute the response of periodic and non-periodic structures to any incident fields, the next step consisted in characterizing the absorption capabilities of some metamaterials taking into account the spatial coherence of the fields.

To do this, we used the formalism proposed in [30], which is based on the fact that a finite structure can only absorb fields through a limited number of independent degrees of freedom: the natural absorption modes of the structure. Computing these modes, the problem of evaluating the absorption in a given structure becomes linear with respect to the intensity of these natural modes, simplifying the whole procedure.

An extension to infinite periodic structures was proposed in [31] for 2D problems with a scalar wave function. In Chapter 3, we extended this formalism to 3D geometries and polarized wave function. It was shown theoretically and through a practical example that characterizing a periodic structure through the way it absorbs incident plane waves for different angles of incidence is not correct, except if the periodicity of the structure is smaller than half the wavelength, if the coupling in the absorption between the two possible polarization of the fields is negligible and if one only wants to

characterize the absorption capabilities for far-field excitations. Note that in the case where these three hypotheses are ensured, it is proven that the natural absorption modes of the structure are corresponding to these plane waves, so that *in fine* the structure is still characterized through its natural absorption modes.

After deriving the formalism, it has been applied to two different plasmonic absorbers: a silver slab and a period array of free-standing silver rods. The absorption mechanisms taking place inside these structures were highlighted. In the silver slab, the absorption is mainly mediated through the evanescent surface plasmon supported by its interface. In the wire medium, we counted three different absorption mechanisms: two slightly evanescent long-range surface modes and a strongly evanescent short-range mechanism.

In order to exploit these absorption mechanisms, a scattering layer with a controlled periodicity has been added on top of the structure. Playing with the periodicity of the scattering layer, propagative incident plane waves can be coupled to the absorption modes, increasing the absorption by one order of magnitude. Long-range surface modes provide angularly selective absorption, while short-range surface modes offer wide-angle absorption.

Concerning the prospects, the most obvious one would be to continue the design of the improved absorber, in order to further increase the absorption and realize a prototype as a proof of concept.

In a more general perspective, the application of EAI to other domains where the absorption has an important role and must be carefully controlled could be highly beneficial, despite its apparent complexity. Such applications can for example be found in the medical domain, where the power absorption inside a body must be carefully limited [143] or sometimes maximized in the region of a tumour [144, 145, 146].

We are also convinced that the EAI formalism can be easily adapted to the reverse problem: the black-body radiation. In that case, this formalism would find many applications such as noise filtering, when the noise is thermal in origin, or the beamforming of incoherent sources.

5.4 Modelling of the Wire Medium

In Chapter 4, a periodic medium made of vertically aligned conducting wires embedded in a dielectric matrix has been studied. As shown by several models proposed in the literature, this medium may support three different propagative modes even for deeply subwavelength periodicity. Most interestingly, one of these modes (TEM mode) is propagative whatever the transverse wavenumber of the excitation. The appearance of such a propagative mode for very high transverse wave vectors can be used to increase the absorption [176].

For that reason, a complete model for the determination of the propagating modes within the wire medium was derived. The proposed model is a trade-off between simplified models available in the literature, which are good at providing an intuitive understanding of the physics, and the full-wave simulation of the wire medium, which is computationally more intensive and provides few physical insights. It was also shown that the eigenmodes within the wire medium are characterized by some orthogonality properties.

This part of the work was stopped too early to provide results in accordance with the objectives of this Thesis, mainly due to the lack of time. However, we believe that this work has been made general enough to be extended to lossy structures and even plasmonic wires by properly adapting the boundary conditions. One possible extension is to use contrast sources to model the scattering by the wires.

Starting from the fast and accurate evaluation of 4D singular integrals involved in the MoM, continuing through impedance matrix manipulations for the simulation of 3D semi-infinite metamaterials or 2D defective arrays, including the theory of spatial coherence and the EAI formalism into the numerical techniques, applying the resulting methods to periodic structures and last optimizing a periodic absorber for wide-angle absorption, this Thesis covered several key aspects of the original objectives. However, there is plenty of room for improvements and innovations and many leads could not be investigated in the limited time of a PhD. The next step will probably consist in testing the observations that have been made on a prototype, closing the loop through an experimental validation.

Appendix A

Detailed proofs

In this Appendix are provided the proofs that were removed from the text for better readability.

A.1 Proof of the Green's formalism

Knowing that

$$\nabla^2 G(\mathbf{r}, \mathbf{r}') + k_0^2 G(\mathbf{r}, \mathbf{r}') = -\delta(\mathbf{r} - \mathbf{r}'), \quad (\text{A.1})$$

we want to prove that, for any scalar function $F(\mathbf{r})$, the $\varphi(\mathbf{r})$ function given by

$$\varphi(\mathbf{r}) = \iiint G(\mathbf{r}, \mathbf{r}') F(\mathbf{r}') dV(\mathbf{r}') \quad (\text{A.2})$$

is a solution to the Helmholtz equation

$$\nabla^2 \varphi + k^2 \varphi = -F(\mathbf{r}) \quad (\text{A.3})$$

where $F(\mathbf{r})$ is acting as the source term.

Starting from (A.1), one can multiply both the RHS and the LHS by the same function without breaking the equality

$$F(\mathbf{r}') (\nabla^2 G(\mathbf{r}, \mathbf{r}') + k_0^2 G(\mathbf{r}, \mathbf{r}')) = -F(\mathbf{r}') \delta(\mathbf{r} - \mathbf{r}'). \quad (\text{A.4})$$

$F(\mathbf{r}')$ being independent from $\mathbf{r}$, it can be distributed and then introduced inside the ∇^2 operator. Since (A.4) is true for any coordinate $\mathbf{r}'$, it can be reformulated in a weaker form by integrating the LHS and RHS over the whole space:

$$\begin{aligned} \iiint \left(\nabla^2 F(\mathbf{r}') G(\mathbf{r}, \mathbf{r}') + k_0^2 G(\mathbf{r}, \mathbf{r}') \right) dV(\mathbf{r}') \\ = - \iiint F(\mathbf{r}') \delta(\mathbf{r} - \mathbf{r}') dV(\mathbf{r}'). \end{aligned} \quad (\text{A.5})$$

Again, it can be noticed that the integral is carried over the $\mathbf{r}'$ coordinates while the ∇^2 operator is applied to the $\mathbf{r}$ coordinates. Distributing the integral, switching the integral and derivation order and using the property of the delta distribution, one obtains

$$\begin{aligned} \nabla^2 \left(\iiint F(\mathbf{r}') G(\mathbf{r}, \mathbf{r}') dV(\mathbf{r}') \right) \\ + k_0^2 \left(\iiint F(\mathbf{r}') G(\mathbf{r}, \mathbf{r}') dV(\mathbf{r}') \right) = -F(\mathbf{r}). \end{aligned} \quad (\text{A.6})$$

Substituting (A.2) into (A.6), one obtains Equation (A.3).

