

A PLATE-ARRAY METAMATERIAL IN CYLINDRICAL GEOMETRIES

A THESIS PRESENTED FOR THE DEGREE OF
DOCTOR OF PHILOSOPHY OF IMPERIAL COLLEGE LONDON
AND THE
DIPLOMA OF IMPERIAL COLLEGE
BY
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THE INVESTIGATION WHICH IS THE SUBJECT OF THIS THESIS
WAS CARRIED OUT UNDER THE TERMS OF QINETIQ
AGREEMENT No: CON11566

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DECEMBER 2023

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A Plate-Array Metamaterial in Cylindrical Geometries

ABSTRACT

A metamaterial composed of closely-spaced, thin metallic plates, sandwiched between layers of dielectric, is modelled for the purposes of engendering hierarchical photonic crystals along one- and two-axes. The plate-array is considered infinite in its depth but is made to occupy a circular cross-section, so as to define a plate-array metamaterial cylinder, or metacylinder. By homogenizing the plate-array in the limit of small inter-plate spacing, we arrive to an effective medium description for the plate-array that describes the motion of waves within the dielectric channels. This model is encapsulated by an effective one-dimensional wave equation in the interior and a pair of continuity equations at the cylindrical surface. The solutions exterior to the metacylinder are provided in terms of expansions in Bessel functions, a treatment referred to as the dynamic multipole method. By writing the interior solutions as sums over regular waves, we arrive to the scattering matrix for an arbitrary arrangement of metacylinders, before considering macroscopic structures of an underlying periodic order. This semi-analytic formalism lends itself to numerical simulations, with which we investigate phenomena such as: the quasi-modes of metacylinder ring resonators, the reflection and transmission of plane-waves by a metacylinder diffraction grating, Rayleigh-Bloch modes of a tunable dispersion, and the effective properties of a 2D plate-array metasurface. We also outline concepts from 2D topological photonics for the purposes of realising the valley-Hall insulator phase in a honeycomb photonic crystal. The overlapping of a non-trivial band gap for both transverse electric and transverse magnetic polarizations corresponds to a complete photonic band gap engendered by the spatial symmetry breaking of the direct lattice. In turn, the honeycomb lattice is shown to host edge modes when two media, of opposite boundary condition but identical symmetry-breaking perturbation, are joined to form an interface.

“It’s the job that’s never started as takes longest to finish”

- J.R.R. Tolkien

ACKNOWLEDGMENTS

I am indebted to so many people for their help in writing this thesis. Foremost to my supervisor Professor Richard Craster for all of his guidance, his patience, his wisdom and the faith he put in me when my code wasn't working. I am so lucky to have worked with you.

To my many colleagues Professor Sébastien Guenneau, Dr. Bryn Davies, Dr. Richard Wiltshaw, Dr. Marie Touboul, Dr. Benjamin Vial, Dr. Marc Martí-Sabaté and Dr. Mario Lázaro. You have all been of tremendous help and a constant source of encouragement. I genuinely could not have completed this PhD without you.

To Dr. Stuart Hawkins and his family, for inviting me to Sydney, taking me to Maroubra beach and introducing me to the Aussie brekkie roll. Also to Professor Christopher Poulton, for being such a kind host at UTS and buying me Sydney rock oysters (they really were the best in the world).

To Professor Richard Porter, for all of his help on the plate-array homogenization model and for inviting me to visit him at the University of Bristol. It was lovely to be back in my old neck of the woods.

To Thivan, Sara, Karina, Jamie, Connor and Maria, for being such wonderful office mates and comrades-in-arms. Also to Dr. Hiroyuki and Anna, for laughing at my jokes (and at me). It was a joy to be around you all.

To my beloved partner Emilie, for giving me more to life than mathematics, and for being such good fun. How could I have done it all without you?

To my mother Elena and brother Michael, for everything they've ever done for me, and for being there through all of the agonies that a PhD entails.

Finally, to my father Jeremy, who would be very pleased to know that his investment in a GCSE maths and physics tutor has finally made a return.

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Journal Papers

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Submitted

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R Wiltshaw, HJ Putley, C Bou Dagher, and MP Makwana. Properties of topologically non-trivial complete photonic band gaps.

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1 Introduction

1.1 Wave Propagation

In their classical sense, waves are described as a propagating disturbance in some quantity, and are synonymous with the transport of energy across space and time. Classical waves can be distinguished as either mechanical (such as seismic, water or acoustic waves) or electromagnetic (light), and are ordinarily accompanied by a partial differential equation (PDE) or *wave equation* governing the motion of the wave. A wave equation deals with either scalar or vector functions, the former pertaining to scalar quantities such as acoustic pressure, and the latter to vector quantities such as unpolarized light or elastic waves. Mechanical waves occur due to the oscillations of matter about an equilibrium position from which they do not greatly deviate, such that energy is transported through the medium over long distances. Electromagnetic waves on the other hand require no underlying medium through which to propagate; they are synchronised oscillations of electric and magnetic fields transverse to the direction of propagation. The motion of light is governed by Maxwell's equations, which under appropriate conditions can be combined to form a pair of second order wave equations for the magnetic and electric fields. Several quantities characterising wave propagation apply regardless of the underlying setting, namely: wavelength λ , wavenumber k , angular frequency ω and amplitude A . As my supervisor has often remarked 'Waves is Waves.'

1.1.1 Linear Waves and Green's Function

Linear waves are waves governed by a linear wave equation, that is a PDE linear in the dependent variable and its higher derivatives. Linear systems benefit from the superposition principle, which asserts that the net response to a collection of stimuli is a sum over the responses to the stimuli individually. Each stimulus can represent the introduction of some instantaneous impulse to the problem, which disturbs the otherwise harmonious

behaviour of the PDE and produces an output or *impulse response*. Examples of stimuli include the load applied by a mass on an elastic body at a point on the body's surface, or the presence of a dielectric medium in the path of propagating light. The impulse response of a linear PDE in a specified boundary value problem is called the *Green's function*, which is the solution to the linear PDE in response to the instantaneous stimulus. Thus for some linear differential operator $L(\mathbf{r})$ with specified boundary conditions, the Green's function $G(\mathbf{r}; \mathbf{r}')$ is the solution to the equation:

$$LG(\mathbf{r}; \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') \quad (1.1)$$

where $\mathbf{r}$ represents any point and the impulse at the point $\mathbf{r}'$ is represented by the Dirac delta function. The net forcing of the problem due to a set of instantaneous sources is therefore a sum over Dirac delta functions, and the net response a sum over Green's functions.

The principle of superposition is essential to the work presented in this thesis, which relies on the summation over fundamental structural elements, and therefore over Green's functions, to describe the net macroscopic scattering of waves. The Green's function for a particular structural element, or *inclusion*, is determined by consideration of the conditions on the inclusion, as well as any conditions applying to the outgoing solution, such as the Sommerfeld radiation condition.

1.1.2 Time-Harmonic Fields

Let us consider one of the most well-known and ubiquitous equations in physics, the two-way scalar linear wave equation:

$$\left(\nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \right) u(\mathbf{r}, t) = 0, \quad (1.2)$$

where ∇^2 is the Laplace operator in spatial coordinates, t is the time coordinate, $u(\mathbf{r}, t)$ is the wavefield as a function of both space and time, and c is the wave speed. Equation (1.2) governs wave motion in a variety of settings, including acoustic waves and light of transverse-electric (TE) or transverse-magnetic (TM) polarizations. Here we introduce the notion of *time-harmonic* waves, which are waves that are assumed to vary periodically in time in a sinusoidal fashion. This allows for the explicit separation of the time

component from the spatial components, such that for a time-harmonic field:

$$u(\mathbf{r}, t) \equiv \text{Re}\{u(\mathbf{r})e^{-i\omega t}\}. \quad (1.3)$$

Equation (1.3) encapsulates the evolution of the solution in time, meaning that solutions to wave scattering problems computed with time-harmonic fields are referred to as being in the ‘frequency domain’, in that they capture the time-averaged wave propagation. Substitution of (1.3) into (1.2) yields the following wave equation, known as the Helmholtz equation:

$$(\nabla^2 + k^2)u(\mathbf{r}) = 0, \quad (1.4)$$

where the time-dependence $e^{-i\omega t}$ has been suppressed and $k = \omega/c$. Solutions to the Helmholtz equation are frequently given in terms of k rather than ω , and this is the convention used in this thesis.

We are concerned with the propagation of linear time-harmonic waves, that is waves with any explicit time dependence fully accounted for in the governing PDE, as in (1.4). Particular focus is paid to scalar flexural waves in thin-elastic plates and light in TE polarization; this reduces the vector wave equation to a scalar wave equation for only a single magnetic field component.

1.1.3 Dispersion

The dispersion of a wave packet describes how waves of different frequencies disperse, or spread out, in space during propagation through a dispersive medium. The *dispersion relation* of a wave describes the angular frequency as a function of wavenumber $\omega = f(k)$, with a linear relationship describing non-dispersive propagation*. To see why, we must define two velocities that characterise wave motion:

$$v_p = \frac{\omega}{k}, \quad \text{and} \quad v_g = \frac{\partial \omega}{\partial k}. \quad (1.5)$$

The first, v_p , is the phase velocity, which describes the velocity at which any phase of the wave, such as a crest or trough, propagates at a given frequency. The second, v_g , is the group velocity, which is the velocity of the energy-carrying envelope of the wave, as outlined by the wave’s amplitudes. In the case $v_p = v_g$ then ω is directly proportional

*The dispersion equation is often equivalently written $f(\omega, k) = 0$.

to k i.e. $\omega/k = \partial\omega/\partial k = c$ where c is a constant, such that waves of any frequency travel at the same speed. More generally $v_p \neq v_g$ so waves of different frequencies travel at different speeds, and it is in this case that a wave packet in propagation through a dispersive medium would spread out. An example of dispersion that most readers will be familiar is that of white light in propagation through a triangular prism; the refractive index of the prism is a function of wavelength, causing white light to split into its spectral components as different wavelengths are deflected at different angles. Of similar nature is the localisation of light of different wavelengths at different locations along a graded structure, a phenomenon known as *rainbow trapping*.

Analytical dispersion relations are uncommon, but can occur in simply-structured media. Waves guided along a linear grating of point-scatterers for example have a semi-analytical dispersion relation relating the free-space wavenumber ka to the Bloch wavenumber βa via a rapidly converging sum over scattering angles [5]. But an analytical or semi-analytical solution is a rarity, particularly for designed composite materials of some underlying complex structure. In the absence of an elegant closed-form expression one must resort to numerical techniques to deduce the dispersive properties of a medium. This is usually carried out by forming a system of equations relating the incident and outgoing fields through a *scattering* matrix, which encapsulates the medium's geometry and boundary conditions. The scattering matrix is most commonly written $\mathbf{S}(\omega, k)$, or as a function of the 'equivalent' variables dictating dispersion. The non-trivial or *eigensolutions* of the scattering matrix are the set of solutions that exist in the absence of an incident field, and are found by searching for the zeros of the matrix, or equivalently the zeros of the absolute matrix determinant or minimum absolute eigenvalue:

$$|\det(\mathbf{S}(\omega, k))| = 0 \quad \text{or} \quad \min\{|\text{eig}(\mathbf{S}(\omega, k))|\} = 0. \quad (1.6)$$

Writing (1.6) explicitly has made it obvious that we have arrived to a dispersion relation between ω and k . Occasionally, such as when our fields in question are approximated to leading order terms in their underlying expansions, (1.6) can be solved analytically, and these approximations are referred to as *dipole* approximations [13]. In most instances however this can only be achieved for structures of a simple construction, or will only apply in some small limit, and for the most part we are forced to solve (1.6) numerically. Other methods to solve for the dispersive nature of a medium are also available, including finite element methods (FEM) or the fast-Fourier transform (FFT) of scattered fields [14]. The work herein largely avoids these methods except in specific circumstances when FEM computations are used to verify semi-analytical models.

The fact that these solutions exist in the absence of an incident field implies that they exist as a result of the properties of the medium itself. The word ‘eigen’ translates to ‘self’ or ‘own’, so the eigensolutions of a complex medium are the solutions permitted by the medium to propagate through it. In more colloquial language, these are the solutions that ‘want’ to exist, and can therefore be excited by an incident field. Just as any wave in motion along a string is a function of tension and mass per unit length, so too are waves in complex media permitted only by the material properties.

1.1.4 Flexural Waves

In a waves context, elasticity refers to the elastic deformations and stresses experienced by a thin plate due to the presence of forces or moments upon the plate’s surface. Models that attempt to describe these elastic deformations are referred to as plate models, the simplest and most widely used of which is classical plate theory or the Kirchhoff-Love (KL) theory of thin plates. KL theory stipulates that a three-dimensional plate can be represented by a two-dimensional mid-surface plane that undergoes deformations normal to the plate’s surface, and for which deformations in-plane can be neglected for plates of isotropic and homogeneous composition. The propagation of waves through KL plates is modelled in a dynamic sense, with the waves themselves being referred to as *bending* or *flexural* waves in that they represent the elastic bending or flexing of the thin plate in the absence or presence of loading. Making the assumption of time-harmonic fields, the fourth-order PDE that arises to govern these dynamics is referred to as the Kirchhoff-Love equation:

$$(\Delta^2 - k^4)u(\mathbf{r}) = 0 \tag{1.7}$$

where $\Delta^2 \equiv \nabla^4$ is the biharmonic operator* and $u(\mathbf{r})$ is the wavefield, or in this case the displacement field normal to the mid-surface plane. Note that in this case the displacement field is a scalar quantity; vector fields in elasticity occur during propagation through a bulk continuum, being elastic deformations in more than one spatial dimension. A discussion on the key assumptions underlining KL theory are provided in the following chapter.

The scattering of waves in KL plates is modelled as the interaction of flexural waves with inclusions treated as point-forcings, the Green’s function of which being the difference of

*The form of the biharmonic operator ∇^4 is provided in Appendix appendix A Eq. (A.19).

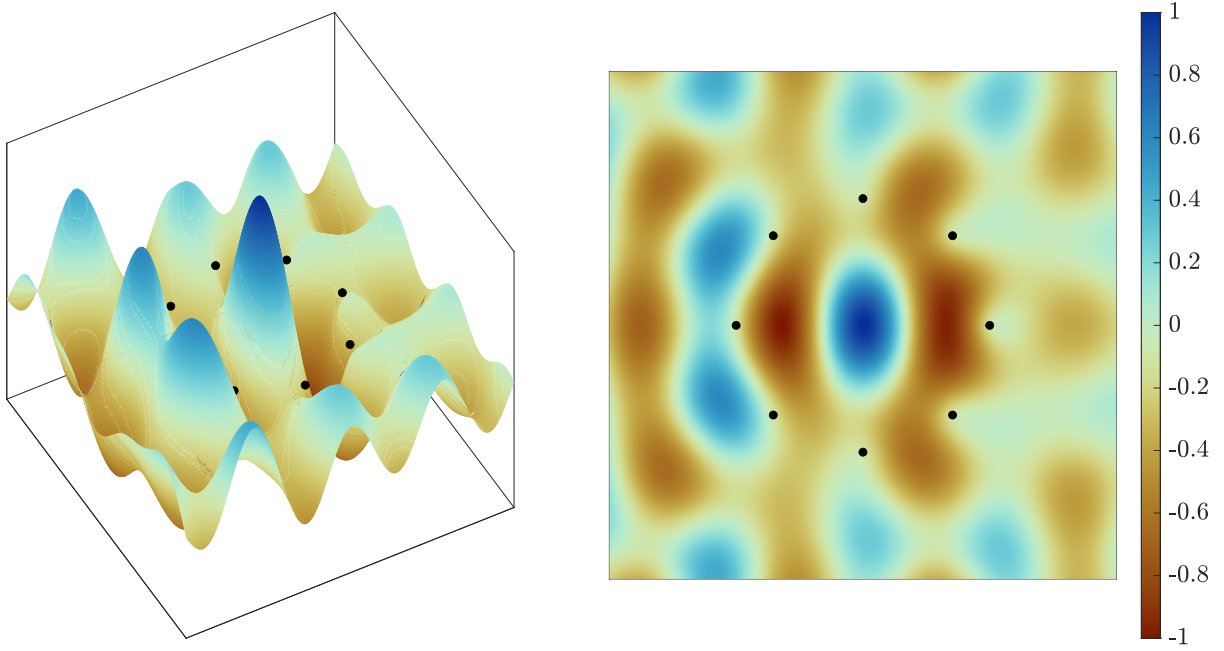


Figure 1.1: (a) Surface and (b) pseudo-colour visualisations of $\text{Re}\{u(\mathbf{r})\}$ in a KL plate due to the scattering of a plane-wave by an arrangement of point-forcings (block dots). Recreation of a result from [5].

two Hankel functions of the first kind. As we shall see in Chapter 2, this Green's function is non-singular even at the point of forcing, and this combined with the necessity of computing only two special functions makes KL theory an excellent model with which to conceive toy problems that translate straightforwardly into acoustic or electromagnetic settings. The displacement field generated by the scattering of a plane-wave by a circular arrangement of point-forcings is visualised in Fig. 1.1 as (a) a surface field and (b) a pseudo-colour field. The periodic arrangement of point-forcings grants the structure a strong resonance at this frequency, which manifests as a large-amplitude displacement field, or rather maximal forcing experienced by the thin-elastic plate.

1.1.5 Electromagnetic Waves

Chapters 3-7 of this thesis are concerned with the propagation of electromagnetic waves in *photonic crystals*, which are structured media characterised by a periodic refractive index n . The motion of an electromagnetic wave in propagation through a photonic crystal, and in the absence of charges and currents, is governed by Maxwell's equations,

written here in time-harmonic form:

$$\left. \begin{aligned} \nabla \cdot \mathbf{E} &= 0, & \nabla \times \mathbf{E} &= ik\sqrt{\frac{\mu_0}{\varepsilon_0}}\mu_r\mathbf{H} \\ \nabla \cdot \mathbf{H} &= 0, & \nabla \times \mathbf{H} &= -ik\sqrt{\frac{\varepsilon_0}{\mu_0}}\varepsilon_r\mathbf{E}. \end{aligned} \right\} \quad (1.8)$$

Here $\mathbf{H} = \mathbf{H}(\mathbf{r})$ is the magnetic field and $\mathbf{E} = \mathbf{E}(\mathbf{r})$ the electric field, μ_0, ε_0 are the permeability and permittivity of free-space and μ_r, ε_r are the relative permeability and permittivity of the medium. In our notation $\mu_r = \mu/\mu_0$ and $\varepsilon_r = \varepsilon/\varepsilon_0$, where μ, ε are the permeability and permittivity of the medium, such that the medium is defined relative to vacuum. Taking the curl of the curl of the magnetic and electric fields, making use of the curl of curl identity (A.18), and eliminating for either $\mathbf{E}$ or $\mathbf{H}$, yields:

$$(\nabla^2 + n^2k^2) \begin{Bmatrix} \mathbf{E} \\ \mathbf{H} \end{Bmatrix} = 0, \quad (1.9)$$

which is just the Helmholtz equation (1.4)*, where $n = \sqrt{\varepsilon_r\mu_r}$. (1.9) can be reduced to a scalar wave equation for the magnetic or electric field by asserting that the electromagnetic wave is of either TE or TM polarization. We follow the notation common to the literature of photonic crystals [15], where in Cartesian coordinates:

$$\underbrace{\mathbf{H} = \begin{pmatrix} 0 \\ 0 \\ H_z \end{pmatrix}}_{\text{TE}}, \quad \mathbf{E} = \begin{pmatrix} E_x \\ E_y \\ 0 \end{pmatrix}, \quad \underbrace{\mathbf{H} = \begin{pmatrix} H_x \\ H_y \\ 0 \end{pmatrix}}_{\text{TM}}, \quad \mathbf{E} = \begin{pmatrix} 0 \\ 0 \\ E_z \end{pmatrix}. \quad (1.10)$$

In the former case there is a scalar wave equation for H_z , and in the latter a scalar wave equation for E_z , with the electric/magnetic field being confined to the xy plane, respectively. We shall see later that when the constituent crystal elements are perfect electrical conductors ($\varepsilon \rightarrow \infty$), a wave of TE polarization need only satisfy a Neumann boundary condition on the longitudinal magnetic field component H_z , with the $\mathbf{E}$ field retrieved via the curl of $\mathbf{H}$ as in (1.8)[†].

A simple example of a periodic crystal in one-dimension is a circular arrangement of cylin-

*Alternatively one can combine the time-dependent Maxwell's equations via the identical method to derive (1.2), before assuming a time-harmonic solution as in §1.1.2.

[†]Equivalently, a wave of TM polarization propagating through a photonic crystal of perfect magnetic conductors ($\mu \rightarrow \infty$) must satisfy a Dirichlet boundary condition for the longitudinal electric field component E_z .

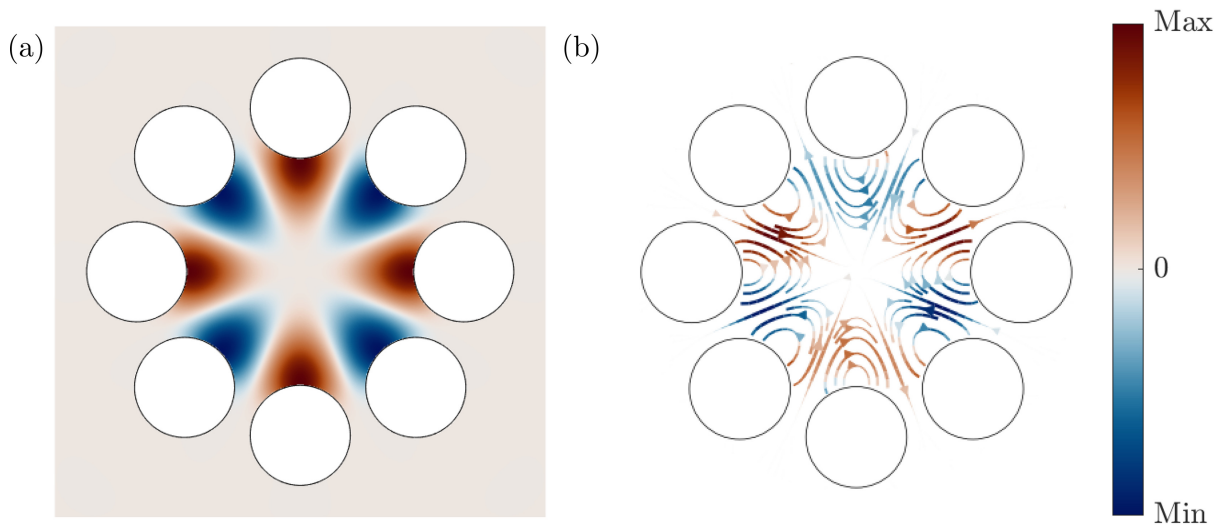


Figure 1.2: (a) $\text{Re}\{\mathbf{H}\}$ and (b) $\text{Re}\{\mathbf{E}\}$ fields of a mode in propagation along a structured ring of metallic cylinders.

dical scatterers, which is invariant in the z -direction and periodic along the circumference. The uniform cylindrical inclusions differ in refractive index from their surrounding medium, with this periodic arrangement giving rise to *grating modes* that propagate along the structure; see Fig. 1.2. The circular cross-section and homogeneity in z allows for the three-dimensional vector problem to be reduced to a description in two-dimensional polar coordinates (r, θ) , with the fields being described in summations of *cylindrical harmonics*; products of Bessel and trigonometric functions. These are generally referred to as *multipole expansions*, in that they are linear combinations of orthogonal modes of increasing order $m \in \mathbb{Z}$, with $m = 0$ denoting the monopole, $m = \pm 1$ the dipole, etc. A full description of the multipole formalism is provided in chapter 3.

1.2 Structured Media and Homogenization

A structured medium refers to a collection of fundamental structural elements repeated periodically, so as to engender a crystal that possesses some underlying long-range order. This uniformity can be exploited for the purposes of determining the crystal's dispersion by reducing the analysis to a fundamental unit cell. A unit cell is, by definition, a fundamental volume of space that can be tessellated, by integer multiples of the crystal's basis vectors, to entirely fill space without gaps or overlaps between cells. A simple one-dimensional example are the rings featured in Fig. 1.2, for which the unit cell is defined as the fundamental wedge that can be rotated through $2\pi/N$ radians about

the ring-centre. Related to this is the notion of homogenization, whereby a structured medium possessing some characteristic lengthscale that is sub-wavelength to a typical wave can be described with *averaged* or *effective* properties in that limit. This enables an ‘effective medium’ description, where the constituent structured building blocks are replaced by an effective wave equation. Likewise, effective material properties, such as the effective electric permittivity or magnetic permeability, can be deduced from an asymptotic analysis of the dispersion relation in the limit of small frequency or small wavenumber.

The mathematical treatment describing the interactions of waves with periodic media requires the language of condensed matter physics, which is concerned with the electronic phases of matter. Concepts such as the Bravais lattice, Bloch’s theorem and topological phases translate identically from systems of ordered matter to structured media in elasticity, acoustics and electromagnetism. In fact, some of the very first topological phases have been realised in photonic systems, rather than in electronic systems, such as the world’s first physically realised 3D Chern insulator [16].

1.2.1 The Direct Lattice and Bloch’s Theorem

A periodic medium is most suitably defined by a set of direct lattice vectors $\{\mathbf{R}_j\}$, where j delineates the j th cell. The dimensionality of $\mathbf{R}_j$ equals the number of dimensions of the crystal, such that in two dimensions:

$$\mathbf{R}_j = n\mathbf{a}_1 + m\mathbf{a}_2, \quad n, m \in \mathbb{Z}, \quad (1.11)$$

where $j = (n, m)$ and the crystal has characteristic primitive lattice vectors $\mathbf{a}_1$ and $\mathbf{a}_2$, which span the lattice. Note that $\mathbf{a}_1$ and $\mathbf{a}_2$ are not collinear, but are not necessarily orthogonal. The direct lattice vectors (1.11) define a *Bravais* lattice: an infinite array of points generated by discrete translations of the primitive lattice vectors. To model the motion of linear waves in this medium we make use of Bloch’s theorem [17], which states that the field $\psi(\mathbf{r})$ at an arbitrary position $\mathbf{r}$ can be written as the product:

$$\psi(\mathbf{r}) = e^{i\mathbf{k}_0 \cdot \mathbf{r}} u(\mathbf{r}), \quad (1.12)$$

where $\mathbf{k}_0$ is the crystal momentum or Bloch wavevector, and $u(\mathbf{r})$ is a periodic function that has the same periodicity as the physical space lattice i.e. $u(\mathbf{r} + \mathbf{R}_j) = u(\mathbf{r})$. Eq. (1.12)

is formally equivalent to:

$$\psi(\mathbf{r} + \mathbf{R}_j) = e^{i\mathbf{k}_0 \cdot \mathbf{R}_j} \psi(\mathbf{r}), \quad (1.13)$$

which asserts that in translating by a direct lattice vector, our solution undergoes a phase shift by an amount proportional to the distance $|\mathbf{R}_j|$. Note that (1.13) applies regardless of the lattice shape. The shape is characterised by defining a primitive cell, that is a unit cell of the lattice that contains a single lattice point, and this in turn is defined by our choice of primitive lattice vectors. Take for example the square and honeycomb lattices depicted in Fig. 1.3a and 1.3b, of primitive lattice vectors:

$$\mathbf{a}_1 = \begin{pmatrix} d \\ 0 \end{pmatrix}, \quad \mathbf{a}_2 = \begin{pmatrix} 0 \\ d \end{pmatrix}, \quad (1.14)$$

in the former case, and:

$$\mathbf{a}_1 = \begin{pmatrix} \sqrt{3}d/2 \\ d/2 \end{pmatrix}, \quad \mathbf{a}_2 = \begin{pmatrix} 0 \\ d \end{pmatrix}, \quad (1.15)$$

in the latter. The cells drawn in Fig. 1.3a and 1.3b* are a special case of primitive cell called the *Wigner-Seitz* cell, of side length d , which is the locus of points of closer proximity to the central lattice point than to any other lattice point. If the point $\mathbf{r}$ denotes any point within the Wigner-Seitz cell, then by (1.13) if we know the form of $\psi(\mathbf{r})$, we know our field everywhere. This is the foundation of all succeeding work in this thesis.

1.2.2 The Reciprocal Lattice

The second variable in determining the phase shift of (1.13) is the Bloch wavevector $\mathbf{k}_0$. By taking the Fourier transform of the direct lattice we generate a Bravais lattice in reciprocal space, or wavenumber space, referred to as the reciprocal lattice. The reciprocal lattice inherits periodicity from the direct lattice, and is defined as:

$$\mathbf{K}_h = n\mathbf{b}_1 + m\mathbf{b}_2, \quad n, m \in \mathbb{Z}, \quad (1.16)$$

where $h = (n, m)$ and the primitive vectors in reciprocal space are defined with respect to those of physical space:

$$\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}, \quad (1.17)$$

*Voronoi diagrams make excellent illustrations for periodic media, as shown by Wiltshaw [18].

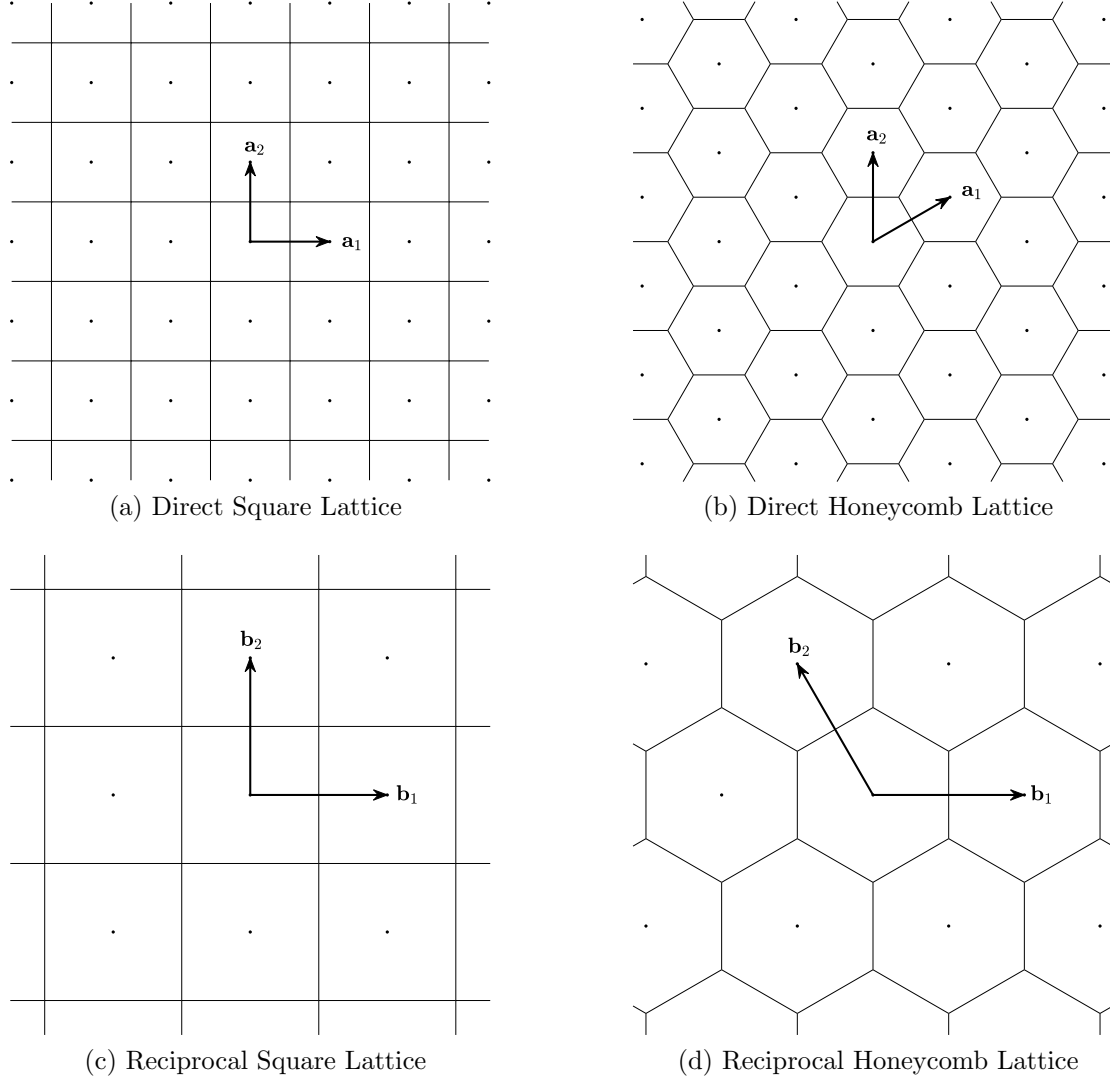


Figure 1.3: The square and honeycomb lattices in (a), (b) physical space and (c), (d) reciprocal space. Lines delineate the (a), (b) Wigner-Seitz cells and (c), (d) Brillouin zones. Labels indicate the primitive lattice vectors, and dots depict the lattice points.

where δ_{ij} is the Kronecker delta. The reciprocal lattices corresponding to the square and hexagonal lattices of primitive vectors (1.14) and (1.15) are depicted in Fig. 1.3c and 1.3d. These possess reciprocal primitive vectors of the form:

$$\mathbf{b}_1 = \begin{pmatrix} 2\pi/d \\ 0 \end{pmatrix}, \quad \mathbf{b}_2 = \begin{pmatrix} 0 \\ 2\pi/d \end{pmatrix}, \quad (1.18)$$

and:

$$\mathbf{b}_1 = \begin{pmatrix} -2\pi/\sqrt{3}d \\ 2\pi/d \end{pmatrix}, \quad \mathbf{b}_2 = \begin{pmatrix} 0 \\ 4\pi/\sqrt{3}d \end{pmatrix}, \quad (1.19)$$

in the square and hexagonal case, respectively. The primitive cell in the reciprocal lattice, that is the locus of wavenumbers closer to the reciprocal lattice point than any other lattice point, is referred to as the Brillouin zone (BZ). In determining the dispersive behaviour of the medium, we need only traverse the Brillouin zone to know the dispersion for any Bloch wavevector $\mathbf{k}_0 + \mathbf{K}_h \forall h \neq 0$. Note that by (1.17), there exists an inverse relationship between the areas of the unit cells in direct space and reciprocal space; a large unit cell in physical space corresponds to a small Brillouin zone in reciprocal space, and vice-versa.

1.2.3 Symmetries

Just as the tessellation of a primitive cell allows us to reduce the scope of wavevectors determining the dispersion of a crystal, so too do the symmetries of the primitive cell reduce this further. Like periodicity, the reciprocal lattice also inherits symmetries belonging to the direct lattice, although not necessarily along the same symmetry planes. The mathematical language characterising the symmetries of structured media is that of group theory, wherein symmetry operations that leave a lattice invariant under transformation collectively define the lattice's *point group*. We omit an analysis of these symmetry operations here, but refer the reader to chapter 7 for a detailed description of the group theory of two-dimensional photonic crystals. For now, we provide an illustrative example that elucidates the point.

The lattice depicted in Fig. 1.4a consists of a single inclusion at the centre of a square Wigner-Seitz cell of characteristic size d . The inclusion is isotropic* in its scattering response, such that a wave incident on the inclusion is scattered uniformly from it, regardless of the angle of incidence. Note that in this example, the underlying physical framework governing the wave motion is irrelevant - the theory applies to elastic, acoustic etc. waves, equally. Thanks to its square shape and the presence of a single inclusion at the origin, the cell has mirror reflections along the x and y axes, as well as along its diagonals. The square cell is also invariant under rotations through $\pi/2$, π , $3/2\pi$ and 2π radians. This invariance under transformation has a profound effect on the behaviour of

*For an anisotropic scatterer, the following arguments do not necessarily apply; see [19] Fig. 3 and Fig. 7.

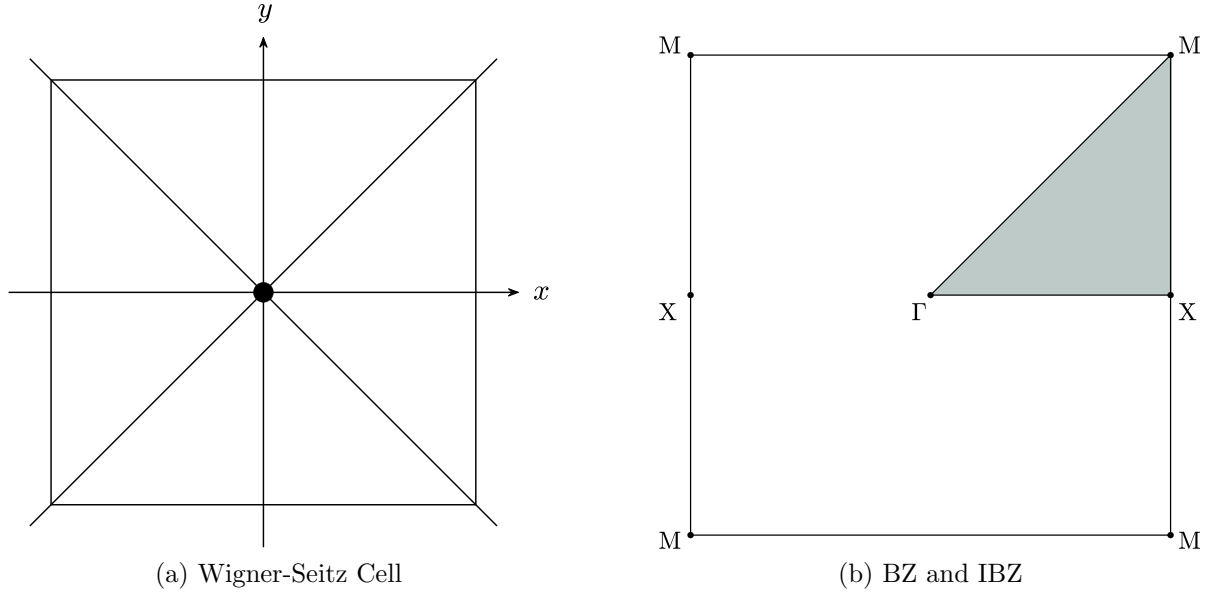


Figure 1.4: Wigner-Seitz cell (a) containing a single isotropic scatterer at the origin. Mirror lines drawn in black. BZ and IBZ (highlighted in grey) (b) for this square lattice.

waves in propagation through the crystal, and one can readily imagine that a wave in propagation from the right edge of the square will have an identical dispersive nature to that propagating from the left edge. Similar observations can be made for the top and bottom edges and the vertices, such that it becomes apparent that we need only consider a certain proportion of propagation directions to unlock the full dispersive picture.

We do this by defining an *irreducible* Brillouin zone (IBZ). The Brillouin zone for this square lattice is depicted in Fig. 1.4b, and is labelled with a set of high-symmetry points $\Gamma = (0, 0)$, $X = (\pm\pi/d, 0)$ and $M = (\pm\pi/d, \pm\pi/d)$ connected by high-symmetry lines. The BZ is found purely by periodic arguments i.e. the primitive lattice vectors, whereas the IBZ is a reduction of the BZ based on the spatial symmetries of the physical lattice, inherited by the reciprocal lattice*. Note that all high-symmetry points labelled in Fig. 1.4b are related by a mirror or rotation operation and/or a reciprocal lattice vector, and we say a point is invariant if its position after a symmetry operation is equivalent to its starting position, as related by a lattice vector. With this in mind, it becomes clear that the grey region indicated in Fig. 1.4b encapsulates the whole dispersive nature of the medium. We have reduced the BZ to an irreducible portion of wavenumber space.

*There is also time-reversal symmetry, but we'll get to that in chapter 7.

1.2.4 Homogenization at Low and High Frequencies

Homogenization is the process by which periodic or nearly periodic structures, that is, inhomogeneous media, are averaged over or homogenized, and is a well established method across many fields of physics and engineering [20–22]. All media are inhomogeneous at some length scale, but the mathematical treatment of most materials involves their averaged material properties such as mass density, Young’s modulus or magnetic permeability. The homogenization of designed composite materials, which are ordinarily characterised by a periodic microstructure, aims to achieve a similar description in terms of effective bulk quantities. This usually facilitates the replacement of the PDE governing the dynamical problem with a simplified differential equation that applies at the macroscale.

Homogenization necessitates a distinction between length scales, one characterised by the period of the microstructure d , and the other by the wavelength of radiation λ , or its wavenumber k . The microstructure period is assumed to be much smaller than the wavelength, to the effect that we may define a non-dimensional small parameter $\epsilon = kd$ or $\epsilon = d/\lambda$, where $\epsilon \ll 1$. The method then involves deriving a leading-order description for the wave motion by means of substitution of ϵ into the governing PDE, before performing a power series expansion in the field. The resultant differential equation describes the averaged medium, and may contain effective material parameters that are deduced by dimensional analysis. Boundary conditions supplied by the microstructure close the problem, to the effect that a composite material is replaced with an ‘effective medium’ description. Solutions pertaining to the homogenized material can be matched with those in the exterior to yield a system of equations for, for example, the scattering of a plane-wave, or the eigenmodes of the microstructure.

The above describes classical homogenization at low frequencies, but a contemporary method that has seen considerable attention across a range of topics is that of high frequency homogenization (HFH). HFH has seen applications in the analysis of periodic media in elastic [8, 23], acoustic [24] and photonic [25] systems. Although this thesis is not primarily concerned with HFH, it is utilised in chapter 2 for the purposes of determining the beat wavelength of array-guided modes along line and ring structures, and so it is pertinent to provide a short definition.

HFH constitutes the asymptotic technique of applying a perturbation to the standing wave eigenmodes of a periodic medium, which correspond to the vertices of the IBZ [7, 26, 27]. These standing waves are of a vanishing group velocity by virtue of the flatness in the dispersion curves close to the band edge. They are characterised by a

rapid short-scale modulation of the wavefield from cell to cell, but a slow modulation in the waveform across the structure. These provide us with a pair of independent coordinates for the short- and long-scales, as well as a small parameter $\epsilon = d/L$, where L is the characteristic length of the structure as a whole. A typical ODE derived using this method is of the form [24]:

$$T f_{0,XX} + \Omega_2^2 f_0 = 0, \quad (1.20)$$

where the variable X denotes the long-scaled variable, $f_0 \equiv f_0(X)$ is a long-scale function, Ω_2 is the second order perturbation to the standing wave frequency, and T is a function of the square of the group velocity [25]. Eq. (1.20) is posed entirely on the long-scale X , wherein the details of the microstructure geometry are encoded in the variable T . The long-scale function $f_0(X)$ determines the beat wavelength of standing wave eigenmodes; this is illustrated in chapter 2 for one-dimensional arrays of point scatterers on an elastic plate.

1.2.5 Quasistatic Approximations of Dilute Media

Quasistatic approximations constitute a particular species of low frequency homogenization problems, wherein a dynamic problem, that is, a problem evolving in time, is analysed under the assumption that the time evolution is very slow. For time-harmonic fields this is equivalent to the limit of $\omega \rightarrow 0$ or $k \rightarrow 0$, such that a Helmholtz problem, for example, is analysed in its approach to the static Laplace's equation. It should come as no surprise then that the static lattice sums, typically featured in array problems under Laplace's equation [13], appear in the asymptotic approximations of the dynamic lattice sums in Appendix B. By analysing periodic media in the quasistatic limit, we recover effective material parameters that capture the medium's response to waves of a wavelength comparable to the length scale of the bulk material. Usually, there exists an additional constraint imposed on the size of the resident scatterers of the periodic medium, which is written in terms of an area fraction f of scatterers in the fundamental cell. Such media are referred to as *dilute* in the limit $f \rightarrow 0$, although, as we will show in chapter 6, quasistatic approximations can often prove accurate at finite values of $f \leq 0.5$.

The effective material parameters of a bulk medium are deduced by assuming a linear relationship between the bulk and Bloch wavenumbers, of the form [13]:

$$k = \alpha k_0, \quad (1.21)$$

where $k_0 = |\mathbf{k}_0|$ and α is the inverse of an *effective phase refractive index* of the medium. If the change in phase of a wave across a fundamental cell is written $\Delta\Phi = k_0 d$, then the effective phase refractive index is defined in:

$$\Delta\Phi = k_0 d = n_{eff} k d, \quad (1.22)$$

such that:

$$n_{eff} = \lim_{k, k_0 \rightarrow 0} \frac{dk_0}{dk} \quad (1.23)$$

$$= \frac{1}{\alpha}. \quad (1.24)$$

Our task then is the evaluation of the gradient α , and this is done by assuming an appropriate ansatz for the form of α in terms of a power series expansion in the Bloch wavenumber, normalised by the characteristic size of the unit cell. This method has been applied to deduce the effective refractive index, and along with it, the effective permittivity, for photonic crystals composed of a dielectric [13], or of scatterers of Neumann or Dirichlet boundary condition [28]. Recent publications have applied this method to anisotropic media consisting of metamaterial inclusions [29]. This is the subject of chapter 6.

1.3 Thesis Outline

This thesis is comprised of six research chapters, one chapter on the multipole method in cylindrical geometries, and an appendix:

- Chapter 2 is concerned with periodic media in linear elasticity, and establishes the methods by which linear waves problems are treated in terms of the superposition of Green's functions. Singly-periodic so-called 'platonic' media consist of linear arrays of point-scatterers or point-forcings, masses or mass-spring pairs, embedded uniformly in a thin-elastic plate. Kinematic assumptions placed on the deformations of the thin plate ensure that the motion of the flexural waves is governed by the KL equation (1.7). The Green's function for the point-forcing is provided as the difference between two Hankel functions, and is non-singular at every point in the computational domain. We construct an infinite linear grating of these point-scatterers and determine the dispersion relation for the array-guided Rayleigh-Bloch modes in terms of a Bloch wavenumber β . The beat wavelength of the grating

modes is inspected by way of HFH, wherein an effective medium ODE describes the long-scale envelope function. Matching integer multiples of beat wavelengths to the circumference of a periodic structured ring resonator, of the same characteristic spacing as the grating, reveals the frequencies of the whispering-Bloch modes of the ring. These quasi-modes are the solutions to a complex dispersion relation, with a negative imaginary component delineating the leakage of energy from the curved structure. Two types of whispering-Bloch modes are classified, and the energy leakage quantified in terms of a quality factor. Finally, we perform ring-array coupling so as to construct macroscopic circuits for the purposes of directing elastic waves. So-called CREAs (coupled resonator elastic arrays) are analogous to the CROWs (coupled resonator optical waveguides) of optical circuits [30].

