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On the effective permittivity of finite inhomogeneous objects

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On the effective permittivity of finite inhomogeneous objects

by

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Preface

This thesis contains the work I performed in the Laboratory for Electromagnetic Research in the EEMCS faculty of Delft University of Technology for the completion of the Masters degree as required by the university. In this thesis, we study a general numerical method, which treats this problem from the inverse scattering point of view and, in principle, determines the effective permittivity of an arbitrary object at any given frequency. We apply this technique to a finite three-dimensional sample of a photonic crystal at different frequencies and compare the results with the predictions from the effective medium theory, the theory of periodic media, and previously known two-dimensional results.

This thesis starts by describing the basic procedure and results of the effective medium theory in Chapter 2. Chapter 3 is devoted to the band gap theory in solid-state physics and photonics. The theory of effective inversion and the reduced-order Arnoldi algorithms are presented in Chapter 4. Finally in Chapter 5 we describe and discuss the numerical experiments.

I would like to express my gratitude towards Dr.Neil Budko for all the time and effort he spent on supervising me, and helping me present the report in the form it is right now. Furthermore, I would also like to thank Dr.ir. Gerard Janssen, Master coordinator Telecom, for his help and support in sorting out a few critical issues during my Masters programme. Finally, I would like to thank all my friends for having put up with me, and helped me immensely during my masters study.

Shreyas Bhargav Raghunathan
Delft, September 2008.

To,
Amma and Appa

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Abstract

In colloidal chemistry, composite (meta)materials, photonics, geophysics and remote sensing, it is often desirable to treat an inhomogeneous object, as a homogeneous with an *effective* permittivity. At the moment, however, there is no general analytical method which estimates this effective permittivity for an arbitrary finite inhomogeneous scatterer. In this thesis, we study a general numerical method, which treats this problem from the inverse scattering point of view and, in principle, determines the effective permittivity of an arbitrary object at any given frequency. We apply this technique to a finite three-dimensional sample of a photonic crystal at different frequencies and compare the results with the predictions from the effective medium theory, the theory of periodic media, and previously known two-dimensional results.

Chapter 1

Introduction

All materials are strongly inhomogeneous at the microscopic level, as they are made up of atoms, molecules and ions. The essence of macroscopic electrodynamics is to average the fields over a fixed volume of atoms and molecules, and introduce constitutive relations in terms of macroscopic quantities, like permittivity ε and permeability μ . The volume considered must be small compared to the geometry of the macroscopic object and the scale on which the macroscopic fields and currents show spatial variations. Yet, it must contain a large number of particles, so that it can be considered an elementary part of a continuum on a macroscopic scale. Thus, the average of the fields over this volume, leads to the macroscopic quantities which vary piecewise continuously with position. This original concept was extended further, to colloids, emulsions, and solid composite materials with fine-scale spatial variations of macroscopic quantities. In these cases we consider another, larger averaging volume, similar to the one defined previously, and introduce constitutive relations in terms of μ_{eff} , ε_{eff} and σ_{eff} . These *effective* parameters are supposed to faithfully reproduce the reaction of the individual elements of the composite medium to an incident electromagnetic field. The effective permittivity of a mixture, for example, however is quite different from the permittivities of the constituent components. An obvious guess for ε_{eff} , would be a volume-average of the true permittivities in the composite. A first order correction to this approximation would then contain the variations between the permittivities of the constituent elements, etc. In this

case, composite medium is usually considered dilute, and the variation in permittivity between the constituent elements small, allowing to neglect the effects of multiple scattering.

The averaging volume used to determine the effective constitutive parameters is unfortunately not well-defined. At lower frequencies where the spatial variation of the fields over the medium is small, such a volume induces a single spatially invariant ε_{eff} for the entire medium. As the frequency of the incident electromagnetic wave increases, while the averaging procedure remains fixed, ε_{eff} may become spatially varying within the medium, and dispersive, i.e. $\varepsilon_{\text{eff}}(\omega)$ will depend on the angular frequency ω , even if the constitutive components of the composite do not. In addition, at higher concentrations and stronger contrasts the multiple scattering effects can no longer be neglected and the averaging procedure becomes much more complicated. This is a very active field of research with applications in studies of optical properties of doped semiconductors, colloids, metallic glasses, aerosols, etc.

The aim of this thesis is to analyse and test an algorithm, [2], which, may in principle, determine ε_{eff} for an arbitrary inhomogeneous medium at any frequency. Here, we use this technique to calculate the effective permittivity of a finite three-dimensional photonic crystal at different frequency ranges. In order to validate our results, we compare them to the predictions of the Effective Medium Theory (EMT), the theory of periodic media, and previous two-dimensional results.

The Effective Medium Theory characterizes an inhomogeneous media as a homogeneous medium with effective permittivity. The Effective Medium Theory (EMT), applicable when the wavelength is larger than the characteristic dimension of the inclusions and gives ε_{eff} in terms of analytical mixing formulas [20, 45, 39, 6]. Such mixing formulas explicitly relate the properties of the constituent elements to the effective electric properties of the medium. Normally these formulas tend to neglect the multiple scattering by assuming a weak contrast or a small concentration of the inclusions. At higher frequencies and smaller wavelengths, the multiple scattering effects cannot be neglected and therefore the effective medium approach has to be extended to include these effects [6].

The strong scattering effects and the mutual interaction of particles, periodically distributed over a background medium, are studied within the theory of infinite periodic media making use of the Bloch theorem. The reaction of these crystals to the incident electromagnetic wave strongly depends on the angular frequency. In other words, periodic structures show strong dispersive behaviour and sometimes even forbid the propagation of the electromagnetic wave of certain frequencies, called photonic band gaps [51, 15, 50, 23]. The appearance of these band gaps depends on the type of the crystal (one-dimensional, two-dimensional or three-dimensional) [48, 28, 13, 52], their lattice constant, and the permittivity of the individual particles. These properties of photonic crystals bear strong similarity with the energy band structures observed in solid state physics [12, 16, 14], which also makes use of the Bloch theorem. More recently, other interesting phenomena, like negative refraction [25, 27, 26, 49] and superprism [17] effects, have also been observed in the vicinity of the first photonic band gap, in two-dimensional crystals.

Metamaterials is another interesting case of periodic structures, but now the individual elements are resonant too. The behaviour of metamaterials is more complex. These structures exhibit negative index of refraction [44] due to a negative effective permittivity [32, 34] and a negative effective permeability [35] at certain frequency bands. Such properties have opened up discussions about the possibility to create perfect lens [31], invisibility cloak [41] and other unusual objects. The theoretical and experimental verifications of Metamaterial properties have constantly been contested and still discussed [36], [9], [46], [8], although a number of authors have experimentally and numerically verified the negative refraction and other phenomena [49], [26], [30].

The effective medium theory approach has been used to explain the properties of not only infinite but finite metamaterials [22, 18, 42, 21] as well. In [22] the authors provide a general theory, which relates the response of the individual resonators to the response of the entire sample. The analysis and the following comparisons, have shown a good agreement between the theoretical predictions and the experimental data. In another approach [43], the effective parameters of the metamaterial with a symmetric unit cell are

calculated by an S-parameter retrieval method. In that paper, the authors observe that the retrieved parameters are not unique, which is also reported in [42]. The possibility of approximating a metamaterial structure by a Periodic Effective Medium (PEM) rather than a homogeneous effective medium, by making use of the inherent periodicity of a metamaterial has also been discussed [19].

In this thesis we present a method which, may be viewed as a generalization of the S-parameter retrieval approach proposed in [43]. We model the problem of determining the effective parameters of a finite sample of periodic inhomogeneous structure, as an inverse scattering problem. Here we invert a finite homogeneous scattering model with the knowledge of the true scattered field measured or simulated by solving the forward problem. This inverse-problem is ill-posed, which leads to a non-unique solution for the effective permittivity, and non-linear, which leads to the increase in the computational complexity. We reduce the complexity, by using the reduced-order Arnoldi algorithm [2]. Numerical experiments performed on a finite three-dimensional photonic crystal with a two-dimensional periodicity, using this method, shows good agreement with the prediction from effective medium theory, the theory for metamaterials and band gaps. The effective permittivity determined from this algorithm is indeed not unique, similar to the observations made in [43]. The results from the numerical experiments have also been compared with the analysis of a two-dimensional photonic crystal [38] and the observed deviations have been discussed.

We start though by describing the basic procedure and results of the effective medium theory in Chapter 2. Chapter 3 is devoted to the band gap theory in solid-state physics and photonics. The theory of effective inversion and the reduced-order Arnoldi algorithms are presented in Chapter 4. Finally in Chapter 5 we describe and discuss the numerical experiments.

Chapter 2

Basics of Effective Medium Theory

The optical properties of inhomogeneous media are described by complex spatially varying electric permittivity and permeability. The characterization of such a medium using an inhomogeneous permittivity is not very useful, as for this one has to know the position of the particles accurately. In such a case, when the wavelength of the electromagnetic wave is much larger than the size of the inclusions, we may treat the otherwise inhomogeneous mixture as a homogeneous scatterer with effective values of permittivity and permeability. These effective parameters depend on the properties of the constituent elements, their volume fraction and sizes.

The *Effective Medium Theory* (EMT) and its approximations are a set of analytical models, describing the macroscopic properties of a medium made up of finer inhomogeneities. The microscopic behaviour of each of the component and their relative volumetric fractions play an important role in the macroscopic properties. In electromagnetics the homogeneous constitutive parameters of a inhomogeneous material, effective permittivity ε_{eff} and conductivity σ_{eff} are usually sought for.

2.1 Permittivity of heterogeneous media

2.1.1 Finely dispersed mixture

We start by reviewing the basic procedure of obtaining the effective permittivity of a finely dispersed mixture in the effective medium theory [20]. This is usually done in the electrostatic approximation, where the fields are presumed to be time independent. On the fine scale the constitutive relation is

$$\mathbf{D}(\mathbf{x}) = \varepsilon(\mathbf{x})\mathbf{E}(\mathbf{x}), \quad (2.1)$$

where $\varepsilon(\mathbf{x})$ is not constant in space. On a somewhat larger scale the medium would look homogeneous and isotropic. The idea is to work with averaged $\mathbf{E}$ and $\mathbf{D}$. The averaging is defined as

$$\langle \mathbf{E}(\mathbf{x}) \rangle = \frac{1}{V} \int_{\mathbf{x} \in V(\mathbf{x})} \mathbf{E}(\mathbf{x}) d\mathbf{x}, \quad (2.2)$$

$$\langle \mathbf{D}(\mathbf{x}) \rangle = \frac{1}{V} \int_{\mathbf{x} \in V(\mathbf{x})} \mathbf{D}(\mathbf{x}) d\mathbf{x}, \quad (2.3)$$

where the averaging volume is unfortunately not at all well-defined, which is perhaps the weakest point of the effective medium theory. It is presumed though, that with respect to this average field $\langle \mathbf{E} \rangle$, the medium can be considered isotropic and homogeneous. The effective permittivity is defined via the following relation:

$$\langle \mathbf{D}(\mathbf{x}) \rangle = \varepsilon_{\text{eff}} \langle \mathbf{E}(\mathbf{x}) \rangle. \quad (2.4)$$

If all the particles making up the mixture are isotropic, and the variation $\delta\varepsilon$ of permittivity between different elements in the mixture is small compared to the values of ε itself, then it is possible to compute ε_{eff} up to the second order in the variation $\delta\varepsilon$.

Let $\mathbf{E}(\mathbf{x})$ be the local value of the electric field strength. It can be expressed as

$$\mathbf{E}(\mathbf{x}) = \langle \mathbf{E}(\mathbf{x}) \rangle + \delta\mathbf{E}(\mathbf{x}). \quad (2.5)$$

The local value of permittivity is similarly expresses as

$$\varepsilon(\mathbf{x}) = \langle \varepsilon \rangle + \delta\varepsilon(\mathbf{x}), \quad (2.6)$$

$$\langle \varepsilon \rangle = \frac{1}{V} \int_{\mathbf{x} \in V(\mathbf{x})} \varepsilon(\mathbf{x}) d\mathbf{x}, \quad (2.7)$$

where $\langle \varepsilon \rangle$ is the volume average of the true permittivity in the medium. Now, substituting (2.6) and (2.5) in (2.4) we obtain

$$\begin{aligned} \langle \mathbf{D}(\mathbf{x}) \rangle &= \langle (\langle \varepsilon \rangle + \delta\varepsilon)(\langle \mathbf{E} \rangle + \delta\mathbf{E}) \rangle, \\ &= \langle \langle \varepsilon \rangle \langle \mathbf{E} \rangle \rangle + \langle \langle \varepsilon \rangle \delta\mathbf{E} \rangle + \langle \delta\varepsilon \langle \mathbf{E} \rangle \rangle + \langle \delta\varepsilon \delta\mathbf{E} \rangle, \\ &= \langle \varepsilon \rangle \langle \mathbf{E} \rangle + \langle \varepsilon \rangle \langle \delta\mathbf{E} \rangle + \langle \delta\varepsilon \rangle \langle \mathbf{E} \rangle + \langle \delta\varepsilon \delta\mathbf{E} \rangle, \\ &= \langle \varepsilon \rangle \langle \mathbf{E} \rangle + \langle \delta\varepsilon \delta\mathbf{E} \rangle, \end{aligned} \quad (2.8)$$

since, by definition,

$$\langle \delta\varepsilon \rangle = 0,$$

$$\langle \delta\mathbf{E} \rangle = 0.$$

Hence, the zero-order approximation can be written as

$$\begin{aligned} \langle \mathbf{D}(\mathbf{x}) \rangle &= \langle \varepsilon \rangle \langle \mathbf{E}(\mathbf{x}) \rangle, \\ \varepsilon_{\text{eff}} &= \langle \varepsilon \rangle. \end{aligned} \quad (2.9)$$

Now, we consider the local non-averaged equation

$$\nabla \cdot \mathbf{D} = 0. \quad (2.10)$$

Substituting (2.6) and (2.5) in (2.10) we obtain

$$\begin{aligned} \nabla \cdot \mathbf{D} &= \nabla \cdot [(\langle \varepsilon \rangle + \delta\varepsilon)(\langle \mathbf{E} \rangle + \delta\mathbf{E})], \\ &= \nabla \cdot (\langle \varepsilon \rangle \langle \mathbf{E} \rangle) + \nabla \cdot (\langle \varepsilon \rangle \delta\mathbf{E}) + \nabla \cdot (\delta\varepsilon \langle \mathbf{E} \rangle) + \nabla \cdot (\delta\varepsilon \delta\mathbf{E}), \\ &= \langle \varepsilon \rangle \nabla \cdot \langle \mathbf{E} \rangle + \langle \varepsilon \rangle \nabla \cdot \delta\mathbf{E} + \delta\varepsilon \nabla \cdot \langle \mathbf{E} \rangle + \langle \mathbf{E} \rangle \cdot \nabla \delta\varepsilon + \nabla \cdot \delta\varepsilon \delta\mathbf{E}. \end{aligned} \quad (2.11)$$

Assuming

$$\nabla \cdot \langle \mathbf{E} \rangle = 0, \quad (2.12)$$

and a weak contrast, we can retain only the terms up to the first order in variations $\delta\varepsilon$ and $\delta\mathbf{E}$, i.e.

$$\nabla \cdot \mathbf{D} = \langle \varepsilon \rangle \nabla \cdot \delta\mathbf{E} + \langle \mathbf{E} \rangle \cdot \nabla \delta\varepsilon. \quad (2.13)$$