A.2 EFIE for div-conformal BF and TF

In this section, the development that allows one to go from (1.46c) to (1.49) using the div-conformality of the BF and TF is detailed.

The starting point is the general formula of the EFIE:

$$\begin{aligned} Z_i^{EJ}[j, k] = \iint_{\partial\Omega} \mathbf{f}_{Tj}(\mathbf{r}) \cdot \left[\frac{-j\eta_i(k_i^2 + \nabla\nabla\cdot)}{k_i} \right. \\ \left. \times \iint_{\partial\Omega} G_i(\mathbf{r}, \mathbf{r}') \mathbf{f}_{Bk}(\mathbf{r}') dS(\mathbf{r}') \right] dS(\mathbf{r}) \end{aligned} \quad (\text{A.7})$$

First of all, since the BF and TF have a limited extend, the integrals over the whole surface $\partial\Omega$ can be limited to the integral over the surface of the BF (S') and the surface of the TF (S). Applying this and distributing the sum in (A.7) leads to

$$\begin{aligned} Z_i^{EJ}[j, k] = \frac{-j\eta_i}{k_i} \left[k_i^2 \iint_S \iint_{S'} \mathbf{f}_{Tj}(\mathbf{r}) \cdot \mathbf{f}_{Bk}(\mathbf{r}') G_i(\mathbf{r}, \mathbf{r}') dS(\mathbf{r}') dS(\mathbf{r}) \right. \\ \left. + \iint_S \mathbf{f}_{Tj}(\mathbf{r}) \cdot \left(\nabla\nabla\cdot \iint_{S'} \mathbf{f}_{Bk}(\mathbf{r}') G_i(\mathbf{r}, \mathbf{r}') dS(\mathbf{r}') \right) dS(\mathbf{r}) \right] \end{aligned} \quad (\text{A.8})$$

Concentrating on the second term, using the identity

$$\mathbf{f} \cdot \nabla g = \nabla \cdot (g\mathbf{f}) - g\nabla \cdot \mathbf{f} \quad (\text{A.9})$$

with $\mathbf{f}_T$ as the vector field and the divergence of the integral of over the BF

as the scalar field, it leads to

$$\begin{aligned}
& \iint_S \mathbf{f}_{Tj}(\mathbf{r}) \cdot \left(\nabla \nabla \cdot \iint_{S'} \mathbf{f}_{Bk}(\mathbf{r}') G_i(\mathbf{r}, \mathbf{r}') dS(\mathbf{r}') \right) dS(\mathbf{r}) \\
&= \iint_S \nabla \cdot \left(\mathbf{f}_{Tj}(\mathbf{r}) \cdot \left(\nabla \cdot \iint_{S'} \mathbf{f}_{Bk}(\mathbf{r}') G_i(\mathbf{r}, \mathbf{r}') dS(\mathbf{r}') \right) \right) dS(\mathbf{r}) \quad (\text{A.10}) \\
&- \iint_S (\nabla \cdot \mathbf{f}_{Tj}(\mathbf{r})) \cdot \left(\nabla \cdot \iint_{S'} \mathbf{f}_{Bk}(\mathbf{r}') G_i(\mathbf{r}, \mathbf{r}') dS(\mathbf{r}') \right) dS(\mathbf{r})
\end{aligned}$$

Using the divergence theorem on each halves of the TF, the first term of the RHS of (A.10) becomes

$$\begin{aligned}
& \iint_S \nabla \cdot \left(\mathbf{f}_{Tj}(\mathbf{r}) \cdot \left(\nabla \cdot \iint_{S'} \mathbf{f}_{Bk}(\mathbf{r}') G_i(\mathbf{r}, \mathbf{r}') dS(\mathbf{r}') \right) \right) dS(\mathbf{r}) \\
&= \oint_{\partial S_1} \hat{\mathbf{n}}_1(\mathbf{r}) \cdot \mathbf{f}_T \left(\nabla \cdot \iint_{S'} \mathbf{f}_{Bk}(\mathbf{r}') G_i(\mathbf{r}, \mathbf{r}') dS(\mathbf{r}') \right) dl(\mathbf{r}) \quad (\text{A.11}) \\
&+ \oint_{\partial S_2} \hat{\mathbf{n}}_2(\mathbf{r}) \cdot \mathbf{f}_T \left(\nabla \cdot \iint_{S'} \mathbf{f}_{Bk}(\mathbf{r}') G_i(\mathbf{r}, \mathbf{r}') dS(\mathbf{r}') \right) dl(\mathbf{r})
\end{aligned}$$

with S_1 and S_2 the surfaces of the two halves of the TF, ∂S_i the boundary of surface S_i , $\hat{\mathbf{n}}_i(\mathbf{r})$ the outer normal to ∂S_i in $\mathbf{r}$ and $\oint$ denoting the integral over a closed contour. Noticing that $\hat{\mathbf{n}}_i \cdot \mathbf{f}_T = 0$ on the external edges of the TF and that the contributions of the internal edge for each half TF cancel out due to the fact that $\hat{\mathbf{n}}_1 = -\hat{\mathbf{n}}_2$ on that edge, one finally obtains that the contribution of that term vanishes. Equation (A.10) becomes

$$\begin{aligned}
& \iint_S \mathbf{f}_{Tj}(\mathbf{r}) \cdot \left(\nabla \nabla \cdot \iint_{S'} \mathbf{f}_{Bk}(\mathbf{r}') G_i(\mathbf{r}, \mathbf{r}') dS(\mathbf{r}') \right) dS(\mathbf{r}) \\
&= - \iint_S (\nabla \cdot \mathbf{f}_{Tj}(\mathbf{r})) \cdot \left(\nabla \cdot \iint_{S'} \mathbf{f}_{Bk}(\mathbf{r}') G_i(\mathbf{r}, \mathbf{r}') dS(\mathbf{r}') \right) dS(\mathbf{r}) \quad (\text{A.12})
\end{aligned}$$