- Chapter 3 constitutes a detailed formulation of the dynamic multipole method for cylindrical geometries in two-dimensions, and is the foundation upon which the succeeding work of chapters 4-6 is built. This is contextualised in terms of electromagnetic waves propagating under transverse incidence in either TE (E_x, E_y, H_z) or TM (H_x, H_y, E_z) polarization. The longitudinal field component is shown to be a superposition of regular and outgoing waves in a language of cylindrical harmonics: Bessel functions of integer order multiplying angular terms. Graf's addition theorem provides a change-of-basis to the singular component of the field. This enables the total field due to the scattering of N cylinders to be written in the polar coordinates of any one cylinder in the local vicinity of that cylinder. We then demonstrate how, by application of a boundary condition on the cylindrical surface, a system of equations can be formed for the total field scattered by an arbitrary arrangement of N cylinders.
- In chapter 4 we consider a metamaterial composed of a plate-array microstructure sandwiched between layers of a dielectric, and its implementation into a cylindrical cross-section. This metamaterial is of interest as it has been shown to exhibit a strong anisotropic response in scattering, making it a good candidate material for reconfigurable structured media. A detailed derivation is provided of the homogenization of the plate-array medium. This provides an 'effective medium' description consisting of a one-dimensional wave equation in the interstitial dielectric channels, and a pair of continuity conditions at the cylindrical surface. We examine the scattering by a single metacylinder of a plane-wave, before considering the scattering by multiple metacylinders arranged in a circle. This structured ring resonator is shown to possess whispering-Bloch modes of a tunable quality factor, and it is shown that

a $\mathcal{O}(10^5)$ increase in this quality factor is possible under appropriate plate-array orientation.

- In chapter 5, the metacylinders are arranged periodically along one axis so as to form a metamaterial diffraction grating, or *metagrating*. The mathematical analysis of this structure necessitated the use of a rapidly convergent form of the grating sum, which was first derived by Twersky [31]. The reflection and transmission of a plane-wave by the metagrating is analysed, and it is shown that the metagrating possesses regions in phase-space of perfect reflection and perfect transmission. The latter of these phenomena is tantamount with the observed Goos-Hänchen shift in the field as it traverses the grating. The metagrating is also shown to host multiple families of Rayleigh-Bloch modes existing beneath the continuum, and the dispersion of these modes is analysed as a function of the uniform plate-array angle and cylinder radius.
- Chapter 6 is concerned with the periodic arrangement of these metacylinders along two axes, so as to engender a metasurface that is reconfigurable at the pixel level. We provide a derivation of the crystal's lattice sum in terms of cylindrical harmonics, and arrive to a rapidly convergent formulation by a comparison between Green's functions in direct and reciprocal space. By formulating the metasurface's dipole matrix, we homogenize the surface in the quasistatic limit of $k \rightarrow 0$, and in doing so derive the surface's effective permittivity tensor. The anisotropy of the metasurface at leading order is shown to be a function of the uniform plate-array angle δ , index n_r and filling fraction f . The model serves as an example to the wider literature as to how a rotational degree of freedom possessed by photonic crystal elements enables an effective anisotropic description at the macro-scale. The asymptotic forms of all constituent dipole matrix elements are provided in appendix B.
- Finally, chapter 7 details my ongoing work on topological photonic phases in two-dimensions. The eigenmodes of photonic crystals possess symmetries engendered by the spatial symmetries of the lattice in real space, and time-reversal symmetry. Spatial symmetries are classified using the language of group theory, whereby the set of operations that leave a lattice point invariant under transformation are collectively known as the lattice's *point group*. We leverage the breaking of these spatial symmetries to crack open associated degeneracies in the photonic band structure, and in doing so realise the 2D photonic topological insulator phase of light. This is demonstrated for both polarizations of light simultaneously i.e. a topologically

non-trivial band gap for both TE and TM polarizations is made to overlap. This facilitates edge modes for both polarizations at the same frequency. We then join two crystals, of the same symmetry breaking perturbations, to realise edge modes between Neumann and Dirichlet media.

- Concluding remarks are provided in chapter 8, and possible extensions to this work are outlined.

2 Toy Problems in Elasticity

The purpose of this chapter is to elucidate the methods by which structured media are treated mathematically. Linear elasticity serves as an uncomplicated setting in which to model so-called ‘toy problems’, which serve as illustrative devices that share traits with analogous problems in other physical realms. Arrangements of point-scatterers placed upon a thin-elastic plate give rise to resonances belonging to the structured arrangement that are synonymous with large-amplitude elastic deformations; in periodic structures these resonances correspond to array-guided modes. We draw from the approach outlined herein in later chapters on structured media in electromagnetism.

The contents of this chapter is adapted from that published in [1], with additional contributions from G.J. Chaplain: Fig. 2.4 and the so-called FHG method, B. Maling: Fig. 2.7, H. Rakotoarimanga-Andrianjaka: the winding number method, and R.V. Craster.

2.1 Introduction to Chapter 2

Thin-elastic plates support flexural waves and have been much studied, particularly in connection with the dynamics of shells [32] and the vibration of periodic engineering structures [33]. More recently, the subject has undergone a renaissance with the analysis of doubly-periodic arrays of supports, [34, 35], revisited from the point of view of phononic crystals [36] with these structured elastic plates being dubbed platonic crystals [37]; the aim being to manipulate and re-direct vibrational wavefields through negative- and ultra-refraction [38, 39], Dirac-like point effects [40, 41] and highly-directive dynamic anisotropy [35, 42] by leveraging Bragg scattering and the interactions due to the periodic structuring.

In the related field of photonics, concerned with structured electromagnetic and optical media, alternative routes for spectral filter design using resonances based on whispering gallery modes have been developed [43]. Micro-Disks, or micro-rings, of one dielectric

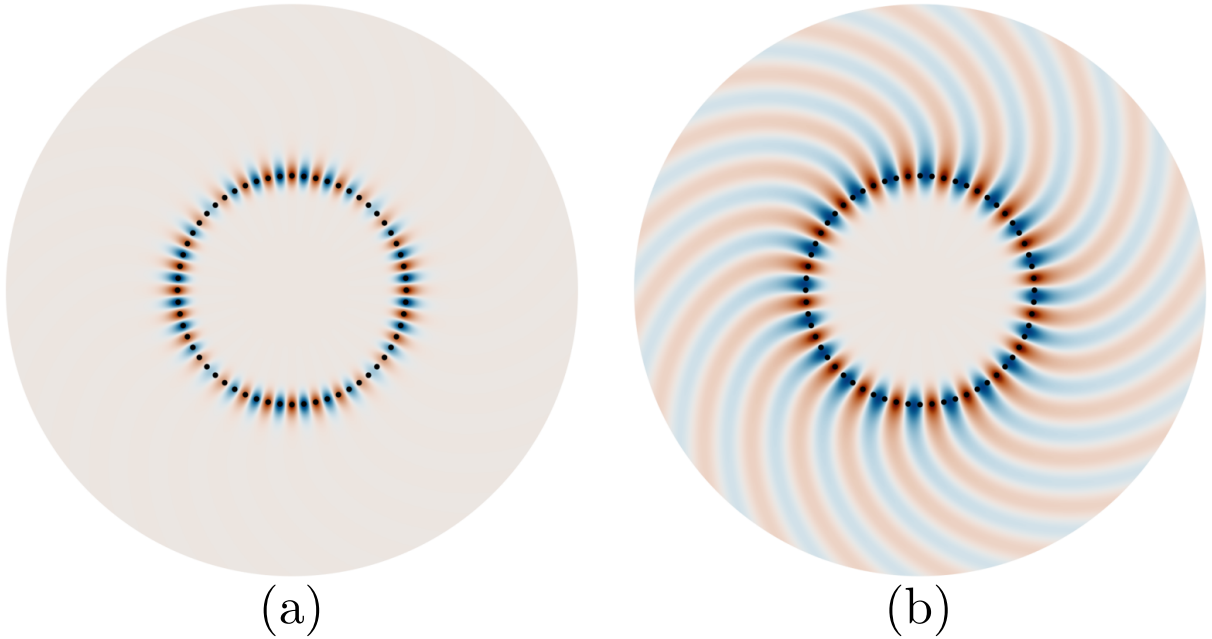


Figure 2.1: Structure-located whispering-Bloch modes of a ring resonator consisting of $N = 60$ uniform point-masses (black dots) arranged in a circle and embedded in a thin-elastic plate obeying KL theory. Panel (a) depicts a standing mode near the band edge, whereas (b) depicts a leaky mode of lower mode number. Normalised wavefield colour scale, red/blue indicating maximum/minimum real displacement. Perceptually uniform colour maps are used throughout [6].

material embedded within another medium have strong resonances, characterized by high quality-factors at discrete frequencies. Coupling, possibly multiple, resonant micro-disks, or micro-ring resonators created by annular waveguides with index mismatch to the surrounding medium, with adjacent waveguides provides a means to filter, or transfer, wave energy within an integrated optical circuit. Whispering gallery mode resonances are highly sensitive and as such they also find application in bio-sensors [44] and even more widely in nonlinear optics [45]. Devices based upon these resonators are well-established [46, 47] and have been widely developed for telecommunications and optical sensing and many other applications [48]. Despite the success of integrated ring resonators based upon material mismatch there are limitations in the quality-factors that can be achieved due to imperfections and roughness at the surface of the micro-disk and in practical terms, for the frequencies desired, small rings on the scale of microns with high material mismatch are required; these are harder to fabricate and limit the range of materials available which motivates alternative approaches to obtaining resonant structures. One recent approach [49] is to note that structured periodic gratings can support Rayleigh-

Bloch waves (RB) that propagate along the grating and exponentially decay away from it [50]. Rayleigh-Bloch waves, engendered by some periodic geometry, have arisen in various guises across different areas of wave mechanics, for example in electromagnetism as spoof surface plasmons [51] or those waves supported by Yagi-Uda antennas [52, 53]. When the array is curved to create a circular structured grating then a strongly localised resonance exists, with high quality-factor, that shares some features of whispering gallery modes but the modes are now created by periodic structuring as in Bloch waves and as such are termed whispering-Bloch (WB) modes [49], as shown in Fig. 2.1.

Given the interest in the filtering and manipulation of flexural waves the focus of this chapter is on the eigensolutions pertaining to singly-periodic structures in elasticity. As in electromagnetism, macrostructures composed of some periodic organization of fundamental point-forcings upon an elastic plate have been shown to possess non-trivial solutions to the governing bi-harmonic wave equation, including Rayleigh-Bloch modes along linear gratings[5] and whispering-Bloch modes in structured ring resonators [54]. In matching the corresponding eigensolutions between line and ring we have shown the analogy between the modes possessed by each structure, and in minimising the impedance mismatch between line and ring we demonstrate that it is feasible to couple both structures together to form flexural wave filters. These filters mimic the design of microring-resonator circuits in optics [30, 55], and as such we term them *CREAs*, or coupled resonator elastic arrays.

This chapter is structured as follows: we start by setting out KL theory and the scattering by N arbitrarily positioned inclusions, before treating an infinite grating of equally-spaced point-masses that supports Rayleigh-Bloch modes, and reproduce the dispersion bands of [5]. Section 2.4 describes the formulation of whispering-Bloch quasi-modes of complex wavenumber determined via the winding number method of [54], and the extraction of the limiting quality-factor $\mathcal{Q}$. Combining these resonant devices in § 2.5 we devise platonic circuits of type drawn schematically in Fig. 2.2 and demonstrate a high level of control in the filtering and directing of flexural waves. We finish by providing our closing remarks, noting several practical applications of these platonic circuits.

2.2 The Kirchhoff-Love Theory of Thin Plates

KL theory [56] models the out-of-plane vibrations of thin-elastic plates, and makes the kinematic assumptions of preservation of both plate thickness and straight lines normal to the mid-surface plane after deformation. KL theory remains valid at vibrational

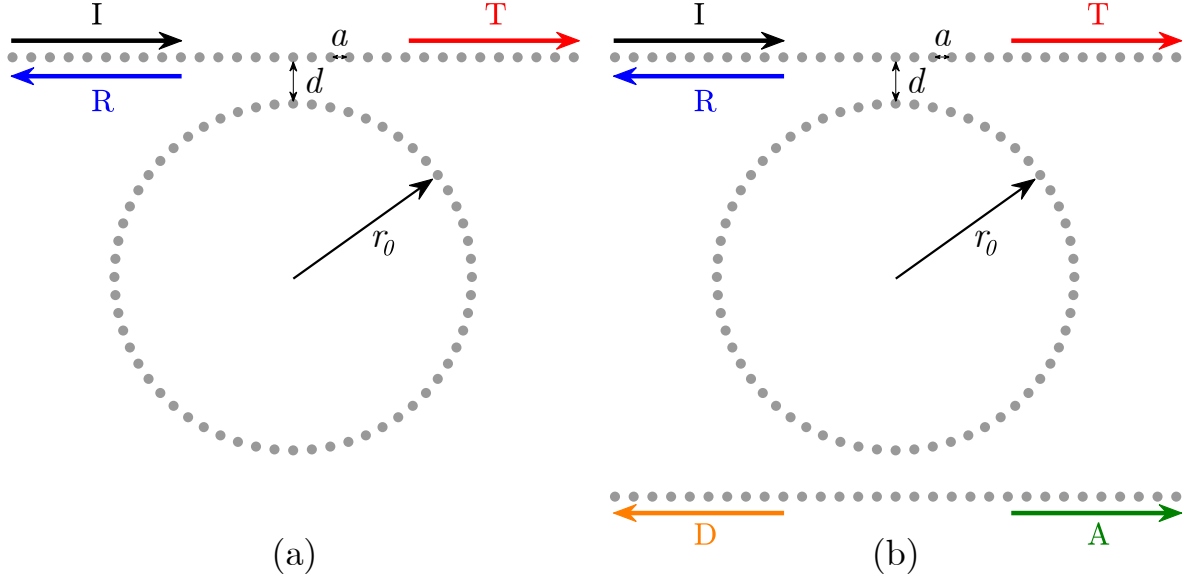


Figure 2.2: Schematic showing a typical platonic circuit geometry. (a) Structured ring-resonator of radius r_0 separated by a distance d from a neighbouring periodic line array. Incident Rayleigh-Bloch modes along the array couple into the ring and this results in a measured fall in through-transmission T . (b) Add-drop filter with the structured ring resonator coupling to two line arrays, with transmission coefficients D and A measuring mode propagation along the drop- and add-ports respectively.

wavelengths greater than 20 times the plate thickness [57], a consideration we avoid in the numerics herein by introducing non-dimensional variables parameterising the plate and embedded inclusions, consistent with [5]. The displacement of a thin-elastic plate perpendicular to the x - y plane under excitation by an incident wavefield, assuming a time-harmonic variation of radian frequency ω , is written as $U(\mathbf{r}, t) = \text{Re}\{u(\mathbf{r})e^{-i\omega t}\}$ where $u(\mathbf{r})$ is the out-of-plane displacement at the in-plane position $\mathbf{r} = (x, y)$. The equation of motion governing the propagation of flexural waves in an isotropic, homogeneous plate, in the absence of external forces, is:

$$(\nabla^4 - k^4)u(\mathbf{r}) = 0 \quad (2.1)$$

where ∇^2 is the two-dimensional Laplacian operator and $k^4 = m_p\omega^2/D$ where k is the wavenumber of free waves in the plate, $D = Eh^3/12(1 - \nu_p^2)$ the bending modulus, E the Young's modulus, h the plate thickness, ν_p the Poisson ratio and m_p the mass per unit area of the plate. Eq. (2.1) is modified by the introduction of time-harmonic point-forcings, for which we introduce the Green's function $g(\mathbf{r}, \mathbf{r}'; k)$, which itself is expressed

in terms of Hankel functions:

$$g(\mathbf{r}, \mathbf{r}'; k) = \frac{i}{8k^2} \{H_0(k\rho) - H_0(ik\rho)\} \quad (2.2)$$

where $\rho = |\mathbf{r} - \mathbf{r}'|$ and H_0 is the Hankel function of the first kind and order zero. The Green's function (2.2) represents the field at point $\mathbf{r}$ due to a point-forcing at $\mathbf{r}'$ upon the plate, and satisfies the modified equation of motion:

$$(\nabla^4 - k^4)g(\mathbf{r}, \mathbf{r}'; k) = \delta(\mathbf{r} - \mathbf{r}'). \quad (2.3)$$

Notably this Green's function is bounded as $\mathbf{r} \rightarrow \mathbf{r}'$, which makes it ideal as a building block to solve for the scattering of flexural vibrations by infinite arrays, or finite numbers, of point-forcings [5]. The non-singular nature of (2.2) allows for the determination of the flexural wavefield globally, with each point-forcing corresponding to a Green's function (2.2) in summation. Following the derivation in [5], for an array of N point-forcings at arbitrary positions $\mathbf{r}_n$, where $n = 0 \dots N - 1$ the displacement $u(\mathbf{r})$ obeys:

$$D(\nabla^4 - k^4)u(\mathbf{r}) = D \sum_{n=0}^{N-1} A_n \delta(\mathbf{r} - \mathbf{r}_n) \quad (2.4)$$

where DA_n is the forcing at $\mathbf{r}_n$; if this is assumed proportional to the displacement at the point then an impedance $\mu_n D$ characterises this and $DA_n = \mu_n Du(\mathbf{r}_n)$. Evans and Porter [5] introduce the impedance parameter:

$$\mu_n = 4k^4 a^2 \tilde{\mu}_n + i4k^2 \tilde{\nu}_n, \quad (2.5)$$

which is related to the mass M at the point, and a characteristic length-scale a via the non-dimensional parameters:

$$\tilde{\mu}_n = \frac{1}{4m_p a^2} M_n, \quad \tilde{\nu}_n = -\frac{1}{\sqrt{16Dm_p}} \nu_n, \quad (2.6)$$

where we introduce point-wise damping ν_n at each loading point; these points are described as mass-loaded with a damping force. The Green's function (2.2) is placed in the summation over point position such that, in the presence of an incident field $u_i(\mathbf{r})$, the total wavefield satisfying (2.4) is:

$$u(\mathbf{r}) = u_i(\mathbf{r}) + \sum_{n=0}^{N-1} A_n g(\mathbf{r}, \mathbf{r}_n; k). \quad (2.7)$$

A system of N equations for the coefficients of the Green's functions follows:

$$A_m = \mu_m u_i(\mathbf{r}_m) + \mu_m \sum_{n=0}^{N-1} A_n g(\mathbf{r}_m, \mathbf{r}_n; k) \quad (2.8)$$

for $m = 0 \dots N-1$.

Noting that $g(\mathbf{r}_m, \mathbf{r}_n; k) = g(\mathbf{r}_n, \mathbf{r}_m; k)$ we introduce a symmetric matrix $\mathbf{G}$ where $G_{i,j} = g(\mathbf{r}_i, \mathbf{r}_j; k)$, the diagonal matrix $\hat{\mu}$ containing the impedances μ_m and the vectors $\mathbf{A} = (A_0, \dots, A_{N-1})^T$ and $\mathbf{U} = (u_i(\mathbf{r}_0), \dots, u_i(\mathbf{r}_{N-1}))^T$. Writing the linear system of (2.8) as:

$$(\mathbf{I} - \hat{\mu}\mathbf{G}) \mathbf{A} = \hat{\mu}\mathbf{U} \quad (2.9)$$

allows for the coefficients of the Green's functions to be solved for numerically, and we refer to this as the scattering matrix method. The formulation above, with each point possibly having its own mass and damping, is general; hereafter we simply take each point to be identically mass-loaded and undamped, unless explicitly stated otherwise.

2.3 Rayleigh-Bloch Modes

2.3.1 Formulation

As also noted in [5] it is possible, instead of applying forcing or an incident field, to look for localised states as solutions and in particular to consider an infinite periodic line array with each mass-loading separated by a characteristic length a , such that $\mathbf{r}_n = (na, 0)$ for $n \in \mathbb{Z}$. The periodicity of the geometry is exploited through the introduction of a Bloch wavenumber β such that there is a phase-shift along the array of $A_n = e^{i\beta a} A_{n-1}$, making $A_n = e^{i\beta a n} A_0$ and $A_0 = \mu u(\mathbf{r}_0)$. A dispersion relation relating this phase-shift to wavenumber emerges from equation (2.7) when one considers the point $\mathbf{r}_0$:

$$\frac{i(ka)^2}{2} \tilde{\mu} \sum_{n=-\infty}^{\infty} e^{i\beta a n} \{H_0(ka|n|) - H_0(ika|n|)\} - 1 = 0 \quad (2.10)$$

where we discard the damping at each point $\tilde{\nu}_n$, and assert that the impedance $\tilde{\mu}_n$ is uniform such that $\tilde{\mu}_n \equiv \tilde{\mu}$. Using the Poisson summation formula (A.20) and the integral

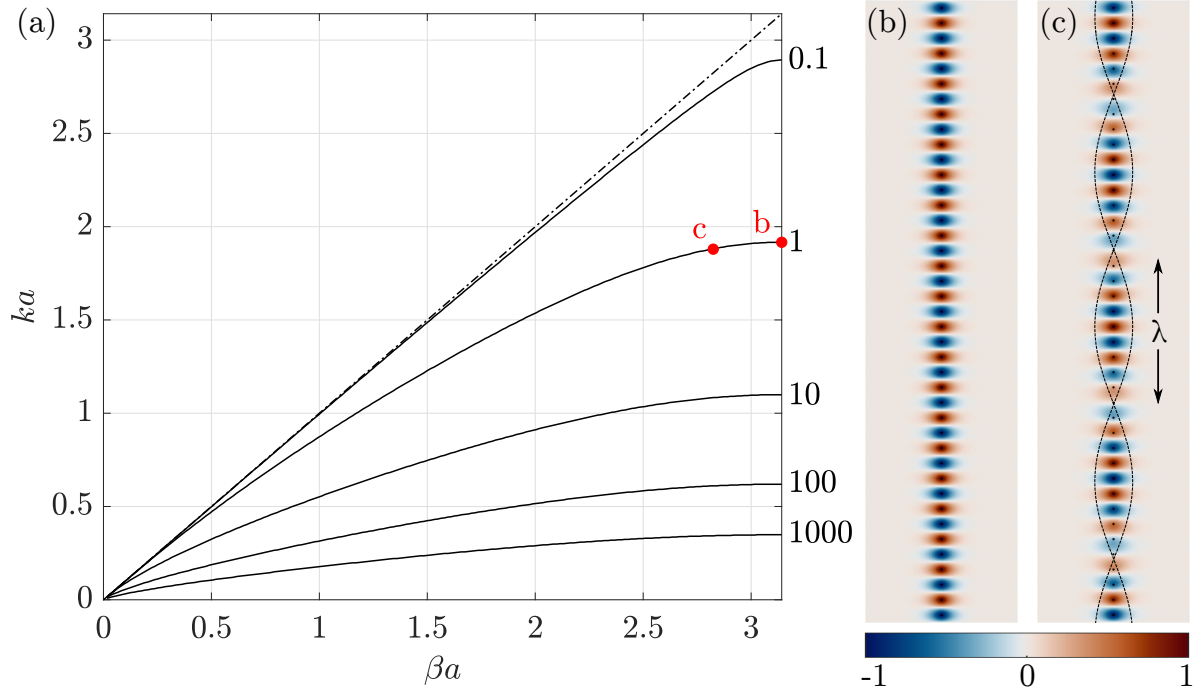


Figure 2.3: (a) Rayleigh-Bloch dispersion bands for an infinite line array of mass-loadings of uniform spacing, mass parameterised with increasing $\tilde{\mu}$ labelled on the right, calculated via eqs. (2.10) and (2.11). (b), (c) Real displacement fields for the corresponding points marked in (a). At the band edge (b), a standing waveform exists, characterised by a uniform long-scale amplitude. For frequencies away from the band edge, e.g. (c), a long scale envelope modulates the oscillations, resembling a beat frequency. The envelope wavelength, λ , is calculated using High Frequency Homogenisation (HFH) [7, 8].

form of the Green's function given in [5], we rewrite the infinite summation as:

$$ka\tilde{\mu} \sum_{n=-\infty}^{\infty} (\lambda_n^{-1} - \gamma_n^{-1}) \quad (2.11)$$

where:

$$\lambda_n = \left(\left(\frac{\beta_n}{k} \right)^2 - 1 \right)^{\frac{1}{2}}, \quad \gamma_n = \left(\left(\frac{\beta_n}{k} \right)^2 + 1 \right)^{\frac{1}{2}} \quad \text{and} \quad \beta_n = \beta + \frac{2n\pi}{a}. \quad (2.12)$$

The infinite sum (2.11) has been shown to converge (see (4.9) of [5]), and herein we evaluate this summation at $N = \mathcal{O}(10^2)$ when calculating the dispersion bands. The dispersion relation (2.10) has a single real solution k corresponding to each β value $\beta \in (0, \pi/a]$ where $\beta > k$ for fixed $\tilde{\mu}$, such that the infinite sum is real valued; infinite $\tilde{\mu}$ corresponds to pinned points and no solution exists in this case. The real solutions to

(2.10), given in [5], correspond to Rayleigh-Bloch (RB) modes that propagate along the array and exponentially decay with distance perpendicular to the array. In Fig. 2.3(a) the dispersion bands describing Rayleigh-Bloch modes upon periodic line arrays are shown for several mass-loading parameters $\tilde{\mu}$, where the pinned limit is approached as $\tilde{\mu} \rightarrow \infty$. Figures 2.3(b) and (c) show the wavefields corresponding to the labels b and c along the $\tilde{\mu} = 1$ dispersion band in Fig. 2.3(a). The band flattens on approach to the band edge, resulting in a group velocity of zero and a standing wave solution in Fig. 2.3(b) with a modulating antisymmetric displacement existing only on a short-scale from point-to-point. Reducing the wavenumber from the band edge, to c, reveals an additional scale of wave propagation along the line array as in Fig. 2.3(c); the short-scale oscillations, as in Fig. 2.3(b), remain, but now are augmented by a long-scale beat envelope of characteristic wavelength, λ , defined by Eq. (11) of [8]. The long-scale is analyzed using the high-frequency-homogenization (HFH) method [7, 8, 23], with the envelope characterisation being useful in the identification of topological edge states [8] and the redirection of modes in multidirectional energy splitters [58]. In § 2.4 analogous beat envelopes arise in the waveforms of whispering-Bloch modes, and their wavenumbers correspond to an integer number of long-scale beat wavelengths circumnavigating the ring. The wavelength of these beats is determined via the high-frequency homogenisation scheme described below.

2.3.2 High Frequency Homogenisation

Here we briefly outline the High Frequency Homogenisation scheme, which follows that in [8], used to approximate several Rayleigh- and whispering-Bloch resonant frequencies by inspecting the beat wavelength of a line array. High Frequency Homogenisation rests on separating the spatial coordinates into two scales to be treated independently. The periodic nature of the singly-periodic array naturally characterises a short scale, defined by the coordinates $\boldsymbol{\xi} = (x/l, y/l)$, with l being commensurate with the periodicity. A long scale $X = x/L$ is then defined on the order of the length of the entire array, characterised by L . Assuming that $\epsilon \equiv l/L \ll 1$, we expand both the wavefield and frequency of the standing wave solutions (at the band edge) to derive an effective medium ODE for the long scale modulated by oscillatory behaviour on the short scale. The resulting equation describes the long-scale envelope function $f(X)$ through:

$$f_{XX} - \tilde{T}f = 0, \quad (2.13)$$

where $\tilde{T} = \left(\frac{k^4 - k_0^4}{T}\right)$: k_0 is the wavenumber at the band edge with k corresponding to the wavenumber of excitation, and T is a quantity that can be evaluated in several ways, depending on how the dispersion relations are obtained. In certain scenarios an exact analytical form relates T to integral quantities of the wavefield [59], whereas here we opt to obtain it from a Fourier-Hermite-Galerkin (FHG) method, specifically developed for calculating the dispersion curves for RB arrays in thin plates [8]. The sign of $\tilde{T}$ then determines the characteristic decay envelope (for $k > k_0$) or beat wavelength (for $k < k_0$). By calculating this wavelength we are able to estimate the frequencies supported along a line array that correspond to a WB resonance around a discrete ring array (assuming the same inter-point spacing), by matching an integer number of wavelengths of the beat wavelength around the ring - shown in Fig. 2.8. The dispersion curves calculated by the FHG method match those calculated as in [5], as shown in Fig. 2.4, which additionally shows the asymptotic approximation of the dispersion relation obtained by the HFH scheme.

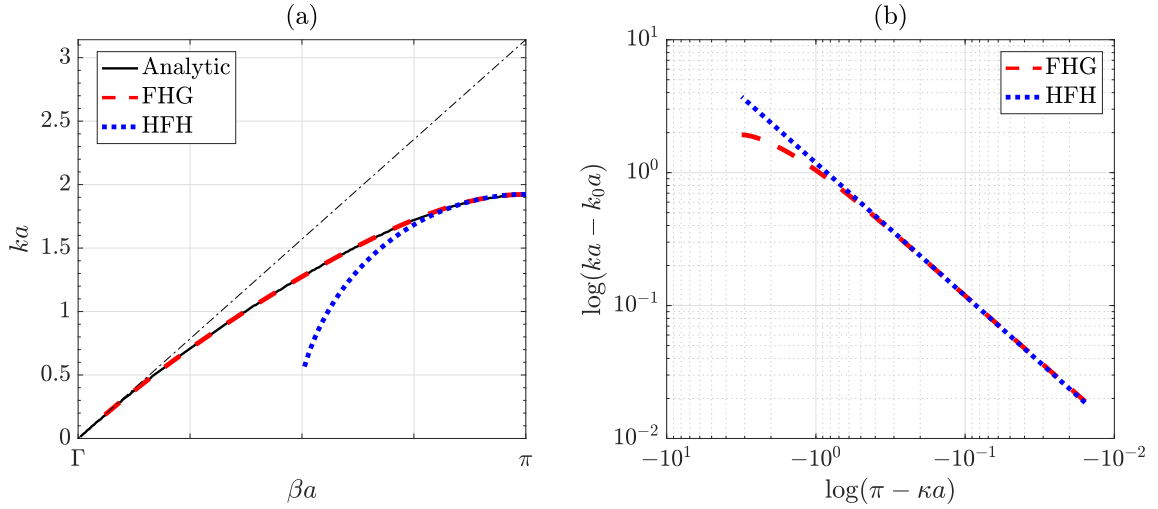


Figure 2.4: (a) Dispersion curves for line RB array ($\tilde{\mu} = 1$) calculated analytically as in [5] (solid black), using the Fourier-Hermite-Galerkin (FHG) scheme as in [8] (dashed red) with the corresponding HFH asymptotics (dotted blue). (b) Log-log plots confirming HFH accuracy.

2.4 Whispering-Bloch Modes

2.4.1 Formulation for Point-Forcings

We consider structured ring resonators, and their resonant behaviours, for which we expect to encounter quasi-modes [60] i.e. complex solutions to a dispersion relation that are interpreted by analogy with the Rayleigh-Bloch modes upon line arrays. We consider the open system of a finite number of masses N placed, equally spaced, around a circle of radius r_0 . From (2.7), (2.8), in the absence of an incident field, the wavefield and coefficients are:

$$u(\mathbf{r}) = \sum_{n=0}^{N-1} A_n g(\mathbf{r}, \mathbf{r}_n; k), \quad A_m = \mu \sum_{n=0}^{N-1} A_n g(\mathbf{r}_m, \mathbf{r}_n; k). \quad (2.14)$$

Bloch's theorem for a circular geometry follows by introducing $\hat{R}$, the discrete rotation operator of angle $2\pi/N$, for any function $f(r, \theta)$, by $\hat{R}f(r, \theta) = f(r, \theta + 2\pi/N)$. From rotational symmetry $u(\mathbf{r}) = u(r, \theta)$ and $\hat{R}u(r, \theta)$ satisfies the same eigenvalue problem as $u(r, \theta)$, and is equal up to a multiplicative constant σ such that $\hat{R}u(r, \theta) = \sigma u(r, \theta)$. Since $\hat{R}^N$ is the identity operator, we must have $\sigma^N = 1$ with σ being one of the N th roots of unity, $\sigma = e^{2\pi i m/N}$ with $m \in \{0, \dots, N-1\}$.

Denoting the coefficients A_n with $n \in \{0, \dots, N-1\}$ and applying this result, in the case where N is even, there exist $m \in \{0, \dots, N/2\}$ such that:

$$A_n = e^{\pm 2\pi i n m/N} A_0 \quad (2.15)$$

where A_0 is an arbitrary constant; the positive and negative signs in the exponential lead to clockwise and anticlockwise spiralling solutions later, and we use the positive solutions hereafter. For a mode $m \in \{0, \dots, N/2\}$ the dispersion relation $\mathcal{D}(k, m) = 0$ is given by (2.14), when considering the point $\mathbf{r}_0$, leading to:

$$\mathcal{D}(k, m) = \mu \sum_{n=0}^{N-1} e^{2\pi i n m/N} g(\mathbf{r}_0, \mathbf{r}_n; k) - 1 \quad (2.16)$$

and we solve for k as a given quasi-mode indexed by $m \in \{0, \dots, N/2\}$. We only consider solutions k such that:

$$\text{Re}(k) > 0 \quad \text{and} \quad \text{Im}(k) < 0. \quad (2.17)$$

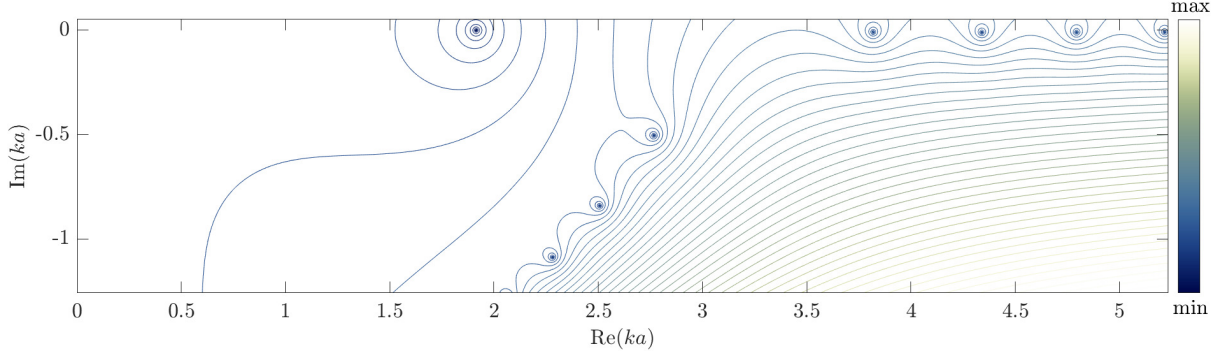


Figure 2.5: The behaviour of the dispersion relation in complex k space using $\log(|\mathcal{D}(k, m)|)$ shown as a contour plot for $N = 60$, $\tilde{\mu} = 1$ and $m = N/2 = 30$. Three types of solutions are immediately apparent; the isolated root of lowest $\text{Re}(k)$ and $\text{Im}(k)$ to the top left, the set of increasing $\text{Re}(k)$ roots to the top right, and the set of increasing $\text{Im}(k)$ roots centre-left. These solutions correspond to, respectively, the structure located, interior and decaying modes of the platonic ring resonator.

These two conditions account for quasi-modes describing outward going solutions with vanishing energy at infinity i.e. $|\mathbf{r}| \rightarrow +\infty$.

In Fig. 2.5 we show a typical contour plot of $\log(|\mathcal{D}(k, m)|)$, for $N = 60$, $\tilde{\mu} = 1$ and $m = N/2 = 30$, that shows the existence of complex roots that are very close to the real axis. In Fig. 2.5 the solutions to the dispersion relation (2.16) are located at the sharp peaks for which $\log(|\mathcal{D}(k, m)|) \rightarrow -\infty$. The complex roots of the dispersion relation are found numerically using the winding number to identify regions that contain a zero and the moments of the winding number to obtain its position [54, 61, 62]; given the high accuracy required to resolve the imaginary component these zeros were then refined using the built-in `fsolve` in `Matlab` that uses a Levenberg-Marquardt algorithm.

Figure 2.5 illustrates the solution space of (2.16) at fixed m , for which three types of solution can be discerned occurring at different wavenumbers. Modes with a wavenumber close to $\text{Im}(k) = 0$ are localised to the ring, whereas those of larger $\text{Im}(k)$ decay too rapidly into the infinite plate to be retained by the structure. From the analysis of whispering-Bloch modes in [49, 54] we anticipate two families of modes belonging to a platonic ring resonator: structure-located whispering-Bloch (WB) modes and interior modes. Structure-located modes, that have the smallest value of $\text{Re}(k)$ and $\text{Im}(k)$ for any given m , are characterised by an antisymmetric field pattern localised to the inclusions defining the ring. The period of antisymmetry is defined by the given mode number m , and in the case of $m = N/2$ equals the arc-spacing between points - see Fig. 2.6(a) and (b). The antisymmetric structured mode $m = N/2$ has special significance, being

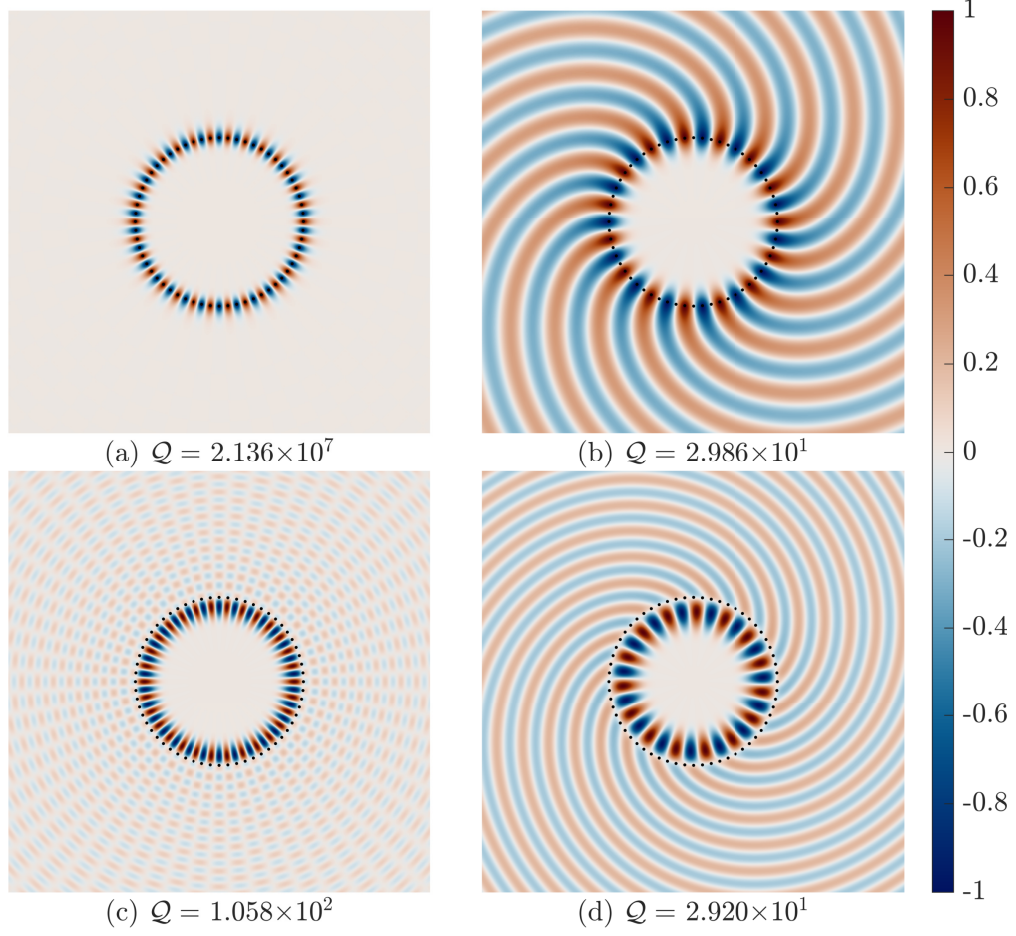


Figure 2.6: Real displacement fields for (a) the structure-located mode at modal value $m = N/2$, (b) the structure-located mode at modal value $m = N/4$, (c) the first interior mode at modal value $m = N/2$ and (d) the first interior mode at modal value $m = N/4$. Ring structure illustrated by black points.

analogous to the standing wave solution of Rayleigh-Bloch modes along the line array of Fig. 2.3(b) and being the most highly confined mode available to the ring.

The other family of modes, the interior modes, are localised to the cavity of the ring - see Fig. 2.6(c) and (d) - and correspond to solutions of greater $\text{Re}(k)$ and $\text{Im}(k)$ components along the top-right of Fig. 2.5. These solutions are characterised by the same antisymmetry of their line array structured counterparts, with an equal periodicity and a modulating field pattern now localised within the ring structure. Upon inspection at these interior wavenumbers, the ring is observed to be acting as a boundary reflector of incoming vibrations, not unlike the reflection of plane-waves by the periodic line arrays

of [5]. In the small m case, these interior patterns begin to resemble whispering gallery modes observed in optical micro-disks [63] or on the interior of rings of infinitely long dielectric rods [64]. The analysis herein on a ring of scatterers is directly comparable to similar work conducted in [65]; the exploration of the complex wavenumber space belonging to a ring of circular inclusions revealed highly symmetric standing mode solutions both interior and exterior to the ring, of a form dependent upon the selected mode number p . This included the identification of a ‘dominant mode’ $p = N/2$ for which the largest forces upon the ring structure were observed.

A key characteristic of both structured and interior solutions is the leakage of energy into the far-field, resulting in radiating Archimedean Spirals [66], as visible in Fig. 2.6(b) and (d). These radiation patterns appear as the wavenumber migrates from that of the antisymmetric $m = N/2$ solution, which itself defines the maximally structure-localised solution of minimal $\text{Im}(k)$ component and hence minimal leakage. The spiralling patterns grow increasingly significant in the wavefields of resonance with growing $\text{Im}(k)$ component as the selected mode decreases, visibly dominating the field pattern as in Fig. 2.9(b). These clockwise modes were selected by taking the positive sign of the exponent in (2.15), and identically reversed solutions exist for the negative sign. These radiation patterns are also visible in ring resonators composed of Neumann-type inclusions [66] and in the context of photonic crystal fibers [64, 67], featuring similar spirals in ‘nearly bound states’. Hammer *et al.* provide the mode profiles of propagating TE modes as a function of bend radius of the waveguide [68], and in the following section we make similar considerations in our investigation of curvature-induced radiative losses.

2.4.2 Curvature-Induced Radiation Loss

The degree to which a quasi-mode of complex frequency is confined to a ring, or decays into the plate, is described quantitatively by the quality-factor, $\mathcal{Q}$, of a WB mode. We define $\mathcal{Q}$ as:

$$\mathcal{Q} = \frac{\text{maximum energy stored in cycle}}{\text{energy lost per radian of cycle}} \sim \frac{\text{Re}(\omega)}{|2\text{Im}(\omega)|}, \quad (2.18)$$

where the expressions on the left- and right-hand-sides coincide in the limit $\text{Im}(\omega)/\text{Re}(\omega) \rightarrow 0$ [9]. Herein we calculate the limiting quality-factor in terms of complex wavenumber components as:

$$\mathcal{Q} = \frac{\text{Re}(k^2)}{|2\text{Im}(k^2)|}, \quad (2.19)$$

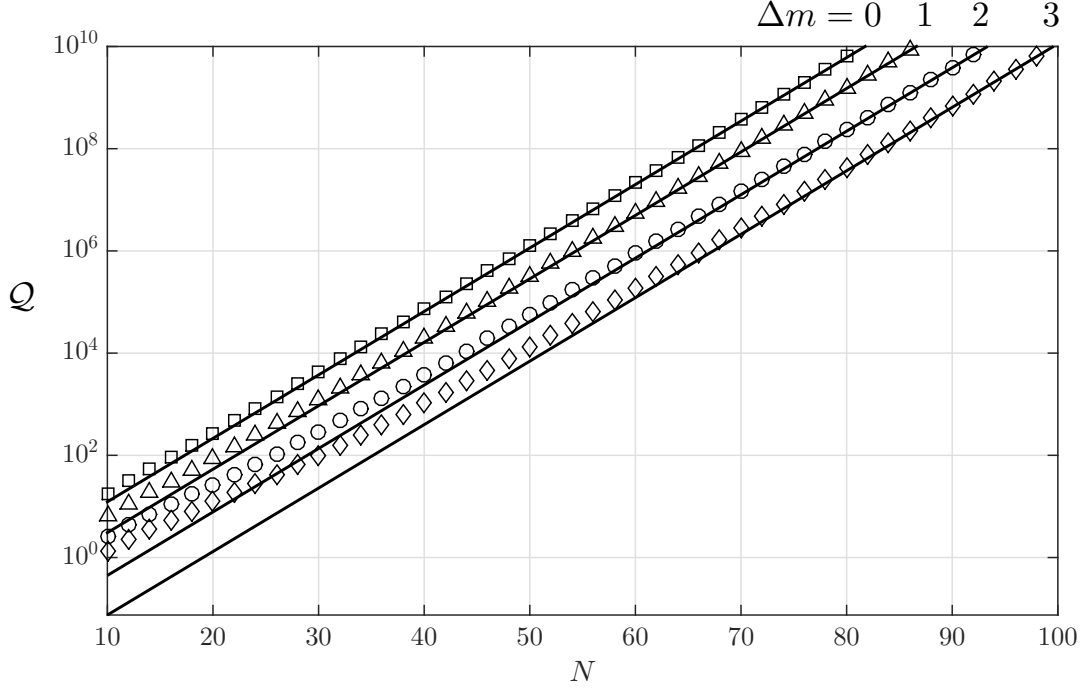


Figure 2.7: $\mathcal{Q}$ dependence belonging to rings of N point-masses of uniform mass-loading $\tilde{\mu} = 1$. Symbols are from calculation via dispersion relation (2.16), with different symbols used for different values of Δm . Solid lines are from asymptotic formula (6.24) of [9], formulated under considerations of the outer solution region. Figure adapted from [9].