To obtain $\langle \delta\varepsilon \delta\mathbf{E} \rangle$ we start by averaging $\delta\mathbf{E}$ over the volume occupied by particles with the same value of $\delta\varepsilon$. Since the medium is isotropic as a whole, we have

$$\begin{aligned} \frac{\partial}{\partial x_1} \langle \delta\mathbf{E} \rangle_{\delta\varepsilon,1} &= \frac{\partial}{\partial x_2} \langle \delta\mathbf{E} \rangle_{\delta\varepsilon,2} = \frac{\partial}{\partial x_3} \langle \delta\mathbf{E} \rangle_{\delta\varepsilon,3} \\ &= \frac{1}{3} \nabla \cdot \langle \delta\mathbf{E} \rangle_{\delta\varepsilon}, \end{aligned} \quad (2.14)$$

where $\langle \delta\mathbf{E} \rangle_{\delta\varepsilon}$ denotes averaging over $\delta\varepsilon$ sub volume. Now, we consider $\langle \mathbf{E} \rangle$ directed along the x_1 axis. In this case

$$\begin{aligned} \langle \varepsilon \rangle \nabla \cdot \langle \delta\mathbf{E} \rangle_{\delta\varepsilon} &= - \langle \mathbf{E} \rangle \cdot \nabla \delta\varepsilon, \\ \langle \varepsilon \rangle \frac{\partial}{\partial x_1} \langle \delta\mathbf{E} \rangle_{\delta\varepsilon,1} + \langle \varepsilon \rangle \frac{\partial}{\partial x_2} \langle \delta\mathbf{E} \rangle_{\delta\varepsilon,2} + \langle \varepsilon \rangle \frac{\partial}{\partial x_3} \langle \delta\mathbf{E} \rangle_{\delta\varepsilon,3} &= \\ &= - \langle \mathbf{E} \rangle_1 \frac{\partial}{\partial x_1} \delta\varepsilon - \langle \mathbf{E} \rangle_2 \frac{\partial}{\partial x_2} \delta\varepsilon - \langle \mathbf{E} \rangle_3 \frac{\partial}{\partial x_3} \delta\varepsilon \end{aligned} \quad (2.15)$$

and from (2.14) we rewrite the above equation as

$$3 \langle \varepsilon \rangle \frac{\partial}{\partial x_1} \langle \delta\mathbf{E} \rangle_{\delta\varepsilon,1} = - \langle \mathbf{E} \rangle_1 \frac{\partial}{\partial x_1} \delta\varepsilon, \quad (2.16)$$

$$\langle \delta\mathbf{E} \rangle_{\delta\varepsilon,1} = - \frac{\langle \mathbf{E} \rangle_1}{3 \langle \varepsilon \rangle} \delta\varepsilon. \quad (2.17)$$

As the choice of the x_1 axis is arbitrary, we may generalise the above equation as

$$\langle \delta\mathbf{E} \rangle_{\delta\varepsilon} = - \frac{\langle \mathbf{E} \rangle}{3 \langle \varepsilon \rangle} \delta\varepsilon. \quad (2.18)$$

Now multiplying the above expression by $\delta\varepsilon$ and averaging over all $\delta\varepsilon$ we get

$$\begin{aligned} \delta\varepsilon \langle \delta\mathbf{E} \rangle_{\delta\varepsilon} &= - \frac{\langle \mathbf{E} \rangle}{3 \langle \varepsilon \rangle} \delta\varepsilon^2, \\ \langle \delta\varepsilon \delta\mathbf{E} \rangle_{\delta\varepsilon} &= - \frac{\langle \mathbf{E} \rangle}{3 \langle \varepsilon \rangle} \delta\varepsilon^2, \\ \langle \delta\varepsilon \delta\mathbf{E} \rangle &= - \frac{\langle \mathbf{E} \rangle}{3 \langle \varepsilon \rangle} \langle \delta\varepsilon^2 \rangle. \end{aligned} \quad (2.19)$$

One important thing to note is that, though $\langle \delta\varepsilon \rangle = 0$, we can see that $\langle \delta\varepsilon^2 \rangle \neq 0$ and thus the first correction to average permittivity is

$$\varepsilon_{\text{eff}} = \langle \varepsilon \rangle - \frac{1}{3\langle \varepsilon \rangle} \langle (\delta\varepsilon)^2 \rangle. \quad (2.20)$$

Having derived a general expression for the effective permittivity in a binary mixture, let us look at some specific results.

2.1.2 Dilute dielectric mixtures

In case of dilute mixtures, the effective permittivity is related to the concentration of individual elements and their dielectric permittivities as [45]

$$\varepsilon = (1 - q)\varepsilon_1 + q\varepsilon_2, \quad (2.21)$$

where ε is the effective permittivity of the mixture, ε_1 and ε_2 are the permittivity of the constituents. Here, q is the volume fraction of elements with ε_2 as the dielectric permittivity. This is a linear relation and is applicable only at very low concentrations.

2.1.3 Clausius-Mosotti relation

At reasonably high concentrations, considering small spherical inclusions inside a homogeneous medium, the effective permittivity of the medium can be expressed as a function of the microscopic parameters of the inclusion. The sizes of these inclusions are such that they are macroscopically small and yet significant. The effective permittivity of a mixture with these particles is given as

$$\frac{\varepsilon - 1}{\varepsilon + 2} = \frac{4\pi}{3} \sum_j N_j \alpha_j, \quad (2.22)$$

which is the Clausius-Mosotti [45] equation. Here, N_j is the number of “molecules” per unit volume and α_j is their respective polarizabilities. This equation provides us with an explicit relation between the macroscopic ε and the microscopic α of the individual molecules. Still, a microscopic model is required to determine α of each molecule.

2.1.4 Maxwell-Garnett relation

As an extension of the Clausius-Mosotti expression, the Maxwell-Garnett theory assumes a convenient model for the microscopic α_j and is in general evaluated using the elementary electrostatics. For a dilute binary medium with spherical inclusions with dielectric constant ε_1 and volume fraction η_1 we have

$$\frac{\varepsilon - 1}{\varepsilon + 2} = \eta_1 \frac{\varepsilon_1 - 1}{\varepsilon_1 + 2}, \quad (2.23)$$

which is the Maxwell-Garnett formula. In this case the inclusions have assumed to be embedded in air. The Maxwell-Garnett formula relates the effective permittivity of a dilute binary mixture to the permittivity of the constituents ε_1 and the volume fraction η_1 inside the host. If a host with permittivity ε_0 , contains inclusions with permittivity ε_1 , of a volume fraction η_1 we have

$$\frac{\varepsilon - \varepsilon_0}{\varepsilon + 2\varepsilon_0} = \eta_1 \frac{\varepsilon_1 - \varepsilon_0}{\varepsilon_1 + 2\varepsilon_0}, \quad (2.24)$$

and conversely as

$$\frac{\varepsilon - \varepsilon_1}{\varepsilon + 2\varepsilon_1} = (1 - \eta_1) \frac{\varepsilon_0 - \varepsilon_1}{\varepsilon_0 + 2\varepsilon_1}. \quad (2.25)$$

It can be easily proved that this approach is not symmetric and interchanging the host medium and inclusions results in different values for ε .

2.1.5 Bruggeman model

The Maxwell-Garnett approach can be extended to a general two component system, without explicitly assuming a host medium. Consider a two-component mixture, with ε_1 and ε_2 denoting the permittivity of the two components and η_1 and η_2 denoting their respective concentrations. The effective permittivity of this system, ε is given by

$$\eta_1 \left(\frac{\varepsilon_1 - \varepsilon}{\varepsilon_1 + 2\varepsilon} \right) + \eta_2 \left(\frac{\varepsilon_2 - \varepsilon}{\varepsilon_2 + 2\varepsilon} \right) = 0, \quad (2.26)$$

which is Bruggeman formula, where $\eta_1 + \eta_2 = 1$. The Bruggeman model is symmetric, unlike the Maxwell-Garnett model, with no distinction between the two inclusion phases in the mixture.

2.1.6 Non-spherical inclusions

Using the same principles as in the Bruggeman model, the formula for cylindrical inclusions inside a mixture is given by [39]

$$\eta_1 \left(\frac{\varepsilon_1 - \varepsilon}{\varepsilon_1 + \varepsilon} \right) + \eta_2 \left(\frac{\varepsilon_2 - \varepsilon}{\varepsilon_2 + \varepsilon} \right) = 0, \quad (2.27)$$

or as an extension of Maxwell-Garnett approach, derived by Lord Rayleigh as

$$\frac{\varepsilon - \varepsilon_2}{\varepsilon_1 + \varepsilon_2} = \eta_1 \frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 + \varepsilon_2}. \quad (2.28)$$

2.2 Variational bounds on permittivity

Difficulties in calculating the effective parameters lead to interest in obtaining bounds on these parameters for validity [45]. The Wiener bound for layered structures with topologies parallel or perpendicular to the applied field is given by

$$\frac{\varepsilon_1 \varepsilon_2}{q \varepsilon_1 + (1 - q) \varepsilon_2} \leq \varepsilon \leq (1 - q) \varepsilon_1 + q \varepsilon_2, \quad (2.29)$$

where ε_1 and ε_2 are the permittivities of the constituents of the binary mixture and q is the concentration of ε_2 . This is a strict bound and the value of ε_{eff} is always between these values for a binary mixture with fixed volume fractions. This bound is general and applicable only with dilute mixtures.

Let us consider a two-component mixture where little information about the spatial distribution of the inclusion is available. If, the medium can be considered macroscopically homogeneous and isotropic the variational bounds on effective permittivity are given by,

$$\varepsilon_1 + \frac{\varepsilon_1 \eta_1}{\frac{\varepsilon_1}{\varepsilon_2 - \varepsilon_1} + \frac{\eta_1}{3}} < \varepsilon < \varepsilon_2 + \frac{\varepsilon_2 \eta_2}{\frac{\varepsilon_2}{\varepsilon_1 - \varepsilon_2} + \frac{\eta_2}{3}}. \quad (2.30)$$

The above bound is called the Hashin-Shtrikman bound [11][10]. By analogy this bound can also be extended to magnetic permeability and conductivity.

The effective medium approximations model an inhomogeneous medium as a homogeneous medium with an effective permittivity. The models described above are all based on the Lorentz approach for small particles which

considers the local field at each inclusion. An important point to be emphasised is the assumption that the local field acting on all molecules is the same. Such an assumption is justified only with periodic structures, like crystals, or randomly oriented particles. The models are applicable only when particle sizes are much smaller than the wavelength of the electromagnetic wave. The Effective Medium Theory approach tends to neglect inter-particle interaction. Carefully calculated rigorous bounds on such models, limit the values of ε that can be determined from these models. Nevertheless, EMT may be used for validating a more general technique at low frequencies.

Chapter 3

Infinite periodic media

The basic effective medium theory formulas tend to underestimate the mutual interaction between particles in the mixture. This is due to the fact that no simple analytic solution to three-dimensional scattering problems with more than one scatterer is known, with one notable exception - an infinite periodic array of scatterers. In this chapter we characterize the field in such infinite periodic media. This solution originates from the solid state physics and hence we first introduce its quantum mechanical version [16, 12]. Further, we treat the one-dimensional electromagnetic case and discuss extensions to two and three dimensions, as well as applications of this theory to metamaterials.

3.1 Motion of electron in a periodic potential

Consider an electron moving along the x -axis, inside an atomic lattice. The one-dimensional wavefunction $\psi(x)$ of such an electron satisfies the Schrödinger wave equation:

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}\mathcal{E}\psi(x) = \frac{2m}{\hbar^2}V(x)\psi(x), \quad (3.1)$$

where $\mathcal{E}$ is the eigenvalue, representing the total energy of the propagating electron. Since the energy is a scalar, we may represent the energy function as

$$f(x) = \mathcal{E} - V(x)\frac{2m}{\hbar^2}, \quad (3.2)$$

and hence (3.1) as

$$\frac{d^2\psi(x)}{dx^2} + f(x)\psi(x) = 0. \quad (3.3)$$

When an electron moves past an ion, it experiences the Coulomb force. If the motion is along a number of ions placed regularly so as to constitute a periodic lattice structure, the potential experienced by the electron can be written as a periodic function. Neglecting the end effects and assuming an infinitely periodic medium, we have the potential in a one dimensional case

$$V(x) = V(x + na), \quad n = 0, 1, 2 \dots \quad (3.4)$$

where $V(x)$ is the potential experienced by the electron and a is the period along the x axis. The scalar function f , by definition, must satisfy the periodicity condition

$$f(x) = f(x + na). \quad (3.5)$$

Equation (3.3) is a second order differential equation, and has two solutions which are denoted as $\psi_1(x)$ and $\psi_2(x)$. Thus, any solution to the equation (3.3) can be expressed as a linear combination of the two solutions $\psi_1(x)$ and $\psi_2(x)$. Using these two solutions we obtain

$$\psi_1\psi_2'' + f\psi_1\psi_2 = 0, \quad (3.6)$$

$$\psi_2\psi_1'' + f\psi_1\psi_2 = 0. \quad (3.7)$$

subtracting the above equations and integrating

$$\psi_1\psi_2' - \psi_2\psi_1' = W = \text{const.} \quad (3.8)$$

By definition, the Wronskian of the functions ψ_1 and ψ_2 is

$$W = \det \begin{pmatrix} \psi_1 & \psi_2 \\ \psi_1' & \psi_2' \end{pmatrix} \quad (3.9)$$

which is independent of x and is a constant from (3.8).

Due to the periodicity of $f(x)$, if $\psi(x)$ is a solution of (3.1), then $\psi(x+a)$ is also a solution. Hence $\psi(x)$ can also be expressed via ψ_1 and ψ_2 as

$$\begin{aligned}\psi_1(x+a) &= A\psi_1(x) + B\psi_2(x), \\ \psi_2(x+a) &= C\psi_1(x) + D\psi_2(x),\end{aligned}\tag{3.10}$$

where A, B, C , and D are some constants. Substituting (3.10) in the (3.9) leads to

$$\begin{aligned}W &= \det \begin{pmatrix} A\psi_1 + B\psi_2 & C\psi_1 + D\psi_2 \\ A\psi'_1 + B\psi'_2 & C\psi'_1 + D\psi'_2 \end{pmatrix}, \\ &= \det \begin{pmatrix} \psi_1 & \psi_2 \\ \psi'_1 & \psi'_2 \end{pmatrix} \det \begin{pmatrix} A & C \\ B & D \end{pmatrix}.\end{aligned}\tag{3.11}$$

Hence, the constants must satisfy

$$\begin{aligned}\det \begin{pmatrix} A & C \\ B & D \end{pmatrix} &= 1, \\ AD - BC &= 1.\end{aligned}\tag{3.12}$$

Instead of looking for a general solution of the form (3.10), we would like to find independent solution ψ_1 and ψ_2 , each satisfying

$$\psi_1(x+a) = \lambda\psi_1(x),\tag{3.13}$$

$$\psi_2(x+a) = \lambda\psi_2(x),\tag{3.14}$$

where λ is some constant. Repeating the steps (3.11) and (3.12) with λ we see that

$$\lambda^2 = 1.\tag{3.15}$$

From (3.13) and (3.10) we obtain

$$\begin{aligned}A\psi_1 + B\psi_2 &= \lambda\psi_1, \\ C\psi_1 + D\psi_2 &= \lambda\psi_2.\end{aligned}\tag{3.16}$$

$$\tag{3.17}$$

Eliminating ψ_1 and ψ_2 from the above equation, assuming $\lambda = e^\alpha$, and solving the equation

$$\det \begin{pmatrix} A - \lambda & B \\ C & D - \lambda \end{pmatrix} = 0, \quad (3.18)$$

we arrive at the following condition on α :

$$\cosh \alpha = \frac{A + D}{2}. \quad (3.19)$$

This leads to the conditions on the existence of a wave function. If $\frac{A+D}{2} > 1$, then α is real and the wavefunctions are represented as

$$\psi_1(x + a) = e^\alpha \psi_1(x), \quad (3.20)$$

$$\psi_2(x + a) = e^{-\alpha} \psi_2(x). \quad (3.21)$$

If $\frac{A+D}{2} < 1$, then α is imaginary and taking $\alpha = ika$, where k is real and a is the lattice period, the solutions are represented as

$$\psi_1(x + a) = e^{ika} \psi_1(x), \quad (3.22)$$

$$\psi_2(x + a) = e^{-ika} \psi_2(x). \quad (3.23)$$

The functions $\psi_1(x)$ and $\psi_2(x)$ are still unknown and depend upon the explicit form of the scalar function f . If this function is a constant, such that $f = p^2$, where p is real, the wavefunctions ψ_1 and ψ_2 are bounded for any value of x and thus $\lambda = e^{ipx}$, $\lambda' = e^{-ipx}$. If the function is a constant, still, such that $f = -p^2$, then the solutions for the Schrödinger wave equation are exponentially decaying or increasing. As wavefunctions must be bounded, such solutions are not acceptable. Hence the wavefunctions satisfying the Schrödinger equation with a periodic potential can be written as

$$\psi_1(x) = e^{ikx} u_1(x), \quad (3.24)$$

$$\psi_2(x) = e^{ikx} u_2(x), \quad (3.25)$$

where u_m are periodic function:

$$u_m(x + Na) = u_m(x), \quad N = 0, 1, \dots \quad (3.26)$$

This is the Bloch theorem. To show that $u(x)$ is indeed periodic, we note that the probability distribution of the electron must also show the same periodicity as the potential, which can be represented as

$$|\psi(x)|^2 = |\psi(x+a)|^2. \quad (3.27)$$

Let C be a scaling acquired by the function $\psi(x)$ at the point $x+a$, and (3.27) implies that $|C| = 1$. Thus we may write $C = e^{ika}$, where k is an arbitrary parameter. The expression for the wavefunction is,

$$\begin{aligned} \psi(x) &= e^{-ika}\psi(x+a), \\ e^{-ikx}\psi(x) &= e^{-ik(x+a)}\psi(x+a). \end{aligned}$$

This shows that $u(x) = e^{-ikx}\psi(x)$ is also a periodic function with period a .