Using a similar reasoning, the second factor of the RHS of (A.12) can be simplified:

$$\begin{aligned}
& \nabla \cdot \iint_{S'} \mathbf{f}_{Bk}(\mathbf{r}') G_i(\mathbf{r}, \mathbf{r}') dS(\mathbf{r}') \\
&= \iint_{S'} \nabla \cdot (\mathbf{f}_{Bk}(\mathbf{r}') G_i(\mathbf{r}, \mathbf{r}')) dS(\mathbf{r}'), \quad (\text{A.13a})
\end{aligned}$$

$$= \iint_{S'} (\nabla \cdot \mathbf{f}_{Bk}(\mathbf{r}')) G_i(\mathbf{r}, \mathbf{r}') dS(\mathbf{r}') \quad (\text{A.13b})$$

$$\begin{aligned}
& + \iint_{S'} \mathbf{f}_{Bk}(\mathbf{r}') \cdot \nabla G_i(\mathbf{r}, \mathbf{r}') dS(\mathbf{r}'), \\
& = - \iint_{S'} \mathbf{f}_{Bk}(\mathbf{r}') \cdot \nabla' G_i(\mathbf{r}, \mathbf{r}') dS(\mathbf{r}'), \tag{A.13c}
\end{aligned}$$

$$\begin{aligned}
& = - \iint_{S'} \nabla' \cdot (\mathbf{f}_{Bk}(\mathbf{r}') \cdot G_i(\mathbf{r}, \mathbf{r}')) dS(\mathbf{r}') \\
& \quad + \iint_{S'} (\nabla' \cdot \mathbf{f}_{Bk}(\mathbf{r}')) G_i(\mathbf{r}, \mathbf{r}') dS(\mathbf{r}'), \tag{A.13d}
\end{aligned}$$

$$= \iint_{S'} (\nabla' \cdot \mathbf{f}_{Bk}(\mathbf{r}')) G_i(\mathbf{r}, \mathbf{r}') dS(\mathbf{r}'), \tag{A.13e}$$

where (A.13b) is obtained using the identity

$$\nabla \cdot (g\mathbf{f}) = \nabla g \cdot \mathbf{f} + g\nabla \cdot \mathbf{f}, \tag{A.14}$$

(A.13c) is obtained considering that $\mathbf{f}_B$ is independent from the $\mathbf{r}$ coordinates, and (A.13e) is obtained using a similar development as in (A.11).

Putting everything together, one obtains Equation (1.49).

A.3 Treatment of singular zones in Section 1.3

In this section, we will show that, most of the time, no particular treatment is required for the possibly singular region where $R \rightarrow 0$. This section follows the same reasoning as [59], but extends it to higher dimensions.

Since the divergence theorem is only valid for sufficiently smooth functions, singular integrands need a special care. Following a “divide-and-conquer” strategy, the integration domain is split into two parts, one corresponding to the singular region of vanishing extent and the other one corresponding to the rest of the domain of integration, over which the integrand is regular.

Consider the regular function f and the vector field $\mathbf{g}_i$ such that

$$f(\mathbf{u})R^{(i-1)}(\mathbf{u}) = \nabla \cdot \mathbf{g}_i(\mathbf{u}), \quad \forall \mathbf{u} \in \{\mathbf{u} | R(\mathbf{u}) \geq R_0\}. \tag{A.15}$$

with R the distance function, $R_0 > 0$ and $i \geq 0$. In the following, we will consider the limit $R_0 \rightarrow 0^+$. We want to solve the following integral over a k -dimensional domain Ω :

$$I_S = \int_{\Omega} f R^{(i-1)} dV_k^k. \tag{A.16}$$

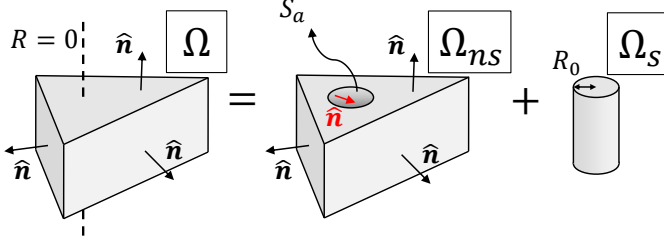


Figure A.1: Singularity treatment of a 3D volume with the R function varying only along two dimensions.

First, we separate the domain of integration Ω into two parts, Ω_{ns} and Ω_s , such that

$$\Omega_s = \Omega \cap \{\mathbf{u} | R(\mathbf{u}) < R_0\}, \quad (\text{A.17a})$$

$$\Omega_{ns} = \Omega \setminus \Omega_s. \quad (\text{A.17b})$$

In Figure A.1, an example is provided for a 3D volume with a distance function varying along two out of the three coordinates. Splitting the integral of (A.16) and substituting (A.15) where the equation is valid gives

$$I_S = \int_{\Omega_{ns}} \nabla \cdot \mathbf{g} \, dV_k^k + \int_{\Omega_s} f R^{(i-1)} \, dV_k^k. \quad (\text{A.18})$$

The goal of this section is to provide a sufficient condition to simply neglect the singular zone, i.e. a sufficient condition for the following identity to hold true:

$$\int_{\Omega_{ns}} \nabla \cdot \mathbf{g} \, dV_k^k + \int_{\Omega_s} f R^{(i-1)} \, dV_k^k = \oint_{\partial\Omega} \mathbf{g} \cdot \hat{\mathbf{n}} \, dV_{k-1}^k, \quad (\text{A.19})$$

with $\partial\Omega$ the surface of Ω and $\hat{\mathbf{n}}$ the outer unit normal of $\partial\Omega$. First, we will derive a sufficient condition for the contribution of the integral over Ω_s to be negligible. Then, we will tackle the contribution of the surface $\{\partial\Omega_{ns}\} \setminus \{\partial\Omega\}$ (surface S_a in Figure A.1).

Singular volume Consider the shape of the volume Ω_s . Along the $\hat{\mathbf{u}}_{1 \rightarrow 3}$ directions, which the R function depends on, it will correspond to a circle (2D) or a sphere (3D) of radius R_0 . Along the $\hat{\mathbf{u}}_{4 \rightarrow 6}$ directions, the volume corresponds to a line (1D), polygon (2D) or polyhedron (3D) whose length, surface or volume will be denoted by h . Figure A.1 depicts the case of a 3D volume, with a R function that only varies along two out of the three dimensions spanned by the volume.