N	Structure k	$\mathcal{Q}$	Interior k	$\mathcal{Q}$
20	$6.058 - 5.6 \times 10^{-3}i$	2.728×10^2	$14.825 - 9.4 \times 10^{-2}i$	3.935×10^1
40	$12.182 - 4.2 \times 10^{-5}i$	7.312×10^4	$25.791 - 9.2 \times 10^{-2}i$	6.987×10^1
60	$18.289 - 2.1 \times 10^{-7}i$	2.136×10^7	$36.480 - 8.7 \times 10^{-2}i$	1.054×10^2
80	$24.393 - 9.6 \times 10^{-10}i$	6.326×10^9	$47.035 - 8.2 \times 10^{-2}i$	1.442×10^2

Table 2.1: Table of complex wavenumbers for the structure-located and first interior modes for $m = N/2$ with corresponding limiting quality-factors $\mathcal{Q}$. Note the exponential growth in $\mathcal{Q}$ as $\pi/N \rightarrow 0$.

for the quasi-mode solutions of (2.16) determined using the winding number method of [54]. As observed in rings consisting of Neumann inclusions embedded in thin-elastic plates [9, 66], the curvature-induced radiation loss experienced by a WB mode of given m rapidly falls as the number of points comprising the ring is increased; Fig. 2.7 shows the dependence of $\mathcal{Q}$ on N plotted on a logarithmic scale for three mode numbers. It is

convenient to introduce an alternative definition of the mode number as:

$$\Delta m = N/2 - m, \quad (2.20)$$

describing the ‘modal distance’ from the WB mode of greatest confinement, $m = N/2$. The $\text{Im}(k)$ component is observed to be exponentially small in angular period (see $\epsilon = \pi/N \rightarrow 0$ discussion in [9]) as the quasi-mode wavenumber migrates towards the real-axis to a corresponding RB wavenumber, and accordingly $\mathcal{Q}$ grows exponentially large in the same limit. The decline in $\mathcal{Q}$ with increasing modal distance corroborates the observed radiation leakage experienced by propagating WB modes; at $N = 60$ specifically, the contrasting spiralling patterns of radiation and lack thereof in Fig. 2.6(b) and (a) respectively illustrate the same decline in $\mathcal{Q}$ with Δm . In Tab. 2.1 we give values of the resonant wavenumbers k for different N corresponding to the structure-located and the first interior modes for which $m = N/2$ and $\tilde{\mu} = 1$.

Intuitively, the physical mechanism behind the leakage can be thought of in terms of direction of the propagating WB mode from point-to-point. Unlike the ring resonators of optical and photonic systems [55, 63], elastic ring resonators are characterised by their inclusion geometry of point- or Neumann-type inclusions equally spaced along a circle, rather than through an effective refractive index and bend radius of a continuous waveguide. Introducing a curvature on the small-scale Bloch-periodic geometry causes a bending of the WB mode as it propagates from point-to-point, and this bending allows for the escape of flexural wave energy into the infinite plate. This is in contrast to the line array, for which propagation of the field perpendicular to the array is exponentially small with distance. In the limit of zero curvature $N \rightarrow \infty$, one expects a return to the RB case of no radiative losses and perfect localisation of the waveform to the structure. However, as the ring is both a finite and open system, one should always expect some leakage of energy into the plate for point-masses. Exponentially localised waveforms have been found by Movchan *et al.* [69] in rings devised of a finite number of mass-spring resonators for which the total mass and stiffness of the structure are set to result in a ‘negative inertia’, with real k identified via a homogenization model.

Mode localisation upon finite structures of resonators is desirable for the purposes of guiding and filtering flexural vibrations to a high-degree of precision and control. In § 2.5 we analyze more geometrically complex elastic circuits of point-masses and the resonant behaviours that lie therein. For the purposes of ease of calculation and demonstration, we have selected rings of $N = 60$ point-masses of $\tilde{\mu} = 1$ and select only the highest $\mathcal{Q}$ modes

available to minimise leakage into the plate. We demonstrate the guiding and filtering of flexural waves through ring resonator circuits and measure the resonant phenomena of the composite systems devised.

2.5 Ring-Array Coupling

2.5.1 Matching Solutions

The existence of Rayleigh- and whispering-Bloch modes upon similarly structured gratings suggests that a coupling between line arrays and ring resonators is feasible for the purposes of directing and manipulating wave motion in elastic plates. The analogy between such modes is made obvious by comparing the structure-located WB modes of lowest $\text{Re}(k)$ for a ring resonator of N inclusions at modal values $m \in \{1, \dots, N/2\}$ to the Rayleigh-Bloch dispersion band of Fig. 2.3(a) at $\tilde{\mu} = 1$. Scaling the spacing along the line array, a , to equal the linear distance between points along the ring, $a = 2 \sin(\pi/N)$, the dispersion band for this ring-scaled array is superposed atop the discretised set of $\text{Re}(k)$ WB solutions of the ring in Fig. 2.8(a). The antisymmetric mode of highest confinement $m = N/2$ corresponds to the standing wave solution $\beta = \pi/a$ located at the band edge, and modes of increasing Δm (and hence increasing leakage) migrate away from the band edge towards lower $\text{Re}(k)$, reflecting the growing dominance of the $\text{Im}(k)$ component and falling $\mathcal{Q}$.

The analogy between the Rayleigh-Bloch waves on the line array and the structured whispering-Bloch modes around the ring is further strengthened by inspecting the form of the wavefields in each regime. For a line array of point-masses there is a marked scale separation between the microstructure of the periodic cell and the macrostructure of the entire array; the supported Bloch waves are characterised by fast oscillatory solutions on the short scale modulated by an envelope function on the long scale, as shown in Fig. 2.3(c). The modulation, or beat wavelength of the RB wave is calculated using the High Frequency Homogenisation (HFH) asymptotic scheme [7], which leverages the multi-scale nature of the system by perturbing about the standing wave solutions present in the Bloch spectra at the edges of the Irreducible Brillouin Zone. This technique has recently been applied to 1D line arrays of point-masses on Kirchhoff-Love elastic plates [8], resulting in the governing equation (4) being reduced to an ODE entirely on the macroscale that incorporates the effects of the microstructure. The array is then homogenised and the resulting ODE captures all the dispersive properties of the bands,

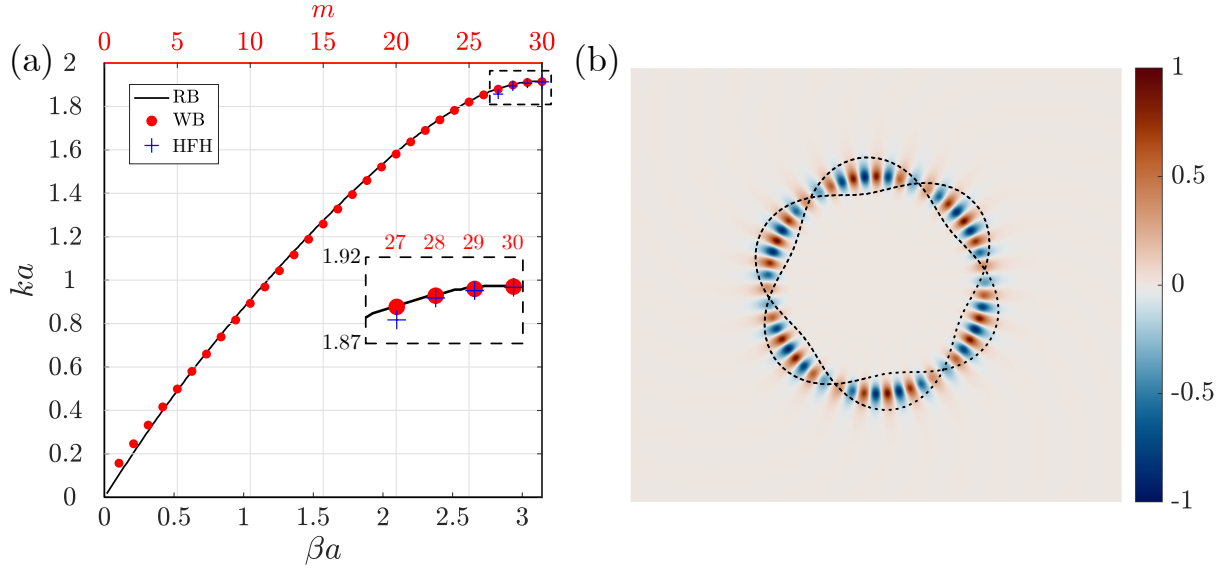


Figure 2.8: (a) The dispersion curve and discrete $\text{Re}\{k\}$ solutions pertaining to a line array (solid line) and ring resonator (red points) at an impedance characterised by $\tilde{\mu} = 1$. Blue crosses correspond to predictions from the HFH calculations for which an integer number of wavelengths fit around the ring. The superposition of the RB curve atop the WB solutions and HFH approximations suggests a strong analogy between the line array and ring structure-located modes. (b) The real displacement wavefield pertaining to the $\Delta m = 3$ WB mode featuring three full beat wavelengths wrapped around the ring, illustrated by the superposed long-scale envelope.

described by the modulation of the strongly oscillating field. By considering a ring with the same inter-point spacings as the line array, this technique is used to estimate several resonance modes of the ring in which integer numbers of the beat wavelength fit around the ring. These correspond to modes near the band edge of the line array as exemplified in Fig. 2.8(b).

The coupling geometry considered is based on that of Yariv [70] and is drawn schematically in Fig. 2.2(a); a line array of ring-scaled spacing is paired a distance d from a ring resonator of N point-masses. To ensure impedance matching (2.5) between line and ring, we assert the following condition on the impedance $\tilde{\mu}$:

$$\tilde{\mu}_{line} a_{line}^2 = \tilde{\mu}_{ring} a_{ring}^2 \quad (2.21)$$

where a_{line} is the linear spacing along the line array and a_{ring} is the arc spacing along the ring, and these separations are equivalent in the limit $N \rightarrow \infty$. The relative angle between the nearest-neighbour points of the line array and ring is set to ensure minimal

through-transmission along the line array downstream of the ring. The line array itself consists of $2M - 1$ points, and a Rayleigh-Bloch mode is triggered upon the array via excitation by a Green's function along the array upstream of the ring. Given that RB modes are modes of real frequency, the frequency of excitation is selected such that it corresponds to the real part only of the lowest $\text{Re}(k)$ solution to the dispersion relation (2.16) for any given m - the structure-located WB modes. Accordingly only these modes will be observed during coupling.

2.5.2 Numerical Damping

The dispersion relation (2.10) corresponds to an infinite line array. For systems lacking a ubiquitous quasi-periodicity, such as the coupled ring-array systems of Fig. 2.2, we cannot determine the coefficients of the Green's functions A_n everywhere through considerations of the geometry, and instead resort to computation via the scattering matrix method (2.9). However, solving for the coefficients introduces a numerical problem; any infinite line array must be truncated for (2.9) to remain finite, and the infinite sum over the line array elements converges extremely slowly, meaning that any finite number of terms cannot accurately describe an array extending *ad infinitum*. This truncation introduces spurious reflections at the extremal points of the array that must be avoided so as to prevent reverse RB propagation. In [71] the authors introduce a filtering method that allows for the slowly convergent summation to be determined analytically, making use of the phase between coefficients to filter out terms at the extremal ends of the array. Similarly, one might consider deriving asymptotic approximations as in [72], folding this expression back into a modified scattering matrix (2.9). While these methods are certainly useful and effective under perfect quasi-periodicity, they are rigid in their application. For ease of computation and efficiency, we prevent spurious reflections using an absorbing layer of inclusions inserted into the scattering matrix (2.9), introducing a point-wise damping $\tilde{\nu}_n$ for inclusions at the extremities of the truncated array in the impedance matrix $\hat{\mu}$.

A line array of forcings placed at $\mathbf{r}_n = (na, 0)$, for $n \in \{-M + 1, \dots, M + 1\}$, has the left- and right-most N_d inclusions characterised by an impedance coefficient composed of an identical mass term $\tilde{\mu}$, but with an additional damping term $\tilde{\nu}(n_d)$ now a function of the position index n_d , such that:

$$\mu_d(n_d) = 4k^4 a^2 \tilde{\mu} + i4k^2 \tilde{\nu}(n_d). \quad (2.22)$$

The dependence of the damping term on position is taken as:

$$\tilde{\nu}(n_d) = \frac{|N_d - n_d|^p}{N_d^p} \tilde{\nu}_0 \quad (2.23)$$

where p determines the rapidity, or rather smoothness, of the damping out of reflected modal energy, $\tilde{\nu}_0$ is an arbitrary damping constant and the index n_d counts from 1 to N_d . Such index-dependent damping is used for guided elastic waves in [73], and in applying the same technique we select $N_d = \mathcal{O}(10^2)$ and $p = \mathcal{O}(10^1)$. These parameter values were determined through the evaluation of $|A_n|$ along the dissipative regions of the line array, for which parameter values corresponding to an observed absence of reflections, and a decay of the coefficients to zero in these regions, were selected. The vector of coefficients $\mathbf{A}$ is found through (2.9) using the impedance matrix:

$$\hat{\mu} = \text{diag}(\mu_d(1), \dots, \mu_d(N_d), \mu, \dots, \mu, \mu_d(N_d), \dots, \mu_d(1)) \quad (2.24)$$

where μ denotes identically all point-wise impedances in the undamped region of the truncated array. Equation (2.9) is augmented by the incident field for which we use excitation at the point $\mathbf{r}_f = ((N_d + 1)a, 0)$ due to a forcing:

$$u_i(\mathbf{r}) = g(\mathbf{r}, \mathbf{r}_f; k); \quad (2.25)$$

the wavenumber k corresponds to a Rayleigh-Bloch solution (2.10). As a validation, solving the new linearised system describing the truncated line array in isolation, the resulting wavefield in the fundamental unit cell matches identically that calculated via the theoretical Bloch wavenumber solution (6.5) of [5]. This method of absorption is implemented into all following line array-ring couplings and platonic circuits, and makes possible the accurate determination of transmission coefficients in the through- and drop-ports of the proposed platonic filters.

2.5.3 Measuring Transmission

The strength of coupling is described through the measurement of power radiated along the line array downstream of the ring. This is calculated using the following expression for the time-averaged flexural wave flux in a Kirchhoff-Love thin-elastic plate [74]:

$$\langle \mathbf{F} \rangle = \frac{k^2}{2} \text{Im} \left(u(\mathbf{r}) \nabla \nabla^2 u^*(\mathbf{r}) - \nabla^2 u^*(\mathbf{r}) \nabla u(\mathbf{r}) \right), \quad (2.26)$$

where $u^*(\mathbf{r})$ denotes the complex conjugate of the displacement field (in fact, (2.26) is a ‘simplified’ flux. See [74]). This form of time-averaged flux is a statement of energy conservation in the plate: the surface integral of the time-averaged flux $\langle \mathbf{F} \rangle$ around any contour not enclosing a source must be zero. The power transmitted along the horizontal line array through a given unit cell ma is determined through integration of the quantity $\langle \mathbf{F} \rangle \cdot \hat{\mathbf{x}}$ along the boundaries of the corresponding infinite unit strip [75], such that:

$$I = \int_{-\infty}^{\infty} (\langle \mathbf{F} \rangle \cdot \hat{\mathbf{x}}) dy. \quad (2.27)$$

This integral of the time-averaged flux provides a measure of the wave energy propagating along the line array. We define the through-transmission coefficient T as the ratio of the radiated powers along the line in the presence of the ring and in isolation respectively - the latter being an unattenuated Rayleigh-Bloch solution - such that:

$$T = \frac{I_T}{I_0}, \quad (2.28)$$

where both I_T and I_0 are measured at the boundary of the same unit strip downstream of the ring. The measurement of transmission over a narrow range of excitation frequencies provides an alternative definition of the quality-factor for a coupled ring-line array of real ω :

$$Q_c = \frac{\omega_r}{\Delta\omega}, \quad (2.29)$$

where Q_c is the quality-factor of coupling, ω_r is the resonant frequency in the measured transmission spectrum and $\Delta\omega$ is the full width at half maximum (FWHM) of the resonance peak. Using the definition $k^4 = m_p\omega^2/D$, (2.29) is rewritten in terms of infinite plate wavenumber:

$$Q_c = \frac{k_r^2}{\Delta(k^2)}, \quad (2.30)$$

where k_r is the wavenumber corresponding to the resonant frequency ω_r and $\Delta(k^2)$ is the FWHM of the resonant peaks in $1 - T$. Definition (2.30) should not be conflated with the limiting Q of the ring; the distinction being that Q quantifies the radiative losses suffered by ring-guided quasi-modes in isolation, whereas Q_c is a measure of the losses suffered by a ring-array coupler during coupling.

Shown in Fig. 2.9 are the transmission spectra in the wavenumber regions about the WB (a) $m = N/2$ and (c) $m = N/4$ modes, WB wavenumbers labelled with vertical dashed lines. The resonances of the line-ring composite system are perturbed with respect to the

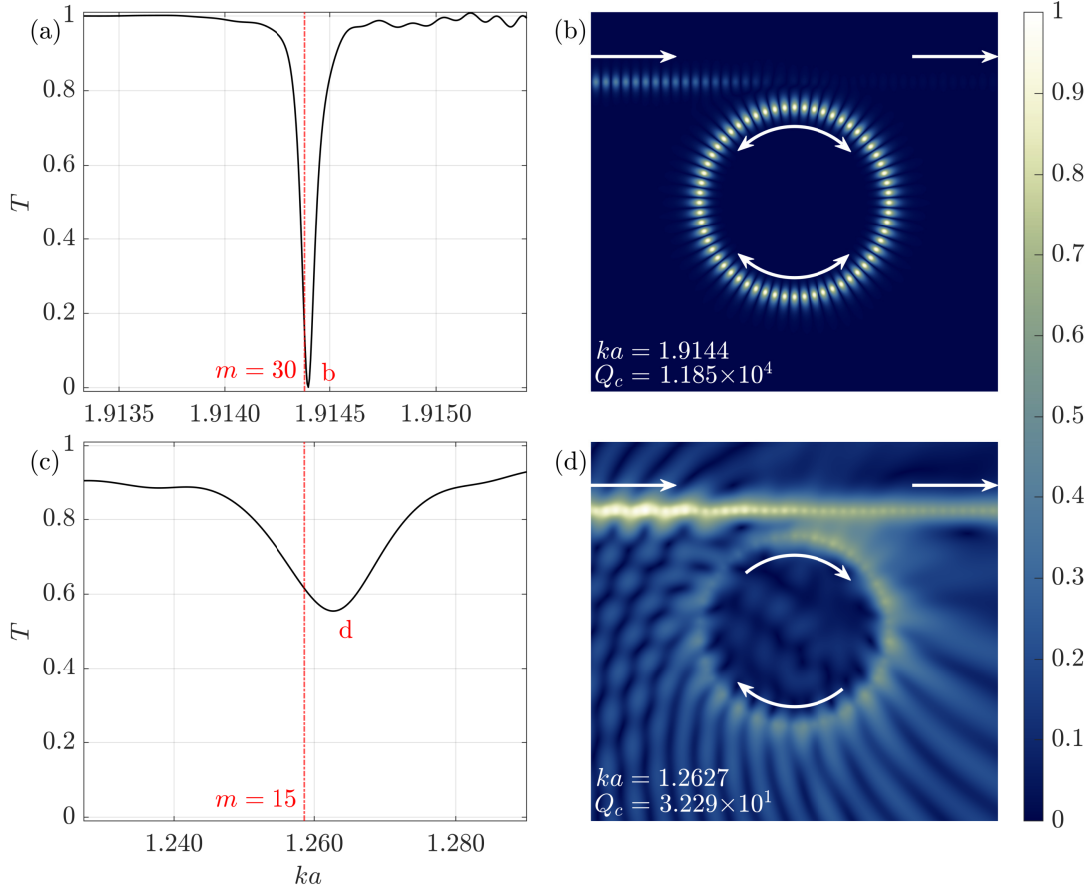


Figure 2.9: Transmission spectra about WB resonances for (a) $m = 30$ and (c) $m = 15$ for a ring of $N = 60$ mass-loadings, red dashed lines indicating WB resonances of (2.16). Minima in T corresponding to paired absolute displacement wavefields (b) and (d) for which $Q_c = 1.185 \times 10^4$ and $Q_c = 3.229 \times 10^1$ respectively.

WB resonances due to the presence of the neighbouring line array, with Fig. 2.9(a) $ka = 1.9144$ and (c) $ka = 1.2627$ corresponding to wavefields Fig. 2.9(b) and (d) respectively, and with Q_c values measured as (a) $Q_c = 1.185 \times 10^4$ and (b) $Q_c = 3.229 \times 10^1$. The wavefields Fig. 2.9(b) and (d) are plotted with absolute displacement values to highlight the attenuation of the propagating RB mode from the left-of-ring source, and the direction of the WB mode in propagation around the ring (ring geometry not shown hereafter for illustrative purposes). As is observed for conventional ring-guide couplers [46], a left-of-ring source produces a clockwise-propagating mode around the ring, with leakage arising due to the curvature of the circular array and spirals emanating from the structure in Fig. 2.9(d) as in Fig. 2.6(b). The coupling differs at the band edge wavenumber, at which the propagating RB mode acts as a standing wave source for flexural vibrations

into the ring, and the propagation around the ring follows no preferential direction, as in Fig. 2.9(b). These mode trajectories can be observed in the time-averaged flux streamline plots of § 2.5.5.

We emphasise that the measure Q_c captures not the curvature induced losses experienced by the mode in propagation about the ring, but rather the radiative losses experienced during coupling. At wavenumbers at, or close to, the band edge the loss during coupling is at a minimum, and this is reflected by the sharp and narrow resonance peak of Fig. 2.9(a). The shallower and broader resonances characterising lower wavenumbers reflect weaker line-ring coupling and greater leakage into the plate, the latter being visible in the wave-field Fig. 2.9(c) as leakage emanating from the coupling region, and corroborated by the measure of Q_c being $\mathcal{O}(10^3)$ smaller at $m = 15$ than at $m = 30$. As energy leakage becomes increasingly characteristic of the coupling process with decreasing wavenumber, the measured Q_c falls towards zero, with the resonances in transmission growing increasingly shallow and broad and the filtering capabilities of the ring diminishing. This limit on the maximum Q_c available to the composite line-ring system has implications for the types of circuit geometries conceivable, and their ability to filter and direct flexural vibrations. In § 2.5.4 we demonstrate the filtering of flexural waves in circuits of conjoined ring resonators, for which the highest Q_c modes were selected in order to minimise radiative losses during both propagation and coupling.

2.5.4 Coupled Resonator Elastic Arrays - CREAs

Like their optical counterparts (see coupled resonator optical waveguides: CROWs [30, 63]), chains of coupled ring resonators in an elastic plate can be utilised as a means of directing and channeling vibrational energy: coupled resonator elastic arrays (CREAs) for the control of flexural wave motion. To this end, the first geometry we consider is the add-drop filter (ADF) of Fig. 2.2(b). The narrow-band nature, and depth of the transmission minima, at high m number - visible in Fig. 2.9(a) - suggests that line-ring coupling could be utilised for the purposes of narrow-band wave filtering. The upper line array defines the input- and through-ports and the lower the add- and drop-ports. The measure of drop-transmission coefficient is akin to that of the through-transmission coefficient:

$$T = \frac{I_T}{I_0}, \quad D = \frac{I_D}{I_0}, \quad (2.31)$$

where I_T and I_D are the radiated powers measured downstream/upstream along the through- and drop-ports of Fig. 2.2(b) respectively, and I_0 the reference RB power in the

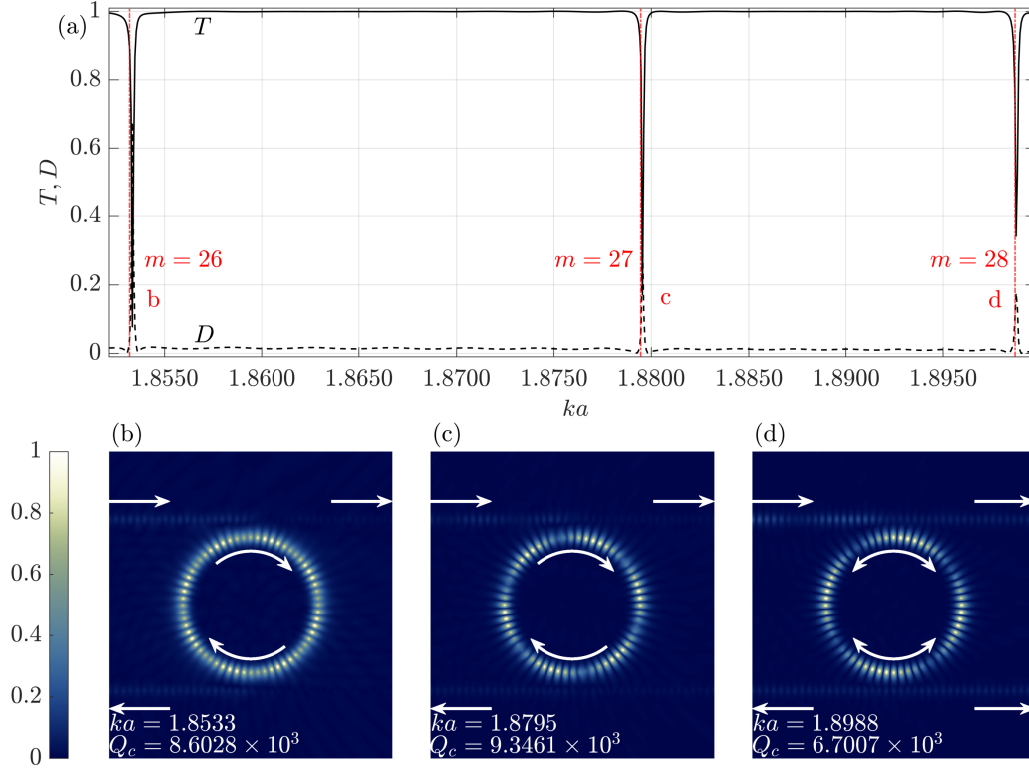


Figure 2.10: (a) T and D spectra in the wavenumber region of WB resonances (b) $m = 26$, (c) $m = 27$ and (d) $m = 28$, wavefields of absolute displacement. White arrows indicating directions of RB and WB propagation in line array and ring. Note that the highest WB modes feature bidirectional propagation in ring and array, (d), whereas lower resonances feature unidirectional propagation, (b) and (c).

absence of the ring.

For strong coupling and optimal wave filtering, hereafter we select only those modes at or near the band edge such that the radiative losses in propagation and the measured through-transmission coefficients are minimised. Shown in Fig. 2.10 are the displacement fields and T and D spectra near three WB resonances: (a) T and D spectra featuring peaks/dips near the WB (b) $m = 26$, (c) $m = 27$ and (d) $m = 28$ modes. The behaviours exhibited by the filter are similar to those exhibited by equivalent optical and photonic crystal ADFs [55, 76]; the transmission spectra Fig. 2.10(a) feature sharp peaks/dips in T and D close to the WB resonances, and the directionality of the WB mode is shown to be dependent on the wavenumber of excitation. Visible in the absolute displacement fields Fig. 2.10(b)-(d) is the attenuation of Through-port RB propagation, WB propagation

around the ring, and the transmission of an RB mode unidirectionally or bidirectionally along the output array. The bidirectional or unidirectional RB propagation in the output array is dependent on the selected resonance, with bidirectional propagation observed at resonances closest to the band edge and unidirectional propagation occurring at resonances at or below the $m = 27$ resonance. Like the coupling of Fig. 2.9(b), at band edge adjacent wavenumbers the RB mode acts as a standing wave source of flexural vibrations into the ring with no preferential direction; both clockwise and anticlockwise WB circulation results in transmission into both the drop- and add-ports of the output array, as in Fig. 2.10(d). In Fig. 2.10(b) and (c) the ring-guided mode is purely clockwise with transmission predominantly into the drop-port, and both fields feature stronger attenuation of RB propagation along the input array, corroborating the sharper dips in through-transmission in Fig. 2.10(a) measured at these resonances.

At these band edge adjacent wavenumbers Fig. 2.10(b)-(d), analogous long-scale envelopes to those along the linear array calculated via HFH (Fig. 2.8(a)) are observed along the ring during coupling, with integer number of beat wavelengths circumnavigating the ring in each case. As in Fig. 2.9(b), the Q_c (measured with the peaks in $1 - T$) are of the order $Q_c = \mathcal{O}(10^3) - \mathcal{O}(10^4)$ and decline with distance from the band edge, reflecting the increase in energy loss during coupling. We note that the highest quality-factor of coupling available to the composite system belongs to the first resonance featuring purely unidirectional motion, in this case the resonance near the $m = 27$ WB mode, and that this is a consequence of the measurement of T (and hence Q_c) being downstream of the ring.

Next we consider CREAs consisting of multiple rings chained horizontally, such that neighbouring rings couple with one-another and the leading and trailing rings couple with the bordering line arrays. By introducing additional rings we expect to observe resonant behaviours that differ from those of the isolated ring or single-ring ADF, including multiple resonances in transmission about each WB resonance [77] and alternating waveforms from ring-to-ring, visible in the field pattern at each resonance [55, 63]. Referred to as ‘supermodes’ in [55, 63], a given WB resonance of the isolated ring splits into a series of peaks/dips about the central WB wavenumber. As stated in [55], a Fourier harmonic system is revealed in the field patterns of the resonances; rings in ‘off-states’ being nodes and neighbouring ‘on-state’ rings antinodes, with the supermode resonances defining the set of observable harmonics and the fundamental harmonic being that of the lowest frequency. The number of rings also determines the direction of add- and drop-ports in the output array, with an even number of rings reversing the drop-port direction relative to

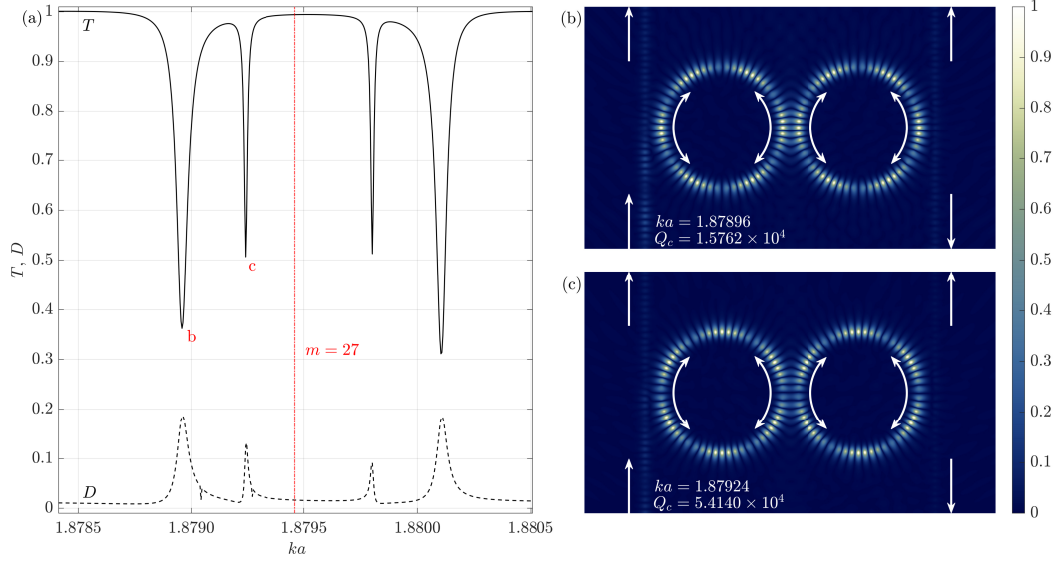


Figure 2.11: (a) Transmission spectrum about the WB $m = 27$ wavenumber for a two-ring CREA, where the left-of-centre resonances correspond to absolute wavefields (b) and (c) from left to right. The mode propagation is bidirectional throughout the CREA system at all resonances.

the ADF and an odd number retaining it. The propagation remains bidirectional at band edge adjacent wavenumbers, as in Figs. 2.9(b) and 2.10(d).

Shown in Figs. 2.11 and 2.12 are the transmission spectra and corresponding resonant wavefields for the CREAs consisting of two and three rings respectively, in the wavenumber region about the WB $m = 27$ wavenumber. This mode was chosen as it corresponds to the highest coupling quality-factor available to the ADF - see Fig. 2.10(b) - for which the output mode propagation was observed to be primarily through the drop-port. In Fig. 2.11, the T and D spectra pertaining to a two-ring system have split into a series of multiple resonances about the central WB wavenumber; four narrow-band resonances are measured, of Q_c values of the order $Q_c = \mathcal{O}(10^4)$, with all resonances corresponding to bidirectional propagation through the CREA system. The absolute displacement wavefields Fig. 2.11(b) and (c) correspond to the left-of-centre resonances from left to right, with each exhibiting a mirror symmetry about the mid-point between the rings. The ring-guided modes feature the long-scale beat-waveform of Fig. 2.8(b), where the waveforms of Fig. 2.11(c) are a rotation of those of Fig. 2.11(b) through half a beat wavelength. Consequently the stronger outer resonances are characterised by waveforms of an antinode at the line-ring interface, whereas the weaker inner resonances are characterised by a node at the line-ring interface. This observation corroborates the shallower measured

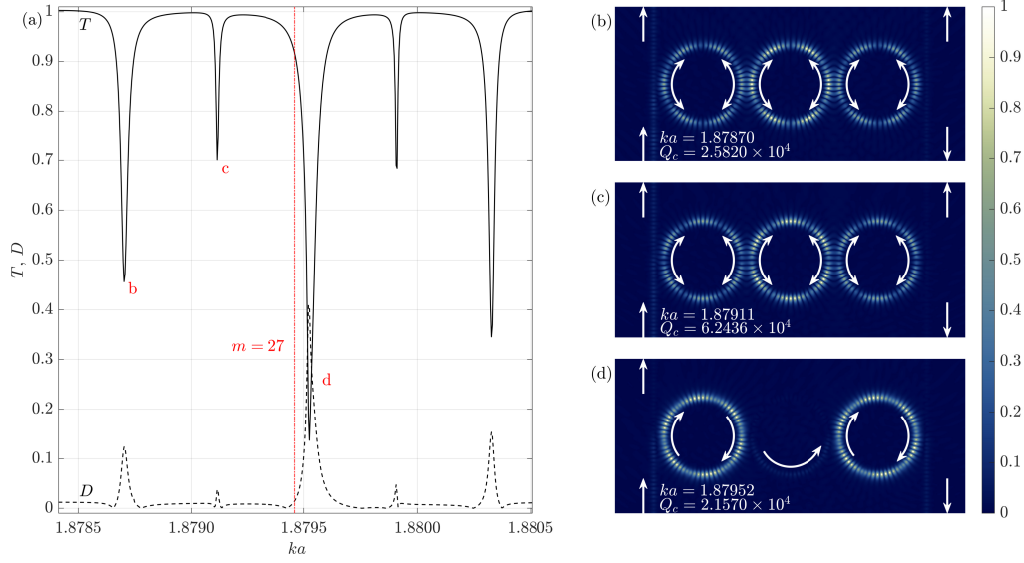


Figure 2.12: (a) Transmission spectrum about the WB $m = 27$ wavenumber for a three-ring CREA, where the left-of-centre resonances correspond to absolute wavefields (b), (c) and (d) from left to right. The mode propagation is (b) bidirectional, (c) bidirectional and (d) unidirectional throughout the CREA system. Note the central ring of (d), with propagation exclusively along the lower arc, is in an ‘off-state’.

dips or peaks in T or D , with an antinode associated with maximal input attenuation and drop-transmission, and a node minimal input attenuation and drop-transmission. The shape of the waveforms are repeated about the central wavenumber, such that the resonances to the right of the central wavenumber are reflections of those on the left about the centroid of each ring (for more detail, see Fig. 2.13).

To emphasise the symmetries available to the CREAs we include a second example with an odd number of rings. In Fig. 2.12 the transmission spectra for a CREA of three rings has split into a set of five resonances over the same wavenumber region about the central WB $m = 27$ wavenumber, of Q_c values again of order $Q_c = \mathcal{O}(10^4)$. The absolute displacement wavefields Fig. 2.12(b)-(d) correspond to the left-of-centre resonances of Fig. 2.12(a) from left to right, and each features a mirror symmetry now about the centroid of the central ring in the chain. The circulating ring modes include the long-scale beat-waveform of the $m = 27$ WB mode, and the inner resonance waveforms are again rotations of the outer resonance waveforms through half a beat wavelength. As for the two-ring CREA the weaker resonances are associated with a node at the line-ring interface and the stronger resonances an antinode, with all four outer resonances corresponding to bidirectional motion throughout the CREA. The strong central peak/dip in transmission is a mode of

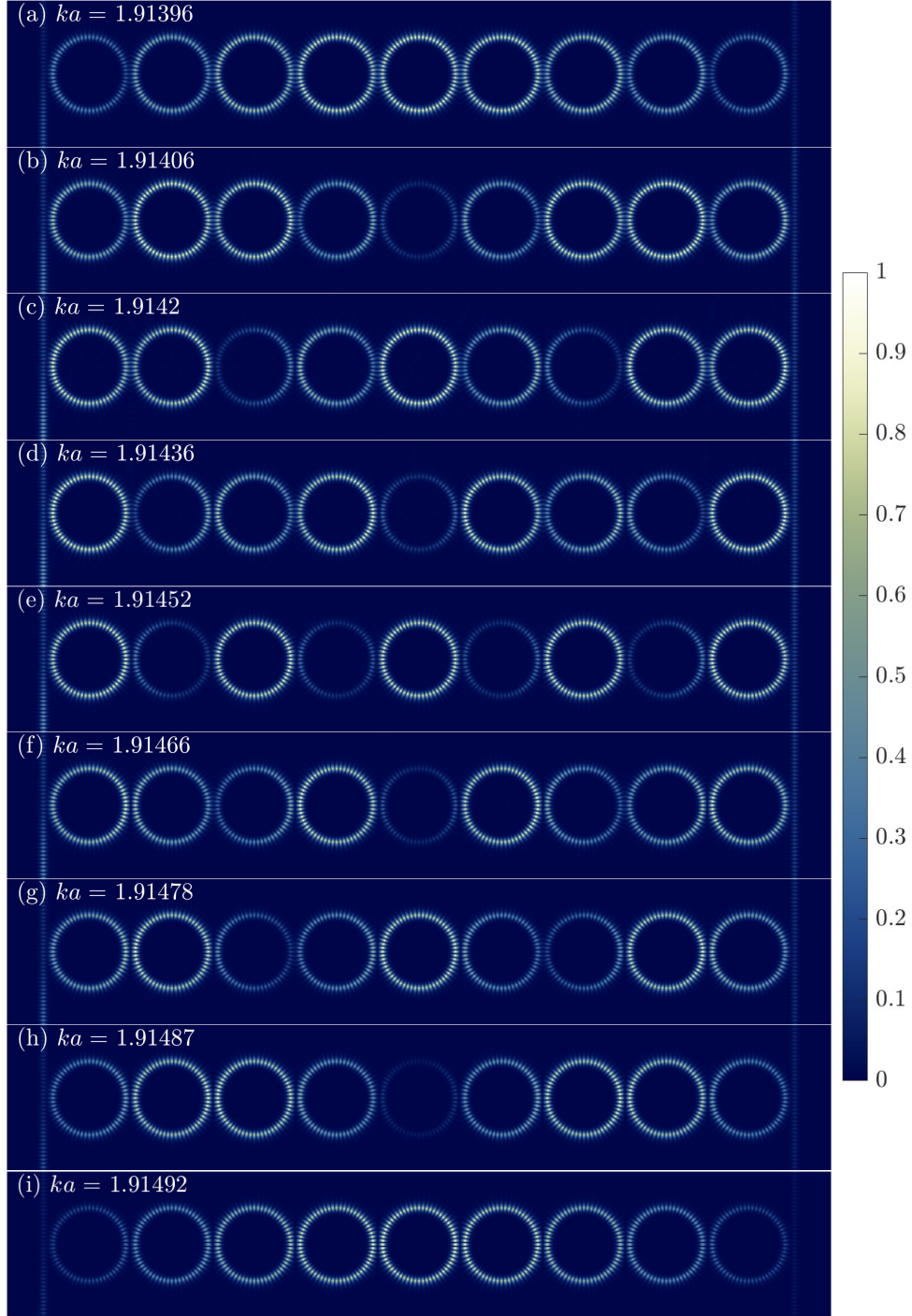


Figure 2.13: Absolute displacement field patterns at supermode resonances about the WB $m = 30$ resonance for a CREA system consisting of nine ring resonators. A similar set of harmonics are observed around all WB modes for the nine-ring CREA.

purely unidirectional motion through the CREA (see Fig. 2.12(d)), akin to the alternating clockwise-anticlockwise ring networks of Hammer *et al.* [55, 63] or Poon *et al.* [78, 79]. This resonance occurs at the same wavenumber as that measured near the WB $m = 27$ resonance of the single ring ADF - see Fig. 2.10(c) for which $ka = 1.8795$ - and like the circulating waves of [79] §2B is interpreted as a superposition of WB modes belonging to the ring resonators. The resulting output transmission is purely into the drop-port to the bottom right, with little leakage of energy into the add-port. The central resonance of Fig. 2.12(a) and lack thereof of Fig. 2.11(a) suggests that odd-numbered CREAs are better candidates for flexural wave filters, with the same shape in transmission spectra observed around other band edge adjacent modes for the two- and three-ring CREAs.

To emphasise the variety of available resonant states belonging to CREA systems, displayed in Fig. 2.13 are the collection of field patterns (a)-(i) belonging to a CREA of nine ring resonators around the $m = 30$ WB mode. The emergent pattern resembles closely that of Hammer [55] Fig. 5 ordered (a)-(i) belonging to a CROW of nine rings. Features include off-state and on-state rings and the strongest output transmission at the central resonance Fig. 2.13(e). The resonant waveforms each hold a mirror symmetry about the central ring, with the waveforms Fig. 2.13(f)-(i) being reflections of those (a)-(d) about the centroid of each ring. The circulation throughout the chain is bidirectional at all wavenumbers of resonance, each ka being adjacent to the band edge of Fig. 2.8(a) at which the standing wave source induces bidirectional coupling.

2.5.5 Flux Vector Fields

The time-averaged flux equation (2.26) describes the flux at any point $\mathbf{r}$ in the x - y plane, averaged over one period. As explained in [74] $\mathbf{F}$ is a simplified flux that is ‘more suitable for use in practice’, and when time-averaged coincides with the time-average of the ‘true’ flux. This makes it an ideal quantity for the purposes of illustrating the average motion of flexural vibrations through the line-ring couplers of § 2.5. The first of these we consider is the single line-ring coupler of Fig. 2.9(b) and (d), with emphasis on the coupling region between line and ring. In Fig. 2.14 we superpose the time-averaged flux streamlines atop the normalised absolute displacement fields of Fig. 2.9(b) and (d). In Fig. 2.14(a) the coupling into the ring is observably bidirectional; the group velocity of the incident Rayleigh-Bloch wave is close to zero, allowing for the incident RB mode to reverse direction during coupling and propagate anticlockwise around the ring. In Fig. 2.14(b) the higher group velocity leads to exclusively clockwise propagation in the

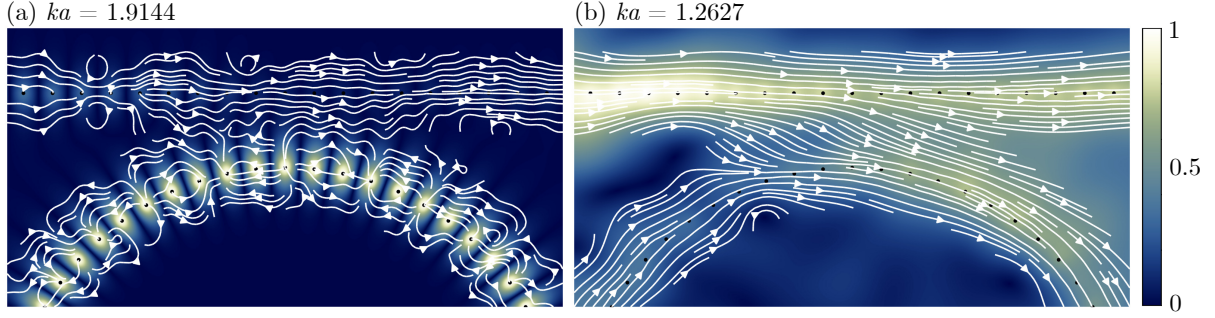


Figure 2.14: Flux streamlines plotted atop absolute displacement fields at wavenumbers of resonance (a) $ka = 1.9144$ and (b) $ka = 1.2627$ for the line-ring coupler. Panel (a) demonstrates the lack of a preferential direction around the ring at the $m = 30$ resonance, whereas (b) demonstrates purely clockwise ring propagation. Geometry included for clarity.

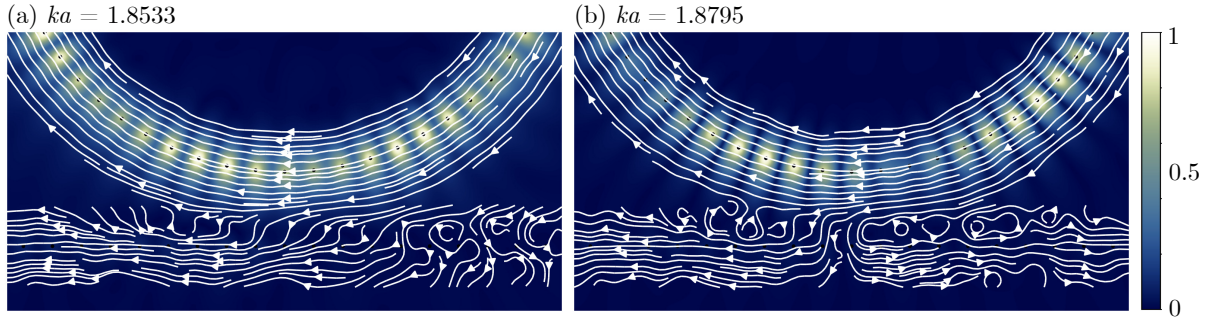


Figure 2.15: Flux streamlines plotted atop absolute displacement fields at wavenumbers of resonance (a) $ka = 1.8533$ and (b) $ka = 1.8795$ for the ADF. Panel (a) displays transmission exclusively through the drop-port whereas (b) displays propagation primarily into the drop-port, with some reversal along the add-port due to the proximity of the $m = 27$ mode to the band edge.

ring with no reversal, and this is the observed case in the field plots at resonances away from the band edge.

Next, the time-averaged flux through the output-port of the ADF is shown superposed atop the normalised absolute displacement fields of Fig. 2.10(b) and (c) in Fig. 2.15. In Fig. 2.15(a) at $m = 26$ the output is almost exclusively through the drop-port due to a clockwise propagating mode in the ring, with flux curves appearing within the add-port due to radiation leakage from the ring. In Fig. 2.15(b) at $m = 27$ the clockwise ring mode couples into the output array primarily through the drop-port to the left, although due to its proximity to the band edge exhibits some reversal into the add-port to the right.