3.1.1 Kronig-Penney model

Let the potential inside the atomic lattice be modulated as a square wave function, with the maximum value being V_0 . Now, the Schrödinger wave equation is defined as

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(\mathcal{E} - V(x))\psi = 0. \quad (3.28)$$

and from the Bloch theorem, we have

$$\psi(x) = e^{ikx}u(x). \quad (3.29)$$

Substituting (3.29) in (3.28) we have

$$\frac{d^2}{dx^2}[e^{ikx}u(x)] + \frac{2m}{\hbar^2}(\mathcal{E} - V(x))e^{ikx}u(x) = 0, \quad (3.30)$$

which on simplification reduces to

$$\frac{d^2u(x)}{dx^2} + 2ik\frac{du(x)}{dx} + \frac{2m}{\hbar^2}\left(\mathcal{E} - V(x) - \frac{\hbar^2k^2}{2m}\right)u(x) = 0. \quad (3.31)$$

We assume that the square-wave modulated $V(x)$ is such that in the interval $0 < x < a$, $V = 0$. Hence, in this interval we have

$$\frac{d^2u(x)}{dx^2} + 2ik\frac{du(x)}{dx} + \frac{2m}{\hbar^2}\left(\mathcal{E} - \frac{\hbar^2k^2}{2m}\right)u(x) = 0.$$

Solving the above equation for $u(x)$ we obtain

$$u(x) = Ae^{i(\alpha-k)x} + Be^{-i(\alpha+k)x}, \quad (3.32)$$

$$\alpha = \sqrt{\frac{2m\mathcal{E}}{\hbar^2}}. \quad (3.33)$$

In the interval $a < x < a + b$ where $V = V_0$ the solution is of the form,

$$u(x) = Ce^{(\beta-ik)x} + De^{-(\beta-ik)x}, \quad (3.34)$$

$$\beta = \sqrt{\frac{2m}{\hbar^2}(V_0 - \mathcal{E})}. \quad (3.35)$$

Now, at the points $x = 0$ and $x = a$, the function $u(x)$ and its derivative must be continuous. Applying the periodicity condition we have $u(a) = u(-b)$, and thus

$$A + B = C + D, \quad (3.36)$$

$$i(\alpha - k)A - i(\alpha + k)B = (\beta - ik)C - (\beta + ik)D, \quad (3.37)$$

$$Ae^{i(\alpha-k)a} + Be^{-i(\alpha+k)a} = Ce^{-(\beta-ik)b} + De^{+(\beta+ik)b}, \quad (3.38)$$

$$\begin{aligned} i(\alpha - k)Ae^{i(\alpha-k)a} - i(\alpha + k)Be^{-i(\alpha+k)a} = \\ (\beta - ik)Ce^{-(\beta-ik)b} - (\beta + ik)De^{+(\beta+ik)b}. \end{aligned} \quad (3.39)$$

from the above set of equations, eliminating the constants, we get

$$\frac{\beta^2 - \alpha^2}{2\alpha\beta} \sinh(\beta b) \sin(\alpha a) + \cosh(\beta b) \cos(\alpha a) = \cos(k(a + b)). \quad (3.40)$$

3.1.2 Energy gaps

Now we can determine the allowed energy values from (3.40). We choose the values of a, b, V_0 and k , and compute the allowed energy states from the above expression. The value of k is varied while other values are kept constant, and the new eigenstates are computed. In order to show the emergence of a energy band gap from the above equation, the value of the Bloch wavenumber k was varied between -2 and 2 with a step of 0.1 . We assume electron energies as in the Bohr model for the hydrogen atom, and choose the values of a and

b in terms of Bohr radius $a_0 = 0.529 \text{ \AA}$. The choice of the parameters was totally arbitrary and they are given as

$$a = 5a_0$$

$$b = 0.3a_0$$

$$V_0 = 6\text{Ry}$$

The energy band structure computed from (3.40) with the specified parameters was calculated as (energy is in Rydbergs)

Figure 3.1: One-dimensional band structure for electron in a periodic potential - from Kronig-Penney model

The energy structure shown in Figure 3.1, reveals the appearance of an Energy gap. The Bloch wave vector for electrons with energies in the band gap are imaginary and non propagating.

3.2 Electromagnetic waves in periodic media

In this section we consider the propagation of the electromagnetic wave in a one-dimensional periodic medium. The purpose of this section is to extend the theory of band gaps to photonic crystals. The theory has strong formal similarities to the quantum theory of electron, described previously, as it also

makes use of the Bloch modes. The configuration and the following analysis are the same as in [55].

3.2.1 The configuration

The scattering configuration is depicted in Figure 3.2. The medium is periodic along the x axis, and the electromagnetic wave is assumed to be propagating along the x axis. We consider a *TEM* mode, with the electric field along the z and the magnetic field along the y axis. Let $E_x(x, \omega)$ and $H_y(x, \omega)$ be the electric and magnetic fields in the (x, ω) domain, respectively.

3.2.2 Regions of analysis

There are two distinct regions of analysis with respect to x as shown, i.e. $\mathcal{R}_1 = \{\mathbf{x} \in \mathbb{R}^3 | (n-2)\Lambda < x < (n-2)\Lambda + b\}$ and $\mathcal{R}_2 = \{\mathbf{x} \in \mathbb{R}^3 | (n-2)\Lambda + b < x < (n-1)\Lambda\}$, where $\Lambda = a + b$. The values a and b are the thickness of the $\mathcal{R}_2$ and $\mathcal{R}_1$ respectively. Each of the sub-regions is considered homogeneous, isotropic, non-conducting and non-magnetic. The region $\mathcal{R}_1$ is characterized by the relative permittivity ε_1 . The region $\mathcal{R}_2$ is characterized by the relative permittivity ε_2 , such that $\varepsilon_1 \neq \varepsilon_2$. In general, the relative permittivity of the entire structure can be described as

$$\varepsilon_r(x) = \begin{cases} \varepsilon_1 & 0 < x < b, \\ \varepsilon_2 & b < x < \Lambda. \end{cases} \quad (3.41)$$

Since we consider a periodic medium the relative permittivity across the medium is periodic, given by

$$\varepsilon_r(x + n\Lambda) = \varepsilon_r(x), \quad n = 0, 1, 2, 3, \dots \quad (3.42)$$

Here, as well as, in many other theoretical investigations of periodic media and photonic crystals a source free configuration is considered. We consider a propagating *TEM* electromagnetic field along the x axis with E_z and H_y as electric and magnetic field quantities respectively.

3.2.3 Maxwell's equations

The evolution of the electromagnetic field in the configuration is governed by the Maxwell equations. In the region $\mathcal{R}_1$ the Maxwell equations in the

frequency domain (x, ω) , with an $e^{-i\omega t}$ time dependence, are

$$\begin{aligned}\frac{\partial \hat{H}_y^{(1)}(x, \omega)}{\partial x} + i\omega \varepsilon_0 \varepsilon_1 \hat{E}_z^{(1)}(x, \omega) &= 0, \\ \frac{\partial \hat{E}_z^{(1)}(x, \omega)}{\partial x} - i\omega \mu_0 \hat{H}_y^{(1)}(x, \omega) &= 0.\end{aligned}\tag{3.43}$$

where $\hat{E}_z^{(1)}$ and $\hat{H}_y^{(1)}$ are the fields inside $\mathcal{R}_1$ in the (x, ω) domain. The elimination of $\hat{H}_y^{(1)}$ from (3.43) leads us to the scalar Helmholtz equation for $\hat{E}_z^{(1)}(x, \omega)$ in $\mathcal{R}_1$:

$$\frac{\partial^2 \hat{E}_z^{(1)}(x, \omega)}{\partial x^2} + k_1^2(\omega) \hat{E}_z^{(1)}(x, \omega) = 0.\tag{3.44}$$

where

$$k_1 = \frac{\omega}{c} \sqrt{\varepsilon_1}.\tag{3.45}$$

The general solution for (3.44) is

$$\hat{E}_z^{(1)}(x, \omega) = a_n^{(1)} e^{ik_1(x-n\Lambda)} + b_n^{(1)} e^{-ik_1(x-n\Lambda)}.\tag{3.46}$$

which is written at the n^{th} unit cell. This represents the field distribution in the region as a sum of incident and reflected plane waves. Similarly the magnetic field can be recovered from (3.43) as

$$\hat{H}_y^{(1)}(x, \omega) = \frac{1}{Z_1} (a_n^{(1)} e^{ik_1(x-n\Lambda)} - b_n^{(1)} e^{-ik_1(x-n\Lambda)}).\tag{3.47}$$

where

$$Z_1 = \sqrt{\frac{\mu_0}{\varepsilon_1}}\tag{3.48}$$

The field quantities $\hat{E}_z^{(2)}$ and $\hat{H}_y^{(2)}$ in $\mathcal{R}_2$ also obey the Maxwell equations

$$\begin{aligned}\frac{\partial \hat{H}_y^{(2)}(x, \omega)}{\partial x} + i\omega \varepsilon_0 \varepsilon_2 \hat{E}_z^{(2)}(x, \omega) &= 0, \\ \frac{\partial \hat{E}_z^{(2)}(x, \omega)}{\partial x} - i\omega \mu_0 \hat{H}_y^{(2)}(x, \omega) &= 0.\end{aligned}\tag{3.49}$$

which leads to the scalar Helmholtz equation

$$\frac{\partial \hat{E}_z^{(2)}(x, \omega)}{\partial x^2} + k_1^2(\omega) \hat{E}_z^{(2)}(x_3, \omega) = 0. \quad (3.50)$$

The general solution for (3.50) is

$$\hat{E}_z^{(2)}(x, \omega) = a_n^{(2)} e^{ik_2(x-n\Lambda)} + b_n^{(2)} e^{-ik_2(x-n\Lambda)}. \quad (3.51)$$

where

$$k_2 = \frac{\omega}{c} \sqrt{\varepsilon_2}. \quad (3.52)$$

Similarly, the magnetic field can be recovered from (3.49) as

$$\hat{H}_y^{(2)}(x, \omega) = \frac{1}{Z_2} (a_n^{(2)} e^{ik_2(x-n\Lambda)} - b_n^{(2)} e^{-ik_2(x-n\Lambda)}). \quad (3.53)$$

where

$$Z_2 = \sqrt{\frac{\mu_0}{\varepsilon_2}} \quad (3.54)$$

To avoid confusion we take

$$\begin{aligned} a_n &= a_n^{(1)}, b_n = b_n^{(1)}, \\ c_n &= a_n^{(2)}, d_n = b_n^{(2)}. \end{aligned} \quad (3.55)$$

Thus rewriting the solutions for $\mathcal{R}_1$ and $\mathcal{R}_2$ in the n^{th} unit cell,

$$\begin{aligned} \hat{E}_z^{(1)}(x, \omega) &= a_n e^{ik_1(x-n\Lambda)} + b_n e^{-ik_1(x-n\Lambda)}, \\ \hat{H}_y^{(1)}(x, \omega) &= \frac{1}{Z_1} (a_n e^{ik_2(x-n\Lambda)} - b_n e^{-ik_2(x-n\Lambda)}), \\ \hat{E}_z^{(2)}(x, \omega) &= c_n e^{ik_1(x-n\Lambda)} + d_n e^{-ik_1(x-n\Lambda)}, \\ \hat{H}_y^{(2)}(x, \omega) &= \frac{1}{Z_2} (c_n e^{ik_2(x-n\Lambda)} - d_n e^{-ik_2(x-n\Lambda)}). \end{aligned} \quad (3.56)$$

3.2.4 Boundary conditions and translation matrix

At the interface between the media, we can impose the boundary conditions for tangential E_z and H_y .

Figure 3.2: One-dimensional periodic medium

At the interface of the $(n-1)^{\text{th}}$ cell we have

$$\begin{aligned} a_{(n-1)} + b_{(n-1)} &= c_n e^{-ik_2 \Lambda} + d_n e^{ik_2 \Lambda}, \\ \frac{1}{Z_1}(a_{(n-1)} - b_{(n-1)}) &= \frac{1}{Z_2}(c_n e^{-ik_2 \Lambda} + d_n e^{ik_2 \Lambda}). \end{aligned} \quad (3.57)$$

Similarly, at the interface within the n^{th} unit cell, we have

$$\begin{aligned} a_n e^{-ik_1 a} + b_n e^{ik_1 a} &= c_n e^{-ik_2 a} + d_n e^{ik_2 a}, \\ \frac{1}{Z_1}(a_n e^{-ik_1 a} - b_n e^{ik_1 a}) &= \frac{1}{Z_2}(c_n e^{-ik_2 a} - d_n e^{ik_2 a}). \end{aligned} \quad (3.58)$$

The equations in (3.57) can be rewritten in the matrix form as

$$\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} a_{n-1} \\ b_{n-1} \end{pmatrix} = \begin{pmatrix} e^{-ik_2 \Lambda} & e^{ik_2 \Lambda} \\ \frac{Z_1}{Z_2} e^{ik_2 \Lambda} & -\frac{Z_1}{Z_2} e^{ik_2 \Lambda} \end{pmatrix} \begin{pmatrix} c_n \\ d_n \end{pmatrix} \quad (3.59)$$

and (3.58) as

$$\begin{pmatrix} e^{-ik_2 a} & e^{ik_2 a} \\ e^{-ik_2 a} & -e^{ik_2 a} \end{pmatrix} \begin{pmatrix} c_n \\ d_n \end{pmatrix} = \begin{pmatrix} e^{-ik_1 a} & e^{ik_1 a} \\ \frac{Z_2}{Z_1} e^{-ik_1 a} & -\frac{Z_2}{Z_1} e^{ik_1 a} \end{pmatrix} \begin{pmatrix} a_n \\ b_n \end{pmatrix}. \quad (3.60)$$

By eliminating $\begin{pmatrix} c_n \\ d_n \end{pmatrix}$ from (3.59) and (3.60), we obtain the expression of the form

$$\begin{pmatrix} a_{n-1} \\ b_{n-1} \end{pmatrix} = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} a_n \\ b_n \end{pmatrix}. \quad (3.61)$$

where

$$A = e^{-ik_1a} \left[\cos(k_2b) - \frac{1}{2}i \left(\frac{Z_1}{Z_2} + \frac{Z_2}{Z_1} \right) \sin(k_2b) \right], \quad (3.62)$$

$$B = e^{ik_1a} \left[-\frac{1}{2}i \left(\frac{Z_1}{Z_2} - \frac{Z_2}{Z_1} \right) \sin(k_2b) \right]. \quad (3.63)$$

$$C = e^{-ik_1a} \left[\frac{1}{2}i \left(\frac{Z_1}{Z_2} - \frac{Z_2}{Z_1} \right) \sin(k_2b) \right]. \quad (3.64)$$

$$D = e^{ik_1a} \left[\cos(k_2b) + \frac{1}{2}i \left(\frac{Z_1}{Z_2} + \frac{Z_2}{Z_1} \right) \sin(k_2b) \right]. \quad (3.65)$$