We introduce $f_{\max}$ such that $\forall \mathbf{u} \in \Omega$, we have $|f(\mathbf{u})| < f_{\max}$. We can then write

$$\left| \int_{\Omega_s} f R^{(i-1)} dV_k^k \right| \leq \int_{\Omega_s} |f R^{(i-1)}| dV_k^k \quad (\text{A.20a})$$

$$< f_{\max} \int_{\Omega_s} R^{(i-1)} dV_k^k. \quad (\text{A.20b})$$

It can be noticed that the integrand of the RHS of (A.20b) is only depending on R , so that the integration over dimensions $\hat{\mathbf{u}}_{4 \rightarrow 6}$ can be done in a trivial way:

$$f_{\max} \int_{\Omega_s} R^{(i-1)} dV_k^k = f_{\max} h \int_{\Omega_s^R} R^{(i-1)} dV_N^3, \quad (\text{A.21})$$

with Ω_s^R the section of Ω_s in the $\hat{\mathbf{u}}_{1 \rightarrow 3}$ space and N the dimensionality of this section ($N = 2$ for a circle, and $N = 3$ for a sphere). Then, performing the integration over a circle or a sphere, one can find that

$$f_{\max} h \int_{\Omega_s^R} R^{(i-1)} dV_N^3 \leq f_{\max} h \frac{4\pi}{i+2} R_0^{(i+N-1)}. \quad (\text{A.22})$$

Since $R_0 \rightarrow 0^+$, the RHS of (A.22) vanishes as long as $(i + N - 1) > 0$, which will always be the case.

Singular surface Since the second term of the LHS of (A.19) vanishes for all the cases encountered in this paper, we want to derive a sufficient condition for the following identity to be true:

$$\int_{\Omega_{\text{ns}}} \nabla \cdot \mathbf{g} dV_k^k = \oint_{\partial\Omega} \mathbf{g} \cdot \hat{\mathbf{n}} dV_{k-1}^k. \quad (\text{A.23})$$

It can be noticed that, removing Ω_s from Ω , the surface of the new volume of integration has been modified in two ways. First, a small part of the surface of Ω corresponding to the part where $R < R_0$ has been removed. In Figure A.1, it corresponds to the top and bottom surfaces of Ω_s . Moreover, a new surface S_a corresponding to the interface between Ω_{ns} and Ω_s has been created. Applying the divergence theorem and splitting the LHS of (A.23) into two parts gives

$$\oint_{\partial\Omega} \mathbf{g} \cdot \hat{\mathbf{n}} dV_{k-1}^k + \int_{S_a} \mathbf{g} \cdot \hat{\mathbf{n}} dV_{k-1}^k = \oint_{\partial\Omega} \mathbf{g} \cdot \hat{\mathbf{n}} dV_{k-1}^k, \quad (\text{A.24})$$

were the Cauchy integral of the LHS appears due to the fact that the singular zone $R = 0$ has been removed from the surface of integration. We can now consider three different cases:

1. $\mathbf{g} \cdot \hat{\mathbf{u}}_{1 \rightarrow 3} = 0$:

Since $\hat{\mathbf{n}}$ is orthogonal to the $\hat{\mathbf{u}}_{4 \rightarrow 6}$ directions on S_a , if $\mathbf{g}$ is a linear combination these directions, (A.24) is always true.

2. $\mathbf{g} \cdot \hat{\mathbf{u}}_{1 \rightarrow 3} \neq 0$, but $\lim_{R \rightarrow 0} (|\mathbf{g}| R^{(N-1)}) = 0$:

Then, (A.24) is again verified. Indeed,

$$\begin{aligned} \int_{S_a} \mathbf{g} \cdot \hat{\mathbf{n}} dV_{k-1}^k &\leq \int_{S_a} |\mathbf{g}| dV_{k-1}^k \\ &\leq h \int_{\partial \Omega_a^R} |\mathbf{g}| dV_N^3 \\ &< h g_{\max} 4\pi R_0^{(N-1)} \rightarrow 0, \end{aligned} \quad (\text{A.25})$$

with $g_{\max}$ that has been chosen such that $\forall \mathbf{u} \in S_a$, we have $g_{\max} > |\mathbf{g}|$.

3. *Otherwise* :

The case where none of the conditions above is verified and thus (A.24) is not true is never appearing throughout the paper for the singular zone $R \rightarrow 0$.

However, in Equation (1.87b), another singular zone appears for $R \neq 0$ and $P_q \rightarrow 0$. Redoing the development of this section for that particular case, it can be seen that the contribution of the small area $P_q < P_{q,0}$, with $P_{q,0} \rightarrow 0^+$, vanishes while the contribution of the additional boundary $P_q = P_{q,0}$ is not negligible and corresponds to the second term of the RHS of (1.88). For a detailed development, the reader is referred to Equation (5) of [59] or Equations (39) and (40) of [62].

A.4 Fields emitted by 3D quasi-periodic currents

Consider an infinite homogeneous medium of permittivity ε and permeability μ . It is excited by an impressed electric current distribution $\mathbf{J}(\mathbf{r})$. The goal of this Sections is to show how the fields generated by the sources can be computed in the spectral domain. One important feature of the spectral solution is that each spectral component of the fields only depends on the corresponding spectral component of the currents.

As always in classical electromagnetics, everything begins with the Maxwell's equations. To take the rotational of (1.1d), substitute (1.1c) and exploit the identity

$$\nabla \times \nabla \times \mathbf{G}(\mathbf{r}) = \nabla \nabla \cdot \mathbf{G}(\mathbf{r}) - \nabla^2 \mathbf{G}(\mathbf{r}) \quad (\text{A.26})$$

leads to

$$\nabla \nabla \cdot \mathbf{H}(\mathbf{r}) - \nabla^2 \mathbf{H}(\mathbf{r}) = \nabla \times \mathbf{J}(\mathbf{r}) - j\omega\varepsilon \mathbf{M}(\mathbf{r}) + \omega^2\varepsilon\mu \mathbf{H}(\mathbf{r}). \quad (\text{A.27})$$

Since the magnetic currents are set to zero, the magnetic charge density is null, so that $\nabla \cdot \mathbf{H} = 0$. Consequently, the formula can be simplified:

$$\nabla^2 \mathbf{H}(\mathbf{r}) + k_0^2 \mathbf{H}(\mathbf{r}) = -\nabla \times \mathbf{J}(\mathbf{r}), \quad (\text{A.28})$$

with k_0 the wavenumber inside the medium, *i.e.* $k_0^2 = \omega^2\mu\varepsilon$.