To illustrate the bidirectional and unidirectional coupling through the larger CREA sys-

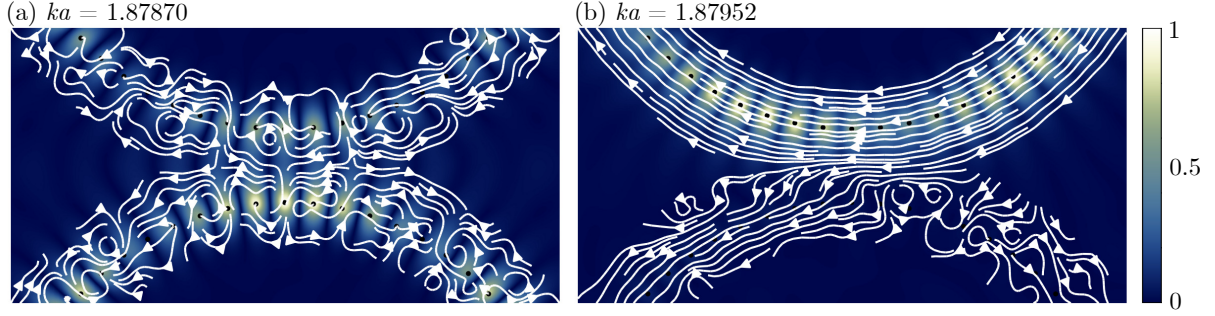


Figure 2.16: Flux streamlines plotted atop absolute displacement fields at wavenumbers of resonance (a) $ka = 1.87870$ and (b) $ka = 1.87952$ at the first ring-ring interface of the three-ring CREA. Panel (a) displaying no preferential direction along either ring and (b) an anticlockwise circulation in the central ring due to a clockwise circulation in the leading ring. Wavefields rotated for consistency with Figs. 2.14 and 2.15.

tems, we include the flux streamlines superposed atop the normalised displacement fields of the three-ring CREA of Fig. 2.12 at a bidirectional wavenumber Fig. 2.16(a) and a unidirectional wavenumber Fig. 2.16(b). Shown at the interface between the leading and central ring, the bidirectional mode of Fig. 2.16(a) corresponds to that of Fig. 2.12(b) and the unidirectional mode Fig. 2.16(b) to Fig. 2.12(d). Note the reversal of flux streamlines in 2.16(a) highlighting the lack of preferential direction.

2.6 Remarks on Chapter 2

Here we have demonstrated a high degree of control in the directing and filtering of flexural waves in thin-elastic plates governed by Kirchhoff-Love thin-plate theory. Arrays of mass-loadings of a high degree of rotational symmetry have been shown to support whispering-Bloch quasi-modes of complex wavenumber, analogous to the Rayleigh-Bloch modes upon infinite line arrays of [5]. These WB modes are characterised by a discrete set of solutions to the dispersion relation (2.16), with imaginary component quantifying the leakage of energy into the far-field. Exploring the complex wavenumber solution space has revealed two families of modes: structure-located modes and interior modes, the former being analogous to RB modes upon linear arrays, the latter provided a detailed analysis in [54]. The achieved limiting quality-factor of the structure-located WB modes is of the order $\mathcal{Q} = \mathcal{O}(10^7)$ for a ring of $N = 60$ point-masses at $m = N/2$, and has been shown to grow exponentially large in the limit $N \rightarrow \infty$ [9]. The analogy between the RB and WB solutions is strengthened by the determination of the long-scale

envelope wavelength via the HFH scheme of [8], demonstrating that the WB solutions adjacent to the band edge correspond to an integer number of wavelengths circumnavigating the ring. Line-ring coupling has allowed for the filtering of flexural waves incoming along the line array, with the measurement of radiated power providing an alternative definition of the quality-factor (2.30) for the line-ring composite systems, herein coined CREAs. The add-drop filter and CREAs of an even and odd number of rings have been conceptualised, with quality-factors of order $Q_c = \mathcal{O}(10^3) - \mathcal{O}(10^4)$, and exhibit both unidirectional and bidirectional mode propagation. The ADF in particular acts as an effective filter for RB output exclusively along the drop-port at those wavenumbers first exhibiting purely clockwise circulation. Similarly, the central resonance of the three-ring CREA corresponds to purely clockwise-anticlockwise circulation, for which the output is exclusively along the drop-port.

Herein we have presented an array of interesting flexural wave phenomena, and this work holds promising extensions to the design of platonic devices. One such example could be the grading of ring radii along the CREA as a means of rainbow trapping [8] for energy harvesting networks like those of [75, 80]. An analogous application in the realm of optics of equivalent CROWs is the slowing of transmission and group velocity of light for the purposes of engineering optical delay lines [78, 81]. In replicating this, exponentially localised waveforms are of particular importance, and in the realm of elasticity this could be achieved through the inclusion of mass-spring ring resonators of negative inertia and real k [69], termed ‘negative inertial circuits’.

3 The Multipole Method in Cylindrical Geometries

3.1 Introduction to Chapter 3

The multipole formulation describing the scattering of waves by cylindrical inclusions was developed independently by several research groups at the turn of the century, namely those of McPhedran [28, 82–85], Felbacq [86, 87] and Evans [65, 88, 89], among others. The derivation provided here is a conglomeration of the essential parts of each of these research papers, provided with additional details so as to ensure that a reader unfamiliar with the subject can straightforwardly comprehend the method. This chapter is self-contained, although draws from the very useful textbook by Yasumoto *et al.* [90]. The formalism established here provides the mathematical backbone to chapters 4-6, with the named formulae and operators appearing again when we consider infinite singly- and doubly-periodic structures.

Our approach in formulating the problem is two-fold. We begin by providing a problem description and discuss the cylinder boundary conditions, before identifying field expressions, in terms of Bessel functions, in a manner grounded in physical arguments. A more rigorous approach in deriving the field is then pursued in terms of integral equations that stem from Green’s theorem. This culminates in an identity relating the regular re-incident field on one cylinder to the singular scattered fields emanating from all of the other cylinders. This, in conjunction with a change-of-basis function, forms the foundation of the method.

3.2 The Dynamic Multipole Method

In waves problems confined to two-dimensions, the multipole method is an elegant formalism with which to describe the multiple scattering of light by cylindrical elements of a circular cross-section. The method leverages the radial periodicity of the cylindrical

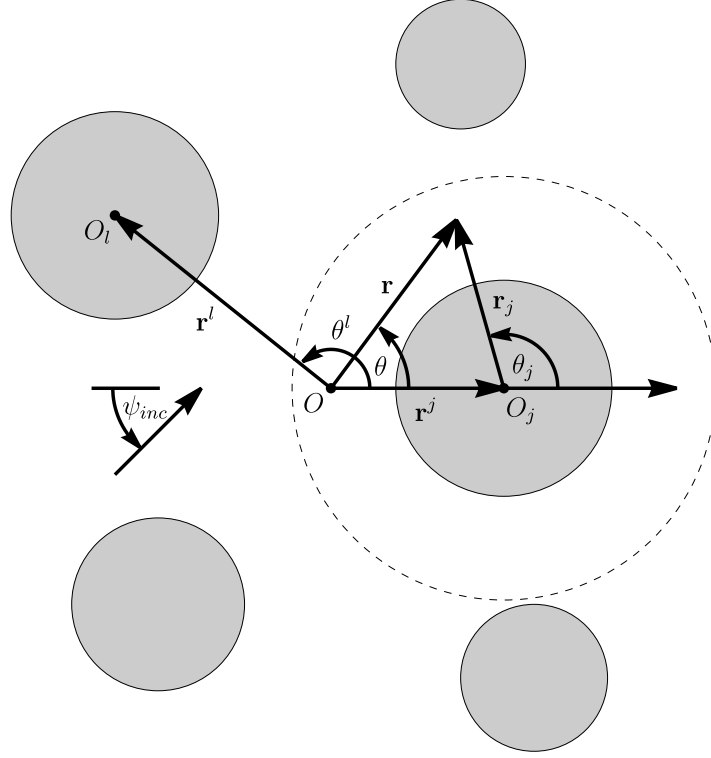


Figure 3.1: Geometry of the scattering inclusions. The dashed region encircling cylinder j indicates the domain of validity of the Fourier-Bessel expansion (3.25).

scatterers to express the electromagnetic field internal and external to the cylinders in terms of Fourier-Bessel series, or rather in terms of *multipole* expansions. A multipole expansion refers to a series of terms of increasingly refined angular characteristics captured by the embedded multipole moments. The zeroth-order moment in the expansion is referred to as the monopole moment, the first-order moment the dipole moment, and so on. In essence, the method reduces the evaluation of the electromagnetic field to the determination of the (unknown) multipole moments, and does so through the construction of a boundary value problem. Generally multipole expansions converge rapidly, requiring fewer than a dozen terms to accurately describe the field, although exceptions do occur, particularly at or close to inherent resonances. Truncating the series expansions allows for a system of equations to be written down and solved.

3.2.1 Geometry

The scattering problem we treat is illustrated in Fig. 3.1, which depicts the horizontal cross-section of a set of cylinders occupying the xy -plane, and which extend infinitely

down the z -axis which is of positive sign into the page. The set of N cylinders are of arbitrary position and radius, and the incident plane-wave is of angle ψ_{inc} with respect to the x -axis. The centre of an arbitrary cylinder j is of position (r^j, θ^j) in *global* coordinates, which defines the coordinate origin O_j of the *local* polar coordinate system (r_j, θ_j) . The radius of the j th cylinder is denoted a_j , and each cylinder consists of a material of a real refractive index, or may be perfectly electrically conducting. The surrounding dielectric medium is assumed to be non-dispersive and is also of real refractive index.

3.2.2 The Helmholtz Wavefield

Assuming an implicit time-harmonic dependence $e^{-i\omega t}$ of the magnetic and electric fields, light in oblique propagation through a medium will be subject to Maxwell's equations (in the sense of distributions):

$$\left. \begin{aligned} \nabla \cdot \mathbf{E} &= 0, & \nabla \times \mathbf{E} &= ik \sqrt{\frac{\mu_0}{\varepsilon_0}} \mu_r \mathbf{H} \\ \nabla \cdot \mathbf{H} &= 0, & \nabla \times \mathbf{H} &= -ik \sqrt{\frac{\varepsilon_0}{\mu_0}} \varepsilon_r \mathbf{E}. \end{aligned} \right\} \quad (3.1)$$

where $k = \omega \sqrt{\mu_0 \varepsilon_0}$ is the vacuum wavenumber, $\mathbf{H} = \mathbf{H}(\mathbf{r})$ is the magnetic field and $\mathbf{E} = \mathbf{E}(\mathbf{r})$ is the electric field. The medium is of permittivity $\varepsilon = \varepsilon_r \varepsilon_0$ and permeability $\mu = \mu_r \mu_0$, where the 0 subscript denotes the vacuum quantities. Making use of the curl of curl identity (A.18) and eliminating for either $\mathbf{E}$ or $\mathbf{H}$ yields the Helmholtz equation:

$$(\nabla^2 + n^2 k^2) \mathbf{V}(r, \theta, z) = 0, \quad (3.2)$$

where $\mathbf{V}$ represents either the electric or magnetic field and n is the refractive index of the medium, $n = c \sqrt{\mu \varepsilon}$. Note that the Laplacian operator ∇^2 is in three-dimensional cylindrical form. By invariance of the cylindrical geometry along the z -axis solutions to (3.2) are of the form:

$$\mathbf{V}(r, \theta, z) = \mathbf{V}(r, \theta) e^{ik_{\parallel} z} \quad (3.3)$$

where $k_{\parallel}$ is the wavenumber component down the cylindrical axis z , and is often referred to as the *propagation constant*. Separating the Laplacian into its polar and longitudinal coordinates, before inserting (3.3) into (3.2), gives:

$$(\nabla_p^2 + k_{\perp}^2) \mathbf{V}(r, \theta) = 0 \quad (3.4)$$

where $k_{\perp} = \sqrt{n^2 k^2 - k_{\parallel}^2}$ and the subscript p denotes the polar Laplacian. In this thesis we are concerned with only the *transverse* incidence of light, defined as $k_{\parallel} = 0$, $k_{\perp} \equiv k$. Then by (3.3) we need only solve for $\mathbf{V}(r, \theta)$, and hence forth drop the p subscript on the Laplacian operator in (3.4).

3.2.3 Boundary Conditions

It is now prudent to distinguish between the regions interior (i) and exterior (e) to the cylindrical inclusions, as well as to distinguish between light of TE (s-) or TM (p-) polarization under transverse incidence. In the former case, the electric field is perpendicular to the plane of incidence, and the magnetic field has one non-zero component which is parallel to the cylinder axis. TE modes are of the form (E_x, E_y, H_z) . In the latter case, the magnetic field is perpendicular to the plane of incidence, and the electric field has a component parallel to the cylinder axis. TM modes are of the form (H_z, H_y, E_z) . In either case the vectorial Helmholtz equation (3.4) reduces to a scalar equation for the longitudinal field component H_z or E_z :

$$(\nabla^2 + (k^i)^2)V^i(r, \theta) = 0 \quad (3.5)$$

in the interior region and:

$$(\nabla^2 + (k^e)^2)V^e(r, \theta) = 0 \quad (3.6)$$

in the exterior region, where $k^i = n^i k$ and $k^e = n^e k$. Note that in the case of transverse incidence it is the convention to scale the wavenumber of the interior region relative to that of the exterior as:

$$k^i = k^e n_r, \quad \text{where} \quad n_r = \frac{n^i}{n^e}. \quad (3.7)$$

The quantity n_r is the *relative index* of the medium. Equation (3.7) is a convenient simplification that leaves only one wavenumber and one refractive index remaining in the problem.

Along with Equations (3.5) and (3.6) the fields are subject to boundary conditions at the cylindrical surface. For a conventional cylinder of dielectric composition, the conserved quantities through the cylindrical boundary are the continuity of the tangential electric and magnetic field components*. By making use of the curl of the electric and magnetic fields in (3.1), the transverse fields can be written in terms of the longitudinal field

*Specifically, conservation of E_{θ} , E_z and H_{θ} , H_z . See [91].

components as:

$$\mathbf{E}_t^\nu = \frac{-iZ_\nu}{k^\nu} \hat{\mathbf{z}} \times \nabla H_z^\nu, \quad (3.8)$$

in TE polarization, and

$$\mathbf{H}_t^\nu = \frac{i}{k^\nu Z_\nu} \hat{\mathbf{z}} \times \nabla E_z^\nu, \quad (3.9)$$

in TM polarization, where ν labels either the interior or exterior medium, and $Z_\nu = \sqrt{\mu_\nu/\varepsilon_\nu}$ is the impedance of the region ν . The angular components of the above are, in polar coordinates (r, θ, z) :

$$E_\theta^\nu = \frac{-iZ_\nu}{k^\nu} \frac{\partial H_z^\nu}{\partial r}, \quad (3.10)$$

$$H_\theta^\nu = \frac{i}{k^\nu Z_\nu} \frac{\partial E_z^\nu}{\partial r}. \quad (3.11)$$

Expressing the tangential components in terms of the normal vector to the cylindrical surface, $\hat{\mathbf{r}} = \mathbf{r}/r$, the conserved quantities are:

$$\hat{\mathbf{r}} \times \mathbf{E}^\nu = -\hat{\boldsymbol{\theta}} E_z^\nu + \hat{\mathbf{z}} \frac{-iZ_\nu}{k^\nu} \frac{\partial H_z^\nu}{\partial r}, \quad (3.12)$$

$$\hat{\mathbf{r}} \times \mathbf{H}^\nu = -\hat{\boldsymbol{\theta}} H_z^\nu + \hat{\mathbf{z}} \frac{i}{k^\nu Z_\nu} \frac{\partial E_z^\nu}{\partial r}. \quad (3.13)$$

The boundary conditions can therefore be written in terms of only the longitudinal field component as:

$$H_z^e|_{r=a} = H_z^i|_{r=a}, \quad \left. \frac{\partial H_z^e}{\partial r} \right|_{r=a} = \frac{\varepsilon_e}{\varepsilon_i} \left. \frac{\partial H_z^i}{\partial r} \right|_{r=a}, \quad (3.14)$$

in the case of TE polarization, and:

$$E_z^e|_{r=a} = E_z^i|_{r=a}, \quad \left. \frac{\partial E_z^e}{\partial r} \right|_{r=a} = \frac{\mu_e}{\mu_i} \left. \frac{\partial E_z^i}{\partial r} \right|_{r=a}, \quad (3.15)$$

in the case of TM polarization, where a is the radius of any given cylinder. The first condition in (3.14) and (3.15) is known as the field continuity, whereas the second condition is known as the flux continuity. Note that if one assumes that both media have a magnetic permeability approximately that of vacuum, then for TE polarized light the continuity of flux condition in (3.14) becomes:

$$\left. \frac{\partial H_z^e}{\partial r} \right|_{r=a} = \frac{1}{n_r^2} \left. \frac{\partial H_z^i}{\partial r} \right|_{r=a} \quad (3.16)$$

where $n_r = \sqrt{\varepsilon_i/\varepsilon_e}$.

These boundary conditions are modified when the cylinders are composed of a perfect electrical conductor. At the boundary between a perfect conductor and an exterior dielectric medium there exists a non-zero surface current density that equals the difference between the tangential magnetic fields in the exterior and interior regions, as given by (3.13)*. The magnetic field inside a perfect conductor is permitted only in the instance that it was present *before* the material transitioned into its perfect conducting state, but for any real conductor the magnetic field remaining after this transition will diffuse on a timescale proportional to the conductivity. It is reasonable then to assume that the interior magnetic field $\mathbf{H}^i = \mathbf{0}$, in which case the tangential components of the magnetic field in the exterior region equal the surface current density:

$$\hat{\mathbf{r}} \times \mathbf{H}^e = \mathbf{J}_s. \quad (3.17)$$

On the other hand, although we know that the electric field inside of a perfect conductor equals zero, $\mathbf{E}^i = \mathbf{0}$, the tangential components of the electric field remain continuous through the perfectly conducting boundary. Hence we have from (3.12):

$$E_z^e|_{r=a} = 0, \quad \left. \frac{\partial H_z^e}{\partial r} \right|_{r=a} = 0. \quad (3.18)$$

The choice of Dirichlet or Neumann boundary condition depends only on the choice of polarization: the former applies to TM polarized light and the latter to TE polarized light.

3.2.4 Fourier-Bessel Series

By circular periodicity, in the local polar coordinates of any given cylinder the field at any point (r, θ) , interior or exterior to the cylindrical boundary, will have the quality of being 2π -periodic: $V(r, \theta + 2\pi) = V(r, \theta)$, and may therefore be represented by a Fourier series:

$$V(r, \theta) = \sum_{m \in \mathbb{Z}} v_m(r) e^{im\theta}. \quad (3.19)$$

*See for example Jones [91] or Jackson [92].

Substitution of (3.19) into the Helmholtz equation (3.4) and making use of the polar Laplacian:

$$\nabla^2 V = \frac{\partial^2 V}{\partial r^2} + \frac{1}{r} \frac{\partial V}{\partial r} + \frac{1}{r^2} \frac{\partial^2 V}{\partial \theta^2}, \quad (3.20)$$

the Fourier coefficients v_m can be shown to satisfy the differential equation:

$$\forall m, \quad \frac{\partial^2 v_m(r)}{\partial r^2} + \frac{1}{r} \frac{\partial v_m(r)}{\partial r} + \left(k_\perp^2 - \frac{m^2}{r^2} \right) v_m(r) = 0. \quad (3.21)$$

Defining $r' = kr$ then (3.21) simplifies to:

$$\forall m, \quad \frac{\partial^2 v_m(r')}{\partial r'^2} + \frac{1}{r'} \frac{\partial v_m(r')}{\partial r'} + \left(1 - \frac{m^2}{r'^2} \right) v_m(r') = 0 \quad (3.22)$$

which is Bessel's differential equation of order m . The solutions of Bessel's differential equation define the Bessel functions, which in cylindrical geometries are of integer order. The general solution of (3.22) is the linear combination of Bessel functions of the first and second kinds:

$$\begin{aligned} v_m &= a'_m J_m(r') + b'_m Y_m(r') \\ &= a'_m J_m(kr) + b'_m Y_m(kr), \end{aligned} \quad (3.23)$$

where $J_m(x)$ is the Bessel function of the first kind and $Y_m(x)$ is the Bessel function of the second kind, each of order m , and the coefficients a_m and b_m are complex valued. This is alternatively expressed in terms of Bessel functions of the first and third kinds (or rather, the Hankel function of the first kind), order m , $H_m^{(1)}(x) = J_m(x) + iY_m(x)$:

$$\begin{aligned} v_m &= (a'_m + ib'_m) J_m(kr) - ib'_m H_m^{(1)}(kr), \\ &= a_m J_m(kr) + b_m H_m^{(1)}(kr). \end{aligned} \quad (3.24)$$

Placing (3.24) back into the Fourier series (3.19) leaves us with an expression for the total field in terms of a Fourier-Bessel series:

$$V(r, \theta) = \sum_{m \in \mathbb{Z}} (a_m J_m(kr) + b_m H_m^{(1)}(kr)) e^{im\theta}. \quad (3.25)$$

The form of (3.25) is also referred to as a multipole expansion in *cylindrical harmonics*^{*}, where the coefficients a_m, b_m are the multipole moments. The zeroth-order term $m = 0$ denotes the monopole moment, the first-order term $m = \pm 1$ the dipole moments, and so on. Whatever the nomenclature, in choosing to express these solutions in the form (3.25), the evaluation of the fields interior and exterior to the cylinders has been reduced to the determination of a set of unknown complex coefficients.

3.2.5 Interior and Exterior Fields

In order to evaluate the multipole moments we make use of both a physical intuition of the problem, as well as the behaviour of the Bessel functions of the first and second kind in the limits of small and large argument. These are, for fixed m :

$$\lim_{x \rightarrow 0} J_0(x) = 1, \quad (3.26a)$$

$$\lim_{x \rightarrow 0} J_m(x) \sim \frac{1}{\Gamma(m+1)} \left(\frac{x}{2}\right)^m, \quad m > 0, \quad (3.26b)$$

$$\lim_{x \rightarrow \infty} J_m(x) \sim \sqrt{\frac{2}{\pi x}} \cos\left(x - \frac{m\pi}{2} - \frac{\pi}{4}\right), \quad \forall m, \quad (3.26c)$$

and

$$\lim_{x \rightarrow 0} Y_0(x) \sim \frac{2}{\pi} \ln(x), \quad (3.27a)$$

$$\lim_{x \rightarrow 0} Y_m(x) \sim -\frac{\Gamma(m)}{\pi} \left(\frac{2}{x}\right)^m, \quad m > 0 \quad (3.27b)$$

$$\lim_{x \rightarrow \infty} Y_m(x) \sim \sqrt{\frac{2}{\pi x}} \sin\left(x - \frac{m\pi}{2} - \frac{\pi}{4}\right), \quad \forall m. \quad (3.27c)$$

The limits for orders $m < 0$ are related to those of $m > 0$ via the Bessel function connection formula (A.1). In considering first the field interior to any cylinder $V^i(r, \theta)$, the appropriate limit is that in which $r \rightarrow 0$. Then by (3.26a) and (3.26b) the Bessel function of the first kind remains finite for all orders m . In the same limit by (3.27a) and (3.27b) the Bessel function of the second kind, and hence the imaginary component

^{*}‘Cylindrical harmonics’ can refer to either the Bessel function in isolation, or the product of three terms, each a function of one cylindrical coordinate alone: the radial term r (the Bessel function), the angular term θ and the longitudinal term z . Alternatively, the Bessel functions of integer order are sometimes referred to as the *cylinder functions* due to their appearance in solutions to Laplace’s equation in cylindrical coordinates. Pick your poison.

of the Hankel function of the first kind, is singular for all orders m . In order to avoid a singularity in the field (3.25) at the origin $r = 0$, and hence satisfy (3.5) in a classical sense, it is imperative that the coefficients b_m of the Hankel functions equal zero. Thus:

$$V^i(r, \theta) = \sum_{m \in \mathbb{Z}} c_m J_m(k^i r) e^{im\theta}, \quad \text{in } r < a, \quad (3.28)$$

where the Fourier coefficients of the interior have been re-labelled c_m . The remaining task is to evaluate these coefficients in order to deduce the interior field.

In the region exterior to the same cylinder the relevant limit in specifying the form of $V^e(r, \theta)$ is that in which $r \rightarrow \infty$; the singularity at $r = 0$ is not an issue as the exterior region excludes the coordinate origin. By (3.26c) and (3.27c) the asymptotic form of the Hankel function of the first kind is:

$$\lim_{x \rightarrow \infty} H_m^{(1)}(x) \sim \sqrt{\frac{2}{\pi x}} e^{i(x - \frac{m\pi}{2} - \frac{\pi}{4})}, \quad \forall m, \quad (3.29)$$

which, along with (3.26c), tells us nothing more than the solution (3.25) remains continuous and differentiable as $r \rightarrow \infty$. In fact, at this point the choice of $H_m^{(1)}(kr)$ in (3.24) and (3.25) appears arbitrary; one could instead choose to express the field anywhere in terms of Hankel functions of the second kind, $H_m^{(2)}(x) = J_m(x) - iY_m(x)$:

$$V(r, \theta) = \sum_{m \in \mathbb{Z}} a_m^* J_m(kr) + b_m^* H_m^{(2)}(kr), \quad (3.30)$$

with the same arguments following for insisting $b_m^* = 0$ in $r < a$ to avoid the singularity in $H_m^{(2)}(0)$. In asymptotic form:

$$\lim_{x \rightarrow \infty} H_m^{(2)}(x) \sim \sqrt{\frac{2}{\pi x}} e^{-i(x - \frac{m\pi}{2} - \frac{\pi}{4})}, \quad \forall m, \quad (3.31)$$

so that like (3.25), (3.30) remains continuous and differentiable as $r \rightarrow \infty$. It would appear then that solutions to the Helmholtz equation in the exterior domain (3.6) are not unique; both (3.25) and (3.30) appear to be valid solutions granted the preceding analysis. What remains is the task of distinguishing between these solutions, given the physical situation being modelled.

The method by which this is achieved is the enforcement of a criterion, or boundary condition, at infinity that singles out a unique solution. This is known as the *Sommerfeld*

radiation condition^{*}, or just *radiation condition*, which states that any solution $u(r, \theta)$ to the Helmholtz equation must satisfy (in two dimensions):

$$\lim_{r \rightarrow \infty} r^{\frac{1}{2}} \left(\frac{\partial}{\partial r} - ik \right) V(r, \theta) = 0 \quad (3.32)$$

uniformly with respect to all angles θ . The radiation condition selects those solutions corresponding to *outgoing* waves at infinity, rather than *incoming* waves from infinity, which is an appropriate assumption given that the field in the neighbourhood of the cylinder is due to the superposition of scattered waves. By (3.26c), (3.27c), (3.29) and (3.31) clearly only the Hankel function of the first kind satisfies the radiation condition. Hence:

$$V^e(r, \theta) = \sum_{m \in \mathbb{Z}} (a_m J_m(k^e r) + b_m H_m^{(1)}(k^e r)) e^{im\theta}, \quad \text{in } r > a, \quad (3.33)$$

is the unique solution for the exterior field about a cylinder in a Helmholtz wavefield.

3.2.6 Interpreting the Solutions

The solutions (3.28) and (3.33) are interpreted by first distinguishing between the sums over the Bessel and Hankel functions of the first kind. In the former case, we have already established that the Bessel function of the first kind does not satisfy the radiation condition (3.32) at any order, and remains regular even at $r = 0$. On the other hand, the Hankel function of the first kind does satisfy (3.32) at all orders, and is singular at $r = 0$. Hence in the interior domain the solution (3.28) is a sum over *regular* waves, whereas the solution in the exterior domain (3.33) is a sum over both regular and outgoing waves[†].

It is necessary now to work in local polar coordinates (r_j, θ_j) of origin O_j at the centre of the j th cylinder. Each field component corresponds to one of three sources: the total field scattered to infinity by the j th cylinder, the field scattered by all of the other cylinders $l \neq j$ towards the j th cylinder, and the field due to any additional incident radiation, such as a plane-wave propagating from infinity. The second sum in (3.33) therefore constitutes the total field scattered by the j th cylinder, as this is a sum over outgoing waves which satisfies (3.32)[‡]. The first sum in (3.33) on the other hand constitutes the total incident

^{*}There is an excellent review article by Schot [93] which details Sommerfeld's motivations for formulating this condition.

[†]Likewise, a sum over Hankel functions of the second kind would be a sum over incoming waves from infinity that are singular at the coordinate origin, although this lacks a physical interpretation in cylindrical geometries (unless the wavenumber is complex).

[‡]Sommerfeld states 'the sources must be *sources*, not *sinks* of energy. The energy which is radiated

field illuminating the j th cylinder from *all* sources. In a similar fashion the interior field (3.28), represented by a sum over regular waves, constitutes the total field penetrating the j th cylinder. In this sense each cylinder acts as a source of scattered (outgoing) waves in its local coordinate system, which in the local coordinate system of any other cylinder will be an additional source of incident (regular) waves. We therefore refer to this component of the field as the re-incident field, which is an apt label given its origin.

Hence, solution (3.33) is of the form:

$$\begin{aligned} V_j^e(r_j, \theta_j) &= V_j^{inc}(r_j, \theta_j) + V_j^{sc}(r_j, \theta_j) \\ &= \sum_{m \in \mathbb{Z}} a_{j,m} J_m(k^e r_j) e^{im\theta_j} + \sum_{m \in \mathbb{Z}} b_{j,m} H_m^{(1)}(k^e r_j) e^{im\theta_j}, \end{aligned} \quad (3.34)$$

where V_j^{inc} is the total incident field on, and V_j^{sc} is the total scattered field by, the j th cylinder, and $a_{j,m}$, $b_{j,m}$ refer to its multipole moments. The contributions to V_j^{inc} by the incident radiation and re-incident fields are separable, and in distinguishing between the two sources we will arrive to a useful identity relating $a_{j,m}$ and $b_{j,m}$. We model the incident radiation as a plane-wave propagating at angle ψ_{inc} from the x -axis of a global coordinate system (r, θ) , and is of wavevector $\mathbf{k}^e = (k^e \cos(\psi_{inc}), k^e \sin(\psi_{inc}))$. The centroid of any cylinder j in this global system is labelled (r^j, θ^j) , not to be confused with the local polar coordinates of the same cylinder (r_j, θ_j) . The plane-wave at an arbitrary point in space can be expressed in terms of a sum over these coordinates:

$$\begin{aligned} V_j^\lambda &= e^{i\mathbf{k}^e \cdot (\mathbf{r}^j + \mathbf{r}_j)} \\ &= e^{ik^e r^j \cos(\theta^j - \psi_{inc})} e^{ik^e r_j \cos(\theta_j - \psi_{inc})}, \end{aligned} \quad (3.35)$$

where the superscript λ denotes the plane-wave. We then make use of the Jacobi-Anger identity (A.7) to write the second exponential function in the form of a sum over regular waves:

$$e^{ik^e r_j \cos(\theta_j - \psi_{inc})} = \sum_{m \in \mathbb{Z}} i^m J_m(k^e r_j) e^{im(\theta_j - \psi_{inc})}. \quad (3.36)$$

The field due to the plane-wave in the local coordinates (r_j, θ_j) is therefore:

$$V_j^\lambda = \sum_{m \in \mathbb{Z}} a_{j,m}^\lambda J_m(k^e r_j) e^{im\theta_j} \quad (3.37)$$

from the sources must scatter to infinity; *no energy may be radiated from infinity into... the field*' [94].

where $a_{j,m}^\lambda$ have been identified by comparison with the first sum in (3.34) as:

$$a_{j,m}^\lambda = i^m e^{ik^e r^j \cos(\theta^j - \psi_{inc}) - im\psi_{inc}}. \quad (3.38)$$

The total exterior field in the local coordinates of the j th cylinder is now of the form:

$$\begin{aligned} V_j^e(r_j, \theta_j) = & \sum_{m \in \mathbb{Z}} a_{j,m}^\lambda J_m(k^e r_j) e^{im\theta_j} \\ & + \sum_{m \in \mathbb{Z}} a_{j,m} J_m(k^e r_j) e^{im\theta_j} + \sum_{m \in \mathbb{Z}} b_{j,m} H_m^{(1)}(k^e r_j) e^{im\theta_j}, \end{aligned} \quad (3.39)$$

where $a_{j,m}$ now denotes those multipole moments due to sources of re-incident waves only. It should be stressed that as $a_{j,m}^\lambda$ are known quantities, the only remaining task in evaluating the exterior field is to deduce $a_{j,m}$ and $b_{j,m}$.

3.3 Green's Theorem Approach

Any discussion of sources of waves and their limiting behaviour would be incomplete without a discussion of Green's theorem. Green's theorem provides us with a rigorous derivation of the field in terms of cylindrical harmonics, as well as a pair of equations for the multipole moments $a_{j,m}$ and $b_{j,m}$. To carry this out, we have to deduce the solution to a Helmholtz equation subject to a point-source: the Green's function. In this we follow the method of Horsley [95].

3.3.1 Green's Function

The Green's function is the solution $g(\mathbf{r} - \mathbf{r}')$ to the Helmholtz equation with a point-source on the right-hand-side, represented by a Dirac delta function:

$$(\nabla^2 + k^2)g(\mathbf{r} - \mathbf{r}') = \delta^2(\mathbf{r} - \mathbf{r}'), \quad (3.40)$$

where $g(\mathbf{r} - \mathbf{r}')$ represents the field at the point $\mathbf{r}$ due to a point-source at the position $\mathbf{r}'$, and $\delta^2(\mathbf{r} - \mathbf{r}')$ is the two-dimensional delta function. There are several methods to go about determining the form of this Green's function, but the simplest involves expressing

it in terms of its Fourier-transform [95]:

$$g(\mathbf{r} - \mathbf{r}') = \int \frac{d^2\boldsymbol{\kappa}}{(2\pi)^2} \tilde{g}(\boldsymbol{\kappa}) e^{i\boldsymbol{\kappa} \cdot (\mathbf{r} - \mathbf{r}')}. \quad (3.41)$$

Likewise the Fourier-transform of the delta function is:

$$\delta^2(\mathbf{r} - \mathbf{r}') = \int \frac{d^2\boldsymbol{\kappa}}{(2\pi)^2} e^{i\boldsymbol{\kappa} \cdot (\mathbf{r} - \mathbf{r}')}. \quad (3.42)$$

Placing these in the Helmholtz equation (3.40) we have:

$$\int \frac{d^2\boldsymbol{\kappa}}{(2\pi)^2} (k^2 - \kappa^2) \tilde{g}(\boldsymbol{\kappa}) e^{i\boldsymbol{\kappa} \cdot (\mathbf{r} - \mathbf{r}')} = \int \frac{d^2\boldsymbol{\kappa}}{(2\pi)^2} e^{i\boldsymbol{\kappa} \cdot (\mathbf{r} - \mathbf{r}')} \quad (3.43)$$

from which it becomes obvious that the Fourier transform of the Green's function is:

$$\tilde{g}(\kappa) = \frac{1}{k^2 - \kappa^2}. \quad (3.44)$$

Placing (3.44) back into (3.41) we have:

$$g(\mathbf{r} - \mathbf{r}') = \int \frac{d^2\boldsymbol{\kappa}}{(2\pi)^2} \frac{e^{i\boldsymbol{\kappa} \cdot (\mathbf{r} - \mathbf{r}')}}{k^2 - \kappa^2}. \quad (3.45)$$

This integral over the wavenumber $\boldsymbol{\kappa}$ is, in polar coordinates (κ, θ_κ) :

$$g(\mathbf{r} - \mathbf{r}') = \int_0^\infty \frac{\kappa}{2\pi} d\kappa \int_0^{2\pi} \frac{1}{2\pi} \frac{e^{i\kappa|\mathbf{r} - \mathbf{r}'| \cos(\theta_\kappa)}}{k^2 - \kappa^2} d\theta_\kappa, \quad (3.46)$$

where the integral over the angular coordinate θ_κ can be trivially solved by making use of the Jacobi-Anger identity (A.7) and noting that due to the orthogonality of the Bessel functions, the only remaining summand after integration is that of order $n = 0$:

$$g(\mathbf{r} - \mathbf{r}') = \int_0^\infty \frac{\kappa}{2\pi} \frac{J_0(\kappa|\mathbf{r} - \mathbf{r}'|)}{k^2 - \kappa^2} d\kappa. \quad (3.47)$$

By writing $J_0(x) = [H_0^{(1)}(x) + H_0^{(2)}(x)]/2$, and making use of the identity relating Hankel functions of zeroth-order (A.4), we arrive to the following integral for the Green's function:

$$g(\mathbf{r} - \mathbf{r}') = \int_{-\infty}^\infty \frac{\kappa}{4\pi} \frac{H_0^{(1)}(\kappa|\mathbf{r} - \mathbf{r}'|)}{k^2 - \kappa^2} d\kappa. \quad (3.48)$$

The form of this integral is beneficial in two ways: the first is that it is now an integral over the entire real κ -axis, and the second is that the integrand is of the form of a Hankel function of the first kind. Equation (3.48) is reminiscent of Cauchy's integral formula, which asserts that:

$$f(z_0) = \frac{1}{2\pi i} \oint_{\mathcal{C}} \frac{f(z)}{z - z_0} dz, \quad (3.49)$$

where the path of integration along $\mathcal{C}$ in the complex z -plane is counterclockwise and encloses the pole z_0 . In order to make use of (3.49) the path of integration over the real κ -axis in (3.48) needs to be modified into that over a closed curve in the complex κ -plane that encloses one of the two poles of the integrand: $+k$ or $-k$. The presence of two poles at $\pm k$ is evocative of the lack of a uniqueness in the solutions encountered in § 3.2.6, and can be remedied with the same application of the Sommerfeld radiation condition. In choosing the $+k$ pole then by (3.49) our solution will be of the form $H_0^{(1)}(k|\mathbf{r} - \mathbf{r}'|)$ i.e. an outgoing wave satisfying (3.32), whereas in choosing the $-k$ pole then by the identity (A.4) the solution will be of the form $H_0^{(2)}(k|\mathbf{r} - \mathbf{r}'|)$ i.e. an incident wave that fails to satisfy (3.32). Once again, we have recovered uniqueness thanks to Sommerfeld.

The remaining task is to construct the curve that encloses only the $+k$ pole. By writing κ as the complex number $\kappa = Re^{i\phi}$, then by (3.29):

$$H_0^{(1)}(\kappa|\mathbf{r} - \mathbf{r}'|) \sim e^{i\kappa|\mathbf{r} - \mathbf{r}'|} = e^{R(i\cos(\phi) - \sin(\phi))|\mathbf{r} - \mathbf{r}'|} \quad (3.50)$$

for large $\kappa|\mathbf{r} - \mathbf{r}'|$. Obviously $|\mathbf{r} - \mathbf{r}'|$ is always positive valued, and so as $R \rightarrow \infty$ the real part of the integrand decays to zero as long as $0 \leq \phi < \pi$. We are permitted therefore to close the path of integration through the union of the real κ -axis with a semi-circular arc in the upper half-plane, and we will label this union $\mathcal{C}_+$; see Fig. 3.2. As the integrand equals zero along the arc so too does its integral, and we may write:

$$g(\mathbf{r} - \mathbf{r}') = -\frac{1}{2\pi i} \oint_{\mathcal{C}_+} \frac{i\kappa H_0^{(1)}(\kappa|\mathbf{r} - \mathbf{r}'|)}{2(\kappa + k)(\kappa - k)} d\kappa. \quad (3.51)$$

In its current form however the path $\mathcal{C}_+$ intersects both poles along the real axis, and in order to retain the validity of (3.49) we must ensure that the integrand remains analytic everywhere along the path of integration. The usual approach here is to deform the path of integration around the poles, but instead we will employ a *regularization* technique*

*Instead of moving the path of integration so as to avoid the pole, we are instead moving the pole so as to avoid the semi-circular path, and in doing so ensure that the integrand in (3.48) remains analytic everywhere along $\mathcal{C}_+$. Hence the term 'regularization'.

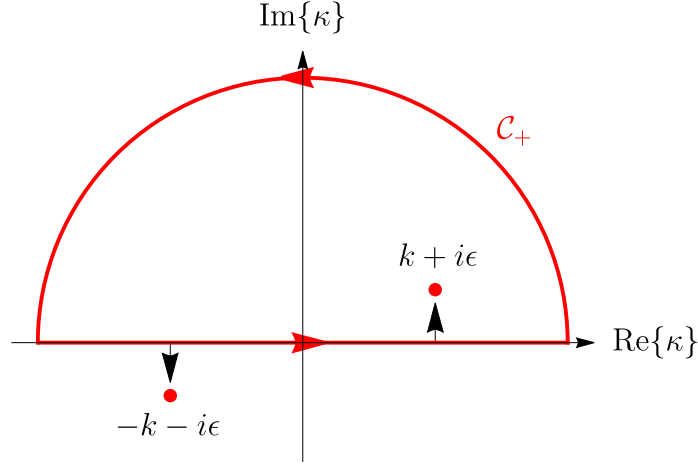


Figure 3.2: The contour of integration $\mathcal{C}_+$ enclosing the pole $\kappa = k + i\epsilon$. The path of integration has been regularized by shifting the poles off-axis.

to shift the poles off-axis. We do this by adding to the wavenumber in (3.40) a small imaginary quantity $i\epsilon$ where $0 < \epsilon \ll 1$. This choice of parameter is pertinent given that the positive sign of ϵ shifts the $+k$ pole upwards into the enclosing semi-circular path and shifts the $-k$ pole downwards into the lower half-plane*. The integral for the green's function now reads:

$$g(\mathbf{r} - \mathbf{r}') = -\frac{1}{2\pi i} \oint_{\mathcal{C}_+} \frac{i\kappa}{2} \frac{H_0^{(1)}(\kappa|\mathbf{r} - \mathbf{r}'|)}{(\kappa + (k + i\epsilon))(\kappa - (k + i\epsilon))} d\kappa, \quad (3.52)$$

where $\mathcal{C}_+$ encloses only the pole $\kappa = k + i\epsilon$. By comparison with (3.49), and taking the limit $\epsilon \rightarrow 0$, the Green's function for the Helmholtz equation subject to a point-source is:

$$g(\mathbf{r}; \mathbf{r}') = \frac{1}{4i} H_0^{(1)}(k|\mathbf{r} - \mathbf{r}'|), \quad (3.53)$$

where the notation $g(\mathbf{r}; \mathbf{r}')$ has been introduced in place of $g(\mathbf{r} - \mathbf{r}')$ for brevity.

3.3.2 Green's Theorem

It is possible, through the application of Green's theorem, to arrive to an integral equation for the field in the local annulus surrounding any cylinder. In constructing an integral equation of the appropriate form, we re-write the Helmholtz equations (3.6) and (3.40)

*A more rigorous derivation that avoids this regularization technique altogether involves integrating along the sections of the real κ -axis sandwiching the poles, and integrating around the poles in arcs of some infinitesimally small radius; we avoid this method here for simplicity.

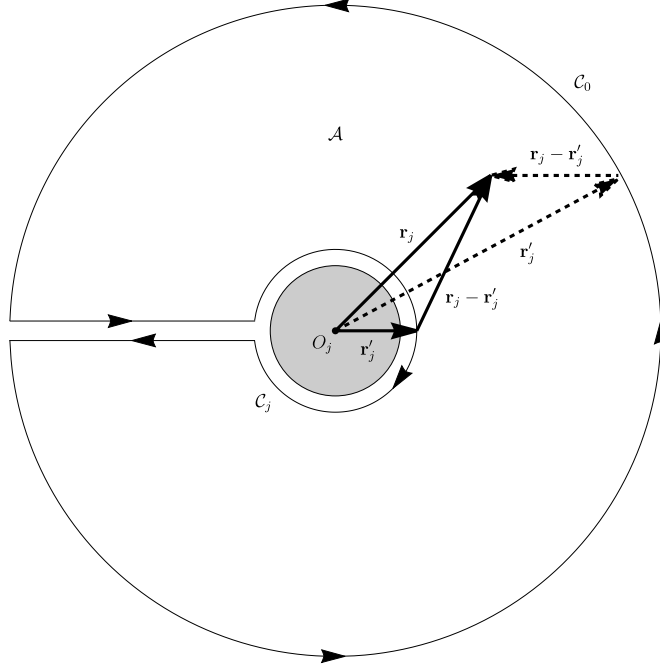


Figure 3.3: Contour of integration defining the annulus $\mathcal{A}$

as:

$$\nabla'^2 V(\mathbf{r}') = -k^2 V(\mathbf{r}'), \quad (3.54)$$

$$\nabla'^2 g(\mathbf{r}; \mathbf{r}') = -k^2 g(\mathbf{r}; \mathbf{r}') + \delta^2(\mathbf{r} - \mathbf{r}'). \quad (3.55)$$

Where the primed operators are acting upon the primed coordinates. Multiplying (3.54) by $g(\mathbf{r}; \mathbf{r}')$ and (3.55) by $V(\mathbf{r}')$, and subtracting the former from the latter, their difference is:

$$V(\mathbf{r}') \nabla'^2 g(\mathbf{r}; \mathbf{r}') - g(\mathbf{r}; \mathbf{r}') \nabla'^2 V(\mathbf{r}') = V(\mathbf{r}') \delta^2(\mathbf{r} - \mathbf{r}'). \quad (3.56)$$

Then by Green's theorem:

$$\begin{aligned} & \iint_{\mathcal{A}} [V(\mathbf{r}') \nabla'^2 g(\mathbf{r}; \mathbf{r}') - g(\mathbf{r}; \mathbf{r}') \nabla'^2 V(\mathbf{r}')] dA \\ &= \oint_{\partial \mathcal{A}} \left[V(\mathbf{r}') \frac{\partial g(\mathbf{r}; \mathbf{r}')}{\partial r'} - g(\mathbf{r}; \mathbf{r}') \frac{\partial V(\mathbf{r}')}{\partial r'} \right] ds' \end{aligned} \quad (3.57)$$

where the area $\mathcal{A}$ refers to the total cross-sectional area enclosed by the contour $\partial \mathcal{A}$. In this case, $\partial \mathcal{A} := \mathcal{C}_j \cup \mathcal{C}_0$, as depicted in Fig. 3.3, where $\mathcal{C}_j$ is the contour of integration around the j th cylinder and $\mathcal{C}_0$ is the contour of integration around an outer ring of

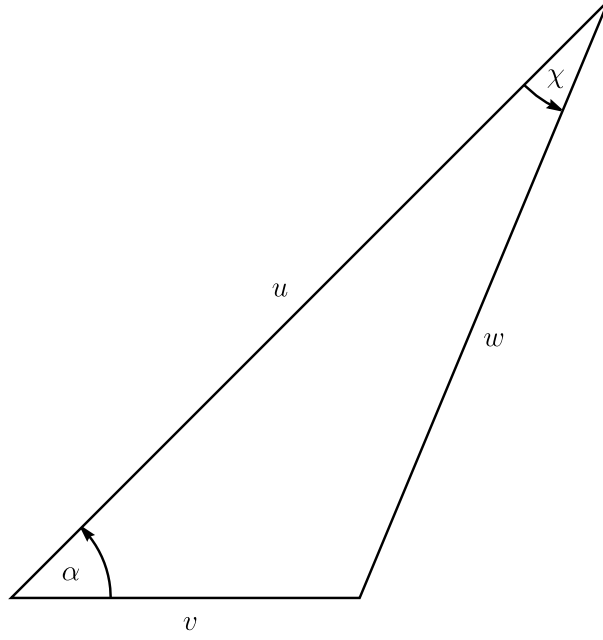


Figure 3.4: Geometry of Graf's addition theorem.

radius equalling the distance to the next nearest-neighbour cylinder*. The contour $\partial\mathcal{A}$ encloses no sources of waves; sources interior to the annulus will be evaluated along $\mathcal{C}_j$, and likewise sources exterior to the annulus will be evaluated along $\mathcal{C}_0$. We have from the right-hand-side of (3.56) that at any point $\mathbf{r}$ within the annulus:

$$\iint_{\mathcal{A}} V(\mathbf{r}') \delta^2(\mathbf{r} - \mathbf{r}') dA = V(\mathbf{r}), \quad (3.58)$$

such that:

$$V(\mathbf{r}) = \oint_{\partial\mathcal{A}} \left[V(\mathbf{r}') \frac{\partial g(\mathbf{r}; \mathbf{r}')}{\partial r'} - g(\mathbf{r}; \mathbf{r}') \frac{\partial V(\mathbf{r}')}{\partial r'} \right] ds'. \quad (3.59)$$

It is sensible to carry out this integration in the local coordinate system (r'_j, θ'_j) rather than the global coordinate system (r', θ') . We have already established that the field at any point in the annulus can be represented by the Fourier series (3.19). As for the Green's function, the vector $\mathbf{r} - \mathbf{r}'$ is equivalent to the vector $\mathbf{r}_j - \mathbf{r}'_j$, which makes the Green's function:

$$g(\mathbf{r}_j; \mathbf{r}'_j) = \frac{1}{4i} H_0^{(1)}(k|\mathbf{r}_j - \mathbf{r}'_j|). \quad (3.60)$$

*Note that the union of these contours defines the annulus depicted in Fig. 3.1.