The equation (3.61) is the translation matrix across a unit cell, which relates the complex amplitudes of the incident and reflected waves in one layer of the unit cell to those in the next. Since the two cells are equivalent, from (3.61) we have

$$\det \begin{pmatrix} A & B \\ C & D \end{pmatrix} = 1. \quad (3.66)$$

3.2.5 Bloch waves and band structures

Here we introduce the lattice translation operator, T such that $T[x] = x + m\Lambda$ where m is any integer. The periodic medium considered here is treated as a one-dimensional lattice, in which case, according to the Bloch theorem, any wave propagating in such a periodic lattice is of the form

$$\hat{E} = E_K e^{ikx} \quad (3.67)$$

where E_K is periodic with the period Λ . The matrix described in (3.61) is a similar representation of a unit cell translation operation. The translation

operation in terms of the Bloch wave is written as

$$\begin{pmatrix} a_{n-1} \\ b_{n-1} \end{pmatrix} = e^{iK\Lambda} \begin{pmatrix} a_n \\ b_n \end{pmatrix}. \quad (3.68)$$

Hence from (3.68) and (3.61) we obtain

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} a_n \\ b_n \end{pmatrix} = e^{-iK\Lambda} \begin{pmatrix} a_n \\ b_n \end{pmatrix}. \quad (3.69)$$

By eliminating $\begin{pmatrix} a_n \\ b_n \end{pmatrix}$ the value of $e^{-iK\Lambda}$ is obtained as

$$e^{-iK\Lambda} = \frac{1}{2}(A + D) \pm \left\{ \left[\frac{1}{2}(A + D) \right]^2 - 1 \right\}^{1/2}. \quad (3.70)$$

Thus, from equation (3.69) we see that $e^{-iK\Lambda}$ is an eigenvalue of the translation matrix. The Bloch waves can thus be considered as the eigenvectors of the translation matrix with eigenvalues given by (3.70), and the Bloch wavenumber K . From (3.70) we can identify two regimes where the Bloch modes exist. If $|\frac{1}{2}(A + D)| < 1$, the values of K are real and correspond to the propagating Bloch mode and if $|\frac{1}{2}(A + D)| > 1$, the values of K are complex with an imaginary K such that Bloch waves are evanescent. The regions where Bloch modes are evanescent are known as the forbidden band for a periodic media, and constitute the band gap. The band edges are where $|\frac{1}{2}(A + D)| = 1$.

Before evaluating the band diagrams for the above configuration, we first calculated the “free photon” diagram for a homogeneous medium with a fictitious period Λ (Figure 3.3). Here, since we assume $\varepsilon_1 = \varepsilon_2 = 4$, the band diagram is described by a linear dispersion relation without any band gaps.

Figure 3.3: Band diagram for a homogeneous medium with $\varepsilon_r = 4$

Let us now consider a specific case, to illustrate the band diagrams in a one-dimensional photonic crystal. Here we use the equation (3.70) to determine the Bloch wave numbers inside the one-dimensional periodic medium. We choose values for $a, b, \Lambda, \varepsilon_1, \varepsilon_2$ and the frequency range ($0 - 22\text{GHz}$) and evaluate the value of K from (3.70). We have seen from the preceding analysis that the Bloch wavenumber K must always be real for the medium to support a propagating Bloch mode. Thus from the computed value of K for each frequency, we remove the values of K which are complex. The parameters were chosen as

$$a = 2.395 \text{ mm}, \quad b = 2.395 \text{ mm}$$

$$f = 0 - 22 \text{ GHz}$$

$$\varepsilon_1 = 1$$

$$\varepsilon_2 = 9.61$$

The band diagram for such a configuration is shown in Figure 3.4, where we

plot wavenumber of the propagating Bloch modes. We notice that the first “forbidden” gap in our medium starts around 12 GHz, with its centre around 15GHz.

Figure 3.4: Band structure for a periodic stratified medium with $\varepsilon_1 = 1$ and $\varepsilon_2 = 9.61$

3.2.6 Two-dimensional and three-dimensional crystals

Analysis of the electromagnetic field in periodic media has been successfully extended to the two-dimensional and three-dimensional structures and photonic crystals [53, 17, 33]. The basic idea of the method is the same: formulate a source-free eigenvalue problem for the Maxwell equations with a periodic coefficient. Further, both the field and the permittivity are expanded in a plane wave basis. Upon subsequent projection, one is left with an algebraic problem of matrix diagonalisation which can be solved numerically. The outcome once again is the frequency-wavenumber diagram. Since in two and three dimensions the wave vector of the plane wave have not only mag-

nitude but also direction, the diagrams become multi-dimensional. In fact, for each particular direction a one-dimensional diagram is obtained similar to the one demonstrated earlier in Figure 3.4. Here too the band gaps may be observed. In [25, 27, 14, 29] the band structures of a two-dimensional photonic crystals have been analysed. In particular, the analysis of a triangular lattice of dielectric rods in air, has shown the existence of a photonic band gap around 15 GHz. The lattice period of the crystal used in this analysis is equal to the lattice period used in our one-dimensional analysis (Figure 3.4). The goal of the two and three-dimensional analysis is to come up with the spatial arrangement which produces overlapping band gaps for majority, if not all directions of wave vectors. It is known, for example, that two-dimensional arrays of dielectrics cylinders forming a square hexagonal lattice do exhibit such a complete band gap. [48], [28], [50], [52].

3.2.7 Periodic resonant structures

Periodicity is a feature also found in metamaterials, which are made up by repeating an unit cell. The unit cell typically is a conducting open resonator much smaller than the free space wavelength of the incident field. An inhomogeneous medium, like metamaterials, can also be modeled as a homogeneous medium with effective parameters derived from the effective medium theory. In many recent publications, for e.g. [22, 18, 42], the problem of determining the effective parameters of a metamaterial structure is addressed. The approach uses the definition of an average field over a unit cell to calculate the *average* effective parameters $\bar{\mu}, \bar{\epsilon}$. Then, the effective parameters of the entire structure are calculated from these average parameters and imposing the periodicity condition. If $\bar{\mu}$ and $\bar{\epsilon}$ are the average permeability and permittivity inside the first unit cell, respectively, and θ is the phase advance across the cell the effective parameters of the whole periodic structure turn out to be:

$$\begin{aligned}\epsilon_{\text{eff}} &= \bar{\epsilon} \frac{\theta/2}{\sin(\theta/2)} [\cos(\theta/2)]^{-S_b}, \\ \mu_{\text{eff}} &= \bar{\mu} \frac{\theta/2}{\sin(\theta/2)} [\cos(\theta/2)]^{S_b}.\end{aligned}\tag{3.71}$$

Here, $S_b = 1$ for electric resonators, while $S_b = -1$ for magnetic resonators. Of course, equations (3.71) are only approximate solutions for the effective permittivity and permeability of a resonant metamaterial. These relations, similar to other effective medium theories, relate the response of a single particle $(\bar{\mu}, \bar{\varepsilon})$ to the effective response of the structure. There are different modes of propagation inside such a medium. The explicit form of θ is obtained in [22] as

$$\sin\left(\frac{\theta}{2}\right) = \frac{S_d \omega \sqrt{\bar{\mu} \bar{\varepsilon}} p}{2} \quad (3.72)$$

where $S_d = 1$ if $\bar{\mu}, \bar{\varepsilon}$ are positive, and $S_d = -1$, if $\bar{\mu}, \bar{\varepsilon}$ are negative, and p is the period of the crystal. We can see that θ depends on $\bar{\mu}$, $\bar{\varepsilon}$, ω and p indicating the presence of both frequency and spatial dispersion.

In case the value of θ is real, there exist a propagating mode inside the crystal. If θ is purely imaginary, our analysis would follow the same line as with the one-dimensional photonic crystal, suggesting the existence of band gaps. The difference between the photonic crystals and the metamaterials is in the *resonant* nature of band gap. If we have $\bar{\mu} \bar{\varepsilon} > \frac{4}{(\omega p)^2}$, from (3.72) we see that θ is a complex number. This does not allow the propagation of the wave inside the medium. By the definition of $\bar{\mu}, \bar{\varepsilon}$ we can see that this phenomenon corresponds to the resonance in the individual elements. In principle such modes exist in a finite structure, but inside an infinitely periodic crystal when the Bloch boundary condition is imposed they do not exist. Hence, the artificial metamaterials are resonant structures, where the periodicity of the resonant elements leads to the band gaps. The resonant nature of the band gaps is a unique feature of metamaterials and is due to the combination of periodicity and resonance.

This approach extends the Effective Medium Theory principles, incorporating the strong multiple scattering effects observed in periodic structures. It seems that periodicity is a necessary condition to obtain a band gap, while the particular frequency range of such band gaps depends explicitly on the period p , and the form of $\bar{\varepsilon}$ and $\bar{\mu}$ of the individual structures. In case of a resonant structure, the band gaps and related phenomena may be tuned to appear at much lower frequencies as compared to a simple photonic crystal

with the same periodicity. Another important result is the appearance of an effective μ , even in cases where the materials are non-magnetic. This has been suggested earlier, that as the size of the scatterer gets large, so that it can sustain a magnetic current, the value of the effective permeability cannot be assumed to be unity [1].

The analysis and the estimation in terms of effective parameters have been mostly developed for infinite periodic media. The case of a finite crystal is obviously different, as the Bloch periodic condition is not satisfied. The presence of evanescent Bloch modes in such crystal is not hard to imagine. Hence, it is important to formulate a rigorous approach to estimate the ε_{eff} of a finite sample.

In [42], once such approach has been proposed. This utilizes the transmission and reflection co-efficients (S-parameters) calculated for a wave normally incident on a finite sample of metamaterial. The scattered field data gathered from the finite slab is inverted, to determine the refractive index n , and the impedance Z of the finite sample. The knowledge of n and Z is used to calculate the effective permittivity and permeability of the finite sample of metamaterial. Further in [43] and [18] this approach is tested systematically on the split ring resonators, thin wire structures and their combination. In both [43] and [42], an inherent ambiguity in determining the effective μ and ε corresponding to the cases where the accurate position of the scattering object is not known has been suggested and discussed.

Nonetheless, the analysis of periodic media reveals to an extent, the form of ε_{eff} which can be expected from such an estimation. In the band gap, we have seen that the Bloch modes of propagation are evanescent. This indicates that, in the band gap the estimated ε_{eff} of a periodic media can be expected to be complex. In addition, the analysis of photonic crystals in [29], [25] has revealed an all angle negative refraction region, just below the first band gap. Though initially it was not attributed to negative effective permittivity or permeability, more recent analysis [24] suggest that the effective permittivity and permeability both have a negative real part, in this region.

Chapter 4

Effective inversion

The method of effective inversion was introduced in [5] as a tool for rapid characterization of compact buried objects. As the scattered field data in subsurface sensing are often aspect-limited, it is impossible to reconstruct an inhomogeneous object completely. Thus it was suggested to represent the unknown two dimensional object as a homogeneous circular cylinder and recover the effective permittivity of this cylinder using an optimization algorithm. Subsequently, this method was extended to three dimensional and arbitrary shaped effective scattering models [2]. The basic idea is very similar to the S-parameter retrieval method [18] where it was first mentioned that the obtained values of ε_{eff} may be non-unique. The effective inversion method may be considered a generalization of the latter approach.

It is not difficult to recognize that effective inversion is a consistent approach to the recovery of the effective permittivity. Indeed, the basic idea behind the effective permittivity is the representation of an arbitrary inhomogeneous object by a homogeneous one having the same outer shape and providing the same scattered field. Let us formulate this problem in more rigorous terms.

4.1 Theory

Consider a finite inhomogeneous isotropic object situated in free space. In the frequency domain with time factor $e^{-i\omega t}$ the electromagnetic field in the

presence of such object satisfies,

$$\begin{aligned} -\nabla \times \mathbf{H}(\mathbf{x}, \omega) - i\omega\varepsilon(\mathbf{x}, \omega)\mathbf{E}(\mathbf{x}, \omega) &= -\mathbf{J}(\mathbf{x}, \omega), \\ \nabla \times \mathbf{E}(\mathbf{x}, \omega) - i\omega\mu_0\mathbf{H}(\mathbf{x}, \omega) &= 0. \end{aligned} \quad (4.1)$$

Here we have presumed that the object has no magnetic contrast with respect to the background medium. The incident field satisfies

$$\begin{aligned} -\nabla \times \mathbf{H}^{\text{in}}(\mathbf{x}, \omega) - i\omega\varepsilon(\mathbf{x}, \omega)\mathbf{E}^{\text{in}}(\mathbf{x}, \omega) &= -\mathbf{J}(\mathbf{x}, \omega), \\ \nabla \times \mathbf{E}^{\text{in}}(\mathbf{x}, \omega) - i\omega\mu_0\mathbf{H}^{\text{in}}(\mathbf{x}, \omega) &= 0, \end{aligned} \quad (4.2)$$

and represents the field produced by the same source as in (4.1), but in free space (without the object). Further, we introduce the scattered field

$$\begin{aligned} \mathbf{E}^{\text{sc}}(\mathbf{x}, \omega) &= \mathbf{E}(\mathbf{x}, \omega) - \mathbf{E}^{\text{in}}(\mathbf{x}, \omega), \\ \mathbf{H}^{\text{sc}}(\mathbf{x}, \omega) &= \mathbf{H}(\mathbf{x}, \omega) - \mathbf{H}^{\text{in}}(\mathbf{x}, \omega). \end{aligned} \quad (4.3)$$

This scattered field satisfies

$$\begin{aligned} -\nabla \times \mathbf{H}^{\text{sc}}(\mathbf{x}, \omega) - i\omega\varepsilon_0\mathbf{E}^{\text{sc}}(\mathbf{x}, \omega) &= -[-i\omega\varepsilon(\mathbf{x}, \omega) - (-i\omega\varepsilon_0)]\mathbf{E}(\mathbf{x}, \omega), \\ \nabla \times \mathbf{E}^{\text{sc}}(\mathbf{x}, \omega) - i\omega\mu_0\mathbf{H}^{\text{sc}} &= 0, \end{aligned} \quad (4.4)$$

and is thus generated by the contrast source. Using the Green's tensor formal solution of (4.4), we can rewrite this problem as an integral equation for the total electric field,

$$\mathbf{E}^{\text{in}}(\mathbf{x}, \omega) = \mathbf{E}(\mathbf{x}, \omega) - \int_{\mathbf{x} \in D} \mathbb{G}(\mathbf{x} - \mathbf{x}', \omega) \chi(\mathbf{x}', \omega) \mathbf{E}(\mathbf{x}', \omega) d\mathbf{x}', \quad (4.5)$$

where

$$\chi(\mathbf{x}, \omega) = \frac{\varepsilon(\mathbf{x}, \omega)}{\varepsilon_0} - 1 = \varepsilon_r(\mathbf{x}, \omega) - 1, \quad (4.6)$$

is the contrast in relative permittivity. The integral is performed over the spatial domain D , where $\chi \neq 0$. The mathematical properties of this integral equation are discussed in [4, 56, 54, 57, 7]. In particular, it is proven that the solution of (4.5) exists if and only if $\varepsilon_r(\mathbf{x}, \omega) \neq 0, \mathbf{x} \in \mathbb{R}^3$. For the solution to be unique it is sufficient that $\text{Im}(\varepsilon(\mathbf{x}, \omega)) > 0, \mathbf{x} \in D$. In operator notation we shall write (4.5) as

$$\mathbf{u} - GX\mathbf{u} = \mathbf{u}^{\text{in}} \quad (4.7)$$

Now let's introduce the effective scattering model. We presume that the illumination condition and the shape of the object are the same, i.e. the same $\mathbf{E}^{\text{in}}(\mathbf{x}, \omega)$ and D . This means that $\mathbf{u}^{\text{in}}$ and G are the same as in (4.7). The effective scatterer, however, is now homogeneous, i.e.,

$$\chi_{\text{eff}} = \frac{\varepsilon_{\text{eff}}(\omega)}{\varepsilon_0} - 1, \quad (4.8)$$

does not depend on $\mathbf{x}$ inside D . The total electric field in the effective scatterer satisfies:

$$\mathbf{u}_{\text{eff}} - GX_{\text{eff}}\mathbf{u}_{\text{eff}} = \mathbf{u}^{\text{in}}. \quad (4.9)$$