At this point, it is useful to introduce the Fourier Transform (FT) of the currents and the magnetic fields, $\tilde{\mathbf{J}}(\mathbf{k}')$ and $\tilde{\mathbf{H}}(\mathbf{k}')$, respectively:

$$\mathbf{J}(\mathbf{r}) = \frac{1}{8\pi^3} \iiint \mathbf{J}_0(\mathbf{k}') \exp(-j \mathbf{k}' \cdot \mathbf{r}) d\mathbf{k}', \quad (\text{A.29a})$$

$$\mathbf{H}(\mathbf{r}) = \frac{1}{8\pi^3} \iiint \mathbf{H}_0(\mathbf{k}') \exp(-j \mathbf{k}' \cdot \mathbf{r}) d\mathbf{k}'. \quad (\text{A.29b})$$

Substituting (A.29) into (A.28), using the identity

$$\nabla \times (\varphi \mathbf{G}) = \nabla \varphi \times \mathbf{G} + \varphi \nabla \times \mathbf{G} \quad (\text{A.30})$$

and rearranging the integration and derivation orders leads to

$$\begin{aligned} & \iiint (k_0^2 - k'^2) \mathbf{H}_0(\mathbf{k}') \exp(-j \mathbf{k}' \cdot \mathbf{r}) d\mathbf{k}' \\ &= \iiint j \mathbf{k}' \times \mathbf{J}_0(\mathbf{k}') \exp(-j \mathbf{k}' \cdot \mathbf{r}) d\mathbf{k}' \end{aligned} \quad (\text{A.31})$$

with $k'^2 = \mathbf{k}' \cdot \mathbf{k}'$.

To isolated the contribution of one spectral component of the currents, one possibility is to multiply both the LHS and RHS by a phase factor $\exp(j \mathbf{k} \cdot \mathbf{r})$ and then integrate on both sides over the whole space, leading to

$$\begin{aligned} & \iiint (k_0^2 - k'^2) \mathbf{H}_0(\mathbf{k}') \iiint \exp[-j (\mathbf{k}' - \mathbf{k}) \cdot \mathbf{r}] d\mathbf{r} d\mathbf{k}' \\ &= \iiint j \mathbf{k}' \times \mathbf{J}_0(\mathbf{k}') \iiint \exp[-j (\mathbf{k}' - \mathbf{k}) \cdot \mathbf{r}] d\mathbf{r} d\mathbf{k}' \end{aligned} \quad (\text{A.32})$$

Noticing that

$$\iiint \exp[-j (\mathbf{k}' - \mathbf{k}) \cdot \mathbf{r}] d\mathbf{r} = \delta(\mathbf{k}' - \mathbf{k}) \quad (\text{A.33})$$

and using the properties of the Dirac's delta function, it finally leads to

$$(k_0^2 - k^2) \mathbf{H}_0(\mathbf{k}) = j \mathbf{k} \times \mathbf{J}_0(\mathbf{k}) \quad (\text{A.34})$$

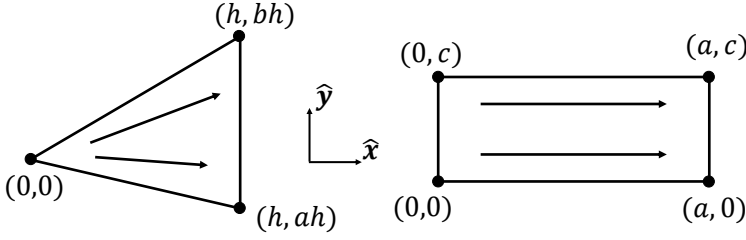


Figure A.2: Local system of coordinates and parametrization used to compute the FT of half-RWG and half-rooftop functions

with $k^2 = \mathbf{k} \cdot \mathbf{k}$. It is important to emphasize that k^2 is not the norm of vector $\mathbf{k}$. Indeed, for non-zero complex $\mathbf{k}$, k^2 may be null or even negative.

Equation (A.34) suggests that the amplitude of a given spectral component of the magnetic field is only depending on the corresponding spectral component of the sources. It is logical considering that, in spatial domain, one has to convolve the sources with the Green's function to obtain the fields. Applying a FT, the convolution becomes a simple multiplication.

In order to find the FT of the electric field generated by the electric sources, one can start from Equation (1.1d):

$$\nabla \times \mathbf{H}(\mathbf{r}) = \mathbf{J}(\mathbf{r}) + j\omega\varepsilon\mathbf{E}(\mathbf{r}) \quad (\text{A.35})$$

Manipulating (A.35), using (A.34) to get rid of the $\tilde{\mathbf{H}}$ term and using the identity

$$-\mathbf{k} \times \mathbf{k} \times \tilde{\mathbf{J}} = k^2 \tilde{\mathbf{J}} - (\mathbf{k} \cdot \tilde{\mathbf{J}})\mathbf{k}, \quad (\text{A.36})$$

one straightforwardly obtains

$$\mathbf{E}_0(\mathbf{k}) = \frac{j\eta_0}{k_0} \frac{1}{(k_0^2 - k^2)} \left[k_0^2 \mathbf{J}_0(\mathbf{k}) - (\mathbf{k} \cdot \mathbf{J}_0(\mathbf{k}))\mathbf{k} \right] \quad (\text{A.37})$$

A.5 Fourier Transform of RWG and rooftop function

The goal of this section is to provide the analytical FT of the rectangles and triangles constituting the RWG, rooftop and hybrid functions. First of all, a local system of coordinates is used and the polygons are characterized through the parameters illustrated in Fig. A.2.

Using these conventions, the FT of the $\hat{\mathbf{x}}$ component of a triangle reads

$$\begin{aligned}
 J_x^{\text{tri}}(k_x, k_y) = & \frac{j}{k_y h} \left[\frac{j h}{k_x + b k_y} \exp(-j(k_x + b k_y)h) \right. \\
 & + \frac{1}{(k_x + b k_y)^2} \left[\exp(-j(k_x + b k_y)h) - 1 \right] \\
 & - \frac{j h}{k_x + a k_y} \exp(-j(k_x + a k_y)h) \\
 & \left. - \frac{1}{(k_x + a k_y)^2} \left[\exp(-j(k_x + a k_y)h) - 1 \right] \right],
 \end{aligned} \tag{A.38}$$

the FT of the $\hat{\mathbf{y}}$ component of a triangle reads

$$\begin{aligned}
 J_y^{\text{tri}}(k_x, k_y) = & \frac{1}{h k_y} \left[-\frac{b h}{k_x + b k_y} \exp(-j(k_x + b k_y)h) \right. \\
 & + \left[\frac{j b}{(k_x + b k_y)^2} + \frac{j}{k_y (k_x + b k_y)} \right] \\
 & \quad \times \left[\exp(-j(k_x + b k_y)h) - 1 \right] \\
 & + \frac{a h}{k_x + a k_y} \exp(-j(k_x + a k_y)h) \\
 & - \left[\frac{j a}{(k_x + a k_y)^2} + \frac{j}{k_y (k_x + a k_y)} \right] \\
 & \quad \times \left[\exp(-j(k_x + a k_y)h) - 1 \right] \Big]
 \end{aligned} \tag{A.39}$$

and the $\hat{\mathbf{x}}$ component of a rectangle reads

$$\begin{aligned}
 J_x^{\text{rect}}(k_x, k_y) = & \frac{\exp(-j k_x a)}{k_y a} \left[-\frac{a}{k_x} + \frac{j}{k_x^2} - \frac{j \exp(j k_x a)}{k_x^2} \right] \\
 & \times \left[\exp(-j k_y c) - 1 \right]
 \end{aligned} \tag{A.40}$$