The r_j and r'_j dependencies are separable by way of Graf's addition theorem [96], which states that for any Bessel function of order m , $\mathcal{S}_m$:

$$\mathcal{S}_m(w)e^{im\chi} = \sum_{q \in \mathbb{Z}} \mathcal{S}_{m+q}(u)J_q(v)e^{iq\alpha}, \quad (3.61)$$

which is valid as long as $v < u$. Here χ and α are the angles between vertices u , w and v , u , respectively, as illustrated in Fig. 3.4 and in appendix A. The choice of source position $\mathbf{r}'_j$ will therefore dictate the choice of u , v and w . In the instance of a source position of $r'_j \in \mathcal{C}_j$ then $r'_j < r_j$ and by (3.61) the Green's function (3.60) is:

$$g(\mathbf{r}_j; \mathbf{r}'_j \in \mathcal{C}_j) = \frac{1}{4i} \sum_{q \in \mathbb{Z}} H_q^{(1)}(kr_j)J_q(kr'_j)e^{iq(\theta_j - \theta'_j)}. \quad (3.62)$$

Note that the primed coordinate is the argument of the Bessel function of the first kind. For a source of position $\mathbf{r}'_j \in \mathcal{C}_0$ on the other hand, $r_j < r'_j$ and by (3.61):

$$g(\mathbf{r}_j; \mathbf{r}'_j \in \mathcal{C}_0) = \frac{1}{4i} \sum_{q \in \mathbb{Z}} H_q^{(1)}(kr'_j)J_q(kr_j)e^{iq(\theta_j - \theta'_j)}, \quad (3.63)$$

where the primed coordinate is now the argument of the Hankel function. Computing first the integral over $\mathcal{C}_j$:

$$\begin{aligned} & \int_{\theta'_j=0}^{2\pi} \left[\sum_{m \in \mathbb{Z}} v_m(r'_j)e^{im\theta'_j} \frac{k}{4i} \sum_{q \in \mathbb{Z}} H_q^{(1)}(kr_j)J'_q(kr'_j)e^{iq(\theta_j - \theta'_j)} \right] \\ & - \left[\sum_{m \in \mathbb{Z}} v'_m(kr'_j)e^{im\theta'_j} \frac{1}{4i} \sum_{q \in \mathbb{Z}} H_q^{(1)}(kr_j)J_q(kr'_j)e^{iq\theta_j - \theta'_j} \right] r'_j d\theta'_j \\ & = \sum_{m \in \mathbb{Z}} \frac{\pi a_j}{2i} (v_m(a_j)kJ'_m(ka_j) - v'_m(a_j)J_m(ka_j)) H_m^{(1)}(kr_j)e^{im\theta_j} \\ & = \sum_{m \in \mathbb{Z}} b_{j,m} H_m^{(1)}(kr_j)e^{im\theta_j}. \end{aligned} \quad (3.64)$$

Here a_j refers to the radius of the j th cylinder and $v'_m(r'_j)$ is the derivative of the Fourier coefficient with respect to the primed coordinate. Crucially the quantity in parentheses on the third line of (3.64) is not a function of position, but of only wavenumber k and cylinder radius a_j . As such, this integral evaluates as a sum over outgoing waves where the multipole moment $b_{j,m}$ has been identified in terms of the Fourier coefficients. Similarly,

the integral over $\mathcal{C}_0$ is:

$$\begin{aligned}
& \int_{\theta'_j=0}^{2\pi} \left[\sum_{m \in \mathbb{Z}} v_m(r'_j) e^{im\theta'_j} \frac{k}{4i} \sum_{q \in \mathbb{Z}} H_q^{(1)}(kr'_j) J_q(kr_j) e^{iq(\theta_j - \theta'_j)} \right] \\
& - \left[\sum_{m \in \mathbb{Z}} v'_m(kr'_j) e^{im\theta'_j} \frac{1}{4i} \sum_{q \in \mathbb{Z}} H_q^{(1)}(kr'_j) J_q(kr_j) e^{iq\theta_j - \theta'_j} \right] r'_j d\theta'_j \\
& = \sum_{m \in \mathbb{Z}} \frac{\pi R_j}{2i} (v_m(R_j) k H_m^{(1)}(kR_j) - v'_m(R_j) H_m^{(1)}(kR_j)) J_m(kr_j) e^{im\theta_j} \\
& = \sum_{m \in \mathbb{Z}} a_{j,m} J_m(kr_j) e^{im\theta_j},
\end{aligned} \tag{3.65}$$

where R_j is the radius of the contour of integration $\mathcal{C}_0$. Clearly this is a sum over regular waves wherein the multipole moments $a_{j,m}$ can be identified by inspection of the third line of (3.65). Summing over these quantities recovers the multipole expansion (3.25) for the field at any point $\mathbf{r}$ within the annulus surrounding the j th cylinder:

$$V(\mathbf{r}) = \sum_{m \in \mathbb{Z}} (a_{j,m} J_m(kr_j) + b_{j,m} H_m^{(1)}(kr_j)) e^{im\theta_j}. \tag{3.66}$$

Green's theorem, in conjunction with the addition theorem, has made it clear that the singular part of the field within this annulus must be due to sources within $\mathcal{C}_j$ i.e. the cylinder*, whereas the regular part of the field must be due to sources external to $\mathcal{C}_0$ i.e. the other cylinders and any other incident field. In fact, it is permissible to instead evaluate the modified contour $\mathcal{C}_0$ that envelopes *all* cylinders. Equating the resulting integral equation with (3.66) produces a very useful expression for the total scattered field at any point in the exterior domain: the Wijnngaard formula.

3.3.3 Wijnngaard's Formula

The following proof provides us with a formula for the total scattered field *at any point* in the exterior domain, known as the *Wijnngaard formula* [97]. It relies on equating the regular re-incident field upon a cylinder j with the sum over the singular scattered fields from all cylinders $l \neq j$. We can use the Green's function (3.53) in conjunction with Green's theorem (3.59) to relate the regular field incident upon cylinder j to the singular

*If one were to instead consider a point-source replacing the enclosed cylinder, the same expansion in outgoing waves would result.

fields scattered by all cylinders $l \neq j$. Stating again the result (3.59) we have:

$$V(\mathbf{r}) = \oint_{\partial\mathcal{A}} \left[V(\mathbf{r}') \frac{\partial g(\mathbf{r}; \mathbf{r}')}{\partial r'} - g(\mathbf{r}; \mathbf{r}') \frac{\partial V(\mathbf{r}')}{\partial r'} \right] ds'. \quad (3.67)$$

In choosing the point $\mathbf{r}$ to lie in the vicinity of the j th cylinder, the field on the left-hand-side can be expressed in terms of the sum of regular and outgoing waves in the (r_j, θ_j) system of coordinates as in (3.25). The right-hand-side is split into three components: the path integral over the j th cylinder, the sum of path integrals over all cylinders $l \neq j$, and the integral over the exterior boundary $\mathcal{C}_0$ that envelopes all cylinders. Then $\partial\mathcal{A} := \mathcal{C}_j \cup \sum_{l \neq j} \mathcal{C}_l \cup \mathcal{C}_0$ and we have:

$$\begin{aligned} & \sum_{m \in \mathbb{Z}} (a_{j,m} J_m(kr_j) + b_{j,m} H_m^{(1)}(kr_j)) e^{im\theta_j} \\ &= \int_{\theta'_j=0}^{2\pi} \left[V_j(\mathbf{r}'_j) \frac{\partial g(\mathbf{r}_j; \mathbf{r}'_j)}{\partial r'_j} - g(\mathbf{r}_j; \mathbf{r}'_j) \frac{\partial V_j(\mathbf{r}'_j)}{\partial r'_j} \right] r'_j d\theta'_j \\ &+ \sum_{l \neq j} \int_{\theta'_l=0}^{2\pi} \left[V_l(\mathbf{r}'_l) \frac{\partial g(\mathbf{r}_l; \mathbf{r}'_l)}{\partial r'_l} - g(\mathbf{r}_l; \mathbf{r}'_l) \frac{\partial V_l(\mathbf{r}'_l)}{\partial r'_l} \right] r'_l d\theta'_l \\ &+ \int_{\theta'=0}^{2\pi} \left[V(\mathbf{r}') \frac{\partial g(\mathbf{r}; \mathbf{r}')}{\partial r'} - g(\mathbf{r}; \mathbf{r}') \frac{\partial V(\mathbf{r}')}{\partial r'} \right] r' d\theta'. \end{aligned} \quad (3.68)$$

In considering first the j th cylinder, we have from (3.62) that when $\mathbf{r}' \in \mathcal{C}_j$, $r'_j < r_j$:

$$g(\mathbf{r}_j; \mathbf{r}'_j) = \frac{1}{4i} \sum_{n \in \mathbb{Z}} H_n^{(1)}(kr_j) J_n(kr'_j) e^{in(\theta_j - \theta'_j)}. \quad (3.69)$$

The integral over $\mathcal{C}_j$ is therefore:

$$\begin{aligned} & \frac{k}{4i} \int_{\theta'_j=0}^{2\pi} \sum_{m \in \mathbb{Z}} (a_{j,m} J_m(kr'_j) + b_{j,m} H_m^{(1)}(kr'_j)) e^{im\theta'_j} \\ & \cdot \sum_{n \in \mathbb{Z}} H_n^{(1)}(kr_j) J'_n(kr'_j) e^{in(\theta_j - \theta'_j)} \\ & - \sum_{m \in \mathbb{Z}} (a_{j,m} J'_m(kr'_j) + b_{j,m} H_m^{(1)'}(kr'_j)) e^{im\theta_j} \\ & \cdot \sum_{n \in \mathbb{Z}} H_n^{(1)}(kr_j) J_n(kr'_j) e^{in(\theta_j - \theta'_j)} r'_j d\theta'_j. \end{aligned} \quad (3.70)$$

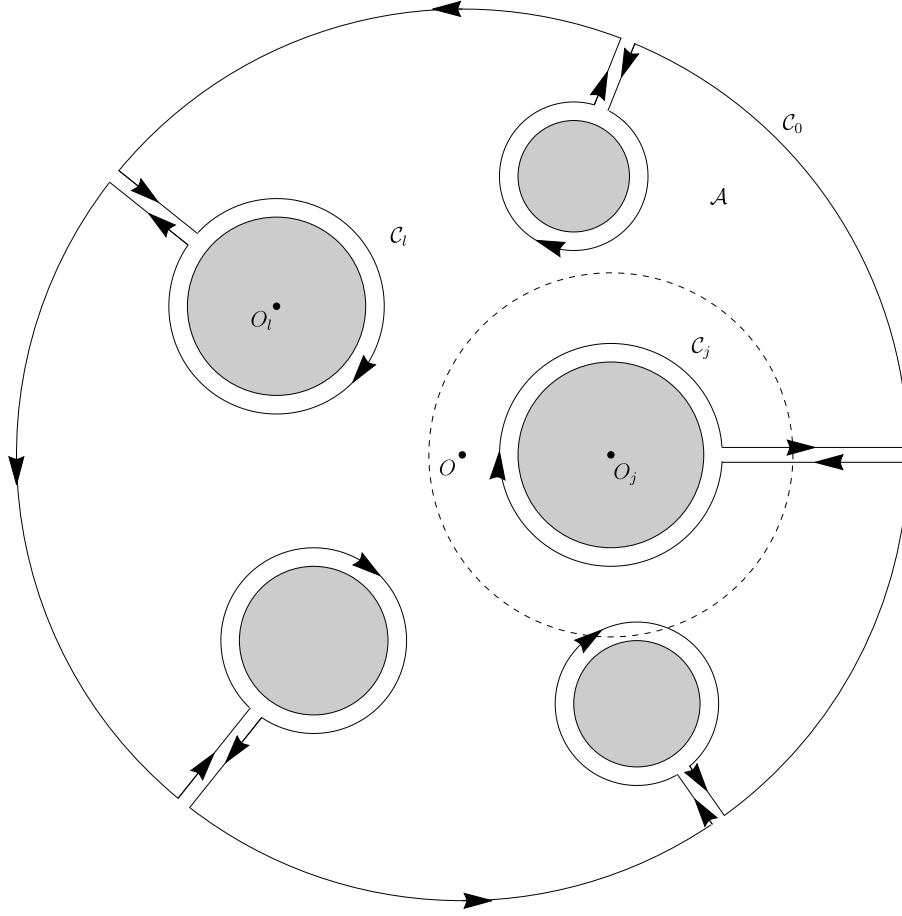


Figure 3.5: Contour of integration $\partial\mathcal{A}$ enveloping all cylinders. The dashed circle indicates the region in which the expansion in local coordinates (3.25) converges.

Due to the orthogonality of the Bessel functions, this is simply:

$$\begin{aligned}
& \frac{\pi k a_j}{2i} \sum_{m \in \mathbb{Z}} \left[a_{j,m} (J_m(k a_j) J'_m(k a_j) - J'_m(k a_j) J_m(k a_j)) \right. \\
& \quad \left. + b_{j,m} (H_m^{(1)}(k a_j) J'_m(k a_j) - H_m^{(1)'}(k a_j) J_m(k a_j)) \right] H_m^{(1)}(k r_j) e^{im\theta_j} \\
& = \frac{\pi k a_j}{2i} \sum_{m \in \mathbb{Z}} W\{J_m(k a_j), H_m^{(1)}(k a_j)\} b_{j,m} H_m^{(1)}(k r_j) e^{im\theta_j}, \tag{3.71}
\end{aligned}$$

where $W\{J_m(x), H_m^{(1)}(x)\}$ is the Wronskian of the Bessel and Hankel functions of the first kind:

$$W\{J_m(k a_j), H_m^{(1)}(k a_j)\} = \frac{2i}{\pi k a_j}. \tag{3.72}$$

Hence, the contribution to the total field due to the integral over $\mathcal{C}_j$ is simply a sum over outgoing waves, as before:

$$V_j^{sc} = \sum_{m \in \mathbb{Z}} b_{j,m} H_m^{(1)}(kr_j) e^{im\theta_j}. \quad (3.73)$$

The integrals over all $\mathcal{C}_l$ for which $l \neq j$ are carried out in identical fashion by swapping j for l . The contribution to the total field from this set of cylinders is therefore a sum over the outgoing waves from each and every cylinder $l \neq j$:

$$\sum_{l \neq j} V_l^{sc} = \sum_{l \neq j} \sum_{m \in \mathbb{Z}} b_{l,m} H_m^{(1)}(kr_l) e^{im\theta_l}. \quad (3.74)$$

The contribution to the total field by the line integral over $\mathcal{C}_0$ will be of the form of a sum over regular waves as in (3.65). Equating only those components of the field arising due to the scattering by cylinders, we have from Green's theorem:

$$\begin{aligned} & \sum_{m \in \mathbb{Z}} a_{j,m} J_m(kr_j) e^{im\theta_j} + \sum_{m \in \mathbb{Z}} b_{j,m} H_m^{(1)}(kr_j) e^{im\theta_j} \\ &= \sum_{m \in \mathbb{Z}} b_{j,m} H_m^{(1)}(kr_j) e^{im\theta_j} + \sum_{l \neq j} \sum_m b_{l,m} H_m^{(1)}(k_\perp r_l) e^{im\theta_l}, \end{aligned} \quad (3.75)$$

or:

$$\sum_{m \in \mathbb{Z}} a_{j,m} J_m(kr_j) e^{im\theta_j} = \sum_{l \neq j} \sum_m b_{l,m} H_m^{(1)}(k_\perp r_l) e^{im\theta_l}. \quad (3.76)$$

In deriving (3.76) we have shown that the regular field incident upon the j th cylinder equals the sum over the singular fields emanating from all of the other cylinders. Substituting the right-hand-side of (3.76) back into the multipole expansion (3.25), then in the absence of any incident radiation the total field at any point $\mathbf{r}$ in the exterior domain $\mathcal{A}$ is:

$$V(\mathbf{r}) = \sum_j \sum_{m \in \mathbb{Z}} b_{j,m} H_m^{(1)}(k^e r_j) e^{im\theta_j}. \quad (3.77)$$

This is the Wijngaard formula. It is a particularly useful formula, as it allows for the total field in the exterior domain to be written in terms of only the set of scattered field multipole moments $b_{j,m}$. The incident field moments $a_{j,m}$ can then be recovered from the scattered field moments via a change-of-basis function.

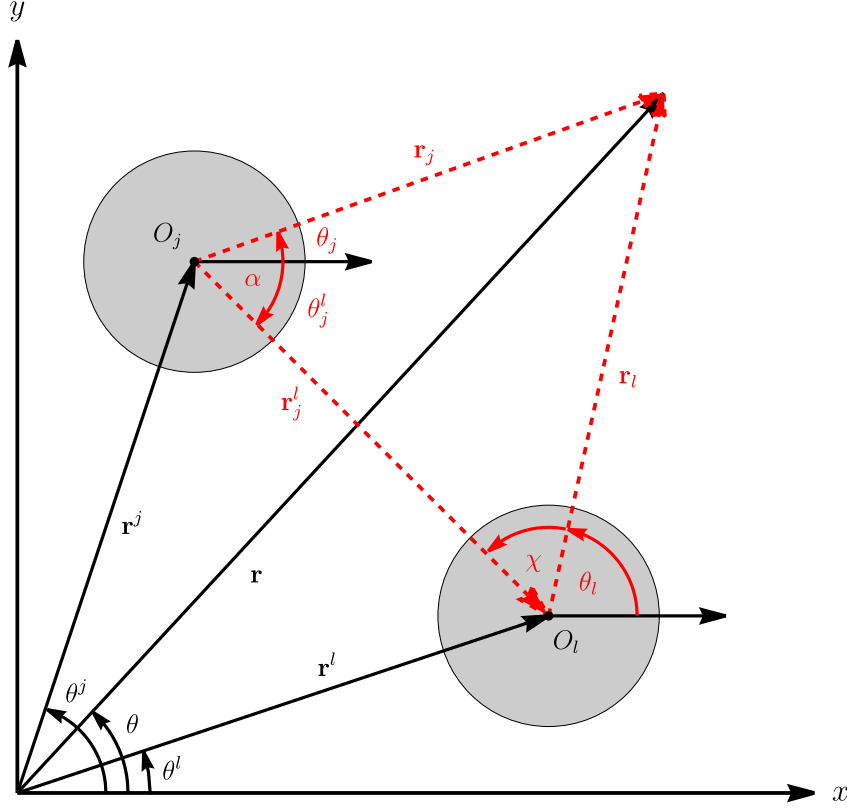


Figure 3.6: The coordinate systems. The red dashed triangle indicates the geometry used by Graf's addition theorem in the change-of-basis. Here $\alpha = \theta_j + \theta_j^l$ and $\chi = \pi - \theta_j^l - \theta_l$.

3.3.4 Change of Basis

We have just shown how the outgoing scattered waves in the coordinate system (r_l, θ_l) of any cylinder $l \neq j$ can instead be regarded as regular waves incident upon another cylinder j in the local coordinate system (r_j, θ_j) . Using the addition theorem again, we carry out a change in basis from the singular Hankel functions of the former coordinate system to the regular Bessel functions of the latter. For outgoing waves in the l th system, the change in basis to regular waves in the j th system takes the form:

$$H_m^{(1)}(k^e r_l) e^{im\theta_l} = \sum_{q \in \mathbb{Z}} H_{q-m}^{(1)}(k^e r_j^l) e^{i(m-q)\theta_j^l} J_q(k^e r_j) e^{iq\theta_j}, \quad (3.78)$$

where (r_j^l, θ_j^l) are the coordinates of O_l relative to O_j , as illustrated in Fig. 3.6. We also note that (3.78) only applies in the region $r_j \leq r_j^l$, which, if one considers all cylinders $l \neq j$, defines the annulus of outer radius equalling the distance to the nearest-neighbour cylinder as in Fig. 3.1. Equation (3.78) is clearly of the form of an expansion in regular

waves in the O_j coordinate system. The field scattered by the l th cylinder towards the j th is then:

$$V_l^{sc}(r_j, \theta_j) = \sum_{m \in \mathbb{Z}} b_{l,m} \sum_{q \in \mathbb{Z}} H_{q-m}^{(1)}(k^e r_j^l) e^{i(m-q)\theta_j^l} J_q(k^e r_j) e^{iq\theta_j}. \quad (3.79)$$

The total field incident on the j th cylinder equals the sum of (3.79) over all $l \neq j$:

$$\sum_{m \in \mathbb{Z}} a_{j,m} J_m(k^e r_j) e^{im\theta_j} = \sum_{l \neq j} \sum_{q \in \mathbb{Z}} b_{l,q} \sum_{m \in \mathbb{Z}} H_{m-q}^{(1)}(k^e r_j^l) e^{i(q-m)\theta_j^l} J_m(k^e r_j) e^{im\theta_j} \quad (3.80)$$

where indices m and q have been swapped on the right-hand-side. Equation (3.80) reveals the following identity:

$$\begin{aligned} a_{j,m} &= \sum_{l \neq j} \sum_{q \in \mathbb{Z}} b_{l,q} H_{m-q}^{(1)}(k^e r_j^l) e^{i(q-m)\theta_j^l} \\ &= \sum_{l \neq j} a_{j,m}^l, \end{aligned} \quad (3.81)$$

where

$$a_{j,m}^l = \sum_{q \in \mathbb{Z}} b_{l,q} \mathcal{H}_{mq}^{jl}, \quad (3.82)$$

$$\mathcal{H}_{m-q}^{jl} = H_{m-q}^{(1)}(k^e r_j^l) e^{i(q-m)\theta_j^l}. \quad (3.83)$$

The quantity (3.82) is the contribution by the l th cylinder to the m th multipole moment of the j th cylinder, $a_{j,m}$, and the embedded quantity (3.83) is the change-of-basis function*.

3.4 Multiple Scattering

This thesis is not concerned with cylinders of ordinary dielectric or metallic composition, but for the purposes of demonstrating how the unknown multipole moments can be evaluated, we provide here a short example. If one considers cylinders of a metallic composition, then for TE polarized light we have a Neumann boundary condition acting upon the longitudinal magnetic field component, specified by (3.18). If the incident field is of the form (3.37) i.e. a plane-wave, then the total field exterior to a set of metallic

*We will see in chapters 5 and 6 how this change-of-basis function plays a role in the sum over periodic infinite lattices.

cylinders is, in the O_j system of coordinates:

$$\begin{aligned}
H_z^e(r_j, \theta_j) &= \sum_{m \in \mathbb{Z}} a_{j,m}^\lambda J_m(k^e r_j) e^{im\theta_j} + \sum_l \sum_{m \in \mathbb{Z}} b_{l,m} H_m(k^e r_l) e^{im\theta_l} \\
&= \sum_{m \in \mathbb{Z}} a_{j,m}^\lambda J_m(k^e r_j) e^{im\theta_j} + \sum_{m \in \mathbb{Z}} b_{j,m} H_m(k^e r_j) e^{im\theta_j} \\
&\quad + \sum_{l \neq j} \sum_{m \in \mathbb{Z}} b_{l,m} \sum_{q \in \mathbb{Z}} \mathcal{H}_{q-m}^{jl} J_q(k^e r_j) e^{iq\theta_j}.
\end{aligned} \tag{3.84}$$

Note that we have dropped the superscript (1) on the Hankel function; any Hankel function from here on will be assumed to be of the first kind unless stated otherwise. Substitution of (3.84) into (3.18), multiplying by $e^{-ip\theta_j}$ and integrating over $d\theta_j$, $\theta_j \in [0, 2\pi]$, gives:

$$a_{j,p}^\lambda J'_p(k^e a_j) + b_{j,p} H'_p(k^e a_j) + \sum_{l \neq j} \sum_{m \in \mathbb{Z}} b_{l,m} \mathcal{H}_{p-m}^{jl} J'_p(k^e a_j) = 0 \tag{3.85}$$

which rearranges to the following system of equations for $b_{j,m}$:

$$b_{j,p} M_p^\infty + \sum_{l \neq j} \sum_{m \in \mathbb{Z}} b_{l,m} \mathcal{H}_{p-m}^{jl} = -a_{j,p}^\lambda. \tag{3.86}$$

Here

$$M_p^\infty = \frac{H'_p(ka_j)}{J'_p(ka_j)} \tag{3.87}$$

is referred to as the *boundary coefficient* for the infinite conductor*, and the quantities $a_{j,m}^\lambda$ are given by (3.38). The system (3.86) comprises a scattering matrix on the left-hand-side multiplying a vector of unknown multipole moments, and a vector on the right-hand-side specifying the incident wave. The multipole moments $b_{j,m}$ are determined for every cylinder $j \in \{1, \dots, N\}$ simultaneously by performing the matrix left divide of system (3.86).

*We will encounter boundary coefficients like this again in chapter 6.

4 Porter’s Plate-Array Metamaterial

The author would like to emphasize that the plate-array effective medium model was developed by R. Porter [98] in a slab arrangement, and later by R. Porter and S. Zheng [99] in a cylinder. The author’s contribution to this literature is the recasting of this homogenization method in electromagnetism. The quasi-modes of the metacylinder ring resonator were also investigated by my summer student Jingyi Ma.

4.1 Introduction to Chapter 4

Recently, Porter *et al.* have published a series of works on plate-array metamaterials, for water waves, that exhibit novel wave interactions [98–102]. In [98] Porter considers a closely-spaced periodic array of thin plates of Neumann boundary condition and identical height and tilt angle, and uses the close spacing of the plates to approximate the plate-array as an effective medium described simply by a one-dimensional wave equation. This continuum model stipulates that the plate-array acts as a perfectly-transmitting negative-refraction metamaterial, capable of perfect waveshifting across the medium as well as being entirely transparent to a plane-wave when the angle of incidence and tilt angle equate. This has been further developed upon by Porter and Zheng to consider cylinders of circular cross-section composed of the same plate-array medium [99, 101, 102], being referred to as metamaterial cylinders or ‘metacylinders’. In particular in [99] the metacylinders have been used to redirect wave energy for the purposes of focusing and blocking water waves, and the capabilities of energy dissipation within the effective medium have been explored. The scattering of incident radiation by the metacylinder has been found to point primarily along the direction at a right angle to the plate-array angle, with little-to-no scattered energy propagation through the exterior domain along the direction of the plate-array.

The purpose of this chapter is to provide the effective medium description of the plate-array metacylinder in an electromagnetic context. By introducing a relative index n_r to

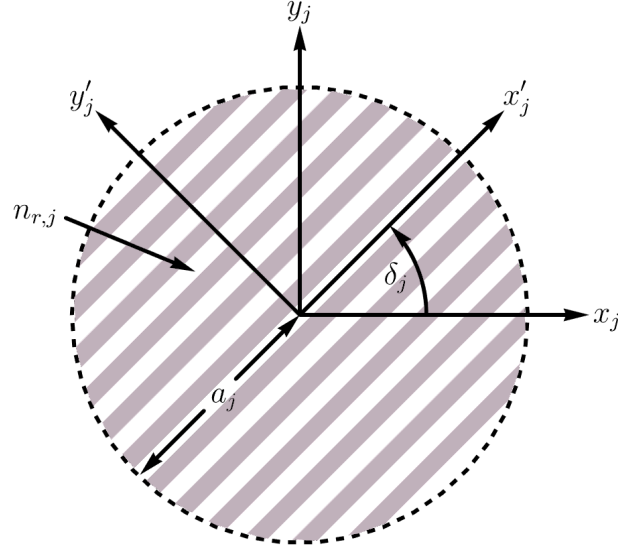


Figure 4.1: Coordinate systems of the j_{th} metacylinder. Cylinder coordinates rotated through δ_j to primed plate-array coordinates. The plate-array is merely illustrative and is not representative of the number of plates, the plate thickness or the inter-plate spacing.

the interstitial medium between the plates, the governing 1D wave equation in the interior is only slightly modified from that in [99]. Once this is carried out, we provide the infinite system of equations for the scattering of light by a set of plate-array cylinders of arbitrary arrangement, radius and orientation angle. Pseudo-colour plots of the magnetic and electric fields reveal the scattering behaviour of the plate-array structure, including at and above the resonant wavenumber of $ka = \pi/2$ for which the homogenization description fails to capture converged solutions. In multiple scattering we also consider a plate-array structured ring resonator, and demonstrate how the quality factor of the structure-located modes is subject to the uniform rotation angle of the metacylinders relative to the polar origin.

4.2 Field Equations

4.2.1 Plate-Array Homogenization

The microstructured plate-array material within the cylindrical inclusions is replaced by an effective medium description encapsulated by three equations; a one-dimensional wave

equation in the interior and a pair of continuity conditions at the surface. The geometry of the plate-array medium is provided in Fig. 4.1. The parallel plate-array is of infinite depth and decreasing length outwards, such that when viewed from above forms a cylinder of circular cross-section of radius a_j , and is aligned at cylinder angle δ_j with respect to the x_j -axis where $\delta_j \in [0, 2\pi)$. We have already established that the fields interior and exterior to the cylinder are subject to the the Helmholtz equations:

$$(\nabla^2 + n_{r,j}^2 k^2) H_{z,j}^i = 0 \quad \text{in} \quad r_j < a_j \quad (4.1)$$

$$(\nabla^2 + k^2) H_z^e = 0 \quad \text{in} \quad r_j > a_j \quad (4.2)$$

where k is the wavenumber in the exterior bulk (we have dropped the superscript e) and $H_{z,j}^i$ refers to the longitudinal magnetic field component interior to the j th cylinder. The Helmholtz equation (4.1) applies exclusively to the interstitial channels between the plates, which are of dielectric composition of relative index $n_{r,j}$ with respect to the exterior medium. The plates themselves are perfectly electrically conducting and are accordingly of Neumann boundary condition. Temporarily dropping the subscript j (we will reintroduce it later), under rotation to the primed cylinder coordinates (x', y') the Helmholtz equation in the interior (4.1) is:

$$\left(\frac{\partial^2}{\partial x'^2} + \frac{\partial^2}{\partial y'^2} + n_r^2 k^2 \right) H_z^i(x', y') = 0 \quad (4.3)$$

and the boundary condition on the perfectly conducting plates is of the form:

$$\frac{\partial}{\partial y'} H_z^i(x', \pm m d_p) = 0 \quad (4.4)$$

for all $m \in \mathbb{Z}$, which represents the continuum* of plates in both directions about the centre of the plate-array, and d_p is the inter-plate spacing, where $n_r k d_p \ll 1$ i.e. the spacing d_p is much smaller than the wavelength of light in the interstitial dielectric. We introduce the new double-primed coordinate y'' where $0 < y'' < 1$, such that any point in the interstitial medium can be written as:

$$(x', y') \equiv (x', m d_p + d_p y''). \quad (4.5)$$

*There is a continuum of channel lengths from the centre of the metacylinder outwards in both directions. Each channel harbours resonances at integer multiples of the first resonant wavenumber $n_r k L_j = \pi/2$, where L_j is the length of channel j .

Labeling $H_z^i(x', y') \equiv H_{m,z}^i(x', y'')$, in double-primed coordinates (4.3) reads:

$$\left(\frac{1}{n_r^2 k^2} \frac{\partial^2}{\partial x'^2} + \frac{1}{\zeta^2} \frac{\partial^2}{\partial y''^2} + 1 \right) H_{m,z}^i(x', y'') = 0 \quad (4.6)$$

with plate boundary condition:

$$\frac{\partial}{\partial y''} H_{m,z}^i = 0 \text{ on } y'' = 0, 1, \quad (4.7)$$

where the subscript denotes the interstitial space between the m_{th} plate and its nearest-neighbour. Note that the small parameter $\zeta = n_r k d_p$ remains small at finite n_r as long as $k d_p \ll 1$. By expanding the solution in powers of the small parameter squared:

$$H_{m,z}^i(x', y'') = H_m^0(x', y'') + \zeta^2 H_m^1(x', y'') + \mathcal{O}(\zeta^4) \quad (4.8)$$

then at leading order (4.6) is $\partial^2 / \partial y''^2 (H_m^0) = 0$. As (4.7) applies at all orders of the field expansion (4.8) we surmise that $H_m^0 \equiv H_m^0(x')$ only. At next order (4.6) reads:

$$\left(\frac{\partial^2}{\partial x'^2} + n_r^2 k^2 \right) H_m^0(x') + \frac{\partial^2 H_m^1}{\partial y''^2} = 0 \quad (4.9)$$

whereby integration over y'' in $0 \leq y'' \leq 1$ and making use of the boundary condition (4.7) yields:

$$\left(\frac{\partial^2}{\partial x'^2} + n_r^2 k^2 \right) H_m^0(x') = 0, \quad (4.10)$$

for all $m \in \mathbb{Z}$. To leading order in ζ , $H_z^i \approx H_m^0(x')$, and we may write:

$$\left(\frac{\partial^2}{\partial x'^2} + n_r^2 k^2 \right) H_z^i(x', y') = 0 \quad (4.11)$$

where the y' dependence has been re-introduced; although the leading order field approximation does not vary over the length-scale $d_p y''$, it is permitted to vary between the disconnected channels of separation $m d_p$, as per the definition (4.5). Solutions of (4.11) comprise the superposition of forwards and backwards travelling waves:

$$H_z^i(x', y') = C(y') e^{i n_r k x'} + D(y') e^{-i n_r k x'} \quad (4.12)$$

where $C(y')$, $D(y')$ are the waves' amplitudes. In polar coordinates:

$$H_z^i(a, \theta) = C(\theta)e^{in_r ka \cos(\theta-\delta)} + D(\theta)e^{-in_r ka \cos(\theta-\delta)} \quad (4.13)$$

where we have used $x' = r \cos(\theta - \delta)$ and replaced the amplitudes $C(y')$, $D(y')$ with equivalent quantities $C(\theta)$, $D(\theta)$ that have an explicit dependence on the angular coordinate. Now, by symmetry about the y' axis,

$$C(\theta) = C(\pi + 2\delta - \theta), \quad (4.14a)$$

$$D(\theta) = D(\pi + 2\delta - \theta), \quad (4.14b)$$

which is an expression of the fact that the surfaces of the semi-circles $\theta \in [\delta - \pi/2, \delta + \pi/2]$ and $\theta \in [\delta + \pi/2, \delta + 3\pi/2]$ are connected by the interior plate-array. By writing $y' = a \sin(\theta - \delta) = a \cos(\theta - \delta - \pi/2)$, we approximate these amplitudes by expansions in Chebyshev polynomials:

$$\begin{aligned} \{C(\theta), D(\theta)\} &= \sum_{n=0}^{\infty} \{c_n, d_n\} T_n\left(\frac{y'}{a}\right) \\ &= \sum_{n=0}^{\infty} \{c_n, d_n\} \cos\left(n\left(\theta - \delta - \frac{\pi}{2}\right)\right) \end{aligned} \quad (4.15)$$

which satisfies (4.14a) and (4.14b)*. Substitution of (4.15) into (4.13) and utilising the Jacobi-Anger identity (A.7) allows for the field on the interior boundary to be expressed as:

$$\begin{aligned} H_z^i(a, \theta) &= \sum_{n=0}^{\infty} c_n \cos\left(n\left(\theta - \delta - \frac{\pi}{2}\right)\right) \cdot \sum_{m \in \mathbb{Z}} i^m J_m(n_r ka) e^{im(\theta-\delta)} \\ &+ \sum_{n=0}^{\infty} d_n \cos\left(n\left(\theta - \delta - \frac{\pi}{2}\right)\right) \cdot \sum_{m \in \mathbb{Z}} (-i)^m J_m(n_r ka) e^{im(\theta-\delta)} \end{aligned} \quad (4.16)$$

for which we note the necessity of the interior field being expressed in sums of multipole expansions in regular waves so as to avoid the occurrence of singular solutions as $a \rightarrow 0$.

We note here that the plate-array cylinders undergo resonance at $n_r ka = \pi/2$, the wavenumber at which an integer number of half-wavelengths equals the length of the central-most channels in the cylinder. Above this wavenumber the resonance moves outwards to channels of shorter length until the central channel reaches its second resonance

*The notation $\{x, y\}$ is shorthand for the respective equations of x and y .

at $n_r ka = \pi$. Hence, the metacylinder undergoes a continuum of resonance in the region $n_r ka \geq \pi/2$, although solutions at and above this threshold fail to converge unless damping is introduced to the interstitial medium. This is discussed at length in § 4.3.3.

Assuming that both the wavenumber k and the interstitial spacing d_p are small, the homogenized wave equation (4.11) will break down under two scenarios. The first is that in which the relative index $n_r \gg 1$, in which case the small parameter $\zeta = \mathcal{O}(1)$ and the homogenization is no longer valid. The second scenario in which (4.11) fails is when $n_r \ll 1$, in which case there is an additional small parameter in the equation (4.6), $n_r k$. Assuming $n_r k \simeq \zeta$ and using ansatz (4.8), one will instead recover Laplace's equation at leading order rather than an equation of the form (4.11). To avoid both scenarios we keep $n_r = \mathcal{O}(1)$ in our computations.

4.2.2 Continuity Conditions

For the purposes of deriving a system of equations, the interior field (4.16) must be connected to the exterior field at the boundary of the metacylinder. In treating the plate-array medium as effectively homogeneous, we have guaranteed that the cylinders retain their circular cross-section and may write the field due to the scattering by N metacylinders, in the presence of an incident plane-wave, as:

$$\begin{aligned} H_z^e(r_j, \theta_j) &= \sum_{m \in \mathbb{Z}} a_{j,m}^\lambda J_m(kr_j) e^{im\theta_j} + \sum_{m \in \mathbb{Z}} b_{j,m} H_m(kr_j) e^{im\theta_j} \\ &+ \sum_{l \neq j}^N \sum_{m \in \mathbb{Z}} b_{l,m} \sum_{q \in \mathbb{Z}} \mathcal{H}_{q-m}^{jl} J_q(kr_j) e^{iq\theta_j}, \end{aligned} \quad (4.17)$$

which is just (3.84). We have already established that the continuity conditions that apply between a dielectric inclusion and the exterior bulk are of the form (3.14) and (3.16), the latter of which has to be modified in this case to account for the metallic plates. This is done by computing the gradient of the interior field along $\mathbf{x}'_j$ before taking its component along $\mathbf{r}_j$; see Fig. 4.2. On the j th metacylinder the continuity conditions read:

$$H_z^e = H_{z,j}^i \quad \text{on } r_j = a_j, \quad (4.18)$$

$$\frac{\partial H_z^e}{\partial r_j} = \frac{1}{n_{r,j}^2} \cos(\theta_j - \delta_j) \frac{\partial H_{z,j}^i}{\partial x'_j} \quad \text{on } r_j = a_j, \quad (4.19)$$

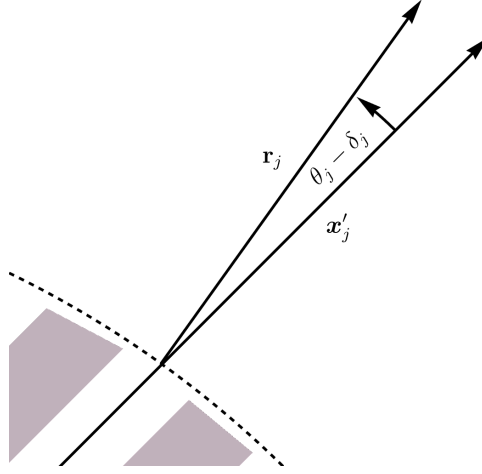


Figure 4.2: Component diagram between $\mathbf{x}'_j$ and $\mathbf{r}_j$.

Substitution of (4.16) and (4.17) into (4.18) and (4.19) describes the continuity of the field and flux through the surface at any point (a_j, θ_j) on the metacylinder. Multiplying by $e^{-ip\theta_j}$ and integrating over $\theta_j \in [0, 2\pi]$ yields:

$$e^{ik(x^j \cos(\psi_{inc}) + y^j \sin(\psi_{inc}))} i^p J_p(ka_j) e^{-ip\psi_{inc}} \quad (4.20)$$

$$+ b_{j,p} H_p(ka_j) + \sum_{\substack{l=1 \\ l \neq j}}^N \sum_{m \in \mathbb{Z}} b_{l,m} \mathcal{H}_{p-m}^{jl} J_p(ka_j)$$

$$= \frac{1}{2} e^{ip(\frac{\pi}{2} - \delta_j)} \sum_{n=0}^{\infty} (c_{j,n} (-1)^n + d_{j,n} (-1)^p) (J_{p-n}(n_{r,j} ka_j) + J_{p+n}(n_{r,j} ka_j)),$$

$$e^{ik(x^j \cos(\psi_{inc}) + y^j \sin(\psi_{inc}))} i^p J'_p(ka_j) e^{-ip\psi_{inc}} \quad (4.21)$$

$$+ b_{j,p} H'_p(ka_j) + \sum_{\substack{l=1 \\ l \neq j}}^N \sum_{m \in \mathbb{Z}} b_{l,m} \mathcal{H}_{p-m}^{jl} J'_p(ka_j)$$

$$= \frac{1}{2n_{r,j}} e^{ip(\frac{\pi}{2} - \delta_j)} \sum_{n=0}^{\infty} (c_{j,n} (-1)^n + d_{j,n} (-1)^p) (J'_{p-n}(n_{r,j} ka_j) + J'_{p+n}(n_{r,j} ka_j)),$$

where prime denotes the derivative of a Bessel function with respect to its argument, and the flux condition (4.21) makes use of Bessel function identities of appendix A for the derivatives on the right-hand-side. Together (4.20) and (4.21) constitute a linear system of equations for the multipole moments and Chebyshev coefficients.

4.2.3 Scattering Matrix

By placing both the interior and exterior field terms on the left-hand-side and the plane-wave on the right-hand-side of Eqs. (4.20) and (4.21), we arrive to the following system of equations for the multiple scattering between all metacylinders:

$$\mathbf{S}\mathbf{A} = \mathbf{Q} \quad (4.22)$$

where

$$\mathbf{S} = \left(\begin{array}{cccc|cccc|cccc} \mathbf{H}_1 & \mathbf{P}_{1,2} & \cdots & \mathbf{P}_{1,N} & \mathbf{C}_1 & \mathbf{0} & \cdots & \mathbf{0} & \mathbf{D}_1 & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{P}_{2,1} & \mathbf{H}_2 & \cdots & \mathbf{P}_{2,N} & \mathbf{0} & \mathbf{C}_2 & \cdots & \mathbf{0} & \mathbf{0} & \mathbf{D}_2 & \cdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{P}_{N,1} & \mathbf{P}_{N,2} & \cdots & \mathbf{H}_N & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{C}_N & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{D}_N \\ \hline \mathbf{H}'_1 & \mathbf{P}'_{1,2} & \cdots & \mathbf{P}'_{1,N} & \mathbf{C}'_1 & \mathbf{0} & \cdots & \mathbf{0} & \mathbf{D}'_1 & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{P}'_{2,1} & \mathbf{H}'_2 & \cdots & \mathbf{P}'_{2,N} & \mathbf{0} & \mathbf{C}'_2 & \cdots & \mathbf{0} & \mathbf{0} & \mathbf{D}'_2 & \cdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{P}'_{N,1} & \mathbf{P}'_{N,2} & \cdots & \mathbf{H}'_N & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{C}'_N & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{D}'_N \end{array} \right) \quad (4.23)$$

is the scattering matrix. Here:

$$\mathbf{A} = (\mathbf{b}_1, \dots, \mathbf{b}_N, \mathbf{c}_1, \dots, \mathbf{c}_N, \mathbf{d}_1, \dots, \mathbf{d}_N)^T, \quad (4.24)$$

and

$$\mathbf{Q} = (\mathbf{Q}_1, \dots, \mathbf{Q}_N, \mathbf{Q}'_1, \dots, \mathbf{Q}'_N)^T. \quad (4.25)$$

The top half of $\mathbf{S}$ corresponds to (4.20) and the bottom half to (4.21). In computation we truncate the infinite multipole and Chebyshev expansions to a size $m, p \in [-M - 1, M]$ and $n \in [0, M]$, respectively for some truncation parameter M . Naturally higher wavenumbers warrant larger truncation parameters for convergent solutions. Accordingly the matrix $\mathbf{S}$ is a square matrix of size $N(4M + 4)$ rows and columns, with submatrices

of the form:

$$H_{j,p,m} = -\delta_{pm}H_p(ka_j), \quad (4.26)$$

$$P_{j,l,p,m} = -\mathcal{H}_{p-m}^{jl}J_p(ka_j), \quad (4.27)$$

$$C_{j,p,n} = \frac{i^p}{2}e^{-ip\delta_j}(-1)^n(J_{p-n}(n_{r,j}ka_j) + J_{p+n}(n_{r,j}ka_j)), \quad (4.28)$$

$$D_{j,p,n} = \frac{i^p}{2}e^{-ip\delta_j}(-1)^p(J_{p-n}(n_{r,j}ka_j) + J_{p+n}(n_{r,j}ka_j)), \quad (4.29)$$

where $P_{j,l,p,m}$ refers to the pm_{th} element of the change-of-basis submatrix $\mathbf{P}_{j,l}$. Similarly $C_{j,p,n}$ and $D_{j,p,n}$ are the pn_{th} elements of the submatrices $\mathbf{C}_j$ and $\mathbf{D}_j$ describing the interior field of metacylinder j as a function of the cylinder angle δ_j . Similarly:

$$H'_{j,p,m} = -\delta_{pm}H'_p(ka_j), \quad (4.30)$$

$$P'_{j,l,p,m} = -\mathcal{H}_{p-m}^{jl}J'_p(ka_j), \quad (4.31)$$

$$C'_{j,p,n} = \frac{i^p}{2n_{r,j}}e^{-ip\delta_j}(-1)^n(J'_{p-n}(n_{r,j}ka_j) + J'_{p+n}(n_{r,j}ka_j)), \quad (4.32)$$

$$D'_{j,p,n} = \frac{i^p}{2n_{r,j}}e^{-ip\delta_j}(-1)^p(J'_{p-n}(n_{r,j}ka_j) + J'_{p+n}(n_{r,j}ka_j)). \quad (4.33)$$

Each metacylinder vector of multipole moments is of the form $\mathbf{b}_l = (b_{l,-M-1}, \dots, b_{l,M})$, $\mathbf{c}_j = (c_{j,0}, \dots, c_{j,N})$ and $\mathbf{d}_j = (d_{j,0}, \dots, d_{j,N})$. Each plane-wave vector $\mathbf{Q}_j$ describes the incident field at the boundary of cylinder j , where:

$$Q_{j,p} = e^{ik(x^j \cos(\psi_{inc}) + y^j \sin(\psi_{inc}))} i^p J_p(ka_j) e^{-ip\psi_{inc}}, \quad (4.34)$$

$$Q'_{j,p} = e^{ik(x^j \cos(\psi_{inc}) + y^j \sin(\psi_{inc}))} i^p J'_p(ka_j) e^{-ip\psi_{inc}}. \quad (4.35)$$

Alternatively the above plane-wave can be replaced by a point-source of form:

$$Q_{j,p} = \frac{1}{4i} \mathcal{H}_{p-o}^{js} J_p(ka_j), \quad (4.36)$$

$$Q'_{j,p} = \frac{1}{4i} \mathcal{H}_{p-o}^{js} J'_p(ka_j), \quad (4.37)$$

of some chosen order o and relative source position (r_j^s, θ_j^s) , where $\mathcal{H}_{po}^{js}$ is the change-of-basis function between the singular source field and the regular incident field upon j .