It is easy to see that a “physical” effective scatterer, such that

$$\mathbf{u}_{\text{eff}} = \mathbf{u}, \quad \text{while } \chi_{\text{eff}} \neq \chi, \quad (4.10)$$

for all $\mathbf{u}^{\text{in}}$, does not exist. By “physical” we mean a scatterer with the permittivity for which the problem (4.9) has a unique solution. Indeed, suppose the χ_{eff} is “physical”, then

$$\begin{aligned} \mathbf{u}_{\text{eff}} &= [I - GX_{\text{eff}}]^{-1}\mathbf{u}^{\text{in}}, \\ \mathbf{u} &= [I - GX]^{-1}\mathbf{u}^{\text{in}} \end{aligned} \quad (4.11)$$

hence from (4.10):

$$\begin{aligned} [I - GX_{\text{eff}}]^{-1}\mathbf{u}^{\text{in}} &= [I - GX]^{-1}\mathbf{u}^{\text{in}}, \\ [I - GX][I - GX_{\text{eff}}]^{-1}\mathbf{u}^{\text{in}} &= \mathbf{u}^{\text{in}}. \end{aligned} \quad (4.12)$$

However, this is possible for all $\mathbf{u}^{\text{in}}$, if and only if

$$\begin{aligned} [I - GX][I - GX_{\text{eff}}]^{-1} &= I, \\ \chi &= \chi_{\text{eff}}, \end{aligned} \quad (4.13)$$

which cannot be the case if X is inhomogeneous and X_{eff} is homogeneous. This shows, that in general an effective homogeneous scatterer, which would produce the same field as the original inhomogeneous one, for all possible incident fields, does not exist. On the other hand, it may be possible to find an effective scatterer, if we consider a limited set of incident fields or relax the condition (4.10).

Suppose that there exist two complementary subsets of the incident field vectors U_1^{in} and U_2^{in} , such that their union is the complete set of all possible incident fields. Suppose also that it is possible to find an effective scatterer for each of these subsets separately, so that $\chi_{\text{eff}} = \chi_1$ for U_1^{in} and $\chi_{\text{eff}} = \chi_2$ for U_2^{in} , with the “strong” condition $\mathbf{u} = \mathbf{u}_{\text{eff}}$. Then it is obvious that $\chi_1 \neq \chi_2$, since otherwise we would have an effective scatterer for all incident fields, which is not possible. This shows that the effective permittivity, if it is found at all, will depend on the illumination conditions.

Now let's weaken the condition, by introducing an operator A , acting on the total field:

$$\mathbf{v} = A\mathbf{u}. \quad (4.14)$$

This could be the averaging operator of the effective medium theory. We, however, prefer to work with the so called “measurement operator”, which defines the actual procedure for measuring the scattered field:

$$\mathbf{E}^{\text{sc}}(\mathbf{x}, \omega) = \int_{\mathbf{x}' \in D} \mathbb{G}(\mathbf{x} - \mathbf{x}', \omega) \chi(\mathbf{x} - \mathbf{x}', \omega) \mathbf{E}(\mathbf{x}, \omega) d\mathbf{x}', \quad \mathbf{x} \in S, \quad (4.15)$$

where S is the data domain. In operator notation this would be

$$\mathbf{u}^{\text{sc}} = RX\mathbf{u}. \quad (4.16)$$

The strong equivalence condition $\mathbf{u} = \mathbf{u}_{\text{eff}}$ is thus replaced by a weaker one

$$\begin{aligned} \mathbf{v} &= \mathbf{v}_{\text{eff}}, \quad A\mathbf{u} = A\mathbf{u}_{\text{eff}}, \\ &\text{or} \end{aligned} \quad (4.17)$$

$$\mathbf{u}^{\text{sc}} = \mathbf{u}_{\text{eff}}^{\text{sc}}, \quad RX\mathbf{u} = RX_{\text{eff}}\mathbf{u}_{\text{eff}}.$$

Let us determine the general mathematical requirements on the operator A or RX , that would guarantee the existence of an effective scatterer. Obviously, A or RX cannot be an invertible operator. Indeed, suppose A is invertible, then

$$\begin{aligned} \mathbf{v} &= \mathbf{v}_{\text{eff}}, \\ A\mathbf{u} &= A\mathbf{u}_{\text{eff}}, \\ A[I - GX]^{-1}\mathbf{u}^{\text{in}} &= A[I - GX_{\text{eff}}]^{-1}\mathbf{u}^{\text{in}}, \\ [I - GX_{\text{eff}}][I - GX]^{-1}\mathbf{u}^{\text{in}} &= \mathbf{u}^{\text{in}}. \end{aligned} \quad (4.18)$$

and we are back to the strong case. Hence, for the existence of the effective scatterer it is necessary that the averaging or measurement operator has a non-trivial null-space. In fact, from (4.18) we see that A should act as some kind of spatial filter, filtering out “inessential” differences between the total fields inside the original and effective scatterer. This shows the importance of the averaging procedure, but also leaves a considerable freedom for choosing A . In particular, the measurement operator (4.15) with a single fixed observation location $\mathbf{x} = \mathbf{x}_r$ is a suitable candidate, as it filters out all functions orthogonal to the tensor-valued function

$$\mathbb{G}(\mathbf{x}_r - \mathbf{x}, \omega) \chi(\mathbf{x}, \omega) \quad (4.19)$$

Thus, the problem of finding the effective permittivity of an inhomogeneous object is an inverse scattering problem, where one looks for ε_{eff} such that

$$\begin{aligned} \chi_{\text{eff}} &= \frac{\varepsilon_{\text{eff}}}{\varepsilon_0} - 1, \\ \chi &= \frac{\varepsilon(\mathbf{x}, \omega)}{\varepsilon_0} - 1, \\ u^{\text{in}} &\text{ is given} \\ D &\text{ is given} \\ u &= [I - GX]^{-1} u^{\text{in}}, \\ u_{\text{eff}} &= [I - GX_{\text{eff}}]^{-1} u^{\text{in}}, \\ Au &= Au_{\text{eff}} \quad \text{or} \quad RXu = RX_{\text{eff}}u_{\text{eff}}. \end{aligned} \quad (4.20)$$

The fact that for the existence of an effective scatterer we need an averaging operator A with a non-trivial null-space leads to the non-uniqueness of ε_{eff} . Indeed, operator A has the property

$$Aw = 0, \exists w \neq 0, \quad (4.21)$$

where function w belongs to the null-space of A . This is required, since, in general

$$w = [I - GX]^{-1} u^{\text{in}} - [I - GX_{\text{eff}}]^{-1} u^{\text{in}} \neq 0. \quad (4.22)$$

Suppose, we have found ε_{eff} such that (4.22) holds. Consider a function

$$\delta w = [I - GX_{\text{eff}}]^{-1} u^{\text{in}} - [I - GX'_{\text{eff}}]^{-1} u^{\text{in}} \neq 0, \quad (4.23)$$

where X'_{eff} defines another homogeneous scatter with $\varepsilon'_{\text{eff}} \neq \varepsilon_{\text{eff}}$. Obviously if

$$A\delta w = 0, \quad (4.24)$$

then this new $\varepsilon'_{\text{eff}}$ is also a suitable effective permittivity. Thus, the very property which makes it possible to find an effective scatterer, may simultaneously lead to its non-uniqueness. Therefore, the null-space of operator A should neither be too small nor too large.

4.2 Numerical solution of the forward problem

The total electric field produced by a finite inhomogeneous object in free space, for the given incident field $\mathbf{E}^{\text{in}}$ and dielectric contrast $\chi(\mathbf{x}, \omega)$, is the solution to the Electric Field Volume Integral Equation (EFVIE) (4.5). In very few cases, the solution for such an equation can be determined analytically. In other cases this equation must be solved numerically. The first step in determining the numerical solution of an integral equation is to construct a finite-dimensional approximation of the problem by discretization. As a result one obtains a system of linear algebraic equations. An integral of form (4.5) is discretized by approximating it as a finite sum. The explicit “strong” form of our singular integral equation is [4]

$$\begin{aligned} \mathbf{E}^{\text{in}}(\mathbf{x}, \omega) = & \left[1 + \frac{1}{3}\chi(\mathbf{x}', \omega) \right] \mathbf{E}(\mathbf{x}, \omega) \\ & - p.v. \int_{\mathbf{x}' \in D} \mathbb{G}(\mathbf{x} - \mathbf{x}', \omega) \chi(\mathbf{x}', \omega) \mathbf{E}(\mathbf{x}', \omega) d\mathbf{x}', \end{aligned} \quad (4.25)$$

where $p.v.$ stands for the principal value of the integral function. The Green’s tensor is now given by,

$$\begin{aligned} \mathbb{G}(\mathbf{x} - \mathbf{x}', \omega) = & \frac{e^{ik_b(\omega)|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x} - \mathbf{x}'|} \left[\left(-k_b^2(\omega) - \frac{i3k_b(\omega)}{|\mathbf{x} - \mathbf{x}'|} + \frac{3(\omega)}{|\mathbf{x} - \mathbf{x}'|^2} \right) \mathbb{Q}(\mathbf{x} - \mathbf{x}') \right. \\ & \left. + \left(k_b^2(\omega) + \frac{ik_b(\omega)}{|\mathbf{x} - \mathbf{x}'|} - \frac{1}{|\mathbf{x} - \mathbf{x}'|^2} \right) \mathbb{I} \right]. \end{aligned} \quad (4.26)$$

The result of integration in (4.25) for a fixed $\mathbf{x}$ is denoted as

$$\begin{aligned}\mathbf{L}(\mathbf{x}) &= p.v. \int_{\mathbf{x}' \in D} \mathbb{G}(\mathbf{x} - \mathbf{x}', \omega) \chi(\mathbf{x}', \omega) \mathbf{E}(\mathbf{x}', \omega) d\mathbf{x}', \\ &= p.v. \int_{\mathbf{x}' \in D} \mathbf{F}(\mathbf{x}') d\mathbf{x}', \quad \mathbf{x} \in D.\end{aligned}\tag{4.27}$$

Now, we divide the domain D into N elementary cells. The integral over the entire domain D can be split into the sum of integrals over elementary cells as:

$$\mathbf{L}(\mathbf{x}) = \sum_{n=1}^{N-1} \int_{\mathbf{x}' \in D_n \setminus D^s(\mathbf{x})} \mathbf{F}(\mathbf{x}') d\mathbf{x}' + \mathbf{L}^s(\mathbf{x}).\tag{4.28}$$

Here D_n is the domain occupied by the n^{th} cell. In the above expression, the integral over specific cell $D_n = D^s(\mathbf{x})$ is taken out of the sum and denoted as $\mathbf{L}^s(\mathbf{x})$. When we integrate over the cell $D^s(\mathbf{x})$, we reach a point where $\mathbf{x} = \mathbf{x}'$, and the Green's tensor is singular. We are going to evaluate this cell separately. Depending on the location of $\mathbf{x}$ different cells play the role of D^s . In the rest of the cells, the integral over each cell is approximated as

$$\int_{\mathbf{x}' \in D_n} \mathbf{F}(\mathbf{x}') d\mathbf{x}' \approx \mathbf{F}(\mathbf{x}_n) V_n,\tag{4.29}$$

where V_n is the volume of the cell D_n and $\mathbf{x}_n$ is the co-ordinate of the centre of mass of the cell. This is given by

$$\mathbf{x}_n = \frac{1}{V_n} \int_{\mathbf{x}' \in D_n} \mathbf{x}' d\mathbf{x}'.\tag{4.30}$$

The approximation in (4.29)-(4.30) is called the mid point rule. If within each cell the Cartesian component $F_i(\mathbf{x}')$ of $\hat{\mathbf{F}}(\mathbf{x})'$ can be expanded in a Taylor series, one can show that the midpoint approximation is of the order h^2 , where h is the effective size of the cell. Thus (4.28) can be rewritten as

$$\mathbf{L}(\mathbf{x}) = \sum_{n=1}^{N-1} \mathbf{F}(\mathbf{x}_n) V_n + \mathbf{L}^s(\mathbf{x}) + \mathcal{O}(h^2).\tag{4.31}$$

Another important point to be emphasized is that the $\mathcal{O}(h^2)$ depends on the volume of the cell V_n and the location of its centre of mass $\mathbf{x}_n$ and not on

the shape of D_n . Thus we may consider the discretization of the domain by cells of arbitrary shape as long as V_n and $\mathbf{x}_n$ remain the same.

The integral over the singular cell, $\mathbf{L}^s(\mathbf{x})$ is given as

$$\mathbf{L}^s(\mathbf{x}) = p.v. \int_{\mathbf{x}' \in D^s(\mathbf{s})} \mathbb{G}(\mathbf{x} - \mathbf{x}', \omega) \chi(\mathbf{x}', \omega) \mathbf{E}(\mathbf{x}, \omega) d\mathbf{x}', \quad (4.32)$$

$$= \lim_{\epsilon \rightarrow 0} \int_{\mathbf{x}' \in D^s(\mathbf{s}) \setminus \delta(\epsilon)} \mathbb{G}(\mathbf{x} - \mathbf{x}', \omega) \chi(\mathbf{x}', \omega) \mathbf{E}(\mathbf{x}, \omega) d\mathbf{x}', \quad (4.33)$$

In view of the above mentioned freedom we may choose $D^s(\mathbf{x})$ to be a spherical cell of radius $a(\mathbf{x})$ and the same volume and centre of mass as the original cell. The value of $\mathbf{L}^s(\mathbf{x})$ is evaluated in the entire cell except for a small spherical area $\delta(\epsilon)$, with radius ϵ and limit $\epsilon \rightarrow 0$ is taken. The result is [3, 37]

$$\mathbf{L}^s(\mathbf{x}) = \frac{2}{3} [(1 - ik_b(\omega)a(\mathbf{x}))e^{ik_b(\omega)a(\mathbf{x})} - 1] \chi(\mathbf{x}_N, \omega) \mathbf{E}(\mathbf{x}_N, \omega) + \mathcal{O}(h^2). \quad (4.34)$$

where $\mathbf{x}_N$ is the centre of mass of the cell.