It can be noticed that for some (k_x, k_y) , the function is undetermined. A study of the value of the function at these limits provide the asymptotic value. Generally, considering the high machine precision of computers, just considering the limit value is sufficient to achieve sufficiently good accuracy for most applications. For that reason, the limits have been properly extracted and are provided hereafter. Note that if a higher precision is needed, the value of the functions around the “singular” points can be extrapolated

using a Taylor expansion. Since these singular points correspond to false singularity (the function is actually smooth on these points), the Taylor expansion is converging nicely.

A.5.1 Particular cases for the triangle, $\hat{\mathbf{x}}$ component

Considering the limit cases of (A.38), four of them can be highlighted:

When $(k_x + bk_y) \rightarrow 0$ and $k_y \neq 0$ In that case, it can be shown that

$$\lim_{(k_x + bk_y) \rightarrow 0} \left(\frac{jh}{k_x + bk_y} \exp(-j(k_x + bk_y)h) + \frac{1}{(k_x + bk_y)^2} \times \left[\exp(-j(k_x + bk_y)h) - 1 \right] \right) = \frac{h^2}{2}, \quad (\text{A.41})$$

which can be straightforwardly substituted into (A.38).

When $(k_x + ak_y) \rightarrow 0$ and $k_y \neq 0$ In a similar way, it leads to

$$\lim_{(k_x + ak_y) \rightarrow 0} \left(-\frac{jh}{k_x + ak_y} \exp(-j(k_x + ak_y)h) - \frac{1}{(k_x + ak_y)^2} \times \left[\exp(-j(k_x + ak_y)h) - 1 \right] \right) = -\frac{h^2}{2}, \quad (\text{A.42})$$

which can be straightforwardly substituted into (A.38).

When $k_y \rightarrow 0$ and $k_x \neq 0$ In that case, the limit is given by

$$J_x^{\text{tri}}(k_x, 0) = \frac{j}{h} \left[2jh \frac{a-b}{k_x^2} + \frac{h^2}{k_z} (b-a) + \frac{2}{k_x^3} (a-b) \left(1 - \exp(jk_x h) \right) \right] \exp(-jk_x h). \quad (\text{A.43})$$

When $k_y \rightarrow 0$ and $k_x \rightarrow 0$ In that case, the limit is given by

$$J_x^{\text{tri}}(0, 0) = (b-a) \frac{h^2}{3} \quad (\text{A.44})$$

A.5.2 Particular cases for the triangle, $\hat{y}$ component

Again, for the FT of the $\hat{y}$ component of the triangle, four distinct particular cases can be highlighted:

When $(k_x + bk_y) \rightarrow 0$ and $k_y \neq 0$ In that case, it can be shown that

$$\begin{aligned} \lim_{(k_x + bk_y) \rightarrow 0} & \left[\frac{jh}{k_x + bk_y} \exp(-j(k_x + bk_y)h) \right. \\ & \left. + \frac{1}{(k_x + bk_y)^2} \left[\exp(-j(k_x + bk_y)h) - 1 \right] \right] \\ & = \frac{h}{k_y} + j \frac{bh^2}{2}, \end{aligned} \quad (\text{A.45})$$

which can be straightforwardly substituted in (A.39).

When $(k_x + ak_y) \rightarrow 0$ and $k_y \neq 0$ In that case, it can be shown that

$$\begin{aligned} \lim_{(k_x + ak_y) \rightarrow 0} & \left[-\frac{jh}{k_x + ak_y} \exp(-j(k_x + ak_y)h) \right. \\ & \left. - \frac{1}{(k_x + ak_y)^2} \left[\exp(-j(k_x + ak_y)h) - 1 \right] \right] \\ & = -\frac{h}{k_y} - j \frac{ah^2}{2}, \end{aligned} \quad (\text{A.46})$$

which can be straightforwardly substituted in (A.39).

When $k_y \rightarrow 0$ and $k_x \neq 0$ In that case,

$$\begin{aligned} J_y^{\text{tri}}(k_x, 0) &= \frac{\exp(-jk_x h)}{h} \left[\frac{jh^2}{2k_x} (b^2 - a^2) + \frac{j}{k_x^3} (a^2 - b^2) \right. \\ & \quad \left. \times \left(1 - \exp(jk_x h) \right) - (a^2 - b^2) \frac{h}{k_x^2} \right]. \end{aligned} \quad (\text{A.47})$$

When $k_y \rightarrow 0$ and $k_x \rightarrow 0$ In that case,

$$J_y^{\text{tri}}(0, 0) = (b^2 - a^2) \frac{h^2}{6} \quad (\text{A.48})$$

A.5.3 Particular cases for the rectangle

Considering the limit cases of (A.40), three of them can be highlighted:

When $k_x \rightarrow 0$ and $k_y \neq 0$ It can be shown that

$$\lim_{k_x \rightarrow 0} \left[-\frac{a}{k_x} + \frac{j}{k_x^2} - \frac{j \exp(jk_x a)}{k_x^2} \right] = \frac{ja^2}{2} \quad (\text{A.49})$$

so that

$$J_x^{\text{rect}}(k_x, k_y) = \frac{1}{k_y a} \frac{ja^2}{2} \left[\exp(-jk_y c) - 1 \right]. \quad (\text{A.50})$$

When $k_x \neq 0$ and $k_y \rightarrow 0$ It can be shown that

$$\lim_{k_y \rightarrow 0} \frac{\exp(-jk_y c) - 1}{k_y} = -jc \quad (\text{A.51})$$

so that

$$J_x^{\text{rect}}(k_x, 0) = -\frac{jc}{a} \exp(-jk_x a) \left[-\frac{a}{k_x} + \frac{j}{k_x^2} - \frac{j \exp(jk_x a)}{k_x^2} \right]. \quad (\text{A.52})$$

When $k_x \rightarrow 0$ and $k_y \rightarrow 0$ Combining the two previous cases, it leads to

$$J_x^{\text{rect}}(0, 0) = \frac{ac}{2}. \quad (\text{A.53})$$

A.6 From Müller to T-matrix

In this section, we will draw the link between the T-matrix based method described in [117] and the eigenmodes determination problem based on the Müller formulation for the Method of Moments [131].