4.2.4 Trick for Numerical Stability

Upon first inspection, it is tempting to simplify the system formed by (4.20) and (4.21) by writing it in terms of boundary coefficients not unlike (3.87). Elegant as this may be, the resulting system grows in its numerical instability as the truncation parameter M is increased; this becomes an issue when the wavenumber of the exterior bulk approaches the resonance value of $n_{r,j}ka_j$, for which an increasing truncation parameter is necessary for convergent solutions. This issue can be circumvented by redefining the multipole moments:

$$b_{j,p} = \frac{\tilde{b}_{j,p}}{H_p(ka_j)} \quad \text{or} \quad b_{j,p} = \frac{\tilde{b}_{j,p}}{H'_p(ka_j)}. \quad (4.38)$$

The resulting system in terms of $\tilde{b}_{j,p}$ remains numerically stable at truncation parameters of $M > 50$ as long as $n_{r,j}ka_j < \pi/2$ for all $j \in N$. The moments $b_{j,p}$ are recovered from $\tilde{b}_{j,p}$ after the matrix-left-divide of the system of equations.

4.3 Single Scattering

4.3.1 Electric and Magnetic Fields

In demonstrating the effects of the plate-array medium on the scattered electromagnetic field, we provide a number of examples in Fig. 4.3 for the magnetic field and Fig. 4.4 for the corresponding electric field, which is computed numerically via the curl of $\mathbf{H}$. A plane-wave of incident angle $\psi_{inc} = \pi/2$ undergoes scattering by a single metacylinder at the origin of the global coordinate system, which is of relative index $n_r = 1$ and radius $a = 1$ in nondescript units. The transparency of the metamaterial to the plane-wave is apparent in panels (a), at which $\delta = \psi_{inc}$ such that the plane-wave is entirely undisturbed by the presence of the metacylinder. Upon rotation this picture changes, with scattering occurring at cylinder angles (b) $\delta = \pi/4$, (c) $\delta = 0$. The resonance at $n_rka = \pi/2$ is plotted in panels (d), for which we note the non-converged solution both inside and outside the metacylinder. In all cases, the maxima of magnetic and electric field strengths occur within the effective medium and dwarf those of the exterior field.

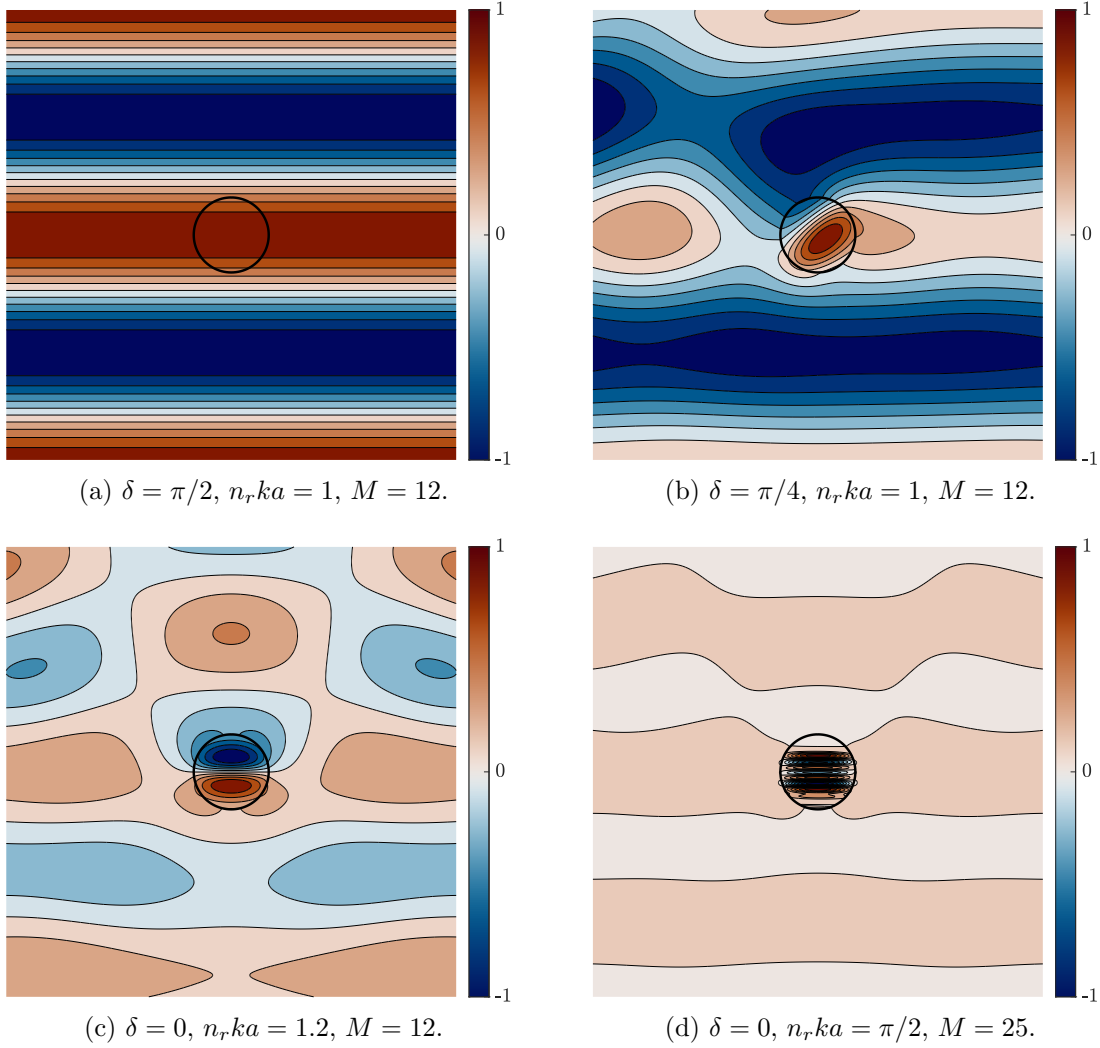


Figure 4.3: Normalised longitudinal magnetic fields H_z due to the scattering by a plane-wave of incident angle $\psi_{inc} = \pi/2$ by a single metacylinder of radius $a = 1$ and relative index $n_r = 1$.

4.3.2 Scattered Energy Flux

The scattering of a plane-wave depicted in Figs. 4.3 and 4.4 is complemented by depictions of the Poynting vector field, which illustrate the directional energy flux of the scattered fields $\mathbf{E}_s$ and $\mathbf{H}_s$ in the immediate vicinity of the metacylinder. For time-harmonic fields the Poynting vector is defined as:

$$\mathbf{S} = \frac{1}{2} \mathbf{E}_s \times \mathbf{H}_s^*, \quad (4.39)$$

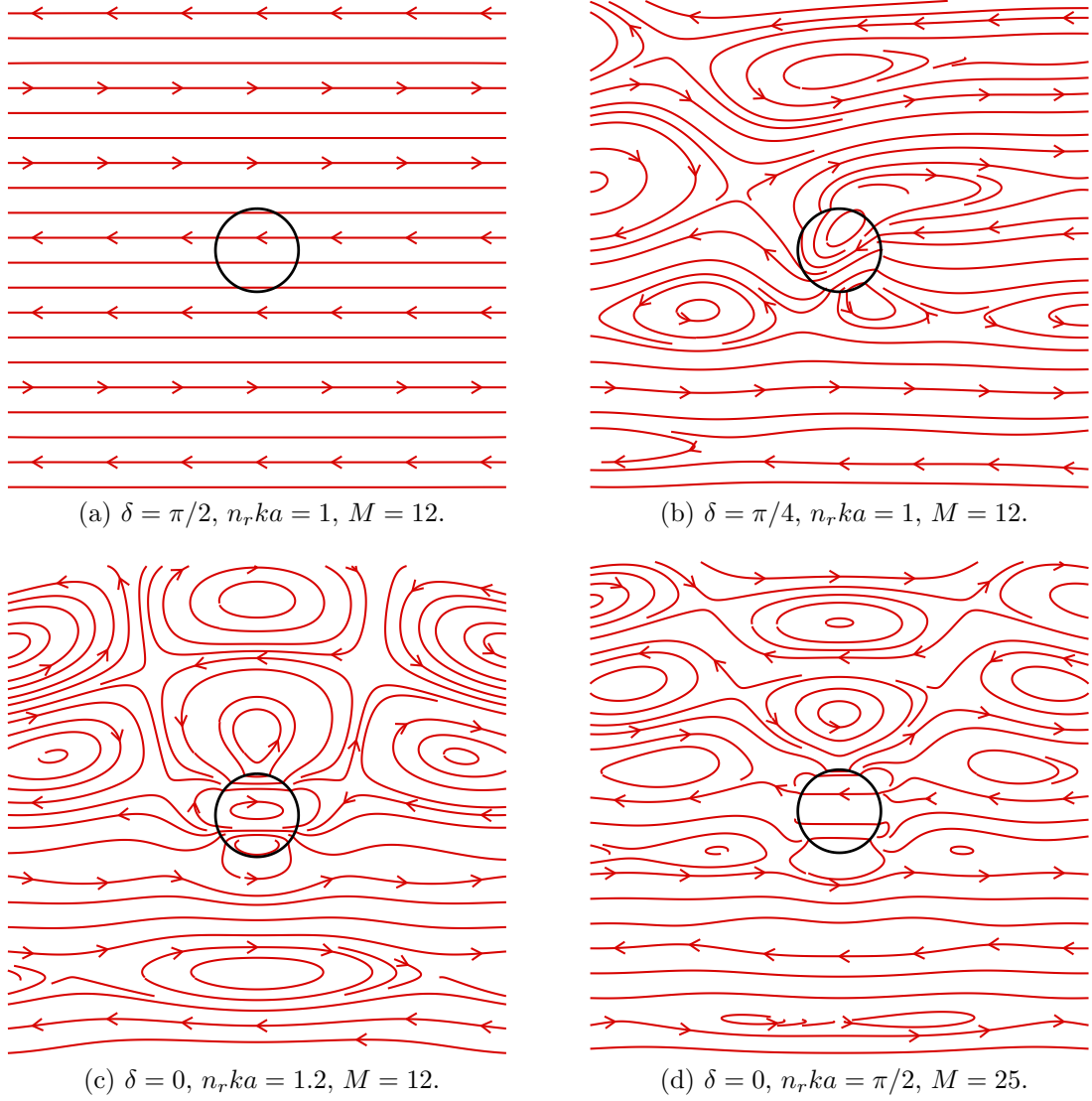


Figure 4.4: Electric fields $(E_x, E_y, 0)$ due to the scattering by a plane-wave of incident angle $\psi_{inc} = \pi/2$ by a single metacylinder of radius $a = 1$ and relative index $n_r = 1$.

such that the time-averaged power flow is by definition $\langle \mathbf{S} \rangle = \text{Re}\{\mathbf{S}\}$, where $*$ denotes the complex conjugate. In Fig. 4.5 we provide the real part of the Poynting vector field normalised by the maximum in time-averaged power flow i.e. $\langle \mathbf{S} \rangle / \langle \mathbf{S} \rangle_{max}$ in the vicinity of the metacylinder at three different wavenumbers and cylinder angles. In all cases the power flow points predominantly along the direction perpendicular to the effective medium with minimal energy propagation along the δ direction. As the wavenumber approaches resonance, strong re-circulation can be observed between the channel mouths, as in panel (c), illustrating how neighbouring channel amplitudes become inter-dependent as

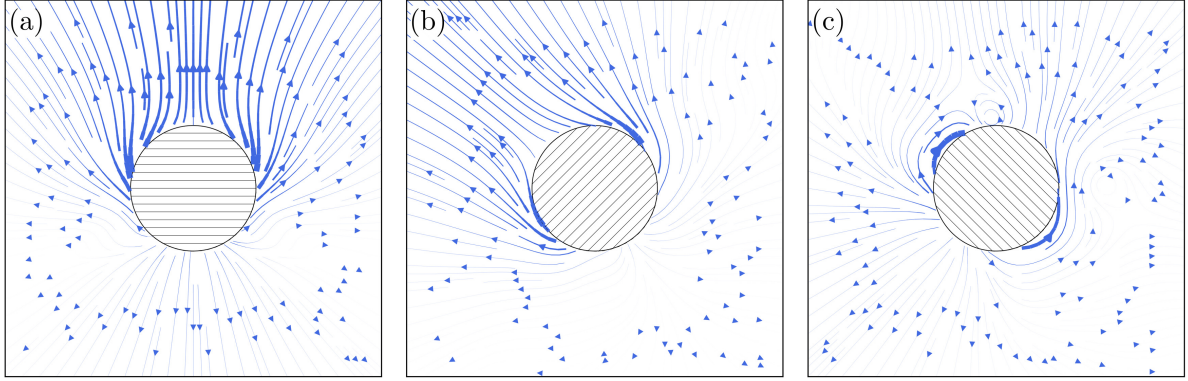


Figure 4.5: The normalised Poynting vector field corresponding to the scattered electric and magnetic fields of an incident plane-wave of angle $\psi_{inc} = \pi/2$. At wavenumber and cylinder angle (a) $n_r ka = 1.2$, $\delta = 0$, (b) $n_r ka = 1.3$, $\delta = \pi/4$ and (c) $n_r ka = 1.4$, $\delta = -\pi/4$. Computations carried out at (a) $M = 20$, (b) $M = 30$ and (c) $M = 40$. Plates drawn in the disc are for illustrative purpose only.

the local wavenumber in the vicinity of the plate-array grows as resonance is approached. The directionality of the scattered energy propagation has ramifications for the types of eigenmodes belonging to periodic structures of metacylinders. We will show later how the long-range uniformity of the plate-array angle in each and every cylinder modifies the dispersion of modes in the macro-structure.

4.3.3 Damping

In previous work [99, 100] it was shown that solutions given by the effective medium model fail to converge at and above the resonant wavenumber of the central channel $n_r ka = \pi/2$, even as the truncation parameter $M \rightarrow \infty$. This lack of convergence manifests as an oscillatory behaviour in the reflection and transmission coefficients of scattered waves, as in Fig. 5.2 of chapter 5 and Figs. 2 and 5 of [100]. In [100] this behaviour is attributed to an increasing frequency in the oscillations in the field between the channel walls, and this in turn is associated with a local wavenumber of oscillations. By writing our Helmholtz equation in the y'' coordinate in (4.6), we have assumed an independence between channel m and its nearest neighbours, and this independence is invalidated when the local wavenumber of oscillations is sufficiently small. This is supported by the reconnecting Poynting vector streamlines of Fig.4.5c, which illustrate the interconnectedness of neighbouring channels as the resonant wavenumber is approached. To resolve the field within the continuum of resonance we introduce a damping component to the interstitial

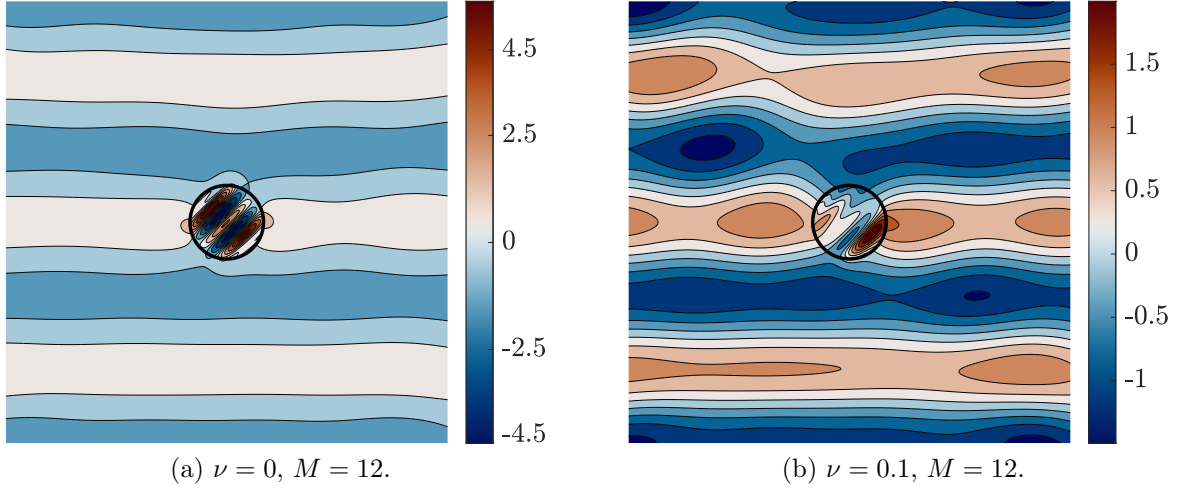


Figure 4.6: The effect of damping on the convergence of scattering computations. Scattering of a plane-wave of resonant wavenumber $n_r ka = \pi/2$ by a metacylinder of damping parameter (a) $\nu = 0$ and (b) $\nu = 0.1$.

dielectric ν , such that:

$$n'_r = n_r(1 + i\nu), \quad (4.40)$$

where n'_r is the damped index. The presence of damping ensures converging solutions at finite truncation parameters M , although not to the solutions that would exist if the effective solutions converged in the absence of damping. Typically ν is of size $\mathcal{O}(10^{-2})$ or $\mathcal{O}(10^{-1})$ in simulation, and we illustrate the effect of damping on the total field in Fig. 4.6. A single metacylinder is depicted of radius $a = 1$ and plate-array angle $\delta = \pi/4$, and is of damping parameter (a) $\nu = 0$, (b) $\nu = 0.1$.

The remainder of this thesis is concerned with wavenumbers below that of the first resonant wavenumber, and so from hereon we assume $\nu = 0$ unless otherwise specified. A discussion of absorption of incident radiation by the plate-array medium is provided in the concluding remarks; this would be achieved by defining an absorption coefficient for the plate-array metamaterial that would vary as a function of ν .

4.4 Metacylinder Ring Resonators

In motivating the succeeding chapters on infinite periodic structures of metacylinders, we consider here a finite periodic arrangement of N metacylinders constituting a ring resonator. As in chapter 2, the eigenmodes of the ring will be Bloch-periodic and manifest

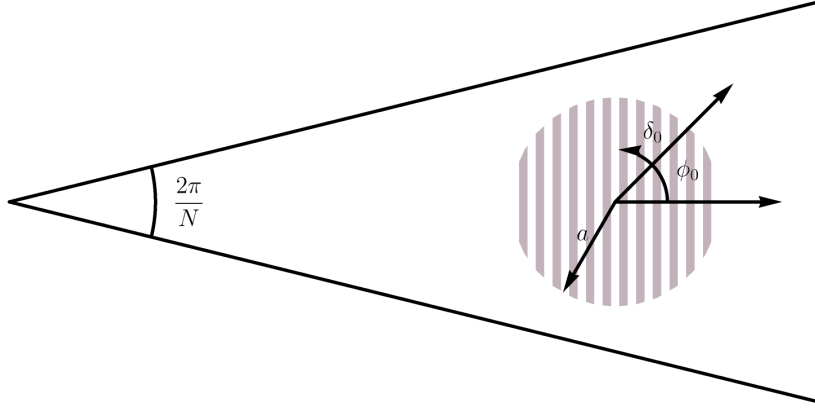


Figure 4.7: Zeroth wedge in the metacylinder ring resonator. The angle ϕ_0 is measured anti-clockwise relative to the global radial direction.

as the non-trivial solutions to a linear system of equations. The cylinders are of positions:

$$x^j = R \cos\left(\frac{2\pi j}{N}\right), \quad (4.41a)$$

$$y^j = R \sin\left(\frac{2\pi j}{N}\right), \quad (4.41b)$$

where $\theta^j = 2\pi j/N$, $j \in [0, N-1]$ and R is the radius of the ring. In order to ensure periodicity around the ring, all cylinder angles must be uniformly oriented relative to the polar origin:

$$\delta_j = \delta_0 + \frac{2\pi j}{N} \quad (4.42)$$

where δ_0 denotes the angle of the 0th cylinder, which is placed on the positive x -axis; see Fig. 4.7. The rotational analogue of Bloch's theorem applies to the field in the j th wedge:

$$H_z(r_j, \phi_j) = e^{\frac{2\pi i j \eta}{N}} H_z(r_0, \phi_0), \quad (4.43)$$

where η is the mode number and

$$\theta_j = \phi_j + \frac{2\pi j}{N} \quad (4.44)$$

where ϕ_j denotes the angular coordinate in clockwise rotation from the line conjoining the ring-centre to the centre of cylinder j , where clearly $\theta_0 \equiv \phi_0$. To proceed we re-write the the field scattered by all cylinders $j \neq 0$ in terms of ϕ_j :

$$\sum_{j=1}^{N-1} \sum_{m \in \mathbb{Z}} b_{j,m} H_m(kr_j) e^{im\theta_j} \equiv \sum_{j=1}^{N-1} \sum_{m \in \mathbb{Z}} f_{j,m} H_m(kr_j) e^{im\phi_j} \quad (4.45)$$

where

$$f_{j,m} = e^{\frac{2\pi i j m}{N}} b_{j,m}, \quad (4.46)$$

and $f_{0,m} \equiv b_{0,m}$. Applying the addition theorem to (4.45) we have:

$$\begin{aligned} H_m(kr_j) e^{im(\frac{3\pi}{2} - \frac{j\pi}{N} - \phi_j)} &= \sum_{q \in \mathbb{Z}} H_{q+m}(kr_0^j) J_q(kr_0) e^{iq(\phi_0 - \frac{\pi}{2} - \frac{j\pi}{N})} \\ \implies H_m(kr_j) e^{im\phi_j} &= \sum_{q \in \mathbb{Z}} H_{q-m}(kr_0^j) J_q(kr_0) e^{iq\phi_0} i^{m-q} e^{-\frac{\pi i j}{N}(m+q)}, \end{aligned} \quad (4.47)$$

where $r_0^j = 2R \sin(j\pi/N)$. The exterior field in (r_0, ϕ_0) coordinates is then:

$$\begin{aligned} H_z^e(r_0, \phi_0) &= \sum_{m \in \mathbb{Z}} f_{0,m} H_m(kr_0) e^{im\phi_0} \\ &+ \sum_{j=1}^{N-1} \sum_{m \in \mathbb{Z}} f_{j,m} \sum_{q \in \mathbb{Z}} H_{q-m}(kr_0^j) J_q(kr_0) e^{iq\phi_0} i^{m-q} e^{-\frac{\pi i j}{N}(m+q)}. \end{aligned} \quad (4.48)$$

Hence, it is clear that by Bloch-periodicity (4.43):

$$f_{j,m} = e^{\frac{2\pi i j \eta}{N}} f_{0,m}, \quad (4.49)$$

such that:

$$\begin{aligned} H_z^e(r_0, \phi_0) &= \sum_{m \in \mathbb{Z}} f_{0,m} H_m(kr_0) e^{im\phi_0} \\ &+ \sum_{j=1}^{N-1} \sum_{m \in \mathbb{Z}} f_{0,m} \sum_{q \in \mathbb{Z}} H_{q-m}(kr_0^j) i^{m-q} e^{\frac{\pi i j}{N}(2\eta - m - q)} J_q(kr_0) e^{iq\phi_0}. \end{aligned} \quad (4.50)$$

As for the interior field, the Helmholtz equation is invariant under rotation, and so our expression for the interior field (4.16) remains unchanged, with (x'_j, y'_j) now aligned with respect to the rotated Cartesian axes (x_j, y_j) , as per (4.42). Along with (4.43) this implies that $\{c_{j,n}, d_{j,n}\} = e^{2\pi i j \eta/N} \{c_{0,n}, d_{0,n}\}$. Applying the continuity conditions (4.18) and (4.19) to the 0th metacylinder, and using the orthogonality of the Bessel functions,

we have:

$$\begin{aligned}
& f_p H_p(ka) + \sum_{j=1}^{N-1} \sum_{m \in \mathbb{Z}} f_m i^{m-p} e^{\frac{\pi i j}{N} (2\eta - m - p)} H_{p-m}(kr_0^j) J_p(ka) \\
& - \frac{1}{2} e^{ip(\frac{\pi}{2} - \delta)} \sum_{n=0}^{\infty} (c_n (-1)^n + d_n (-1)^p) (J_{p-n}(n_r ka) + J_{p+n}(n_r ka)) \\
& = 0
\end{aligned} \tag{4.51}$$

and

$$\begin{aligned}
& f_p H'_p(ka) + \sum_{j=1}^{N-1} \sum_{m \in \mathbb{Z}} f_m i^{m-p} e^{\frac{\pi i j}{N} (2\eta - m - p)} H_{p-m}(kr_0^j) J'_p(ka) \\
& - \frac{1}{2n_r} e^{ip(\frac{\pi}{2} - \delta)} \sum_{n=0}^{\infty} (c_n (-1)^n + d_n (-1)^p) (J'_{p-n}(n_r ka) + J'_{p+n}(n_r ka)) \\
& = 0
\end{aligned} \tag{4.52}$$

where we have dropped the 0 subscript for brevity. Together (4.51) and (4.52) form a system of equations of size $(4M + 4) \times (4M + 4)$, the solutions of which constitute the whispering-Bloch quasi-modes of the metacylinder ring resonator.

As in chapter 2 the whispering-Bloch modes are of two types: structure-located modes that are akin to Rayleigh-Bloch modes along linear gratings, and leaky interior modes of poor quality factor; both types are plotted in Fig. 4.8. The locations of the zeros of the matrix determinant can be observed to shift towards the $\text{Re}\{k\}$ -axis as N is increased for a ring of constant radius, and this shift is quantified by the quality factor $\mathcal{Q}$, which we remind the reader is of the form:

$$\mathcal{Q} = \frac{\text{Re}\{k^2\}}{|2\text{Im}\{k^2\}|}. \tag{4.53}$$

Naturally the quasi-modes, and so too the quality factor, will be a function of the uniform cylinder angle, and a physical intuition of this dependence is provided by the scattered Poynting vector fields of Fig. 4.5. When $\delta = \pi/2$ the direction of energy propagation points outwards from the ring, meaning that the quasi-modes of this configuration will be very leaky relative to those of the $\delta = 0$ configuration for which the energy propagates tangentially to the ring. This is shown plainly in Fig. 4.9 for which the quality factor of the structure-located whispering-Bloch modes is plotted against increasing N for three δ values and for Neumann inclusions. In keeping with the results of Maling *et al.* [9, 49, 66]

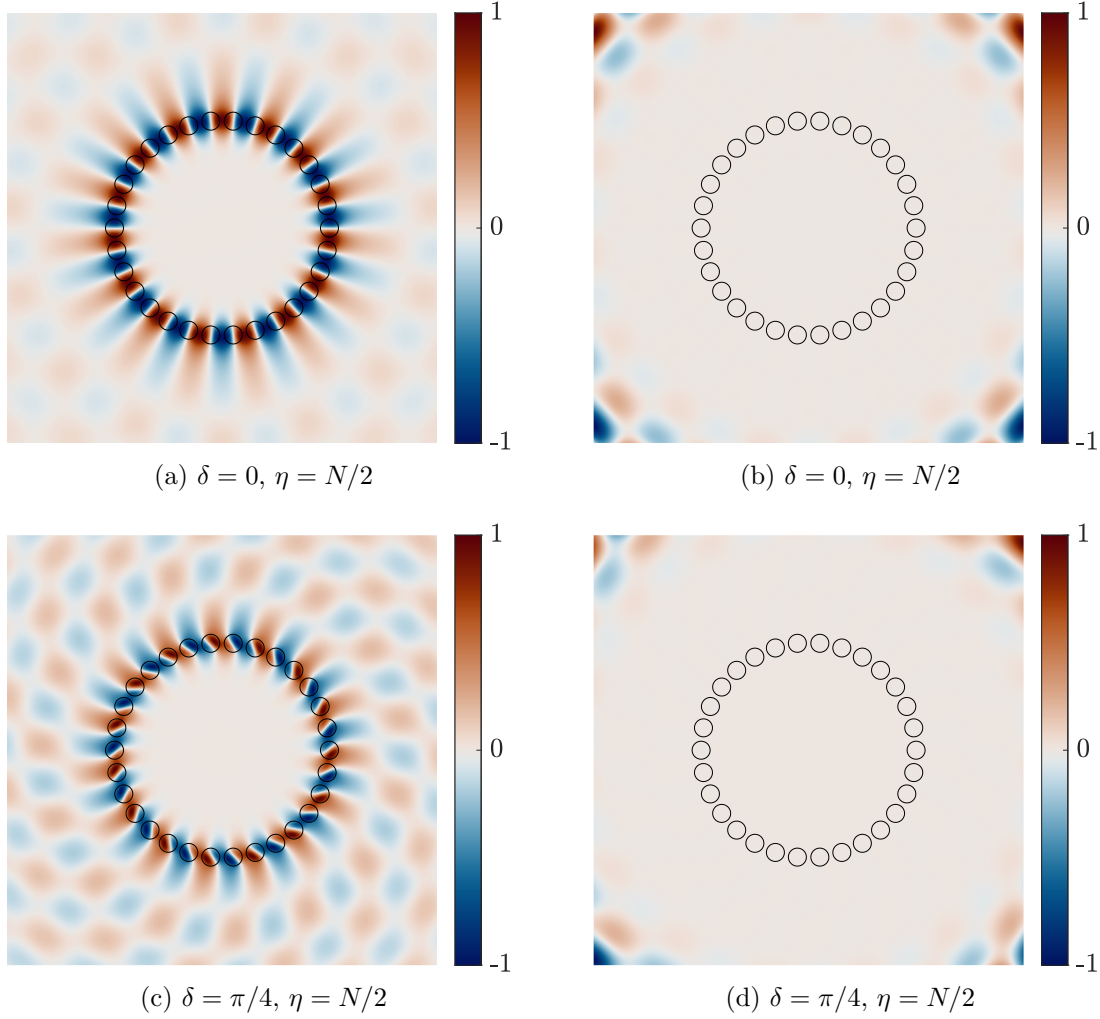


Figure 4.8: Whispering-Bloch quasi-modes of the structured ring resonator of $N = 30$ metacylinders. Panels (a) and (c) depict structure-located modes and panels (b) and (d) depict leaky interior modes.

so as to make an appropriate comparison, the radius of the cylinders is set to $a = 0.8 \sin(\pi/N)$, which ensures that the ratio of cylinder radius to inter-cylinder spacing is a constant. We observe that the quality factor of the $\delta = 0$ orientation is always the largest no matter the number of inclusions, and that rotating the cylinders through $\pi/2$ radians results in a $\sim O(10^7)$ fall in the quality factor of the structure-located modes at $N = 100$. In comparing to the Neumann ring we have observed a $\sim O(10^5)$ increase in the quality factor at $N = 100$ and $\delta = 0$, and hence conclude that the structure-located whispering-Bloch modes are far more confined to the structured ring by way of the plate-array metamaterial. The same cannot be said of the interior modes however, which are

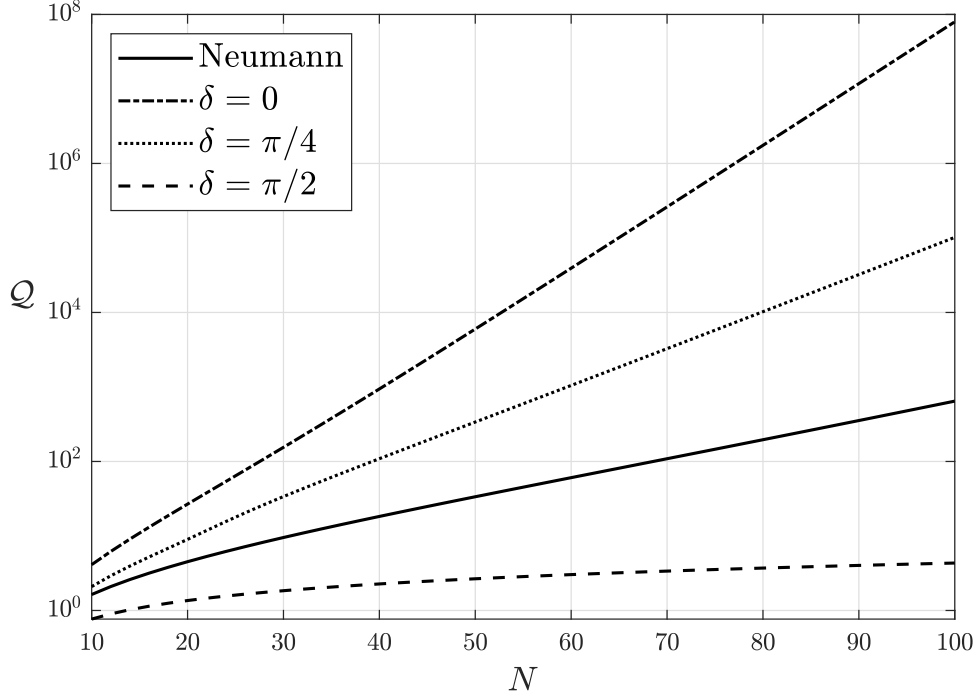


Figure 4.9: Quality factor of the structure-located whispering-Bloch modes of mode number $\eta = N/2$ as a function of N .

all of a quality factor of $\mathcal{Q} \simeq O(10^0)$ no matter the orientation of the plate-array medium. The inclusions, being penetrable, cannot readily trap energy within the structured ring, and this is visualised by the pseudo-color plots of Fig. 4.8 panels (b) and (d), which are dominated by the ‘leaked’ field exterior to the ring resonator.

4.5 Remarks on Chapter 4

In homogenizing the plate-array in the limit of vanishing inter-plate spacing, we have replaced the plates and dielectric channels with an effective medium description. This is encapsulated by a one-dimensional wave equation for the channels and a pair of continuity conditions between the channels and the exterior domain. By writing the interior field as a sum over regular waves, we have slotted the effective description into a multipole formalism that lends itself to numerical simulation. In turn, we have seen how the metacylinders can be implemented as the building blocks of a structured ring resonator, the eigenmodes of which are quasi-modes of a complex wavenumber. The energy leakage has been quantified in terms of a quality factor $\mathcal{Q}$, which has been shown to be a function of the uniform plate-array angle with respect to the ring centre. Under appropriate

orientation, the plate-array grants the structure-located whispering-Bloch modes a quality factor of $\mathcal{O}(10^8)$ for a ring of $N = 100$ cylinders, which is a $\mathcal{O}(10^5)$ increase with respect to a ring resonator of perfectly conducting cylinders.

The main benefit of this effective description over a finite element implementation is the speed with which we can determine the scattering by, and eigenmodes of, macroscopic periodic media. Assuming Bloch-periodic fields grants us the ability to form semi-analytic descriptions of periodic metacylinder structures along one and two directions. We consider the first of these periodic structures in chapter 5 in the form of a tunable metamaterial diffraction grating. We move on to a 2D metasurface in chapter 6, for which we derive the effective permittivity tensor in the quasistatic limit. The study of both structures is however restricted to the wavenumber region below that of the first channel resonance, unless a negative imaginary damping component is introduced to the channel dielectric. The latter could see use in the absorption of an incident field, and this is discussed in the concluding remarks.

5 A Diffraction Grating of Plate-Array Metacylinders

The work presented in this chapter is adapted from the publication [2]. S. Guenneau performed the FEM computations featured in Figs. 5.5 and 5.6. R. Porter and R.V. Craster contributed to the modelling of the problem in discussions and notes.

5.1 Introduction to Chapter 5

Given the highly anisotropic scattering of light by a single metacylinder in isolation, we are interested in structured media that are composed of these fundamental plate-array building-blocks. In particular, we investigate the dispersive nature and effective material parameters of macroscopic periodic structures, and how these behaviours can be tuned via uniform rotation of the plate-array cylinders. The simplest structured medium that can be composed of these plate-array metacylinders is a linear diffraction grating, or so-called metagrating, of evenly spaced and uniform inclusions.

The mathematical treatment of this problem is straightforward; of particular relevance to this aim are the articles by Evans, Porter, Linton and the McIvers *et al.* on the guiding and scattering of waves by singly-periodic arrays, i.e. gratings, of impermeable cylinders [65, 71, 103–105], which we can draw upon and exploit. An important feature of some periodic gratings is the presence of the array-guided modes; the existence of array-guided or Rayleigh-Bloch surface-waves along gratings of impermeable cylinders of Neumann boundary condition was proven in [104, 105] and for general structures in [106], whereas those of Dirichlet boundary condition do not host Rayleigh-Bloch modes [107]. As in elasticity, Rayleigh-Bloch modes in electromagnetism propagate solely along the grating and experience exponential decay with perpendicular distance from the grating axis. Given the existence of Rayleigh-Bloch modes for both gratings of impermeable plates [106] and impermeable circular cylinders [103], and their importance for scattering and energy

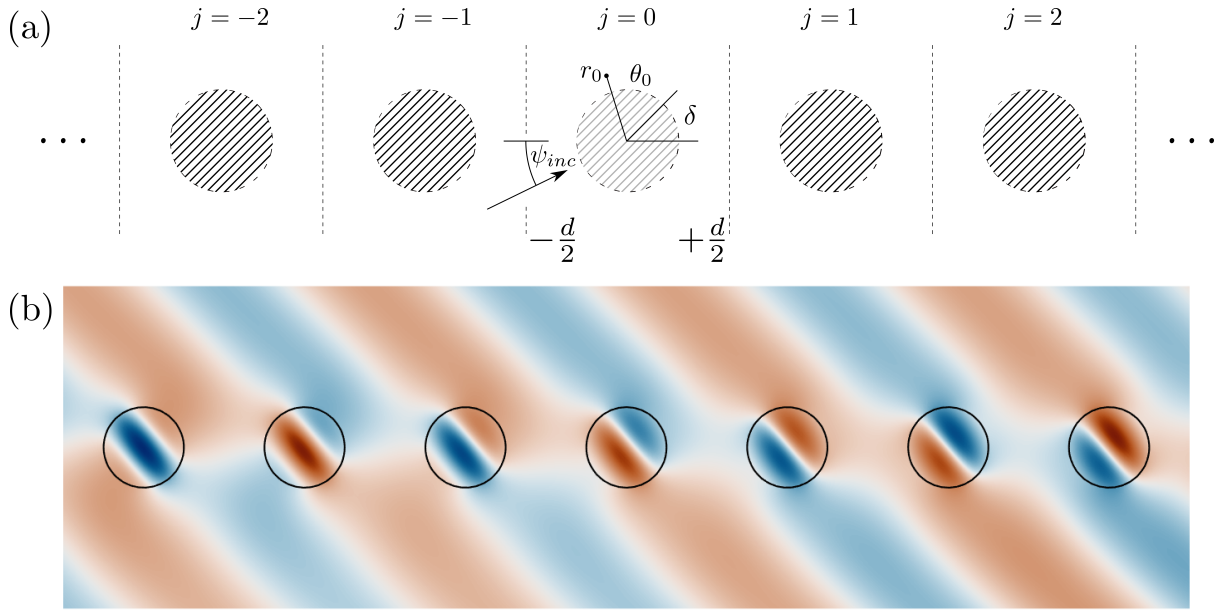


Figure 5.1: (a) Cross-section of the infinite metagrating. (b) A negative Goos-Hänchen shift in the transmitted field due to the scattering of a plane-wave of incident angle $\psi_{inc} = \pi/4$ by a metagrating of uniform angle $\delta = -0.926$.

transport, one expects the metagrating to host Rayleigh-Bloch modes, and moreover that they could be tunable through rotation of the uniform cylinder angle. Their existence has implications for the kinds of solutions that will be observed in the scattering of light by truncated gratings, particularly the forcing experienced by the constituent inclusions at wavenumbers close to the Rayleigh-Bloch wavenumbers [103, 108]. As before, these modes manifest as the non-trivial solutions to the system of equations for the grating; the sums over the infinite structure can be dealt with without too much trouble.

We are also motivated to explore the diffraction grating's reflection and transmission spectra and its dependence on the choice of uniform cylinder angle; the spectra should reveal that the grating is entirely transparent to an incident wave in motion parallel to the plate-array medium. Looking to previous work [101] the diffraction grating should also permit so-called ‘waveshifting’ across its axis, and we explore the possibilities of extraordinary reflection and transmission when the cylinders are close to touching.

This chapter is outlined as follows. We begin by providing the equations of the field due to the scattering by the infinite structure, and define the embedded grating sums in terms of change-of-basis functions. These grating sums are treated via the rapidly convergent representation of Twersky [31]. Following this we provide the infinite system of equations for the grating and consider the scattering of an incident plane-wave. Our

treatment of this is that of a diffraction problem; we derive the reflection and transmission coefficients using Linton's method [71], verifying the implementation computationally by use of the power-balance criterion of Achenbach [109], before analysing the spectra. In a similar fashion, we search for Rayleigh-Bloch modes belonging to the infinite metagrating, and find that the metagrating hosts exclusively symmetric (under vertical orientation) Rayleigh-Bloch modes that are tunable by rotation of the uniform cylinder angle. We finish by providing our concluding remarks, as well as a short discussion on possible applications. Note that in this chapter, we assume $n_r = 1$.

5.2 The Infinite Grating

The diffraction grating consists of an infinite set of plate-array metacylinders of uniform radius a , spacing d and plate-array angle δ positioned along the x -axis with coordinates $(dj, 0)$ for $j \in \mathbb{Z}$, as drawn in Fig. 5.1. The solution at any point in the domain exterior to the grating is of the form:

$$H_z^e = H_z^\lambda + \sum_{j \in \mathbb{Z}} \sum_{m \in \mathbb{Z}} b_{j,m} H_m(kr_j) e^{im\theta_j} \quad (5.1)$$

where the λ superscript denotes the incident plane-wave. The periodicity of the grating and the plane-wave ensures that the field will be Bloch-periodic:

$$H_z^e(r_0 + dj, \theta_j) = H_z^e(r_0, \theta_0) e^{i\beta dj} \quad (5.2)$$

and likewise for the interior field, where β is the Bloch wavenumber along the grating. Applying the condition (5.2) to the local scattered field (3.73) reveals the following identity between the multipole moments of the j th and 0th cylinders:

$$b_{j,m} = e^{i\beta dj} b_{0,m} \quad (5.3)$$

where $b_{0,m}$ is the m th multipole moment of the 0th metacylinder. The total scattered field in the coordinates of the 0th cylinder is found by applying Graf's theorem to (5.1) under consideration of the grating geometry. Clearly $r_0^j = d|j|$ and $\theta_0^j = 0$ for $j \geq 0$ or $\theta_0^j = \pi$ for $j < 0$ so that:

$$\mathcal{H}_{m-q}^{0j} = \text{sgn}(j)^{q-m} H_{m-q}(kd|j|). \quad (5.4)$$

Accordingly in $r_0 < d$:

$$\begin{aligned}
H_z^{sc}(r_0, \theta_0) &= \sum_{m \in \mathbb{Z}} b_{0,m} H_m(kr_0) e^{im\theta_0} \\
&+ \sum_{\substack{j \in \mathbb{Z} \\ j \neq 0}} e^{i\beta dj} \sum_{m \in \mathbb{Z}} b_{0,m} \sum_{q \in \mathbb{Z}} \text{sgn}(j)^{m-q} H_{q-m}(kd|j|) J_q(kr_0) e^{iq\theta_0} \\
&= \sum_{m \in \mathbb{Z}} b_{0,m} H_m(kr_0) e^{im\theta_0} + \sum_{m \in \mathbb{Z}} b_{0,m} \sum_{q \in \mathbb{Z}} \sigma_{m-q}(\beta) J_q(kr_0) e^{iq\theta_0}
\end{aligned} \tag{5.5}$$

where H_z^{sc} denotes the scattered field in the exterior domain and

$$\sigma_l(\beta) = \sum_{j=1}^{\infty} H_l(kdj) ((-1)^l e^{i\beta dj} + e^{-i\beta dj}) \tag{5.6}$$

is the *lattice sum* or *grating sum*^{*}, and constitutes the sum over the infinite grating of the change-of-basis functions of order l multiplied by the Bloch phase. Note that:

$$\sigma_{-l} = (-1)^l \sigma_l,$$

such that we need only compute the grating sums of order $l \geq 0$.