The spatial variable $\mathbf{x}$ is still continuous, and has to be discretized. Similar to $\mathbf{x}'$, which now takes values $\mathbf{x}_n$ at the centers of the elementary cells, we also allow $\mathbf{x}$ to take values $\mathbf{x}_m$, $m = 1, 2, \dots, N$ at the same locations. This method is called *collocation*, since both spatial variables $\mathbf{x}$, and $\mathbf{x}'$ take the value at the same location. In addition, the grid we choose is homogeneous i.e. all the elementary cells D_n are identical cubes of side h . Thus the original integral equation problem in (4.25) is reduced to the following discrete problem

$$\begin{aligned} \mathbf{E}^{\text{in}}(\mathbf{x}_m, \omega) = & \mathbf{E}(\mathbf{x}_m, \omega) - \sum_{n=1}^{N-1} \mathbb{G}(\mathbf{x}_m - \mathbf{x}_n, \omega) \chi(\mathbf{x}_n, \omega) \mathbf{E}(\mathbf{x}_n, \omega) h^3|_{\mathbf{x}_n \neq \mathbf{x}_m} \\ & - \left[\frac{2}{3} (1 - ik_b(\omega)a)e^{ik_b(\omega)a} - 1 \right] \chi(\mathbf{x}_m, \omega) \mathbf{E}(\mathbf{x}_m, \omega)|_{\mathbf{x}_n = \mathbf{x}_m} \\ & + \mathcal{O}(h^2). \end{aligned} \quad (4.35)$$

We still need to choose h and N . Since the dimensions D of the domain are given, the choice of the grid step h determines the fineness of the grid with respect to the function we integrate $\mathbf{F}(\mathbf{x}')$. This function is actually the

product of three functions namely $\mathbb{G}(\mathbf{x} - \mathbf{x}', \omega)$, $\chi(\mathbf{x}, \omega)$ and the unknown total field $\mathbf{E}(\mathbf{x}, \omega)$. Unfortunately, we do not know the function we are trying to integrate. We may expect though, that $\mathbf{E}(\mathbf{x}, \omega)$, resembles a wave and oscillates in space with wavelength, that shrinks proportionally to the permittivity inside $\mathbf{D}$. It is a common practise to choose the grid step h in such a way that, there are at least 20 points per medium wavelength. In case of an inhomogeneous medium, this wavelength is obtained from the largest permittivity $\lambda_{\min} = c/(f\sqrt{\varepsilon_{\max}})$, where f is the frequency and c is the velocity of light in vacuum.

The discrete problem in (4.35) can be reduced to a linear algebraic form as

$$\mathbf{u}^{\text{in}} = \mathbf{u} - GX\mathbf{u}. \quad (4.36)$$

Here, $\mathbf{u}$ and $\mathbf{u}^{\text{in}}$ contain the grid values of the total electric field $\mathbf{E}(\mathbf{x}_n, \omega)$ and the incident field $\mathbf{E}^{\text{in}}(\mathbf{x}_n, \omega)$ respectively. There are totally N grid points where $\mathbf{E}^{\text{in}}(\mathbf{x}_n, \omega)$ is known and $\mathbf{E}(\mathbf{x}_n, \omega)$ is determined. In addition at each grid point, the fields have three Cartesian components. Thus $\mathbf{u}, \mathbf{u}^{\text{in}} \in \mathbb{C}^{3N}$ and each have $3N$ entries written in lexicographical order as

$$\begin{aligned} \mathbf{u} &= \begin{bmatrix} E_1(\mathbf{x}, \omega) \\ E_2(\mathbf{x}, \omega) \\ E_3(\mathbf{x}, \omega) \end{bmatrix} \\ \mathbf{u}^{\text{in}} &= \begin{bmatrix} E_1^{\text{in}}(\mathbf{x}, \omega) \\ E_2^{\text{in}}(\mathbf{x}, \omega) \\ E_3^{\text{in}}(\mathbf{x}, \omega) \end{bmatrix} \end{aligned} \quad (4.37)$$

The matrix X in (4.36) represents the contrast function $\chi(\mathbf{x}_m, \omega)$. The equation (4.35) indicates that it is a point wise multiplier of each Cartesian component of the total field. Therefore we introduce the diagonal matrix X with the entries of $\chi(\mathbf{x}_m, \omega)$ repeated thrice along the main diagonal as

$$X = \begin{bmatrix} \text{diag}(\chi) & O & O \\ O & \text{diag}(\chi) & O \\ O & O & \text{diag}(\chi) \end{bmatrix} \quad (4.38)$$

where O denotes a $N \times N$ matrix filled with zeros. Since $\chi \in \mathbb{C}^N$, we have $X \in \mathbb{C}^{3N \times 3N}$.

The grid values of the Green's tensor is stored in a matrix of the following type

$$G = \begin{bmatrix} G_{11} & G_{12} & G_{13} \\ G_{21} & G_{22} & G_{23} \\ G_{31} & G_{32} & G_{33} \end{bmatrix} \quad (4.39)$$

here each sub matrix $G_{ij} \in \mathbb{C}^{N \times N}$ is given by (4.26). The algebraic problem in (4.36) can be rewritten as

$$[I - GX]\mathbf{u} = \mathbf{u}^{\text{in}}. \quad (4.40)$$

or equivalently as

$$A\mathbf{u} = \mathbf{u}^{\text{in}}. \quad (4.41)$$

The solution for (4.40) is obtained numerically by an iterative algorithm, to avoid the inversion of the large matrix A . The most work in such a computation is the $GX\mathbf{u}$ product. Here $X\mathbf{u}$ is the product of a diagonal matrix and a vector which does not take large computational time. The matrix G generated from the integral operator is of convolution type, and the product of such a matrix with a vector can be computed efficiently with the help of FFT. After the usual circular extension of the matrix G the product $GX\mathbf{u}$ is computed as

$$GX\mathbf{u} = \mathcal{F}^{-1}[\mathcal{F}(G) \cdot \mathcal{F}(X\mathbf{u})], \quad (4.42)$$

and requires $\mathcal{O}(3N \log(3N))$ operations.

4.2.1 Memory requirements

Let us now consider the memory requirements for solving a forward problem as described in (4.40). The input and the output vectors of the problem $\mathbf{u}^{\text{in}}$ and $\mathbf{u}$ are both $3N \times 1$, containing complex values. The number of bytes required to store a complex value in MATLAB are 16, which brings the amount of bytes required to store $\mathbf{u}^{\text{in}}$ and $\mathbf{u}$ to $48N$ bytes each. The matrix X is of the order $3N \times 3N$ and the memory required to store X would be $144N^2$ bytes. Since the values in the matrix X are mostly zeros and the

matrix has only diagonal entries, the total memory required to store X would be equal to the size of χ , which would be $16 \times N$ bytes. The largest matrix in this problem is the one containing the Green's tensor. Since we perform a matrix vector product using FFT, we circularly extend the Green's tensor array $\tilde{G}$ to $2NX \times 2NY \times 2NZ \times 3 \times 3$ array and this array has to be computed once and stored in the memory. The memory required to store this extended $\tilde{G}$ matrix is $1152N$ bytes. If we consider a medium with the dimensions

$$NX = 30,$$

$$NY = 30,$$

$$NZ = 30,$$

then the minimum amount of memory required to solve the forward problem would be

$$\begin{aligned} \text{memory}(\mathbf{u}) &= 1296000 \text{ bytes} \\ \text{memory}(\mathbf{u}^{\text{in}}) &= 1296000 \text{ bytes} \\ \text{memory}(X) &= 216000 \text{ bytes} \\ \text{memory}(\tilde{G}) &= 31104000 \text{ bytes} \\ \text{Total} &\approx 35 \text{ MB.} \end{aligned}$$

These arrays constitute the major chunk of data to be handled, and the other variables occupy insignificant amount of memory.

Such an analysis of the memory requirement is important to determine whether the problem is solvable on a given computer. If we consider the current version of MATLAB(7.1) running on Microsoft Windows XP, the total memory allocated to the MATLAB as a single contiguous block, by Windows XP, is 1.5 GB. Therefore, any problem which requires a storage of more than 1.5 GB cannot be solved using the 32-bit version of MATLAB on a Microsoft Windows XP system.

4.2.2 Numerical experiments

In this section we demonstrate the solution of the forward problem in the linear algebraic form as described in (4.40) using an iterative solver. We consider two configurations: a homogeneous cube and an inhomogeneous cube. The configuration details for the homogeneous cube are shown in

Figure 4.1: Scattering configuration with a homogeneous cube

Figure 4.1. Here, the source is a dipole placed at a distance 6.85 mm away from the cube which has a side of 13.7 mm. The relative permittivity of the homogeneous cube is $\varepsilon_r = 4$ and the frequency of the incident electromagnetic

Figure 4.2: The incident field intensity produced by a point dipole

radiation is 10 GHz. This structure is discretized into $N = NX \times NY \times NZ$ cubic cells, where NX , NY and NZ are the number of cubic cells along the x , y and z -axis respectively. The grid step h , for this medium was chosen as 0.45714 mm, from which the amount of cells required to properly describe the medium is given as $NX = 30$, $NY = 30$, $NZ = 30$ and hence $N = 27000$. The properties of the system matrix described in (4.40) determine the type of iterative method that has to be used. The matrix A is not Hermitian. This rules out the possibility of using a conjugate gradient based iterative method, unless we resort to normal equations [57]. In addition, the matrix A is also not normal, which leaves us with most robust iterative schemes, like GMRES [40] and BiCGstab [47]. The problem was solved using both GMRES and BiCGstab algorithms available in MATLAB. The GMRES algorithm was used with different restarts, and the results of the convergence of the algorithms are shown in Figure 4.4. Now, we consider an inhomogeneous

Figure 4.3: The total field intensity inside a homogeneous cube

Figure 4.4: The total field intensity inside a homogeneous cube

Figure 4.5: Scattering configuration with an inhomogeneous cube

cube shown in Figure 4.5. The total field in the cross-section as indicated in the figure is plotted. Both GMRES and BiCGstab algorithms were tested on the inhomogeneous cube as well. The convergence of the algorithms is plotted in Figure 4.7.

The convergence plot from the above experiments show that the GMRES iterative algorithm with restarts works better in case of a inhomogeneous scatterer. Although there is not much of a difference between the convergence obtained by GMRES and BiCGstab algorithms, the capability of applying restarts and reducing the iterations required to converge to a acceptable residual influenced the usage of GMRES in solving the forward problem.

Figure 4.6: Total field intensity in an inhomogeneous cube

Figure 4.7: Convergence of GMRES and BiCGstab

4.3 Arnoldi inversion

In the preceding section we have shown that the numerical solution of the forward scattering problem is a formidable task even for a homogeneous finite object. Our goal though, is to solve the effective inversion problem, that normally would require solutions of many forward problems. Indeed, consider the following formulation of our problem:

Given.

- An inhomogeneous object of finite extent with $\chi(\mathbf{x})$, occupying known spatial domain $D : \chi(\mathbf{x}) \neq 0, \mathbf{x} \in D$.
- Incident field $\mathbf{E}^{\text{in}}(\mathbf{x})$, $\mathbf{x} \in D$.
- Scattered field $\mathbf{E}^{\text{sc}}(\mathbf{x})$, $\mathbf{x} \in S$ (this can be just a single cartesian component of $\mathbf{E}^{\text{sc}}$ at a single spatial location. Both the amplitude and phase are measured.)

Find.

- $\chi_{\text{eff}} = \frac{\varepsilon_{\text{eff}}}{\varepsilon_0} - 1$ or ε_{eff} such that $RX_{\text{eff}}[I - GX_{\text{eff}}]^{-1}\mathbf{u}^{\text{in}} = \mathbf{u}^{\text{sc}}$

As we saw in the previous section, in discrete form the involved functions and operators become vectors and matrices with the following dimensions

$$\begin{aligned} \mathbf{u}^{\text{in}} &\in \mathbb{C}^{3N} \\ \mathbf{u}^{\text{sc}} &\in \mathbb{C} \quad \text{single data point} \\ \mathbb{R} &\in {}^{1 \times 3N} \\ \mathbb{G} &\in \mathbb{C}^{3N \times 3N} \end{aligned} \tag{4.43}$$

$$\chi_{\text{eff}} = \tilde{\chi}P, \text{ where } \tilde{\chi} \in \mathbb{C}, P \in \mathbb{R}^{3N \times 3N}.$$

P is a diagonal matrix indicating the spatial support of the object, here $P = I$. I is a $3N \times 3N$ identity matrix. Hence, matrix $[I - GX_{\text{eff}}]$ is from $\mathbb{C}^{3N \times 3N}$, and its straight-forward numerical inversion is not possible. The problem is also nonlinear with respect to ε_{eff} and if a Newton-type algorithm was applied to solve it, one would need to compute $[I - GX_{\text{eff}}]^{-1}$ for many

different values of ε_{eff} . On the other hand there exist a few efficient numerical algorithms that compute the vector $\mathbf{u}$:

$$\mathbf{u} = [I - GX_{\text{eff}}]^{-1} \mathbf{u}^{\text{in}}, \quad (4.44)$$

for a fixed χ_{eff} . Actually these iterative algorithms construct a reduced-order approximation of $\mathbf{u}$, which may be re-used with a different value of χ_{eff} . This is the idea behind the method proposed in [5]. Substituting $X_{\text{eff}} = \tilde{\chi}P$ in (4.44), we obtain the following problem

$$[I - \tilde{\chi}GP]\mathbf{u} = \mathbf{u}^{\text{in}}. \quad (4.45)$$

Note that the matrix vector products involving GP can be computed by using FFT as a result of the convolution structure of the equations. The approximate solution for $\mathbf{u}_m$ is constructed as

$$\mathbf{u}_m \in \mathcal{K}_m(GP, \mathbf{q}_1) = \text{span}\{\mathbf{q}_1, GP\mathbf{q}_1, \dots, (GP)^{m-1}\mathbf{q}_1\}, \quad (4.46)$$

where $\mathbf{q}_1$ is some vector. The space $\mathcal{K}_m$ is the Krylov subspace of the matrix GP with respect to the starting vector $\mathbf{q}_1$. The orthonormal basis for such a space is obtained by applying the Arnoldi algorithm with $\mathbf{q}_1$ as the starting vector. The algorithm given below generates from the vector $\mathbf{q}_1, GP\mathbf{q}_1, \dots, (GP)^{m-1}\mathbf{q}_1$ a set of vectors $\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_m$ which are orthonormal by construction.

```

for  $j = 1$  to  $m$ 
   $z = GP\mathbf{q}_j$ 
  for  $i = 1$  to  $m$ 
     $h_{i,j} = \mathbf{q}_i^H z$ 
     $z = z - h_{i,j}\mathbf{q}_i$ 
  end
   $h_{j+1,j} = \|z\|$ 
  if  $h_{j+1,j} = 0$  quit
     $\mathbf{q}_{j+1} = z/h_{j+1,j}$ 
end
```

By arranging the Arnoldi vectors $\mathbf{q}_i$ as columns in matrix Q_m , where m is

the number of iterations, the Arnoldi process can be summarized as

$$GPQ_m = Q_m H_m + h_{m+1,m} \mathbf{q}_{m+1} \mathbf{e}_m^T, \quad (4.47)$$

where H_m is an $m \times m$ upper Hessenberg matrix containing the recurring coefficients and $\mathbf{e}_m$ is the m th column of the $m \times m$ identity matrix I_m . The equation (4.47) is the Arnoldi decomposition of the matrix GP . Since the generated Arnoldi vectors are orthonormal, we have

$$Q_m^H Q_m = I_m, \quad (4.48)$$

and from $Q_m^H GPQ_m = H_m$ it follows that

$$Q_m^H \mathbf{q}_{m+1} = \mathbf{0}. \quad (4.49)$$

Now that we have constructed an orthonormal basis for the Krylov sub-space, we can expand the approximation in terms of the basis vectors as

$$\mathbf{u}_m = \alpha_1 \mathbf{q}_1 + \alpha_2 \mathbf{q}_2 + \dots + \alpha_m \mathbf{q}_m = Q_m \alpha_m, \quad (4.50)$$

where $\alpha_m = [\alpha_1, \alpha_2, \dots, \alpha_m]^T$ is a vector of the expansion coefficients. The residual corresponding to this approximation is

$$\mathbf{r}_m = \mathbf{u}^{\text{in}} - (I - \tilde{\chi} GP) \mathbf{u}_m. \quad (4.51)$$

We know that $\mathbf{u}_m \in \mathcal{K}_m$ and hence the residual $\mathbf{r}_m \in \mathcal{K}_{m+1}$. Expanding the residual using the Arnoldi vectors, we have

$$\mathbf{r}_m = \beta_1 \mathbf{q}_1 + \beta_2 \mathbf{q}_2 + \dots + \beta_{m+1} \mathbf{q}_{m+1} = Q_{m+1} \beta_{m+1}, \quad (4.52)$$

where $\beta_{m+1} = [\beta_1, \beta_2, \beta_3, \dots, \beta_{m+1}]^T$. The norm of the residual is given by

$$\|\mathbf{r}\| = (|\beta_1|^2 + |\beta_2|^2 + \dots + |\beta_{m+1}|^2)^{1/2}. \quad (4.53)$$