Using the PMCHWT formulation of the MoM, the equivalent currents on the interfaces between different media are found by imposing the continuity of the tangential electric and magnetic fields on both sides of the testing functions. Using the Müller formulation, however, the equivalent currents along the interfaces separating different media are found imposing on both sides of the interface:

$$\hat{n} \times \mathbf{E}^{\text{in}} + \hat{n} \times \mathbf{E}^{\text{sc}} = -\mathbf{M}_{\text{eq}} \quad (\text{A.54a})$$

$$\hat{n} \times \mathbf{H}^{\text{in}} + \hat{n} \times \mathbf{H}^{\text{sc}} = \mathbf{J}_{\text{eq}} \quad (\text{A.54b})$$

with $\hat{n}$, the direction normal to the surface toward the side of the interface that is tested, $\mathbf{E}^{in}$ and $\mathbf{H}^{in}$ the incident electric and magnetic fields and $\mathbf{E}^{sc}$ and $\mathbf{H}^{sc}$ the electric and magnetic fields radiated on the interface by $\mathbf{J}_{eq}$ and $\mathbf{M}_{eq}$, the unknown equivalent electric and magnetic currents.

To apply Müller formulation to the geometry illustrated in Fig. 2.11, it is necessary to impose (A.54) on both side of both interfaces.

Below, we concentrate on the inner part of the layer. The surfaces are discretized and (A.54) is applied to both interfaces on their inner side. The system of equations to solve then reads

$$\tilde{\underline{\underline{Z}}}_{M,11}^{\uparrow} \mathbf{x}_{l1} - \tilde{\underline{\underline{Z}}}_{M,12} \mathbf{x}_{l2} = \mathbf{x}_{l1} \quad (\text{A.55})$$

$$-\tilde{\underline{\underline{Z}}}_{M,22}^{\downarrow} \mathbf{x}_{l2} + \tilde{\underline{\underline{Z}}}_{M,21} \mathbf{x}_{l1} = -\mathbf{x}_{l2} \quad (\text{A.56})$$

with $\tilde{\underline{\underline{Z}}}_{M,pq}$ the impedance matrix specific to the Müller formulation. This impedance matrix describes the transverse fields generated on Plane p by currents on Plane q using the periodic Green's function, and the $\uparrow$ and $\downarrow$ symbols indicate if fields are tested just above or just below the interface.

As well known, the use of the equivalence principle produces twice as many equations as unknowns. The Müller formulation can be chosen to avoid a non-linear eigenmode formulation by involving only two consecutive interfaces.

In that case, half of the unknowns will drop using Equation (2.60). We then obtain

$$\tilde{\underline{\underline{Z}}}_{M,12}^{-1} (\tilde{\underline{\underline{Z}}}_{M,11}^{\uparrow} - \underline{\underline{I}}) \mathbf{x}_{l1} = g \mathbf{x}_{l1} \quad (\text{A.57})$$

$$(\tilde{\underline{\underline{Z}}}_{M,22}^{\downarrow} - \underline{\underline{I}})^{-1} \tilde{\underline{\underline{Z}}}_{M,21} \mathbf{x}_{l1} = g \mathbf{x}_{l1} \quad (\text{A.58})$$

As always when using Müller formulation, these two system of equations have to be combined somehow [131]. One possibility is to simply add them together. However, to keep the eigenvalue g constant, we will define the $\underline{\underline{T}}$ -matrix as

$$\underline{\underline{T}} = \frac{\tilde{\underline{\underline{Z}}}_{M,12}^{-1} (\tilde{\underline{\underline{Z}}}_{M,11}^{\uparrow} - \underline{\underline{I}}) + (\tilde{\underline{\underline{Z}}}_{M,22}^{\downarrow} - \underline{\underline{I}})^{-1} \tilde{\underline{\underline{Z}}}_{M,21}}{2} \quad (\text{A.59})$$

such that

$$\underline{\underline{T}} \mathbf{x}_{l1} = g \mathbf{x}_{l1} \quad (\text{A.60})$$

We can notice, as mentioned previously, that the T-matrix formulation has to deal with back-propagation, which is illustrated by term $\tilde{\underline{\underline{Z}}}_{M,12}^{-1}$ in formula (A.59).

With this definition, the eigenmodes inside the structure correspond to the eigenvectors and eigenvalues of $\underline{\mathcal{T}}$ and can be computed all at once. However, because of the back-propagation term, $\underline{\mathcal{T}}$ is ill-conditioned and the results may be inaccurate.

A.7 Decay of modes due to loss

A more formal proof of Equation (2.73) is presented here, based on energy conservation. The physical origin of the constant ρ_α is also investigated.

Consider an infinitely 3D periodic metamaterial made of an infinite superposition of layers. A mode α is excited at the bottom interface of a layer, say Plane 0 and Layer 0, and propagates upward. Due to the fact that this mode is, by definition, a homogeneous solution to Maxwell's equations for the periodic geometry of the metamaterial, this mode will propagate without coupling with other modes, unless there is some defect in the periodic geometry. As we are considering an infinite metamaterial, such defect does not exist and therefore the modes α can be treated independently of the other modes, with which it cannot interact. In the following, we will consider that the direction of propagation of a mode is defined as the direction of its energy flow. For evanescent modes, which do not carry energy, the direction is given by the energy flow transported by the mode if infinitesimal losses are introduced.