5.2.1 Elementary Function Representation of Schlömilch Series

In its current form the grating sum (5.6) is slow to converge and is not suitable for computation. Twersky [31], referring to (5.6) as a ‘Schlömilch series’, derived an elementary function representation which is more amenable to computation, and we provide this here

^{*}We reserve the term ‘lattice sum’ for the sum over the doubly-periodic lattice in Chapter 6.

in our notation:

$$\sigma_{2l} = 2(-1)^l \sum_{n \in \mathbb{Z}} \frac{e^{i2l \operatorname{sgn}(n)\psi_n}}{kd \sin(\psi_n)} + \frac{i}{\pi} \sum_{n=0}^l \frac{(-1)^n 2^{2n} (l+n-1)!}{(2n)!(l-n)!} \left(\frac{2\pi}{kd}\right)^{2n} B_{2n}\left(\frac{\beta d}{2\pi}\right) \quad (5.7)$$

$$\sigma_{2l-1} = 2(-1)^l i \sum_{n \in \mathbb{Z}} \frac{e^{i(2l-1) \operatorname{sgn}(n)\psi_n}}{kd \sin(\psi_n)} + \frac{2}{\pi} \sum_{n=0}^{l-1} \frac{(-1)^n 2^{2n} (l+n-1)!}{(2n+1)!(l-n-1)!} \left(\frac{2\pi}{kd}\right)^{2n+1} B_{2n+1}\left(\frac{\beta d}{2\pi}\right) \quad (5.8)$$

for $l \geq 1$ and

$$\sigma_0 = -1 - \frac{2i}{\pi} \left(C + \ln \left(\frac{kd}{4\pi} \right) \right) + \frac{2}{kd \sin(\psi_0)} + \sum_{\substack{n \in \mathbb{Z} \\ n \neq 0}} \left(\frac{2}{kd \sin(\psi_n)} + \frac{i}{|n|\pi} \right) \quad (5.9)$$

for $l = 0$. Here C refers to Euler's constant and $B_n(x)$ refers to the Bernoulli polynomial, which can be written as a finite sum [110]. Essentially, the grating sum (5.6) has been recast as a sum over propagating and evanescent modes of scattering angles $\psi_m(\beta)$ for $n \in \mathbb{Z}$, where:

$$\psi_n = \arccos \left(\frac{\beta_n}{k} \right) \quad \text{and} \quad \beta_n = \beta + \frac{2\pi n}{d}, \quad (5.10)$$

such that $\psi_0 \equiv \psi_{inc}$ in the case of the scattering of an incident plane-wave. When $|\beta_n| < k$ we say $n \in \mathcal{M}$ for which all ψ_n are real and of value $0 < \psi_n < \pi$. Whereas when $|\beta_n| > k$, $n \in \mathcal{N}$ for which all ψ_n are no longer real and one must use the following branches of the inverse cosine:

$$\arccos(x) = \begin{cases} i \operatorname{arccosh}(x) & \text{if } x > 1, \\ \pi - i \operatorname{arccosh}(-x) & \text{if } x < -1, \end{cases} \quad (5.11a)$$

$$(5.11b)$$

where $\operatorname{arccosh}(x) = \ln(x + \sqrt{x^2 - 1})$ for $x > 1$; see [71, 111]. The set $\mathcal{M}$ refers to the modes that are permitted to propagate into the far-field, whereas the set $\mathcal{N}$ refers to the evanescent modes that decay exponentially with perpendicular distance from the grating.

5.2.2 Reflection and Transmission

In the case of reflection and transmission of a plane-wave by the diffraction grating the Bloch wavenumber is simply the incident wavenumber component along the diffraction grating i.e. $\beta = k \cos(\psi_{inc})$. Naturally there will always be at least one ($n = 0$) propagating mode of real ψ_n , with higher-modes cutting-on as the incident wavenumber and propagation angle are altered. By inspection of (4.20)-(4.21) the equivalent continuity conditions on the 0th metacylinder in the infinite grating are:

$$\begin{aligned} i^p J_p(ka) e^{-ip\psi_{inc}} + b_p H_p(ka) + J_p(ka) \sum_{m \in \mathbb{Z}} b_m \sigma_{m-p}(\beta) \\ = \frac{1}{2} e^{ip(\frac{\pi}{2}-\delta)} \sum_{n=0}^{\infty} (c_n (-1)^n + d_n (-1)^p) (J_{p-n}(ka) + J_{p+n}(ka)), \end{aligned} \quad (5.12)$$

$$\begin{aligned} i^p J'_p(ka) e^{-ip\psi_{inc}} + b_p H'_p(ka) + J'_p(ka) \sum_{m \in \mathbb{Z}} b_m \sigma_{m-p}(\beta) \\ = \frac{1}{2} e^{ip(\frac{\pi}{2}-\delta)} \sum_{n=0}^{\infty} (c_n (-1)^n + d_n (-1)^p) (J'_{p-n}(ka) + J'_{p+n}(ka)), \end{aligned} \quad (5.13)$$

where we have written $b_{0,m} \equiv b_m$ etc. and assumed $n_r = 1$. Note that the δ -dependence is present only on the right-hand-side of (5.12) and (5.13) in the form of a $e^{-ip\delta}$ term. Together (5.12) and (5.13) form a system of equations for the plane-wave scattering by the infinite grating. The reflection and transmission coefficients are extracted from the expressions for the the far-field in $y < 0$ and $y > 0$ respectively, and are determined in the manner following Linton *et al.* [71]. We begin by implementing the following integral representation of the cylindrical harmonic:

$$H_m(kr_j) e^{im\theta_j} = \frac{(-i)^{m+1}}{\pi} \int_{-\infty}^{\infty} \frac{e^{-k\gamma(t)|y_j|}}{\gamma(t)} e^{ikx_j t} e^{im \operatorname{sgn}(y_j) \arccos(t)} dt \quad (5.14)$$

into (5.1), where:

$$\gamma(t) = \begin{cases} -i\sqrt{1-t^2} & \text{if } |t| \leq 1, \\ \sqrt{t^2-1} & \text{if } |t| > 1. \end{cases} \quad (5.15a)$$

$$(5.15b)$$

Hence:

$$H_z^{sc} = \int_{-\infty}^{\infty} dt \sum_{m \in \mathbb{Z}} b_m \frac{(-i)^{m+1}}{\pi} \frac{e^{-k\gamma(t)|y_0|}}{\gamma(t)} e^{im \operatorname{sgn}(y_0) \arccos(t) + ikx_0 t} \sum_{j \in \mathbb{Z}} e^{i(\beta-kt)dj} \quad (5.16)$$

where we have made use of (5.3) and written $x_j = x_0 - jd$ and $y_j = y_0$. To proceed we make use of the Poisson summation formula in distributional form (A.21):

$$\sum_{j \in \mathbb{Z}} e^{iju} = 2\pi \sum_{n \in \mathbb{Z}} \delta(2\pi n + u) \quad (5.17)$$

where in our case $u = \beta d - kdt$. Performing the integration over $u \in \mathbb{R}$ and noting that $du/dt = -kd$, the variable t is discretised:

$$t = \frac{\beta}{k} + \frac{2\pi n}{kd} = \frac{\beta_n}{k}. \quad (5.18)$$

such that:

$$H_z^{sc} = \sum_{n \in \mathbb{Z}} \frac{2e^{ikr \cos(|\theta| - \psi_n)}}{kd \sin(\psi_n)} \sum_{m \in \mathbb{Z}} (-i)^m b_m e^{im \operatorname{sgn}(\theta) \psi_n}. \quad (5.19)$$

The far-field is encapsulated by only those terms for which $|\beta_n| < k$ i.e. for real ψ_n , the set of propagating plane-waves of scattering angles $\theta = \pm\psi_n$. Thus as $y \rightarrow \pm\infty$:

$$H_z \sim H_z^\lambda + \sum_{n \in \mathcal{M}} \frac{2e^{ikr \cos(\theta \mp \psi_n)}}{kd \sin(\psi_n)} \sum_{m \in \mathbb{Z}} (-i)^m b_m e^{\pm im \psi_n} \quad (5.20)$$

where the reflection and transmission coefficients are identified as:

$$R_n = \frac{2}{kd \sin(\psi_n)} \sum_{m \in \mathbb{Z}} (-i)^m b_m e^{-im \psi_n}, \quad (5.21)$$

$$T_n = \delta_{0n} + \frac{2}{kd \sin(\psi_n)} \sum_{m \in \mathbb{Z}} (-i)^m b_m e^{+im \psi_n}, \quad (5.22)$$

for the diffraction orders $n \in \mathcal{M}$, where δ_{0n} accounts for the incident plane-wave. According to Achenbach *et al.* [109] and later Linton and Evans [89], by considering the time-averaged net power flow through the fundamental cell, the reflection and transmission coefficients form the criterion:

$$\sum_{n \in \mathcal{M}} \frac{t_n}{t_0} (|R_n|^2 + |T_n|^2) = 1 \quad \text{where} \quad t_n = \left(1 - \left(\frac{\beta_n}{k}\right)^2\right)^{\frac{1}{2}}. \quad (5.23)$$

Although this was originally derived under the assumption of a Neumann condition on the cylindrical boundary, we may omit the integral over the metacylinder surface by asserting that due to the permeability of the effective medium, integrating over the cell walls encapsulates the flow through the metacylinder. Thus (5.23) describes the conservation

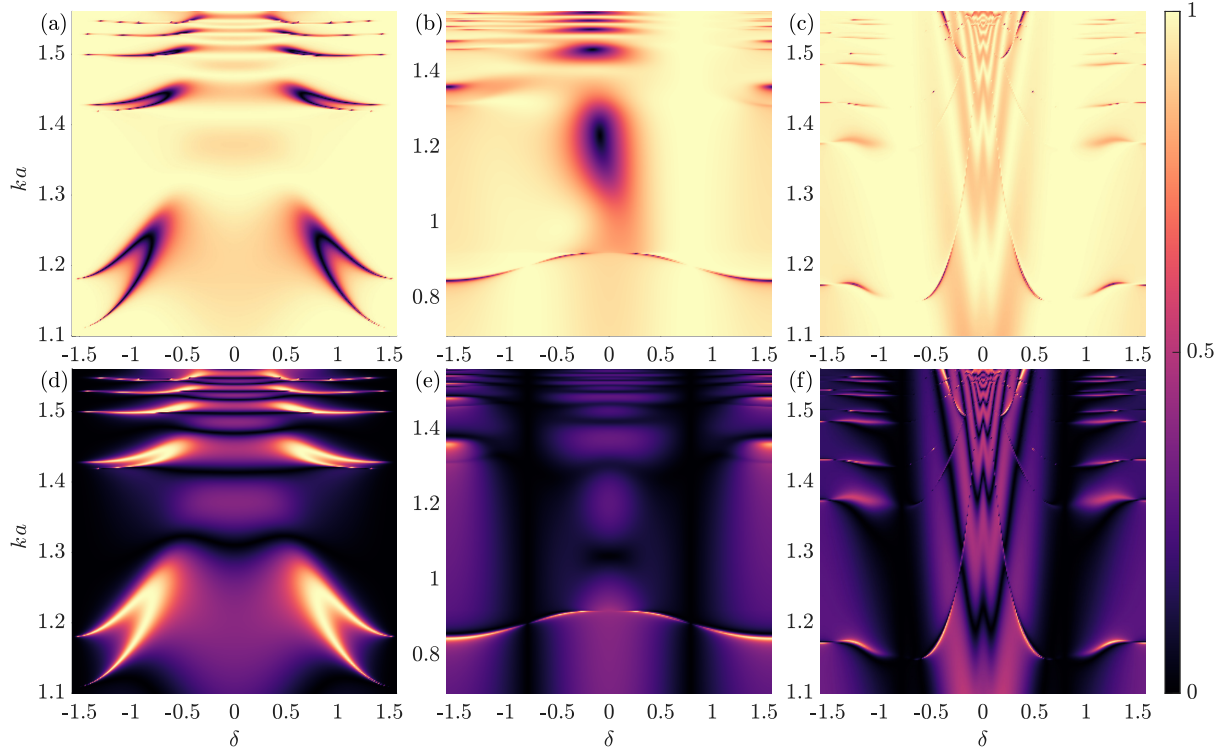


Figure 5.2: Phase-space portraits delineating $|\bar{T}_0|$ (top row) and $|\bar{R}_0|$ (bottom row) for which (a, d) $\psi_{\text{inc}} = \pi/2$ and $a = 0.25d$, (b, e) $\psi_{\text{inc}} = \pi/4$ and $a = 0.25d$ and (c, f) $\psi_{\text{inc}} = \pi/4$ and $a = 0.49d$. The symmetrical features are reminiscent of the Hofstadter butterfly [10, 11] that is generated by the angles δ .

of energy of the metagrating as expressed by the coefficients denoting the reflected and transmitted mode energies in the far-field. As was pointed out in [72] however condition (5.23) implies that R_n and T_n do not represent the physical quantities of reflection and transmitted mode energy, but rather coefficients that require rescaling by a 'normalising factor' to obtain:

$$\bar{R}_n = \sqrt{\frac{t_n}{t_0}} R_n, \quad \bar{T}_n = \sqrt{\frac{t_n}{t_0}} T_n \quad (5.24)$$

that therefore satisfy:

$$\sum_{n \in \mathcal{M}} (|\bar{R}_n|^2 + |\bar{T}_n|^2) = 1. \quad (5.25)$$

Equation (5.25) has been used to verify the correct computational implementation of the system formed by (5.12) and (5.13), and we observe sufficient convergence in computation

at wavenumbers up to $ka = \pi/2$ for $M \geq 20$ for which (5.25) is satisfied to 9 s.f.

We are now in a position to determine the far-field scattering behaviour of the meta-grating, and illustrate these results by providing portraits in phase-space of the rescaled coefficients (5.24) in Fig. 5.2. These phase portraits reveal the behaviour of the meta-grating as both δ and ka are varied, and therefore offer a more complete description of the scattering of wave energy. Beginning with Fig. 5.2(a, d), which respectively delineate $|\bar{T}_0|$ and $|\bar{R}_0|$ under $\psi_0 = \pi/2$ incidence, we provide the phase portrait in the space $\delta \in [-\pi/2, \pi/2]$ and $1.1 \leq ka < \pi/2$ (beneath which the wave undergoes little reflection, leaving the phase-space uniformly monochromatic) for a grating of uniform cylinder radius $a = 0.25d$. The immediate observation is that of symmetry about $\delta = 0$ as well as exact inversion between the portraits as the zeroth order mode is the only mode cut-on; this includes the expected result of transparency at $\delta = \pm\pi/2$, at which the metagrating permits perfect transmission at all wavenumbers. From panels (a, d) we also identify regions of perfect reflection $|\bar{R}_0| = 1$ that, to the authors' knowledge, do not occur for gratings of homogeneous, Neumann-type (be they perfect conductors in EM, sound-hard in acoustics, etc.) cylinders of any radius, cross-section or angle of incidence [89, 109, 112], with the exception being touching cylinders when $\psi_0 = \pi/2$ in Fig. 3 of [89]. In emphasising this result we take a horizontal slice of phase-space at $ka = 1.2$ over all δ and plot the reflection and transmission spectra in Fig. 5.3(a), making clear the points in the spectra at which there is perfect reflection. We plot an accompanying scattering computation illustrating perfect reflection in panel 5.3(b), for which the meta-grating is of finite size, consisting of $N = 101$ metacylinders of angle $\delta = 0.868$ (equation (5.5) is valid only in $r_0 < d$, and so in plotting the total field at distances $r_0 \geq d$ we resort to scattering by finite gratings). At this cylinder angle and wavenumber there is no visible propagation of wave energy into the region above the metagrating.

In addition, these portraits reveal symmetry in δ , and hence ψ_0 , as long as the wavenumber of incidence is below that of the cut-on wavenumber for higher-order modes. In Fig. 5.2 panels (b, e) the phase portraits of $|\bar{T}_0|$ and $|\bar{R}_0|$ are provided for $\psi_0 = \pi/4$ incidence on a grating of $a = 0.25d$, in the region $\delta \in [-\pi/2, \pi/2]$ and $0.7 \leq ka < \pi/2$. The same symmetry about $\delta = 0$ as Fig. 5.2(a, d) is exhibited until the cut-on wavenumber is reached at $ka \approx 0.92$ at which the $m = -1$ modes are cut-on. By once again making a slice along $ka = 1.2$ and plotting the reflection and transmission spectra for all δ in panel 5.3(c), which now additionally features $|\bar{R}_{-1}|$ and $|\bar{T}_{-1}|$, we can see how mode energies of different order compete for dominance in the phase-space. The point labelled d lies at the maximum of the $m = -1$ transmission curve, with corresponding wavefield (d)

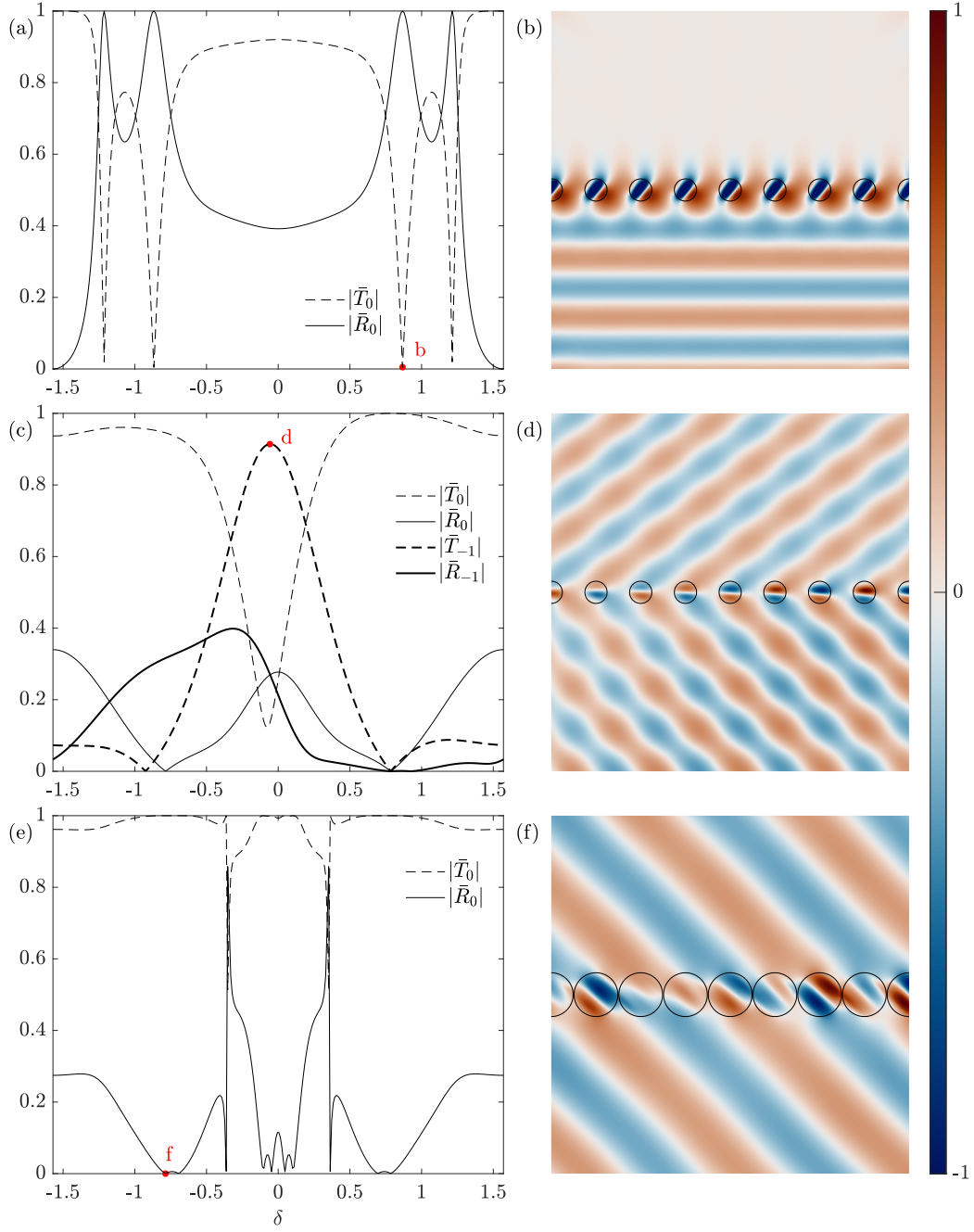


Figure 5.3: (a) Slice of phase-space at $ka = 1.2$ under $\psi_0 = \pi/2$ incidence on a grating of $a = 0.25d$. The wavefield (b), labelled in (a) at $\delta = 0.868$, is an example of perfect reflection of the incident plane-wave for which $|\bar{R}_0| = 1$. (c) Slice of phase-space at $ka = 1.2$ under $\psi_0 = \pi/4$ incidence on a grating of $a = 0.25d$. The wavefield (d), labelled in (c) at $\delta = -0.058$ delineates maximum transmission of the $|\bar{T}_{-1}|$ mode. (e) Slice of phase-space at $ka = 1.2$ under $\psi_0 = \pi/4$ incidence on a grating of $a = 0.49d$. The plane-wave undergoes perfect transmission at the point labelled (f), resembling a negative Goos-Hänchen shift [12] in the transmitted field.

demonstrating the ‘reversed’ transmission apparent in the total wavefield. This mode competitiveness accounts for the modulation of the wavefield in both the reflection and transmission regions, with the mode of largest magnitude dominating the image. At angles of incidence away from $\psi_0 = \pi/2$, the field distribution in and around each metacylinder need not be periodic as different metacylinders along the grating interact with different wavefronts at any instant in time.

With the onset of higher-order modes spoiling the perfect symmetry in phase-space, we look to gratings of a larger radius such that at all wavenumbers in $ka < \pi/2$ lie below the cut-on wavenumber. A grating of $a = 0.49d$, such that the cylinders are close to touching, retains its phase-space symmetry in this region, see Fig. 5.2(c, f), exhibiting perfect transmission at all wavenumbers at $\delta = -\psi_0$. To see how this is feasible, we refer the reader back to Fig. 4.5 and the observation therein that the scattered wave energy always points primarily along the direction perpendicular to δ , even when the angle of incidence is co-linear with this direction as in Fig. 4.5(a). With this picture in mind, the non-intuitive result of perfect transmission when $\delta = -\psi_0$ becomes obvious; any wave energy not scattered by the metagrating continues to point along ψ_0 , and any wave energy that is scattered by the metagrating points along the same direction. This perfect transmission at $\delta = -\psi_0$ can be observed in Fig. 5.3(e, f), and manifests as a negative translational shift in the transmitted field, or a Goos-Hänchen shift [12]. This can be likened to the waveshifting exhibited by Porter’s singly-periodic plate-array metamaterial [101], which allows for exact translation of a plane-wave across the metamaterial without scattering. The Goos-Hänchen shift has been observed in both TE and TM polarizations in subwavelength gratings of dielectric cylinders [113] (although in that case two neighbouring gratings were required to achieve the effect), as well as in TM polarization under reflection by a metallic saw-tooth grating [114], occurring near Wood anomalies and being associated with leaky surface waves. Goos-Hänchen shifting can also be observed along a metagrating of $a = 0.25d$ in Fig. 5.1(b), being imperfect due to competing higher-order modes.

The self-similar oscillatory patterns of Fig. 5.2, evident as $ka \rightarrow \pi/2$, can be likened to those of [100] Fig. 2 on the transmission and reflection of waves by a metamaterial cavity sharing a similar plate-array microstructure. Interestingly, the phase portraits’ symmetries share features to those seen in [11, 115] on localised modes in linear clusters of scatterers. The symmetric pattern is known as the Hofstadter butterfly [10], and is strictly defined as a region in phase-space absent of eigenmodes. In our case these regions instead illustrate areas in phase-space absent of transmitted or reflected modes

contributing to the far-field, and so we make this analogy between the two only lightly.

5.2.3 Tunable Rayleigh-Bloch Modes

Thus far solutions satisfying (5.3) have assumed that the Bloch wavenumber β is the incident wavenumber component along the grating, to the effect that $\beta < k$. If we relax this condition and insist $\beta > k$ then ψ_0 is no longer real by definition (5.11a) and the set $\mathcal{M} = \{\}$ such that there is no reflection or transmission in the directions perpendicular to the grating; all modes are evanescent modes and nothing propagates into the far-field. This regime describes solutions that satisfy continuity conditions (4.18) and (4.19) in the absence of an incident wave: the Rayleigh-Bloch modes. These modes manifest as the non-trivial solutions to the truncated system of equations formed by the following continuity conditions on the 0th cylinder:

$$\begin{aligned} & -b_p H_p(ka) - J_p(ka) \sum_{m \in \mathbb{Z}} b_m \sigma_{m-p}(\beta) \\ & + \frac{1}{2} e^{ip(\frac{\pi}{2}-\delta)} \sum_{n=0}^{\infty} (c_n (-1)^n + d_n (-1)^p) (J_{p-n}(ka) + J_{p+n}(ka)) = 0, \end{aligned} \quad (5.26)$$

$$\begin{aligned} & -b_p H'_p(ka) - J'_p(ka) \sum_{m \in \mathbb{Z}} b_m \sigma_{m-p}(\beta) \\ & + \frac{1}{2} e^{ip(\frac{\pi}{2}-\delta)} \sum_{n=0}^{\infty} (c_n (-1)^n + d_n (-1)^p) (J'_{p-n}(ka) + J'_{p+n}(ka)) = 0, \end{aligned} \quad (5.27)$$

which follow from conditions (5.12) and (5.13). The non-trivial solutions correspond to the zeros of the resulting grating matrix $\mathbf{M}$ or the matrix eigenvalues closest to zero, which are complex in this case and so we must solve for $\min(|\text{eig}(\mathbf{M})|) = 0$ i.e. the minimum absolute eigenvalue. This computation benefits from the small number of terms required by our multipole formalism for a converged solution. Additionally, the numerical stability of the grating matrix can be improved by redefining the multipole moments in (5.26) and (5.27) as in (4.38). For guided modes on infinite linear gratings of Neumann cylinders, RB wavenumbers have been shown to be real [103, 105], with an imaginary component being introduced only when a curvature is present in the periodic structure [66]. Thus we expect that the wavenumbers pertaining to RB modes for the metagrating to occur along the $\text{Re}\{k\}$ axis and with imaginary component equalling zero due to the exponential decay of the RB mode in the directions perpendicular to the grating axis.

It is clear from the periodicity condition (5.3) that we need only consider the range

$0 < \beta d \leq 2\pi$. Replacing βd with $2\pi - \beta d$ (representing a wave propagating in the opposite direction) in (5.6) we have $\sigma_{m-p}(2\pi - \beta d) = (-1)^{p-m} \sigma_{m-p}(\beta d)$ and find that

$$kd(2\pi - \beta d) = kd(\beta d), \quad (5.28)$$

such that we need only consider the range $0 < \beta d \leq \pi$. Similarly, if one considers a wave travelling along a grating of equal and opposite cylinder angle $\delta \rightarrow -\delta$ then by symmetry of the geometry,

$$kd(-\delta) = kd(\delta). \quad (5.29)$$

The dispersion curves relating β and k for gratings of equal and opposite cylinder angle will therefore be indistinguishable, and we need only consider the range $0 \leq \delta \leq \pi/2$. In computation we find that metagratings host RB modes at discrete values of k that satisfy

$$0 < kd < \beta d \leq \pi \quad (5.30)$$

for all βd values, with the exception of the grating at cylinder angles at and approaching $\delta = 0$ for which no RB modes are found to exist. The numerical method carried out to determine $\min(|\text{eig}(\mathbf{M})|) = 0$ goes as follows: find an initial guess for the Rayleigh-Bloch wavenumber by sweeping through $\text{Re}\{k\}$ in the range $0 < kd < \beta d$ for each $\beta d \in (0, \pi]$. The wavenumber corresponding to the smallest $\min(|\text{eig}(\mathbf{M})|)$ is subsequently fed to the built-in `Matlab` function `fsolve` that utilises the Levenberg-Marquardt algorithm to further minimise $\min(|\text{eig}(\mathbf{M})|)$, and returns the Rayleigh-Bloch wavenumber to a predefined tolerance.

At all cylinder angles in the range $\pi/36 \lesssim \delta \leq \pi/2$ we identify a Rayleigh-Bloch wavenumber beneath the light-line $k = \beta$ for any β , and provide the dispersion curves relating kd and βd in the range $\beta d \in (0, \pi]$ in Fig. 5.4 for (a) various δ and (b) various a (labelled). At any and all βd values the corresponding RB wavenumber approaches the light-line in 5.4(a) as $\delta \rightarrow 0$, dovetailing with Fig. 4.5 in showing that as there is no energy propagation along the δ direction, no RB modes may propagate when $\delta = 0$. Similarly as $a \rightarrow 0$ we observe a shift upwards of the RB bands in 5.4(b), as was the case for arrays of circular cylinders [103] of Neumann boundary condition. In both panels 5.4(a) and 5.4(b) all dispersion curves flatten at the band-edge where $\beta d = \pi$, being standing wave solutions with energy localised to the vicinity of the metacylinders.

For arrays of impermeable circular cylinders Rayleigh-Bloch modes are conventionally

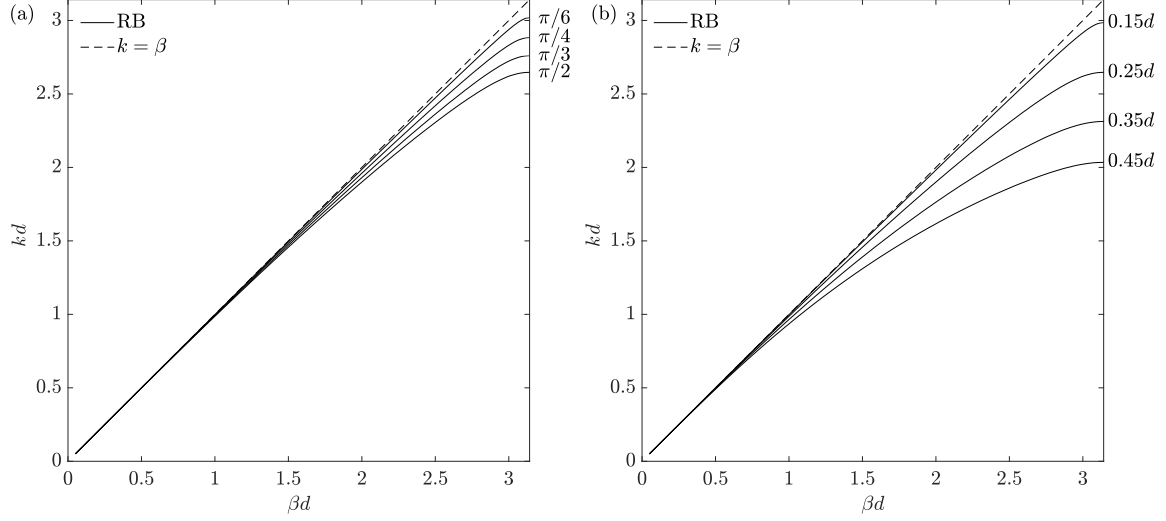


Figure 5.4: (a) RB dispersion bands belonging to a metagrating of radius $a = 0.25d$ at various cylinder angles δ (labelled). (b) RB dispersion bands belonging to a metagrating of $\delta = \pi/2$ at various radii (labelled).

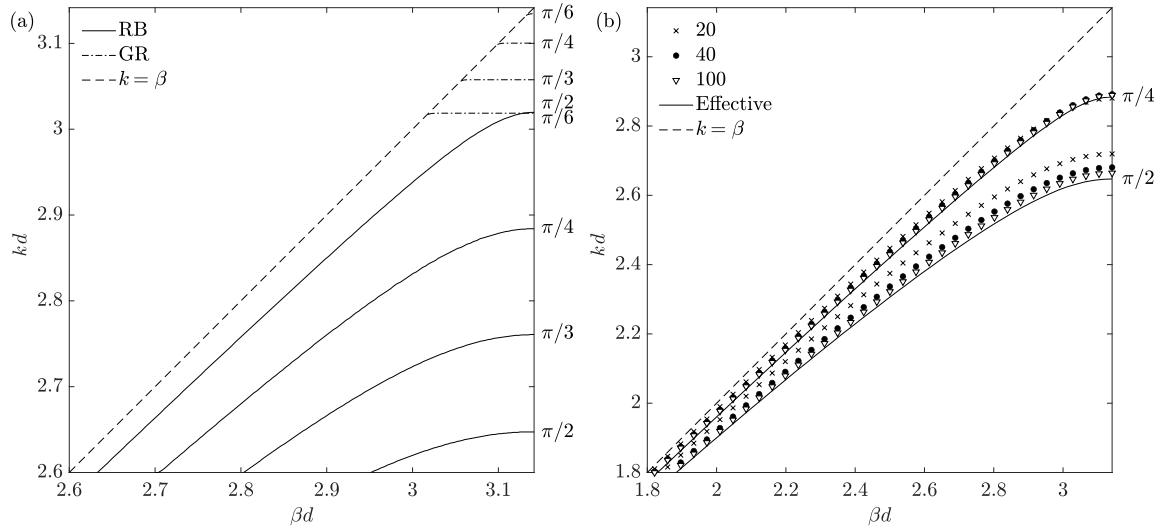


Figure 5.5: (a) Zoom-in of RB bands for $\beta d \in [2.6, \pi]$ with neighbouring grating resonances labelled by δ for a metagrating of uniform radius $a = 0.25d$. (b) Finite element computations (labelled with plate number) in comparison with the effective medium at two cylinder angles (labelled).

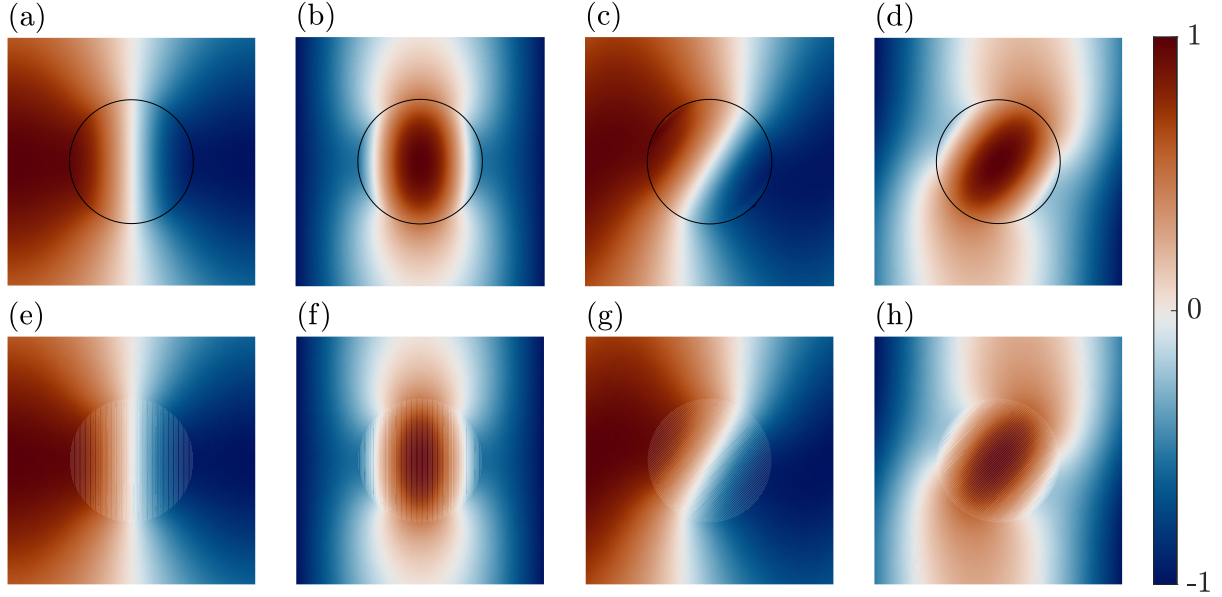


Figure 5.6: (a)-(d) Eigenfields corresponding to standing waves hosted by a metagrating of uniform $a = 0.25d$. (a) RB mode at $kd = 2.6475$ and $\beta d = \pi$ along a grating of $\delta = \pi/2$, paired with (b) a grating resonance along the flat-band at $kd = 3.0172$. Similarly (c, d) RB mode and grating resonance at (c) $kd = 2.8841$ and $\beta d = \pi$ and (d) $kd = 3.0996$ along a grating of cylinder angle $\delta = \pi/4$. (e)-(h) FEM calculations corresponding to standing waves hosted by a metagrating of uniform $a = 0.25d$, with metacylinders consisting of 100 evenly spaced plates. Wavenumbers βd equalling those of (a)-(d).

distinguished by the symmetry of their waveform [103], being symmetric or antisymmetric about the grating axis by virtue of the symmetry of the geometry. This distinction arises from the signs of the Fourier coefficients of the scattered field, with denotation [71]

$$b_m = \begin{cases} (-1)^m b_{-m} & \text{Symmetric} \\ -(-1)^m b_{-m} \text{ and } b_0 = 0 & \text{Antisymmetric.} \end{cases} \quad (5.31a) \quad (5.31b)$$

In the context of the herein metacylinders however, a discussion on symmetry is only meaningful in the instance $\delta = \pi/2$ ($\delta = 0$ being symmetric in geometry but devoid of permissible RB propagation), with all other angles exhibiting RB modes that lack any describable symmetry about the grating axis. In the special case of $\delta = \pi/2$ then we find only symmetric solutions satisfying (5.31a), with no antisymmetric solutions permitted even at cylinder radii approaching $a = 0.5d$. This represents a clear distinction to gratings of impermeable cylinders, themselves having been shown to exhibit antisymmetric RB modes when the cylinder radius $a \gtrsim 0.403d$ [71]. This discrepancy likely arises from the greater connectedness between the neighbouring regions of the metagrating, with

the interstitial channels between the plates being unable to host the requisite zero-field condition along $y = 0$ that is characteristic of antisymmetric modes [103]. Hence all RB solutions at cylinder angle $\delta = \pi/2$ are symmetric and satisfy (5.31a).

Conversely however there can be found an additional species of Rayleigh-Bloch modes satisfying (5.30) for all $\beta d \gtrsim 3.019$ for $\delta = \pi/2$ and $a = 0.25d$. These symmetric solutions lie along an (approximately) flat-band at $kd \simeq 3.0172$ with a group velocity near zero. Naturally this distinguishes them from the conventional RB modes which have a non-zero group velocity up to $\beta d = \pi$, at which the conventional RB modes are standing wave solutions by virtue of the flattening of the dispersion bands towards the band-edge. In waveform the two permitted solutions are distinguished by the position of maxima and minima in the fundamental cell, with maxima/minima at the cell boundaries being characteristic of the first species of RB modes, and maxima/minima within the effective medium for the flat-band grating resonances (GRs). These conditions rotate along with the effective medium, an effect illustrated in Fig. 5.6 in which we provide a gallery of RB and GR modes at $\delta = \pi/2$ and $\delta = \pi/4$. The flat-band grating resonance rises to larger kd like the Rayleigh-Bloch band as $\delta \rightarrow 0$ or $a/d \rightarrow 0$, always lying above the corresponding Rayleigh-Bloch band for any cylinder angle or radius. We provide both dispersion bands for a metagrating of radius $a = 0.25d$ in Fig. 5.5(a) at the same cylinder angles as in Fig. 5.4(a) (labelled). At larger cylinder radii, it is the case that the GRs are not necessarily standing waves in that their bands are not entirely flat, but may curve upwards or downwards close to the light-line. Multiple GR bands have also been observed to occur at $a = 0.45d$ and correspond to multiples of maxima/minima occurring within the effective medium, although this is not shown here.

We now check that the solutions computed by the above RB theory for the effective model translate into RB modes hosted by a metagrating of finite plate number and spacing. We make a comparison to a metagrating modelled with finite element method via software COMSOL Multiphysics [116], of constituent metacylinders of a finite number of plates, plate thickness and interstitial spacing. RB solutions are then computed by inserting a Bloch condition on the walls of the fundamental cell and performing a scan through wavenumber space, with the resulting predicted RB wavenumbers provided in Fig. 5.5(b), being the discrete sets of points superposed atop the continuous dispersion bands of the continuum model. The finite element computations are found to converge to those of the continuum model as the number of plates is increased, with solutions at smaller cylinder angle converging to the continuum model with a smaller number of plates than those of larger cylinder angle. The discrepancy between the FEM and the continuum model

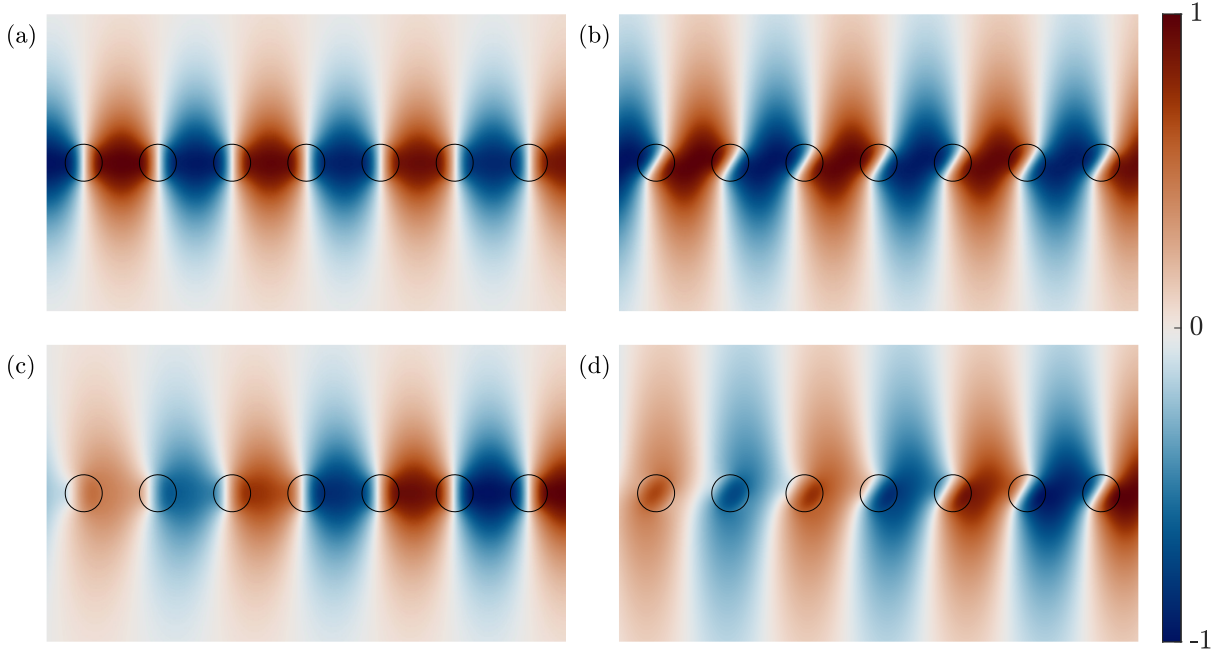


Figure 5.7: Standing (a, b) and propagating (c, d) RB modes along a grating of $a = 0.25d$, excited in a scattering simulation via a monopole line-source of wavenumbers (a) $kd = 2.6475$, $\delta = \pi/2$ and (b) $kd = 2.8841$, $\delta = \pi/4$, (c) $kd = 2.5993$, $\delta = \pi/2$ and (d) $kd = 2.7974$, $\delta = \pi/4$.

computations is largest towards the band-edge, with all FEM computations converging to one-another and the continuum model at smaller wavenumber. The close resemblance of the two methods validates the approximation of the metamaterial cylinder with the continuum model of Porter, and this confirmation is equivalently carried out by Zheng *et al.* through comparison of scattered wavefields [99]. Like Zheng, we point out that the continuum model is advantageous in that it offers a highly efficient method for the computation of wave scattering, and now additionally in the computation of the non-trivial solutions belonging to the grating.

In Fig. 5.6(a)-(d) we provide several eigenfields of the fundamental grating cell corresponding to standing wave solutions taken at the band-edges of Figs. 5.4 and 5.5. Each solution was retrieved from the nullspace of the grating matrix as the basis vector of smallest singular value, with constituent elements equalling the field coefficients. Figure. 5.6(a) depicts the RB wavefield at the band-edge of the $\delta = \pi/2$ curve of Fig. 5.4(a), and can be distinguished from the neighbouring grating resonance of 5.6(b) by the discrepancy in the waveforms between the two; the RB mode having a characteristic zero-field region bisecting the metacylinder and the grating resonance a characteristic maxima or min-

ima condition along the same line. This remains the case in panels (c) and (d), which in turn depict an RB modes and a grating resonance at $\delta = \pi/4$. This illustrates the fact that solutions (a, c), and similarly (b, d), of equal wavenumber βd , are equivalent solutions under rotation. These eigenfields should be compared to the neighbouring panels (e)-(h) which depict waveforms in the fundamental grating cell as calculated using a FEM implementation in COMSOL Multiphysics [116]. Metacylinders consisting of 100 plates of thickness $0.0005d$ and interstitial spacing $0.0045d$ are shown to host identical array-guided solutions, being of equal βd to those of panels (a)-(d).

Lastly, we demonstrate the excitation of RB modes in truncated metagratings in Fig. 5.7, retrieved by following the method set out in [71] of exciting RB modes along a finite grating by placing a monopole line-source of RB wavenumber at one end of the array and performing a scattering computation. We plot these scattered fields about the centroid of a grating of $N = 201$ metacylinders for gratings of Fig. 5.7(a, c) $\delta = \pi/2$ and 5.7(b, d) $\delta = \pi/4$. The standing wave field patterns 5.7(a, b) are dominated by the $|m| = 1$ expansion components which comprise approximately (a) 97.0% and (b) 94.9% of each image respectively, with the remaining leading order components $|m| = 0, 2, 3$ contributing (a) 0.5%, 0.5%, 0.5% and (b) 1.0%, 1.1%, 0.8%. Terms $|m| \neq 1$ contribute a growing percentage of the total field pattern as k falls away from the band-edge, as in 5.7(c, d), for which the $|m| = 1$ components contribute (c) 91.5% and (d) 85.3% respectively, with the remaining leading order components $|m| = 0, 2, 3$ contributing approximately (c) 3.5%, 3.6%, 0.4% and (d) 6.2%, 6.3%, 0.6% respectively. In all cases the sum of terms of $|m| \geq 4$ constitutes less than 0.02% of the total field. The close resemblance between the eigenfields of Fig. 5.6(a, c) to the scattered fields of Fig. 5.7(a, b) reaffirms that the RB theory is accurate in finding the array-guided modes, and that these modes are readily tuned through rotation of the uniform cylinder angle.