It can be shown that by choosing the first Arnoldi vector $\mathbf{q}_1$ and α_m properly, all the β_i vanish except for β_{m+1} . We now rewrite (4.51) by applying (4.50) as

$$\mathbf{r}_m = \mathbf{u}^{\text{in}} - Q_m (I_m - \tilde{\chi} H_m) \alpha_m + \tilde{\chi} h_{m+1,m} \mathbf{q}_{m+1} \mathbf{e}_m^T \alpha_m. \quad (4.54)$$

We still have not chosen the first Arnoldi vector, which is done now as

$$\mathbf{q}_1 = \|\mathbf{u}^{\text{in}}\|^{-1}\mathbf{u}^{\text{in}}, \quad (4.55)$$

and if $I_m - \tilde{\chi}H_m$ is invertible, we choose

$$\alpha_m = \|\mathbf{u}^{\text{in}}\|(I_m - \tilde{\chi}H_m)^{-1}\mathbf{e}_1, \quad (4.56)$$

and thus $\beta_m = \mathbf{0}$. Substituting (4.56) in (4.55) we have

$$\mathbf{u}_m = \|\mathbf{u}^{\text{in}}\|Q_m(I_m - \tilde{\chi}H_m)^{-1}\mathbf{e}_1, \quad (4.57)$$

in which the effective contrast ($\tilde{\chi}$) appears as a parameter, and neither Q_m nor H_m depend on $\tilde{\chi}$. Thus we can see that the Arnoldi vectors generated with respect to this starting vector are shift invariant. The computation of the solution for a new value of $\tilde{\chi}$ is essentially the inversion of a $m \times m$ matrix, where m is the number of iterations. Such an inversion is definitely a lot easier than the complete solution of the new forward problem. The residual of such an approximation can be written as

$$\mathbf{r}_m = \beta_1\mathbf{q}_1 + \beta_2\mathbf{q}_2 + \dots + \beta_{m+1}\mathbf{q}_{m+1} = Q_{m+1}\beta_{m+1}, \quad (4.58)$$

and the reduced-order cost functional as

$$F_m(\tilde{\chi}) = \frac{\|\rho_m\|}{\|\mathbf{u}^{\text{sc}}\|}. \quad (4.59)$$

Usually, the solution for the inverse scattering problem is such that $\tilde{\chi}$ minimizes the above cost functional. The reduced order residual ρ_m of the inverse problem is related to the residual of the forward problem as

$$\rho_m = \tilde{\chi}RP[I - \tilde{\chi}GP]^{-1}\mathbf{r}_m. \quad (4.60)$$

We conclude that ρ_m is small on a set of χ if r_m is small enough on that set. The practical implementation of this algorithm also will involve either measuring or computing the scattered field with the actual inhomogeneous values of permittivity. This is done using the GMRES algorithm described in the section on the forward problem. In addition, it is important to choose a finite set of $\tilde{\chi}$ on which the inverse problem is solved. This is specific to each problem, and is defined so that the set $\tilde{\chi}$ is appropriate from the physical and mathematical points of view.

Chapter 5

Numerical experiments

In the previous chapter, we have described a model-based inversion technique for estimating the effective permittivity of inhomogeneous objects. This iterative scheme first constructs a reduced-order approximation for $\mathbf{u}$, for a particular $\tilde{\chi}$. This can be reused for different values of $\tilde{\chi}$ due to the shift-invariance property of the Krylov subspace constructed using an Arnoldi decomposition. The cost functional generated for different values of $\tilde{\chi}$ is represented as a two-dimensional function of ε the value of $\tilde{\chi}$ which minimizes the cost function (4.59) is considered the solution for the inverse scattering problem. In essence, this scheme generates a homogeneous scatterer which produces the same scattered field as the original inhomogeneous scatterer and has exactly the same spatial dimensions as the true scatterer. In this chapter, we implement this model in MATLAB, and estimate the effective permittivity of a finite two-dimensional photonic crystal.

5.1 Regions of analysis

Before describing the actual configuration, we first fix the set of $\tilde{\chi}$ or in our case ε_{eff} , based on the analysis carried out in the previous chapters. We have identified three sections where the form of ε_{eff} for a periodic media like a finite photonic crystal can be predicted.

- At low frequencies, where the wavelength of the electromagnetic wave is large compared to the individual cylinders. In this region we have

identified that the effective permittivity would be given by (2.28).

- At frequencies close to the first band gap, the permittivity of the photonic crystal is negative.
- In the band gap frequencies, where as a result of evanescent modes the permittivity of the crystal is complex.

On the basis of these observation we define the set of ε_{eff} for which the reduced-order model is applied. The permittivity of the dielectric cylinders making up the finite photonic crystal is 9.61. Since the photonic crystal is constructed by placing such cylinders in air, the effective permittivity of the crystal will not exceed 9.61. Thus we now fix $\text{Re}(\varepsilon_{\text{eff}})_{\text{max}} = 10$. The analysis of periodic media in [22], has indicated the presence of both a positive and a negative loss region. As a result we consider $-10 \leq \text{Im}(\varepsilon_{\text{eff}}) \leq 10$, where the value 10 was an arbitrary choice. Similarly the presence of a negative refraction region, where the effective dielectric permittivity of the medium can be assumed negative is also considered. Therefore we have $\text{Re}(\varepsilon_{\text{eff}})_{\text{min}} = -10$, where the value 10 was a choice prompted by the dielectric permittivity of the individual cylinders.

5.2 Interpretation of results

Before describing the configuration, we analyse the behaviour of the reduced-order functional after 30 Arnoldi iterations. We plot the image of the residual $\log_{10}(\frac{\|\mathbf{r}_{30}\|}{\|\mathbf{u}^{\text{sc}}\|})$ as a two-dimensional function of $\text{Re}(\varepsilon_{\text{eff}})$ and $\text{Im}(\varepsilon_{\text{eff}})$ in Fig 5.1.

Here we observe that the residual has a minimum at $\varepsilon_r = 1$, and that it grows outwards. In this configuration, the residual reaches 1 in a few regions. In order to avoid these regions and to make sure that the estimates are fairly accurate, we shall draw a boundary of the region where the residual reaches 3×10^{-3} . The plot of a cost functional $(\log_{10}(\|u_{\text{eff}}^{\text{sc}} - u_{\text{true}}^{\text{sc}}\|/\|u_{\text{true}}^{\text{sc}}\|))$, is also, a two dimensional function of $\text{Re}(\varepsilon_{\text{eff}})$ and $\text{Im}(\varepsilon_{\text{eff}})$, with a blue line denoting the above mentioned trust region, shown in Figure 5.2. The blue line in this figure, was generated from the residual plot in Figure 5.1 and superimposed

Figure 5.1: $\log_{10}(\frac{\|\mathbf{r}_{30}\|}{\|\mathbf{u}_{\text{in}}\|})$ as a function of $\text{Re } \varepsilon_{\text{eff}}$ and $\text{Im } \varepsilon_{\text{eff}}$. This figure shows the residual after 30 Arnoldi iterations.

Figure 5.2: The cost function $\log_{10}(\frac{\|\rho_{30}\|}{\|\mathbf{u}_{sc}\|})$ as a function of $\text{Re } \varepsilon_{\text{eff}}$ and $\text{Im } \varepsilon_{\text{eff}}$ for homogeneous cylinder. The minimum of the cost function indicated by the dark spot, shows the effective permittivity of the homogeneous cylinder.

on the cost functional. Since this was done for a homogeneous scatterer, we observe that the trust region includes nearly the entire domain. The minima inside this region have been used as estimates of the effective permittivity. Though the minima outside this region may also be a valid estimate of ε_{eff} , we only consider the ones inside the trust regions where the residual of the forward problem is acceptable low.

In the plots of cost functionals shown in Figure 5.2, we consider 100 discrete values for both the real and imaginary parts of effective permittivity. In fact, we actually solve 10,000 separate forward problems in each of the plots shown for the corresponding value of ε , using the reduced-order algorithm. In the absence of the reduced-order algorithm, we would actually solve 10,000 forward problem, where for the photonic crystal described later in this chapter, it would take 120 seconds per problem and hence 1,200,000 seconds (nearly 14 days) in total. Whereas using the reduced-order algorithm, we spend approximately 12,000 seconds (3 hours and 20 minutes) in total, which obviously is a huge gain of 100.

5.3 Effective permittivity of a single dielectric cylinder

The reduced-order model was first tested on a homogeneous object. Here we consider a single finite dielectric cylinder with a square cross section of side 3.2 mm and $\varepsilon_r = 9.61$. The cylinder is 6.86 mm long and is illuminated by a dipole source placed 18.66 mm from one of the faces of the cylinder. The scattering configuration is shown in the Figure 5.3. As can be seen, we consider a monostatic configuration, where the source and the receiver are placed at the same location. The source frequency is varied from 1GHz to 16GHz in steps of 1GHz. We first construct the cost functional for the above configuration at all frequencies in our range. The Figure 5.4- 5.7 shows this cost functional and its minimum occurs at just one value of permittivity. This is the value ε_{eff} for the cylinder, reconstructed by the Arnoldi method. It was observed from this experiments that the value of “effective” permittivity of the single cylinder is obviously the true permittivity of the material.

Figure 5.3: The scattering configuration with a single cylinder

Figure 5.4: The cost functional $\log_{10}(\frac{\|\rho_{30}\|}{\|\mathbf{u}^{\text{sc}}\|})$ as a function of $\text{Re } \epsilon_{\text{eff}}$ and $\text{Im } \epsilon_{\text{eff}}$ for a single dielectric cylinder, indicating the absence of dispersion in a single homogeneous cylinder.

Figure 5.5: The cost functional $\log_{10}(\frac{\|\rho_{30}\|}{\|\mathbf{u}^{\text{sc}}\|})$ as a function of $\text{Re } \varepsilon_{\text{eff}}$ and $\text{Im } \varepsilon_{\text{eff}}$ for a single dielectric cylinder, indicating the absence of dispersion in a single homogeneous cylinder.

Figure 5.6: The cost functional $\log_{10}(\frac{\|\rho_{30}\|}{\|u^{sc}\|})$ as a function of $\text{Re } \varepsilon_{\text{eff}}$ and $\text{Im } \varepsilon_{\text{eff}}$ for a single dielectric cylinder, indicating the absence of dispersion in a single homogeneous cylinder.

Figure 5.7: The cost functional $\log_{10}(\frac{\|\rho_{30}\|}{\|\mathbf{u}^{\text{sc}}\|})$ as a function of $\text{Re } \varepsilon_{\text{eff}}$ and $\text{Im } \varepsilon_{\text{eff}}$ for a single dielectric cylinder, indicating the absence of dispersion in a single homogeneous cylinder.

In addition there is no change in ε_{eff} reconstructed by the Arnoldi method, in the frequency range from 1GHz to 18GHz. This behavior was expected, as for a homogeneous object, an effective scatterer is indeed the object itself. Since we had assumed a non-dispersive permittivity for the dielectric cylinder, the reconstructed permittivity remains a constant for all the frequencies in the range.

5.4 Effective permittivity of two dielectric cylinders

Next, we consider two dielectric cylinders in free space. We again use a monostatic configuration, but now with a pair of dielectric cylinders with a square cross-section, suspended in air. The distance between the cylinders was fixed as 4.79 mm, and the position of the dipole source and receiver is indicated in the Figure 5.8. The reduced-order Arnoldi algorithm was used to calculate the effective permittivity of the medium, for frequencies from 1GHz to 16GHz. The plot of the cost functional from such estimates is shown in Figure 5.9-Figure 5.12. At lower frequencies, where the wavelength of the incident electromagnetic radiation was much larger than the cylinders, the permittivity estimated by inversion did not change. At such low frequencies, like 3 GHz, where the effective medium approximations are valid the value of ε_{eff} predicted by (2.28) was calculated to be 6.699. The Figure 5.9 shows the permittivity plot for 1GHz, and we can observe that the permittivity reconstructed is $\varepsilon_{\text{eff}} = 7.5$ (minimum of the cost functional).

A number of such plots were generated in the frequency range of 1GHz to 18GHz, and the minima from these plots were noted. This effective permittivity of two dielectric cylinders in space at different frequencies was plotted as a function of frequency in Figure 5.13. Each point in this graph is, in fact a collection of various cost functionals for different frequencies. As the frequency increases, and the wavelength of the incident electromagnetic wave becomes comparable to the length of the structure, we find significant deviations from the values predicted by (2.28). At the frequency of 13 GHz we find a sharp increase in the imaginary part of reconstructed permittivity and

Figure 5.8: The scattering configuration with two cylinders

Figure 5.9: The cost functional $\log_{10}(\frac{\|\rho_{30}\|}{\|\mathbf{u}^{\text{sc}}\|})$ as a function of $\text{Re } \varepsilon_{\text{eff}}$ and $\text{Im } \varepsilon_{\text{eff}}$ two dielectric cylinders, indicating the dispersion of the effective permittivity constructed by the Arnoldi algorithm.

Figure 5.10: The cost function $\log_{10}(\frac{\|\rho_{30}\|}{\|\mathbf{u}_{sc}\|})$ as a function of $\text{Re } \varepsilon_{\text{eff}}$ and $\text{Im } \varepsilon_{\text{eff}}$ two dielectric cylinders, indicating the dispersion of the effective permittivity constructed by the Arnoldi algorithm.

Figure 5.11: The cost function $\log_{10}(\frac{\|\rho_{30}\|}{\|\mathbf{u}_{sc}\|})$ as a function of $\text{Re } \epsilon_{\text{eff}}$ and $\text{Im } \epsilon_{\text{eff}}$ two dielectric cylinders, indicating the dispersion of the effective permittivity constructed by the Arnoldi algorithm.

Figure 5.12: The cost function $\log_{10}(\frac{\|\rho_{30}\|}{\|\mathbf{u}_{sc}\|})$ as a function of $\text{Re } \varepsilon_{\text{eff}}$ and $\text{Im } \varepsilon_{\text{eff}}$ two dielectric cylinders, indicating the dispersion of the effective permittivity constructed by the Arnoldi algorithm.

(a)

(b)

Figure 5.13: Dispersion of the effective permittivity of two dielectric cylinders

Figure 5.14: The cost functional $\log_{10}(\frac{\|\rho_{30}\|}{\|\mathbf{u}^{\text{sc}}\|})$ as a function of $\text{Re } \epsilon_{\text{eff}}$ and $\text{Im } \epsilon_{\text{eff}}$ for two cylinders at 13GHz, showing the non-uniqueness of the effective permittivity.

a sharp fall in the real part. Moreover, at this frequency the permittivity reconstructed by the Arnoldi inversion exhibits is not unique. Though the non-unique nature of the effective permittivity does not come as surprise, the appearance of non-uniqueness with just two finite scatterers was unexpected.

To illustrate the position dependence of the effective permittivity determined from the Arnoldi algorithm, the simulation for two dielectric cylinders was performed with a different source receiver configuration. The scattering configuration for is shown in Figure 5.16. The corresponding cost functional, at a frequency of 13 GHz is shown in Figure 5.17. The comparison of this with Figure 5.14 shows that the permittivity constructed by the Arnoldi algorithm depends on the spatial position of the source and the receiver. The Arnoldi

Figure 5.15: The cost functional $\log_{10}(\frac{\|\rho_{30}\|}{\|\mathbf{u}^{\text{sc}}\|})$ as a function of $\text{Re } \epsilon_{\text{eff}}$ and $\text{Im } \epsilon_{\text{eff}}$ for two cylinders at 16GHz, showing the non-uniqueness of the effective permittivity.

Figure 5.16: The scattering configuration with two cylinders

Figure 5.17: The cost functional $\log_{10}(\frac{\|\rho_{30}\|}{\|\mathbf{u}^{\text{sc}}\|})$ as a function of $\text{Re } \epsilon_{\text{eff}}$ and $\text{Im } \epsilon_{\text{eff}}$ for two cylinders at 13GHz. A comparison with Figure 5.14 shows the position dependence of the effective permittivity

algorithm inverts the scattered field data available at the receiver to determine the effective permittivity of the medium. Thus at different positions, different values of the scattered field are inverted which leads to difference in the constructed effective permittivity.