This mode α is characterized by the fields distribution $(\mathbf{E}_\alpha(\mathbf{r}), \mathbf{H}_\alpha(\mathbf{r}))$ and a transfer coefficient g_α . The power transported by that mode crossing Plane p , between slabs $p - 1$ and p , is given by

$$P_\alpha^p = \Re \left\{ \iint_{S_p} \frac{\mathbf{E}_\alpha(\mathbf{r}) \times \mathbf{H}_\alpha^*(\mathbf{r})}{2} \cdot \hat{n} dS \right\} \quad (\text{A.61})$$

with $\Re\{A\}$ the real part of A , $\hat{n}$ the normal to the interface p toward layer p and S_p the surface of that interface limited to one unit cell of the metamaterial. Using Equation (2.60) provides:

$$P_\alpha^p = |g_\alpha|^{2p} \Re \left\{ \iint_{S_0} \frac{\mathbf{E}_\alpha(\mathbf{r}) \times \mathbf{H}_\alpha^*(\mathbf{r})}{2} \cdot \hat{n} dS \right\} \quad (\text{A.62})$$

with the integration that is now performed over S_0 . The medium being lossy, the power crossing two consecutive interfaces has to fade accordingly to the losses, i.e:

$$P_\alpha^p - P_\alpha^{p+1} = P_{\alpha, \text{loss}}^p > 0 \quad (\text{A.63})$$

with $P_{\alpha, \text{loss}}^p$ the losses due to mode α inside layer p if the amplitude of the other modes is null. Using Equation (A.62) and noticing that the power crossing the interface has to be positive due to causality, one can find

$$1 - |g_\alpha|^2 > 0 \quad (\text{A.64})$$

which corresponds to the physical constraint that the amplitude of the mode has to decrease from layer to layer ($|g_\alpha| < 1$).

Now, consider that losses are introduced using a non-zero conductivity σ . The amount of losses due to mode α inside layer p , $P_{\alpha,loss}^p$, can be computed using:

$$P_{\alpha,loss}^p = \iiint_{V_p} \sigma \frac{|\mathbf{E}_\alpha|^2}{2} dV \quad (\text{A.65})$$

with σ the local conductivity and V_p the volume corresponding to the intersection between the layer p and one unit cell of the metamaterial. Note that $\mathbf{E}$ depends on the value of σ . Indeed, changing the value of σ modifies the Green's function of the lossy medium and therefore the solution to the scattering problem. However, if the losses are small enough, the change in the shape of the fields for decreasing losses becomes negligible and a perturbation based approach can be used. If we consider that σ is small and constant in the whole lossy parts of the metamaterial, we can introduce the constant D_α that is independent of the conductivity such that

$$D_\alpha \equiv \iiint_{V_0^{loss}} \frac{|\mathbf{E}_\alpha(\sigma = 0)|^2}{2} dV \quad (\text{A.66})$$

with V_0^{loss} , the volume corresponding to the lossy part of the first layer limited to one unit cell of the metamaterial. Then the power loss will asymptotically reach

$$\lim_{\sigma \rightarrow 0} \frac{P_{\alpha,loss}^p}{\sigma} = |g_\alpha|^{2p} D_\alpha \quad (\text{A.67})$$

Combining this expression with (A.62) and (A.63), it provides:

$$|g_\alpha|^2 \simeq 1 - 2\rho_\alpha \sigma \quad (\text{A.68})$$

with

$$\rho_\alpha = \frac{D_\alpha}{\Re \left\{ \iint_{S_0} (\mathbf{E}_\alpha \times \mathbf{H}_\alpha^*) \cdot \hat{n} dS \right\}} \quad (\text{A.69})$$

which is proportional to the ratio between the power dissipated and the power transported by one mode.

If the conductivity is small enough, from (A.68), the transmission coefficient can be expressed using a first-order Taylor series:

$$|g_\alpha| \simeq 1 - \rho_\alpha \sigma \quad (\text{A.70})$$

List of publications

Journal papers

- J1** D. Tihon, V. Sozio, N.A. Ozdemir, M. Albani and C. Craeye, “Numerically stable eigenmode extraction in 3-D periodic metamaterials,” *IEEE Transactions on Antennas and Propagation*, Vol. 64, no. 7, pp. 3068-3079, 2016.
- J2** D. Tihon, S. Withington, C.N. Thomas and C. Craeye, “Characterization of power absorption response of periodic three-dimensional structures to partially coherent fields,” *Journal of Optical Society of America A*, Vol. 33, no. 12, pp. 2459-2469, 2016.
- J3** D. Tihon and C. Craeye, “All-analytical evaluation of the singular integrals involved in the method of moments,” *IEEE Transactions on Antennas and Propagation*, Vol. 66, no. 4, pp. 1925-1936, 2018.
- J4** D. Tihon, S. Withington, C.N. Thomas and C. Craeye, “Improving absorption in periodic plasmonic structures through a scattering interface layer,” *To be submitted to Journal of Optical Society of America A*.

Conference papers

- C1** D. Tihon, N.A. Ozdemir and C. Craeye, “Krylov subspace-based and MBF-based analysis of large finite arrays of silver nanorods in the presence of a scatterer,” *Numerical Electromagnetic Modeling and Optimization for RF, Microwave, and Terahertz Applications (NEMO)*, 2014 *International Conference on*, pp. 1-4, 2014.
- C2** D. Tihon, S. Hubert, C. Craeye and N.A. Ozdemir, “SVD post-compression combined with shielded-block preconditioner,” *Electromagnetics in Advanced Applications (ICEAA)*, 2014 *International Conference on*, pp. 503-506, 2014.

- C3** D. Tihon, V. Sozio, N.A. Ozdemir, M. Albani and C. Craeye, "Efficient numerical analysis of 3D periodic metamaterials: Multilayer approach and eigenmode analysis," *Antennas and Propagation (EuCAP), 2015 9th European Conference on*, pp. 1-5, 2015.
- C4** D. Tihon, C. Craeye, C. Guclu, F. Capolino and S. Withington, "Orthogonality properties of eigenmodes inside z-invariant periodic structures," *Advanced Electromagnetic Materials in Microwaves and Optics (METAMATERIALS), 2015 9th International Congress on*, pp. 505-507, 2015.
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- C6** D. Tihon and C. Craeye, "Fast computation of the impedance matrix for the periodic method of moments using a plane wave decomposition," *Antennas and Propagation (EuCAP), 2016 10th European Conference on*, pp. 1-4, 2016.
- C7** D. Tihon, S. Withington, C.N. Thomas and C. Craeye, "Computation of the absorption of partially coherent fields using traditional coherent solvers," *Numerical Electromagnetic and Multiphysics Modeling and Optimization for RF, Microwave, and Terahertz Applications (NEMO), 2017 IEEE MTT-S International Conference on*, pp. 329-331, 2017.
- C8** D. Tihon and C. Craeye, "Fast FMIR-MoM implementation using analytical singularity evaluation," *Electromagnetics in Advanced Applications (ICEAA), 2017 International Conference on*, pp. 1361-1364, 2017.
- C9** D. Tihon and C. Craeye, "Closed-form evaluation of the singular terms in electric field integral equations," *Antennas and Propagation (EuCAP), 2017 11th European Conference on*, pp. 520-524, 2017.

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