5.5 Effective permittivity of a finite photonic crystal

In this section, we finally simulate a finite two dimensional photonic crystal. The photonic crystal is constructed by placing a set of dielectric cylinder in air such that they form a triangular lattice. Each cylinder has a square cross-section of side 3.2 mm, and dielectric permittivity of $\epsilon_r = 9.61$, and the

Figure 5.18: The scattering configuration with a finite photonic crystal

period of the triangular lattice $a = 4.79$ mm. This medium was illuminated by a dipole source, placed 18.66 mm from one of the sides of the crystal. The schematic setup of the system is shown in Figure 5.18.

5.5.1 Length of the dielectric cylinder

In general, a two dimensional photonic crystal has permittivity periodically modulated along two of the co-ordinate axis and is homogeneous along the third. The analysis of such crystals is performed considering the length of the cylinder along the homogeneous side to be infinite, allowing a two dimensional analysis. Being closer to reality, in our case, the individual elements making up the crystal are considered to be finite in length. This length of the cylinder is a very important factor in determining the number of grid points N and hence the amount of memory used. It is therefore important to choose it carefully. Usually, the height cylinder is taken to be at least two times the wavelength of the incident field in air. In our case, this would mean, for the frequency of 14 GHz, the height of the structure must be 4.28 cm. With the grid step $h = 4.5714 \times 10^{-4}m$, this would mean at least 94 grid points for the height. Note that in order to compare the results from the three-dimensions analysis with the two-dimensional analysis in [38], the other two dimensions have been conserved. This results in a structure with $NX = 139, NY = 107, NZ = 94$ and $N = 1398062$. The memory requirement for such a configuration is given as

$$\begin{aligned}\text{memory}(\mathbf{u}) &= 67,106,976 \text{ bytes} \\ \text{memory}(\mathbf{u}^{\text{in}}) &= 67,106,976 \text{ bytes} \\ \text{memory}(X) &= 22,368,992 \text{ bytes} \\ \text{memory}(G) &= 1,610,567,424 \text{ bytes} \\ \text{Total} &\approx 1.65 \text{ GB.}\end{aligned}$$

The amount of memory required to simulate such a photonic crystal arrangement is out of range of what MATLAB is capable of handling under Microsoft Windows XP. In addition, the amount of time required to simulate such a medium would be extremely high and the application of effective-inversion

to such a system is out of the question. For this reason, the height of the crystal had to be curtailed to a much lower “acceptable” value. An “acceptable” height, in this case, would be one where the memory requirements are not that high while the volume of the scatterer is significant to produce the desired scattering effects. For this reason, we considered a simple dielectric parallelepiped with a relative permittivity ε_r and varying thickness (NZ) as a scattering object. The frequency of the incident beam was fixed, and the scattering by the object was observed. When the thickness of the object was extremely small, $0.5 - 0.15\lambda_{\text{med}}$, there was no significant scattering or refraction effects observed. As the thickness of the object reached $0.5\lambda_{\text{med}}$, the effects of refraction and scattering on a homogeneous slab appeared. Though such a length is way shorter than the free space wavelength, it appears to be sufficient to produce significant scattering effects. It is therefore advisable to choose the length of at least $0.5\lambda_{\text{med}}$ in the case of photonic crystals.

The analysis of Luo et al [25] show that, for a crystal similar to what we use, the photonic band gap appeared at around 15 GHz. Incidentally we obtain the same estimate in our one-dimensional analysis in Chapter 3. In the vicinity of this first band gap, at nearly 14GHz, the phenomenon of negative refraction was observed. For this reason we compute the total field inside the crystal at frequencies from 14GHz to 18 GHz, and apply the reduced-order inversion from the backscattered data to determine the effective permittivity of the medium. In addition, the ε_{eff} of the crystal at lower frequencies is analysed in order to verify the compliance of the method with the effective medium theory approach. Therefore, for the simulation of our photonic crystal, the length was fixed at λ_{med} at 14GHz, which is 6.86 mm.

5.5.2 Frequencies below the band gap

We first start by looking at frequencies way below the band gap. The photonic crystal was illuminated by the dipole source, with the frequency of the electromagnetic wave being 1 GHz. The forward problem for such a scattering configuration was solved and the backscattered field at the source was calculated. This scattered field was then inverted using the reduced-order

Figure 5.19: The cost functional $\log_{10}(\frac{\|\rho_{30}\|}{\|\mathbf{u}^{\text{sc}}\|})$ as a function of $\text{Re } \varepsilon_{\text{eff}}$ and $\text{Im } \varepsilon_{\text{eff}}$ for the photonic crystal at 1GHz. The effective permittivity of a photonic crystal at low frequencies is close to the predictions from effective medium theory

Figure 5.20: $\log_{10}(\frac{\|\rho_{30}\|}{\|u^{sc}\|})$ as a function of $\text{Re}\epsilon_{\text{eff}}$ and $\text{Im}\epsilon_{\text{eff}}$ for a finite photonic crystal at 300MHz. The effective permittivity of a photonic crystal at low frequencies is close to the predictions from effective medium theory

Arnoldi algorithm, described in Chapter 4. The number of Arnoldi iterations was fixed to 30, and the cost functional after 30 iterations is shown in Figure 5.19. At this frequency, the wavelength of the incident electromagnetic wave is much larger than the size of the individual elements. At this situation, the effective medium approximation in (2.28) is applied and the effective permittivity of the medium is obtained as $\epsilon_{\text{eff}} = 4.8$. We can see from Figure 5.20 that the value obtained by our method is close to the value predicted by the effective medium approximations. Any frequency below this would also have the same effective permittivity, as the effective medium approximations hold for larger wavelengths. This was verified by performing the same experiment with the incident field at 300 MHz.

5.5.3 Frequencies in the vicinity of the band gap

From [25] we know that the all angle negative refraction region, occurs just below the first photonic band gap. In case of an infinite photonic crystal with a lattice constant of $a = 4.79$ mm, this would be around 14-15 GHz. Since the band structure of a finite crystal follows closely the infinite case, a negative effective permittivity is expected around this frequency range. Therefore the incident field was set at a frequency of 14 GHz, and the forward problem was solved for the finite photonic crystal. The incident and the scattered field intensities in the horizontal cross-section of the photonic crystal are shown in Figure 5.23. The intensity of the total field resembles the focusing by a lens, though not much can be made out of it. Since the wavelength of the incident electromagnetic wave is larger than the height of the crystal, the energy flowing around the crystal also attributes to the effect seen on the plane in Figure 5.23.

A negative refraction phenomenon implies that the reconstructed ε_{eff} should have a negative real part. Figure 5.21 shows the cost functional at 14 GHz, after 30 Arnoldi iterations. Though the cost functional shows more than one minima inside the domain, we trust only the one inside the trust region. We observe that the real part of this effective permittivity, at this frequency is indeed negative. In addition, the effective permittivity is complex indicating loss in a lossless medium.

5.5.4 Inside the band gap

The band gap frequencies are a set of frequencies which are blocked by the photonic crystal. As we have seen in the one-dimensional analysis, at these frequencies the Bloch wave vector is imaginary, indicating a decaying electromagnetic wave inside the crystal. This can be interpreted as a loss and thus we may expect a complex effective permittivity. Also, since we are outside the all angle negative refraction region, the real part of the effective permittivity is expected to be positive. The cost functional of the reduced-order Arnoldi algorithm after 30 iterations is plotted in Figure 5.24. Not surprisingly the reconstructed effective permittivity is not purely imaginary, but also has a

Figure 5.21: The cost functional $\log_{10}(\frac{\|\rho_{30}\|}{\|\mathbf{u}^{\text{sc}}\|})$ as a function of $\text{Re}\varepsilon_{\text{eff}}$ and $\text{Im}\varepsilon_{\text{eff}}$ for a finite photonic crystal at 14GHz indicating a negative effective permittivity.

Figure 5.22: The cost functional $\log_{10}(\frac{\|\rho_{30}\|}{\|\mathbf{u}_{sc}\|})$ as a function of $\text{Re } \varepsilon_{\text{eff}}$ and $\text{Im } \varepsilon_{\text{eff}}$ for a finite photonic crystal at 15GHz indicating a negative effective permittivity.

(a) Incident Field Intensity

(b) Total Field Intensity

Figure 5.23: Field intensities inside the finite photonic crystal at the “negative” refraction frequency

Figure 5.24: The cost functional $\log_{10}(\frac{\|\rho_{30}\|}{\|\mathbf{u}^{\text{sc}}\|})$ as a function of $\text{Re}\varepsilon_{\text{eff}}$ and $\text{Im}\varepsilon_{\text{eff}}$ for a finite photonic crystal at 16GHz, inside the band gap.

positive real part. The effective permittivity of the photonic crystal shows non-uniqueness at this frequency as we find more than one minima inside the trust region. This again does not come as a surprise, as this was observed already with just two dielectric cylinders. The effective permittivity of the medium comprising of just two dielectric cylinders at this frequency had negative loss, while no such negative loss is seen even outside the trust region. This suggests that the crystal is in fact lossy, from the effective permittivity.

5.6 Comparison with the two-dimensional analysis

A two dimensional photonic crystal, with identical cross-section and parameters was analyzed in [38] using a similar effective inversion technique. Their crystal consists of a triangular lattice of lossless infinite dielectric cylinders of relative permittivity $\varepsilon_r = 9.61$, suspended in air. The cylinders have a square cross-section of $3.2mm$ and a lattice period of $4.79mm$. The schematic set up of this configuration is shown in Figure 5.25. In the numerical experiments a line source was used, which was placed $18.66mm$ below the configuration shown in the Figure 5.25. In the Figure 5.26 the $\log_1 0$ of the cost function over the domain of interest for a photonic crystal is shown. The frequency of the incident electromagnetic wave generated by the line source was $14GHz$. The white spot in the figure indicates the minimum of this cost-function and corresponds to the effective permittivity. In addition we also observe other maxima and minima around the positive real axis. These correspond to the eigenvalues of the two-dimensional scattering operator. Figure 5.27 shows that the effective permittivity of the crystal is complex with a negative real part. Thus, the dispersion laws of the effective permittivity in two-dimensional and three-dimensional cases are similar, though there is a marked difference in their particular values. An interesting observation about the three-dimensional analysis as compared with the two-dimensional case, is the occurrence of the band gap. Figure 5.27 below shows the reconstructed permittivity of the photonic crystal from [38] at $15GHz$. This is already a band gap frequency, as seen with the permittivity. In addition we observe

Figure 5.25: Scattering configuration for a two-dimensional infinite photonic crystal

Figure 5.26: Base 10 logarithm of the multi-frequency objective function on the domain of interest at 14GHz, showing negative effective permittivity.

Figure 5.27: Base 10 logarithm of the multi-frequency objective function on the domain of interest at 15GHz, inside the band gap. The figure shows that the effective permittivity of the crystal at this frequency is purely imaginary.

that the permittivity is purely imaginary indicating no transmission through the crystal. This is confirmed by the field intensities inside the crystal. The Figure 5.28 below shows the attenuation of the electromagnetic field inside a two dimensional photonic crystal at the band gap. While in the three dimensional analysis, the band gap occurred at $16GHz$, and the effective permittivity of the photonic crystal was complex with a positive real part.

Figure 5.28: Field intensity at 15GHz, from two dimensional analysis, showing the decaying electromagnetic field inside the crystal at the band gap.

Chapter 6

Conclusions and recommendations

6.1 Conclusions

In this thesis, we have tested the model-based Arnoldi algorithm which estimates the effective permittivity of a finite three-dimensional structure. This was tested on a finite inhomogeneous object, i.e. a three dimensional photonic crystal, at different frequencies. This algorithm models the problem of determining this effective permittivity as an inverse-scattering problem. Here a finite homogeneous model is inverted with the knowledge of the scattered field measured or simulated at a point. This scattered field data, at the given point, was calculated by numerically solving the forward problem for the finite inhomogeneous object.

The analysis of the effective inversion technique used in the Arnoldi algorithm, shows that the reconstructed effective permittivity ε_{eff} is not unique, as the inverse problem is ill-posed. The computational complexity of this problem, due to its non-linearity, is circumvented by using the reduced-order model and the shift invariant property of the Krylov, in the Arnoldi algorithm. The system matrix used in the forward problem is not Hermitian and not normal and hence a general iterative scheme, GMRES, is applied to solve the forward problem. The memory constraints of MATLAB operating under Windows XP dictates the dimensions of the photonic crystal which can be used in our simulations. Since, the length and breadth of the crystal was

fixed in order to compare the results with a two-dimensional analysis, the height had to be curtailed to λ_{med} at 14GHz, such that scattering volume of this sample is significant. The number of iterations used in the Arnoldi algorithm was fixed at 30, again due to the memory constraints on the MATLAB implementation.

This model was implemented in a computer program in MATLAB running on Windows XP. The numerical implementation of this model shows good agreement with the previously known theoretical prediction.

- At low frequencies, when the wavelength of the incident electromagnetic wave is larger than the dimensions of the photonic crystal, the effective permittivity calculated by the Arnoldi algorithm is close to the prediction of Effective Medium Theory in (2.28). This effective permittivity, at low frequencies, is unique.
- At higher frequencies, when the wavelength is comparable to dimension of the medium, the permittivity calculated by the Arnoldi algorithm, for the three-dimensional photonic crystal, is not unique. This non-uniqueness was observed even with just two-homogeneous scatterers.
- As the frequency approaches the band gap, i.e. at 14GHz and 15GHz, we observe the appearance of the negative real part of permittivity as predicted in [25].
- In the band gap region of the photonic crystal, we observe that the effective permittivity of the crystal given by the Arnoldi algorithm is positive and complex with a significant imaginary part.

However, the comparison of these results from the three-dimensional analysis with the two-dimensional results, reveals a few deviations.

- The band gap, in the two-dimensional analysis starts at 15 GHz as compared with 16 GHz with the three-dimensional results.
- The values obtained for effective permittivity obtained from the two-dimensional and the three-dimensional models are of the same form, yet quite different.

- Inside the band gap, the effective permittivity constructed by the two-dimensional analysis is purely imaginary, while the effective permittivity from the three-dimensional analysis has a positive real part.

Thus the reduced-order Arnoldi algorithm, used to determine the effective permittivity of a finite three-dimensional photonic crystal, shows good agreements with the effective medium theory, and the theory of periodic media. However, owing to the finite size of the individual elements making up the photonic crystal, we observe variations from the results given by the two-dimensional analysis. In addition, the effective permittivity given by the Arnoldi algorithm is not unique even with just two homogeneous scatterers placed close to each other. Therefore the Arnoldi algorithm can be used to determine the effective permittivity of a finite inhomogeneous medium at any given frequency.

6.2 Recommendations

As described in the section on dimensions of the photonic crystal in chapter 5, the memory constraints play an important role in determining size of the object that can be used in the simulation. In addition, the number of iterations of the Arnoldi approximation used in the implementation of the algorithm described in [2], in MATLAB was fixed to 30, due to the same memory constraints. Thus with a higher available memory, a more accurate simulation of a much larger objects can be achieved.

The Arnoldi algorithm used in [2], stores the $\mathbf{u}_m$ vectors in memory, where m is the number of iterations. This increases the memory requirements for implementing a more accurate system with higher number of iterations. Instead, if this system could be replaced by a recursive system, which does not require the storage of a large number of vectors, the accuracy of the calculation can be increased with no additional memory cost.

In this thesis, we have considered a finite inhomogeneous object made out of a lossless material. This can be extended to a lossy material, and a more complex medium, like a finite sample of metamaterial with resonant components, can be simulated. Also, the inverse scattering problem was

formulated to determine effective permittivity of the inhomogeneous objects. This problem can be reformulated in terms of the magnetic field equations to calculate the effective permeability of finite structures.

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