5.3 Remarks on Chapter 5

To summarise, we have developed the grating theory necessary to describe the scattering and guiding of light by an infinite metagrating of uniform cylinder angle and radius. Painting portraits in phase-space has revealed symmetries reminiscent of the Hofstadter butterfly, which here depicts regions of zero reflected or transmitted mode energies. Both the transparency to, and perfect reflection of, an incident plane-wave by a linear arrangement of non-touching scatterers are results that, to the authors' knowledge, cannot be found in the existing literature on singly-periodic gratings of two-dimensional scatterers

[72, 89, 109, 112]. We have also shown how the symmetry in phase-space manifests as a negative Goos-Hänchen shift in the transmitted field when $\delta = -\psi_{\text{inc}}$. Additionally, we have found that the metagrating hosts RB modes at all cylinder radii, with the dispersion of the RB modes contingent on the choice of both the uniform cylinder angle and radius. We have found that RB modes exist for all $0 < \beta d \leq \pi$, with the RB bands approaching the light-line as $\delta \rightarrow 0$ or $a/d \rightarrow 0$. Our RB theory has been shown to be in good agreement with FEM calculations, with RB wavenumbers as calculated by our FEM implementation approaching those of the continuum model as the number of plates inside a metacylinder is increased from 20 to 100; the smaller the δ , the fewer number of plates required to reach a convergence of FEM to RB theory. A second species of Rayleigh-Bloch solutions have also been found to exist along flat-bands in the band scheme at wavenumbers above those of the conventional Rayleigh-Bloch bands. The two permissible solutions are distinguished by the swapping of a zero-field condition in the fundamental cell.

We remark that in both the scattering and guiding of waves, the key variable in determining the wave interaction is the cylinder angle. Through uniform rotation of the constituent metacylinders it is possible to bring about all of the aforementioned wave interactions, and this bears testament to our claim that the metagrating behaves as a tunable structure. Indeed, the metagrating has the ability to host array-guided modes in a wide region of wavenumber space, as well as permit the antipodal phenomena of perfect transmission and perfect reflection, through just uniform rotation. This makes the metagrating considerably advantageous over gratings of impermeable cylinders that have no such degree of freedom, conventionally relying on altering the geometry itself to bring about novel wave effects. As the mathematical framework here is not unique to light, we foresee that metagratings in acoustics and water waves will exhibit analogous results.

6 Asymptotic Analysis of a Doubly-Periodic Plate-Array Crystal

This chapter consists of work published in [4], for which S. Guenneau performed the FEM computations plotted in Fig. 6.6. The asymptotic forms of the dipole matrix elements were determined using the methodology of C.G. Poulton, and B. Davies and R.V. Craster contributed to discussions of the model.

6.1 Introduction to Chapter 6

Composite materials can be treated as effectively continuous and homogeneous media when the characteristic cell, and hence the crystalline elements therein, are of a subwavelength scale. The long-range uniformity of the crystalline elements gives rise to effective properties at the macro-scale, a process not dissimilar to magnetism induced by the long-range ordering of magnetic dipoles. One such example is the classical photonic crystal of dielectric cylinders, for which the leading order estimate of the effective permittivity is given by the Lorentz-Lorenz formula [13, 117]. The same analysis can be applied to metamaterials, for which the uniformity of the constituent ‘meta-atoms’ gives rise to exotic effective properties. These include negative effective permeability μ_{eff} and a magnetic response [118], negative effective permittivity ε_{eff} [119], and hence left-handed materials [120–122]. These in turn have been proposed to facilitate a myriad of devices, including flat lenses [123], invisibility cloaks [124, 125] and a super-lens utilising all-angle negative refraction [126].

Of recent interest have been metamaterials that allow for a tunable response [127–129], particularly active metasurfaces that hold pixel-level programmability [130]. One such example are 2d crystals of meta-atoms of a multilayered cylindrical geometry [29, 131]. The hyperbolic metamaterial of [131] can be tuned to significantly enhance the scattering cross-section compared to a cylinder of homogeneous composition. Very recently, the

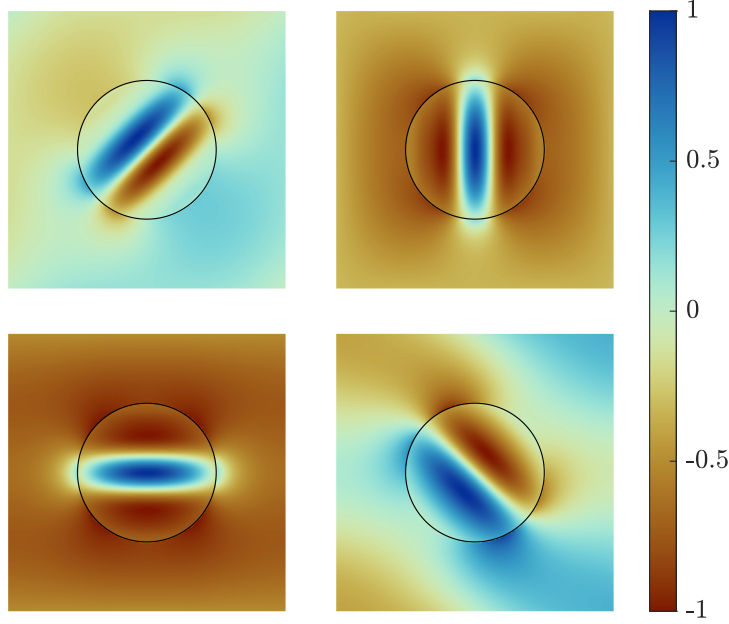


Figure 6.1: Longitudinal magnetic fields H_z of the plate-array crystal in the zeroth cell for different plate-array orientations, corresponding to the Eigenmodes of (6.37)-(6.38).

authors of [29] considered a crystal of metamaterial cylinders consisting of both graphene and multilayered metasurfaces, and were able to demonstrate a number of exotic features, including a tunable hyperbolic dispersion relation and a double negative response. In [29, 131] the tunability is demonstrated by changing the material parameters to modify the macroscopic response. The review articles [132, 133] discuss alternative methods for achieving tunability, including geometrical or structural tuning of the crystalline elements or unit cell. The macroscopic response of a composite metasurface depends on the size and orientation of its constituent elements, providing scope to alter the effective material parameters actively via mechanical adjustment. As pointed out in [133], such mechanical adjustments can be challenging because a physical mechanism is necessary to manipulate the crystalline elements. A number of methods have been proposed to do this, including mechanical deformation of an elastic substrate or matrix [134–137], whereas another uses pneumatic actuators [138]. Alternative methods include thermo-mechanical [139], electro-mechanical [140] and photo-responsive [141] control, among others.

In this chapter, we present an analysis of a 2D periodic medium that is composed of plate-array cylinders; see Fig. 6.1 for typical eigenmodes of the crystal and Fig. 6.2a for a 3D schematic. The analysis is performed in the quasistatic limit of vanishing wavenumber, such that the wavelength is much larger than the characteristic cell dimension. The acoustic mode is used to determine the homogenized properties of the crystal, and for

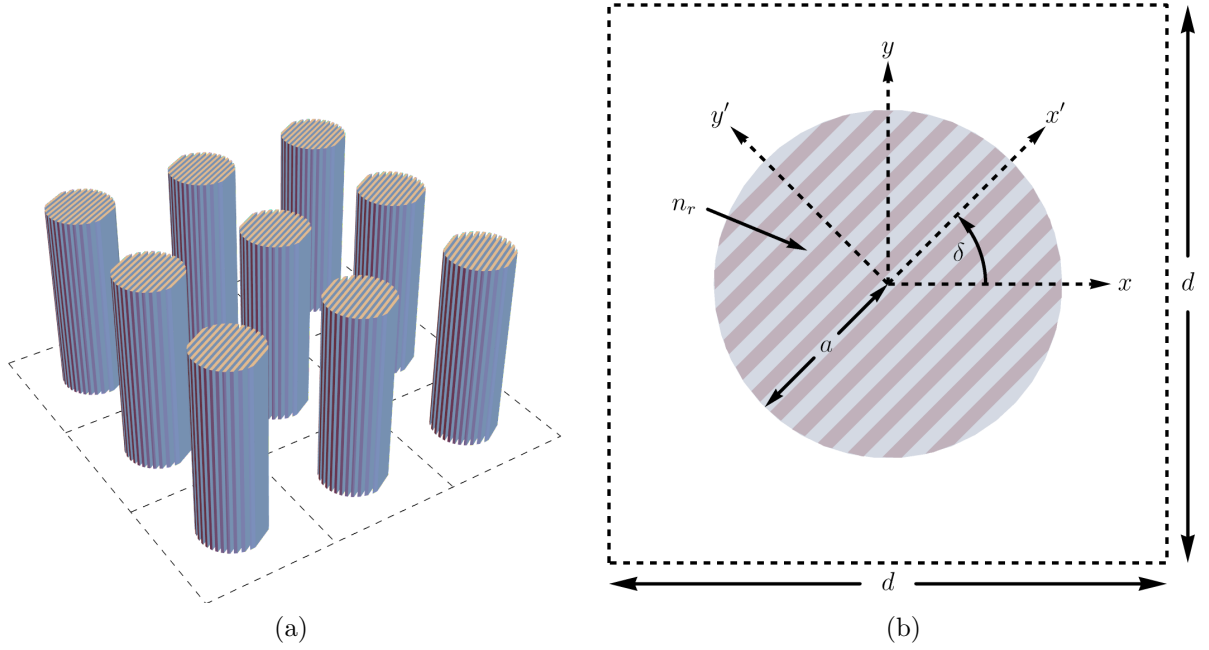


Figure 6.2: (a) A portion of the crystal consisting of plate-array metacylinders arranged in a square lattice. (b) Metacylinder geometry: plates depicted in dark gray and interstitial dielectric in light blue. Plate number and thickness are for illustrative purposes only.

this mode it is assumed that there exists a linear relationship $k \propto k_0$ as $k_0 \rightarrow 0$, where k is the wavenumber in the bulk exterior and k_0 is the Bloch wavenumber of the eigenmodes, as in [13, 142, 143]. The plate-array medium induces anisotropic dispersion of light through the crystal which, due to the long-range uniformity of the crystalline elements, manifests as an acoustic branch that is elliptical. The eccentricity of these elliptical solutions is a function of the effective permittivities along the principal crystalline axes; a result of the metacylinder favouring scattering in a direction perpendicular to the plate-array as in Fig. 4.5. Here it is shown that the effective electrical permittivity is a function of the crystalline filling fraction, the material contrast and, crucially, the difference in angle between the Bloch mode and the uniform plate-array. It is due to this angular dependence that we label this crystal a mechanically programmable metasurface.

This chapter is organised as follows: § 6.2 defines the structure of the periodic medium and the zeroth cell. The crystal is homogenized in § 6.3, in which the infinite system is truncated to form an 8×8 ‘dipole’ matrix. § 6.4 details the expansion of the dipole matrix determinant, from which a pair of Maxwell Garnett equations for the permittivity are recovered at leading order for the cases of no material contrast and non-unity material contrast. This is followed by comparison with numerics conducted using both a multipole

implementation and FEM computations. We state our conclusions in § 6.5. Appendix B provides the small wavenumber expansions of the dipole matrix elements.

6.2 The Infinite Lattice

The infinite lattice, depicted in Fig. 6.2a, consists of the plate-array metacylinders arranged periodically in the (x, y) plane. The metacylinders are of uniform radius a , uniform angle δ and are filled with interstitial dielectric of index n_r ; the zeroth cell is provided in Fig. 6.2b. Here we use the nomenclature that a *large* material contrast refers to $n_r \ll 1$ or $n_r \gg 1$, and a *small* material contrast refers to $n_r \approx 1$. We add that in homogenizing the periodic medium in the quasistatic limit, we will assume that the crystalline structure is dilute; this corresponds to the area fraction of the cylinders $f \ll 1$. In fact, we find that it is possible with our method to consider area fractions $f \leq 0.5$.

As along the diffraction grating, the periodicity of the lattice ensures that there exist solutions of Bloch-periodic form:

$$H_z^e(\mathbf{r} + \mathbf{R}_j) = H_z^e(\mathbf{r})e^{i\mathbf{k}_0 \cdot \mathbf{R}_j} \quad (6.1)$$

where $\mathbf{k}_0$ is the Bloch wavevector and:

$$\mathbf{R}_j = d(n, m), \quad n, m \in \mathbb{Z} \quad (6.2)$$

is the lattice vector delineating the positions $j = (n, m)$ of the infinite set of cylinders. Here $|\mathbf{R}_j| = R_j$ and $\arg\{\mathbf{R}_j\} = \phi_j$. At this stage one could make use of Graf's addition theorem to derive an expression for the total field, but for reasons that will become clear, we will first provide the Green's function for the infinite lattice in direct space. This Green's function is subject to the same Bloch-periodicity as the field, and is the solution to the Helmholtz equation:

$$(\nabla^2 + k^2)G_d(\mathbf{r}; \mathbf{r}') = \sum_j \delta(\mathbf{r} - \mathbf{r}' - \mathbf{R}_j)e^{i\mathbf{k}_0 \cdot (\mathbf{r} - \mathbf{r}')}, \quad (6.3)$$

such that:

$$G_d(\mathbf{r} + \mathbf{R}_j; \mathbf{r}') = G_d(\mathbf{r}; \mathbf{r}')e^{i\mathbf{k}_0 \cdot \mathbf{R}_j}. \quad (6.4)$$

As was the case in chapter 2, the Green's function of the infinite lattice is just the sum

over the Green's functions of each scatterer. Hence:

$$G_d(\mathbf{r}; \mathbf{r}') = \frac{1}{4i} \sum_j H_0(k|\mathbf{r} - \mathbf{r}' - \mathbf{R}_j|) e^{i\mathbf{k}_0 \cdot \mathbf{R}_j}. \quad (6.5)$$

Writing $\boldsymbol{\xi} = \mathbf{r} - \mathbf{r}'$ and noting that:

$$|\boldsymbol{\xi}| < |\mathbf{R}_j|, \quad \forall j \neq 0 \quad (6.6)$$

then from Graf's addition theorem:

$$H_0(k|\boldsymbol{\xi} - \mathbf{R}_j|) = \sum_{l \in \mathbb{Z}} H_l(kR_j) J_l(k\xi) e^{il(\phi_j - \vartheta)} \quad (6.7)$$

where $\boldsymbol{\xi} = (\xi, \vartheta)$. Thus:

$$G_d(\mathbf{r}; \mathbf{r}') = \frac{1}{4i} H_0(k\xi) + \frac{1}{4i} \sum_{l \in \mathbb{Z}} S_l(k, \mathbf{k}_0) J_l(k\xi) e^{-il\vartheta} \quad (6.8)$$

where the $j = 0$ term has been separated from the sum over $j \neq 0$ and

$$S_l(k, \mathbf{k}_0) = \sum_{j \neq 0} H_l(kR_j) e^{il\phi_j} e^{i\mathbf{k}_0 \cdot \mathbf{R}_j} \quad (6.9)$$

is the dynamic* lattice sum.

6.2.1 The Dynamic Lattice Sum

Like the grating sum (5.6) the dynamic lattice sum (6.9) is a sum over the change-of-basis functions $\forall j \neq 0$ multiplied by the Bloch-phase. The lattice sum converges very slowly in direct space, the terms being $\mathcal{O}(R_j)^{-1/2}$ [13]. There are several methods to go about computing faster converging forms of (6.9). One is to treat the 2d lattice as an infinite stack of 1d gratings [144, 145] and to sum over (5.6) using Eqs. (5.7)-(5.9) [31]. Another method, which is preferred here for its simplicity and ease of implementation, is to convert the sum over the direct lattice into a sum over the reciprocal lattice [13, 83, 146] which is rapidly convergent. The convergence of the reciprocal lattice sum can be accelerated by successive integrations as in [147][†].

*Being a function of k .

[†]This method of accelerating the convergence has been described by the authors as a 'dark art'.

To arrive to the lattice sum in reciprocal space, we begin by determining the reciprocal space Green's function. The sites $h = (n, m)$ in the reciprocal lattice are given by the set of reciprocal lattice vectors:

$$\mathbf{K}_h = \frac{2\pi}{d}(n, m), \quad n, m \in \mathbb{Z}. \quad (6.10)$$

Here $|\mathbf{K}_h| = K_h$ and $\arg\{\mathbf{K}_h\} = \theta_h$. The Green's function in the reciprocal domain can be written as the series expansion [146]:

$$G_r(\boldsymbol{\xi}) = \sum_h \tilde{g}(\mathbf{Q}_h) e^{i\mathbf{Q}_h \cdot \boldsymbol{\xi}} \quad (6.11)$$

where $\mathbf{Q}_h = \mathbf{K}_h + \mathbf{k}_0$. Now $G_r(\boldsymbol{\xi})$ remains subject to the Helmholtz equation (6.3), which has right-hand-side:

$$\sum_j \delta(\boldsymbol{\xi} - \mathbf{R}_j) e^{i\mathbf{k}_0 \cdot \mathbf{R}_j} = e^{i\mathbf{k}_0 \cdot \boldsymbol{\xi}} \sum_j \delta(\boldsymbol{\xi} - \mathbf{R}_j). \quad (6.12)$$

To proceed, we turn to the Poisson summation formula [13]:

$$\sum_j \delta(\boldsymbol{\xi} - \mathbf{R}_j) = \frac{1}{A} \sum_h e^{i\mathbf{K}_h \cdot \boldsymbol{\xi}}, \quad (6.13)$$

where A is the area of the unit cell. Hence:

$$\begin{aligned} e^{i\mathbf{k}_0 \cdot \boldsymbol{\xi}} \sum_j \delta(\boldsymbol{\xi} - \mathbf{R}_j) &= \frac{1}{A} e^{i\mathbf{k}_0 \cdot \boldsymbol{\xi}} \sum_h e^{i\mathbf{K}_h \cdot \boldsymbol{\xi}} \\ &= \frac{1}{A} \sum_h e^{i\mathbf{Q}_h \cdot \boldsymbol{\xi}}. \end{aligned} \quad (6.14)$$

Placing (6.14) along with (6.11) into the Helmholtz equation (6.3) gives:

$$\sum_h (k^2 - Q_h^2) \tilde{g}(\mathbf{Q}_h) e^{i\mathbf{Q}_h \cdot \boldsymbol{\xi}} = \frac{1}{A} \sum_h e^{i\mathbf{Q}_h \cdot \boldsymbol{\xi}} \quad (6.15)$$

from which we can identify the reciprocal form of the Green's function:

$$G_r(\boldsymbol{\xi}) = -\frac{1}{A} \sum_h \frac{e^{i\mathbf{Q}_h \cdot \boldsymbol{\xi}}}{Q_h^2 - k^2}. \quad (6.16)$$

The task now is to equate the direct and reciprocal space representations of the Green's

function. First, it is sensible to rewrite (6.16) in the same special functions as its direct counterpart:

$$G_r(\boldsymbol{\xi}) = -\frac{1}{A} \sum_{l \in \mathbb{Z}} \sum_h \frac{i^l J_l(Q_h \xi) e^{il(\theta_h - \vartheta)}}{Q_h^2 - k^2} \quad (6.17)$$

where we have made use of the Jacobi-Anger identity (A.7). Equating (6.17) and (6.8) we have:

$$\begin{aligned} \frac{1}{4i} H_0(k\xi) + \frac{1}{4i} \sum_{l \in \mathbb{Z}} S_l(k, \mathbf{k}_0) J_l(k\xi) e^{-il\vartheta} \\ = -\frac{1}{A} \sum_{l \in \mathbb{Z}} \sum_h \frac{i^l J_l(Q_h \xi) e^{il(\theta_h - \vartheta)}}{Q_h^2 - k^2}, \end{aligned} \quad (6.18)$$

then by equating powers of $e^{i\vartheta}$ we obtain the rapidly convergent form of the lattice sum:

$$S_l(k, \mathbf{k}_0) J_l(k\xi) = -H_0(k\xi) \delta_{l,0} - \frac{4}{A} i^{l+1} \sum_h \frac{J_l(Q_h \xi)}{Q_h^2 - k^2} e^{il\theta_h} \quad (6.19)$$

which converges as $\mathcal{O}(Q_h)^{-5/2}$ [146]. Note that (6.19) is valid for $l \geq 0$ and applies for a 2d lattice of any shape; we need only define the appropriate lattice vectors in direct and reciprocal space. We can simplify (6.19) by noting $H_l(x) = J_l(x) + iY_l(x)$ and rewriting the lattice sum as:

$$S_l = S_l^J + iS_l^Y, \quad (6.20)$$

where:

$$S_l^J(k, \mathbf{k}_0) = \sum_{j \neq 0} J_l(kR_j) e^{il\phi_j} e^{i\mathbf{k}_0 \cdot \mathbf{R}_j} \quad (6.21)$$

$$S_l^Y(k, \mathbf{k}_0) = \sum_{j \neq 0} Y_l(kR_j) e^{il\phi_j} e^{i\mathbf{k}_0 \cdot \mathbf{R}_j}. \quad (6.22)$$

Eq. (6.21) is often referred to as a Bessel series and Eq. (6.22) as a Neumann series. To evaluate the Bessel series we again turn to the Poisson summation formula [146]:

$$\sum_j e^{i\mathbf{R}_j \cdot \mathbf{s}} = \frac{(2\pi)^2}{A} \sum_h \delta(\mathbf{s} - \mathbf{K}_h) \quad (6.23)$$

where $\mathbf{s} = \mathbf{k} + \mathbf{k}_0$. In the first Brillouin zone $\mathbf{s} \neq \mathbf{K}_h$, $\forall h$ as long as $\mathbf{s} \neq \mathbf{0}$, hence:

$$\sum_j e^{i\mathbf{R}_j \cdot \mathbf{s}} = 0. \quad (6.24)$$

Using the Jacobi-Anger identity (A.7) we find:

$$\sum_j \sum_{l \in \mathbb{Z}} i^l J_l(kR_j) e^{il(\phi_j - \theta)} e^{i\mathbf{k}_0 \cdot \mathbf{R}_j} = 0 \quad (6.25)$$

or:

$$\sum_{j \neq 0} \sum_{l \in \mathbb{Z}} i^l J_l(kR_j) e^{il(\phi_j - \theta)} e^{i\mathbf{k}_0 \cdot \mathbf{R}_j} = -1. \quad (6.26)$$

Integrating over $\theta \in [0, 2\pi]$ we obtain:

$$S_l^J(k, \mathbf{k}_0) = -\delta_{l,0}, \quad (6.27)$$

and placing this into (6.19) we find that the lattice sums S_l^Y are of the form:

$$S_l^Y(k, \mathbf{k}_0) J_l(k\xi) = -Y_0(k\xi) \delta_{l,0} - \frac{4}{A} i^l \sum_h \frac{J_l(Q_h \xi)}{Q_h^2 - k^2} e^{il\theta_h}. \quad (6.28)$$

The convergence of (6.28) can be accelerated by successive integrations over the variable ξ , as in [146, 147]. Using the recurrence formulae [148]:

$$\int_0^\eta \xi^{l+1} J_l(k\xi) d\xi = \eta^{l+1} \frac{J_{l+1}(k\eta)}{k} \quad (6.29)$$

$$\int_0^\eta \xi^{l+1} Y_l(k\xi) d\xi = \eta^{l+1} \frac{Y_{l+1}(k\eta)}{k} + \frac{2^{l+1} l!}{\pi k^{l+2}}. \quad (6.30)$$

then after p integrations:

$$\begin{aligned} S_l^Y(k, \mathbf{k}_0) J_{l+p}(k\xi) = & \left[Y_p(k\xi) + \frac{1}{\pi} \sum_{n=1}^p \frac{(p-n)!}{(n-1)!} \left(\frac{2}{k\xi} \right)^{p-2n+2} \right] \delta_{l,0} \\ & - \frac{4}{A} i^l \sum_h \left(\frac{k}{Q_h} \right)^p \frac{J_{l+p}(Q_h \xi)}{Q_h^2 - k^2} e^{il\theta_h}. \end{aligned} \quad (6.31)$$

Numerically we have set $p = 5$, which ensures that the sums converge rapidly with terms of order $\mathcal{O}(Q_h)^{-15/2}$ as Q_h grows large [13].

Lastly, the following relation of S_l^Y can be seen from (6.9):

$$S_{-l}^Y = S_l^{Y*} \quad (6.32)$$

where $*$ denotes the complex conjugate. This is an extremely useful formula, as we need

only compute lattice sums of positive order.

6.2.2 Analogue to the Rayleigh System

We can derive a system of equations for the infinite lattice which is analogous to the so-called ‘Rayleigh identity’ for cylinders of dielectric or metallic composition [13]. Substituting the local scattered field (3.73) into (6.1) we arrive to the following condition on the multipole moments:

$$b_{j,m} = b_m e^{i\mathbf{k}_0 \cdot \mathbf{R}_j} \quad (6.33)$$

as was the case for the infinite diffraction grating Eq. (5.3), where $b_m \equiv b_{0,m}$ refers to the zeroth cell of coordinates (r, θ) . Separating the $j = 0$ and $j \neq 0$ terms in the Wijngaard formula (3.77) and applying the addition theorem, the total field in the absence of incident radiation in the exterior domain is:

$$H_z^e(k, \mathbf{r}) = \sum_{m \in \mathbb{Z}} b_m H_m(kr) e^{im\theta} + \sum_{m \in \mathbb{Z}} b_m \sum_{q \in \mathbb{Z}} S_{m-q} (-1)^{m-q} J_q(kr) e^{iq\theta}, \quad (6.34)$$

which, having deduced (6.20) and (6.27), can be simplified to:

$$H_z^e(k, \mathbf{r}) = \sum_{m \in \mathbb{Z}} i b_m Y_m(kr) e^{im\theta} + \sum_{m \in \mathbb{Z}} i b_m \sum_{q \in \mathbb{Z}} S_{m-q}^Y (-1)^{m-q} J_q(kr) e^{iq\theta}. \quad (6.35)$$

The continuity conditions across the zeroth cylinder are, from (4.18) and (4.19):

$$H_z^e = H_z^i \quad \text{on} \quad r = a, \quad (6.36a)$$

$$\frac{\partial H_z^e}{\partial r} = \cos(\theta - \delta) \frac{1}{n_r^2} \frac{\partial H_z^i}{\partial x'} \quad \text{on} \quad r = a. \quad (6.36b)$$

Substitution of (6.35) and (4.16) into (6.36a) and (6.36b) we arrive to:

$$ib_p \frac{Y_p(ka)}{J_p(ka)} + \sum_{m \in \mathbb{Z}} ib_m S_{m-p}^Y (-1)^{m-p} - \frac{1}{2} e^{ip(\frac{\pi}{2}-\delta)} \sum_{n=0}^{\infty} (c_n (-1)^n + d_n (-1)^p) \frac{J_{p-n}(n_r ka) + J_{p+n}(n_r ka)}{J_p(ka)} = 0, \quad (6.37)$$

$$ib_p \frac{Y'_p(ka)}{J'_p(ka)} + \sum_{m \in \mathbb{Z}} ib_m S_{m-p}^Y (-1)^{m-p} - \frac{1}{2} e^{ip(\frac{\pi}{2}-\delta)} \sum_{n=0}^{\infty} (c_n (-1)^n + d_n (-1)^p) \frac{J'_{p-n}(n_r ka) + J'_{p+n}(n_r ka)}{n_r J'_p(ka)} = 0. \quad (6.38)$$

Here, the prime refers to the derivative with respect to the radial coordinate. The first two terms in both (6.37) and (6.38) resemble the Rayleigh system under Dirichlet and Neumann boundary conditions, respectively [13, 149]. The system formed by Eqs. (6.37) and (6.38) is truncated as $(m, p) \in [-M-1, \dots, M]$ and $n \in [0, \dots, M]$ where M is the truncation point of the multipole and Chebyshev expansions, so as to arrive to a system of equations of dimension $(4M+4)$. Setting the determinant of the truncated system to zero recovers the dispersion relation between k and k_0 .

6.3 Dipole Approximation

6.3.1 The Dipole System

Under the assumption that the crystal is dilute it is reasonable to approximate the solutions (6.35) and (4.16) by the first few terms in their respective expansions. Truncating (6.37) and (6.38) at $M = 1$ we are left with only the $(m, p) \in [-2, -1, 0, 1]$ and $n \in [0, 1]$ terms (we retain one quadrupole moment to ensure that the matrix is square), which

form the following 8×8 system of equations:

$$\mathbf{T} := \left(\begin{array}{cccc|cccc} M_2 + S_0^Y & -S_1^Y & S_2^Y & -S_3^Y & C_{-2,0} & C_{-2,1} & D_{-2,0} & D_{-2,1} \\ -S_1^{Y*} & M_1 + S_0^Y & -S_1^Y & S_2^Y & C_{-1,0} & C_{-1,1} & D_{-1,0} & D_{-1,1} \\ S_2^{Y*} & -S_1^{Y*} & M_0 + S_0^Y & -S_1^Y & C_{0,0} & C_{0,1} & D_{0,0} & D_{0,1} \\ -S_3^{Y*} & S_2^{Y*} & -S_1^{Y*} & M_1 + S_0^Y & C_{1,0} & C_{1,1} & D_{1,0} & D_{1,1} \\ \hline M'_2 + S_0^Y & -S_1^Y & S_2^Y & -S_3^Y & C'_{-2,0} & C'_{-2,1} & D'_{-2,0} & D'_{-2,1} \\ -S_1^{Y*} & M'_1 + S_0^Y & -S_1^Y & S_2^Y & C'_{-1,0} & C'_{-1,1} & D'_{-1,0} & D'_{-1,1} \\ S_2^{Y*} & -S_1^{Y*} & M'_0 + S_0^Y & -S_1^Y & C'_{0,0} & C'_{0,1} & D'_{0,0} & D'_{0,1} \\ -S_3^{Y*} & S_2^{Y*} & -S_1^{Y*} & M'_1 + S_0^Y & C'_{1,0} & C'_{1,1} & D'_{1,0} & D'_{1,1} \end{array} \right) \begin{pmatrix} b_{-2} \\ b_{-1} \\ b_0 \\ b_1 \\ c_0 \\ c_1 \\ d_0 \\ d_1 \end{pmatrix} = \mathbf{0}. \quad (6.39)$$

Here, the following quantities have been defined:

$$M_p = \frac{Y_p(ka)}{J_p(ka)}, \quad M'_p = \frac{Y'_p(ka)}{J'_p(ka)}, \quad (6.40a)$$

$$\{C_{p,n}, D_{p,n}\} = \mathcal{I}_{p,n} \frac{J_{p-n}(n_r ka) + J_{p+n}(n_r ka)}{2J_p(ka)}, \quad (6.40b)$$

$$\{C'_{p,n}, D'_{p,n}\} = \mathcal{I}_{p,n} \frac{J'_{p-n}(n_r ka) + J'_{p+n}(n_r ka)}{2n_r J'_p(ka)}, \quad (6.40c)$$

where:

$$\mathcal{I}_{p,n} = (-1)^{\{n,p\}} i^{p+1} e^{-ip\delta}. \quad (6.41)$$

M_p and M'_p are the boundary coefficients, akin to Eq. (3.87) for the infinite conductor, and $C_{p,n}$, $C'_{p,n}$, $D_{p,n}$ and $D'_{p,n}$ are the interior coefficients. Examining (6.40a) it is clear from the Bessel function relations [150] that $M_{-p} = M_p$ and $M'_{-p} = M'_p$. Lattice sums of a negative order have been replaced by the complex conjugate of lattice sums of positive order by (6.32).

6.3.2 Homogenization

In homogenizing an isotropic medium the standard approach [13, 28, 143, 151–153] is to examine the behaviour of the lowest wavenumber band in the limit $k_0 \rightarrow 0$, for which it is assumed that there exists a proportionality between the bulk exterior wavenumber and Bloch wavenumber of the form:

$$k = \alpha k_0 \quad (6.42)$$

where $k_0 = |\mathbf{k}_0|$ and α is a scalar coefficient. The physical interpretation of α comes from a consideration of the phase difference across the unit cell [151], with a corresponding phase refractive index:

$$n_{eff} = \frac{1}{\alpha} \quad (6.43)$$

for which the label *effective* asserts that the periodic medium can be described as effectively continuous with macroscopic material parameter n_{eff} . Thus,

$$k = \frac{1}{n_{eff}} k_0. \quad (6.44)$$

The form of α , and hence n_{eff} , is deduced by utilising the following expansion [117]:

$$\alpha = \alpha_0 + \alpha_2(k_0 d)^2 + \mathcal{O}(k_0 d)^4 \quad (6.45)$$

where classically the leading order term α_0 encapsulates the dependence on the area fraction f of the cylinders, or the dielectric contrast across the cylindrical surface [13]. α_2 specifies the wavenumber dependence of α and provides the first dynamic correction term to the medium's effective permittivity. At finite frequency this dependence is assumed to be quadratic, hence $\alpha_1 = 0$. Herein we seek to determine only the leading order term α_0 and hence only the leading order effective permittivity in the form of a Maxwell Garnett equation.

For an anisotropic medium on the other hand, the meaning of α is connected with the definition of the effective dielectric tensor, which when diagonalized along the principal axes is of the form:

$$\boldsymbol{\varepsilon}_{eff} = \begin{pmatrix} \varepsilon_1 & 0 \\ 0 & \varepsilon_2 \end{pmatrix} \quad (6.46)$$

where ε_1 and ε_2 are the principal permittivities of the crystal. Assuming that the material is magnetically isotropic, (6.46) can be recast in terms of an effective refractive index tensor:

$$\mathbf{n}_{eff} = \begin{pmatrix} n_1 & 0 \\ 0 & n_2 \end{pmatrix} \quad (6.47)$$

where n_1 and n_2 are the principal refractive indices of the crystal such that $n_1 = \sqrt{\varepsilon_1}$, $n_2 = \sqrt{\varepsilon_2}$. The relationship (6.44) in vector form is:

$$\mathbf{k} = \mathbf{n}_{eff}^{-1} \mathbf{k}_0 = \begin{pmatrix} \frac{1}{\sqrt{\varepsilon_1}} & 0 \\ 0 & \frac{1}{\sqrt{\varepsilon_2}} \end{pmatrix} \mathbf{k}_0. \quad (6.48)$$

To obtain an equation of the form (6.42) we take the magnitude of the left- and right-hand-sides:

$$|\mathbf{k}| = \left(\frac{1}{\varepsilon_1} \cos^2(\theta_0 - \delta) + \frac{1}{\varepsilon_2} \sin^2(\theta_0 - \delta) \right)^{\frac{1}{2}} |\mathbf{k}_0| = \alpha |\mathbf{k}_0| \quad (6.49)$$

where we have written the Bloch vector $\mathbf{k}_0$ as:

$$\mathbf{k}_0 = \begin{pmatrix} k_0 \cos(\theta_0 - \delta) \\ k_0 \sin(\theta_0 - \delta) \end{pmatrix}. \quad (6.50)$$

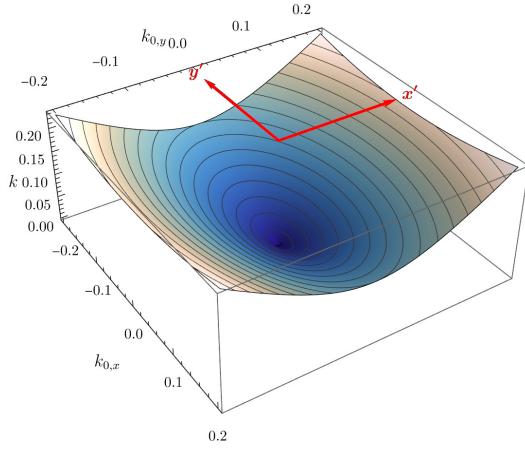
The definition (6.50) aligns the principal axes of the crystal with the rotated plate-array coordinates. Denoting the principal axes' directions as $1 \equiv x'$ and $2 \equiv y'$, then the principal permittivities can be recovered from (6.49) by choosing $\theta_0 = \delta$ for $\varepsilon_{x'}$ and $\theta_0 = \delta + \pi/2$ for $\varepsilon_{y'}$. The remaining challenge is to deduce the form of α by substitution of (6.49) into the dipole system (6.39), and examining the behaviour of $|\mathbf{T}| = 0$ in the limit $k_0 \rightarrow 0$, where $\mathbf{T}$ is the 8×8 matrix given in (6.39).

In determining the small k_0 expansion in α the coefficients (6.40) and lattice sums (6.28) require series expansions in small k and k_0 . The boundary coefficients (6.40a) occur for orders $p \in [0, 1, 2]$, for which the small k expansions are available in Appendix B.1. The interior coefficients (6.40b) and (6.40c) occur for orders $p \in [-2, \dots, 1]$, $n \in [0, 1]$, and like the boundary coefficients require small k expansions for ratios of Bessel functions. These can be found in Appendix B.2.

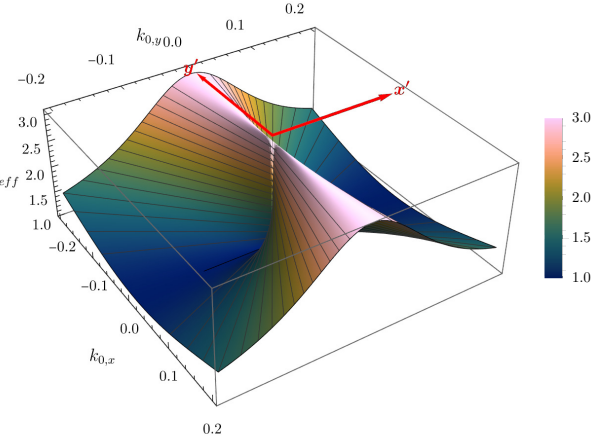
The method by which the lattice sums are approximated requires a series expansion of (6.28) to order k^0 for orders $l \in [0, \dots, 3]$. This involves separation of the $h = 0$ and $h \neq 0$ terms before using Graf's addition theorem [96] on the latter sum to yield an expansion in terms of k_0 . Subsequently, the method makes use of a set of recurrence relations for the lattice sums inherent in the expression to arrive to leading order approximations. This is carried out in Appendix B.3, and follows the method set out in [143].

6.4 Results

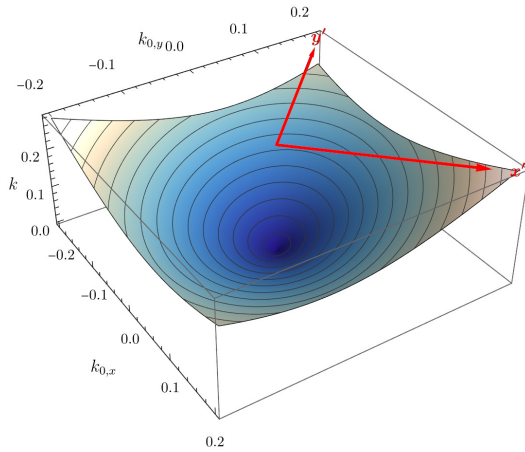
We seek the leading order terms for small k , k_0 in the expansion of $|\mathbf{T}| = 0$. This is achieved by implementing the approximations (B.1)-(B.4), (B.18), (6.49) and (6.45) into (6.39). Computing the determinant of this 8×8 matrix by hand is intractable, so we



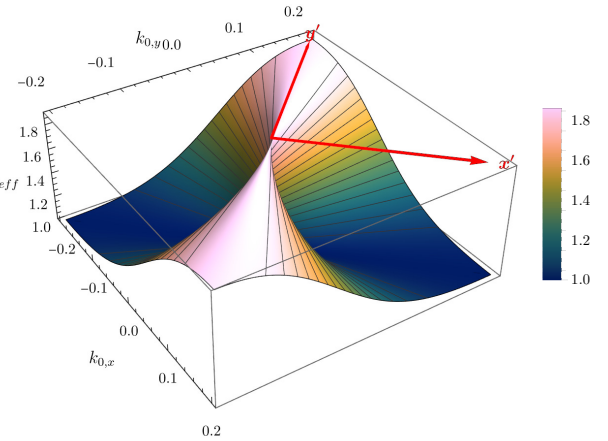
(a) $\delta = \frac{\pi}{2}$, $f = 0.5$, $e = 0.816$



(b) $\delta = \frac{\pi}{2}$, $f = 0.5$



(c) $\delta = \frac{\pi}{4}$, $f = 0.3$, $e = 0.679$



(d) $\delta = \frac{\pi}{4}$, $f = 0.3$

Figure 6.3: First dispersion surface $k = \alpha k_0$ and corresponding effective permittivity ε_{eff} for parameters (a, b) $\delta = \pi/2$, $f = 0.5$ and (c, d) $\delta = \pi/4$, $f = 0.3$ in the portion of the Brillouin zone $(k_{0,x}, k_{0,y}) \in [-0.2, 0.2]$. The eccentricity e is given by (6.56). Principal axes labelled in red.

make use of *Wolfram Mathematica* [154] to carry out the expansion of $|\mathbf{T}|$ analytically. By replacing a with the area fraction of the metacylinders f , according to $a = \sqrt{fd^2/\pi}$, then solving for α_0 we arrive at a Maxwell Garnett equation that describes the leading order behaviour of the crystal. We distinguish between the cases **A.** $n_r = 1$ and **B.** $n_r \neq 1$ in the following two sections, since the resulting effective material parameters take a much more elegant form in the first case.

6.4.1 The Case $n_r = 1$

In the case of $n_r = 1$ the leading order term in the expansion of $|\mathbf{T}|$ is of the form:

$$T_{-12} = \frac{2^{15} 3 e^{2i\delta} \pi^2 ((1+f)\alpha_0^2 - 1 - f \cos(2(\delta - \theta_0)))}{f^6 k_0^{12} d^{12} \alpha_0^{12} (\alpha_0^2 - 1)} \quad (6.51)$$

where T_ν denotes the $\mathcal{O}(k_0)^\nu$ term. Setting (6.51) to zero and solving for α_0 , we have:

$$\alpha_0 = \sqrt{\frac{1 + f \cos(2(\delta - \theta_0))}{1 + f}}. \quad (6.52)$$

The form of (6.52) makes clear that the anisotropy of the crystal is a leading order effect and is due to the interplay of the difference in incident and plate-array angles and the area fraction of the cylinders. We can also define an associated *scalar* effective permittivity:

$$\varepsilon_{eff}^0 = \frac{1 + f}{1 + f \cos(2(\delta - \theta_0))}. \quad (6.53)$$

Eq. (6.53) has the form of a Maxwell Garnett equation, and is related to the elements of the effective permittivity tensor by way of (6.49):

$$\varepsilon_{x'} = 1, \quad (6.54a)$$

$$\varepsilon_{y'} = \frac{1 + f}{1 - f}. \quad (6.54b)$$

Accordingly, light propagating through the crystal will find it to be transparent along the x' direction and will undergo refraction along the y' direction as a function of f . It is interesting to note that in this case the permittivity along the y' direction is the inverse of the scalar effective permittivity for an array of perfect magnetic conductors [13] (that is, cylinders with Dirichlet boundary conditions). Eqs. (6.54) correspond to the square

of the semi-minor and semi-major axes of the index ellipse [155]:

$$\frac{x'^2}{\varepsilon_{x'}} + \frac{y'^2}{\varepsilon_{y'}} = 1. \quad (6.55)$$

From this, we expect elliptical solutions for the dispersion of light with eccentricity:

$$e = \sqrt{\frac{2f}{1+f}} \quad (6.56)$$

which increases with larger area fraction f . Eq. (6.56) tends to zero as $f \rightarrow 0$, meaning isotropy is recovered at small area fraction because the scattering is so weak.

The anisotropy of the crystal is visualized by the first dispersion surfaces in Fig. 6.3 (a, c) and the corresponding effective permittivities in Fig. 6.3 (b, d) for parameters (a, b) $\delta = \pi/2$, $f = 0.5$ and (c, d) $\delta = \pi/4$, $f = 0.3$. Examining first the dispersion surfaces (a, c) we observe that the eccentricity of the elliptical surface contours falls from $e = 0.816$ when $f = 0.5$ to $e = 0.679$ when $f = 0.3$, a consequence of the scattering by the metacylinders being weaker at smaller area fraction. Complementary to these are the permittivity surfaces (b, d), which illustrate how the transport of light through the crystal is subject to its propagation direction, with the values along the x' and y' axes equalling those calculated by (6.54) i.e. transparent along x' and at a maximum along y' .

6.4.2 The Case $n_r \neq 1$

In the case of $n_r \neq 1$ the leading order term in the expansion of $|\mathbf{T}|$ is of the form:

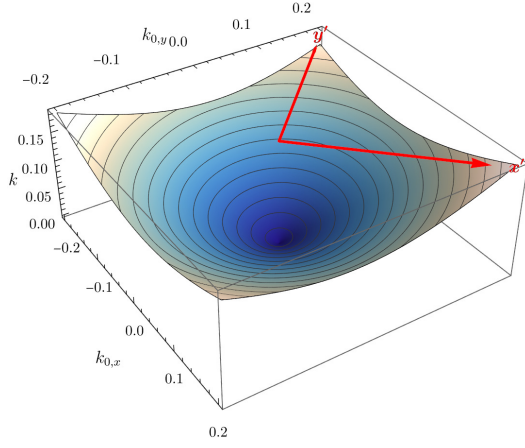
$$T_{-12} = \frac{2^{14}\pi^2 e^{2i\delta} (2n_r^2+1)(n_r^2(f^2-1)-f^2-1-2f\cos(2(\delta-\theta_0)))+(1+f)(n_r^2+1+f(n_r^2-1))\alpha_0^2}{n_r^2 f^6 k_0^{12} d^{12} \alpha_0^{12} (\alpha_0^2-1)}. \quad (6.57)$$

Setting this to zero and solving for α_0 gives:

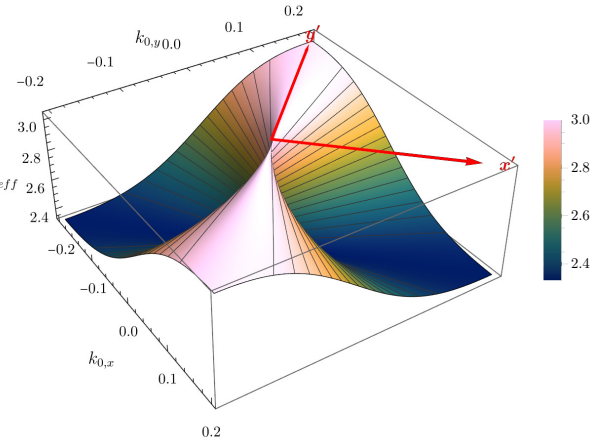
$$\alpha_0 = \sqrt{\frac{n_r^2 + 1 - f^2(n_r^2 - 1) + 2f\cos(2(\delta - \theta_0))}{n_r^2(1+f)^2 - f^2 + 1}}. \quad (6.58)$$

The corresponding Maxwell Garnett equation is:

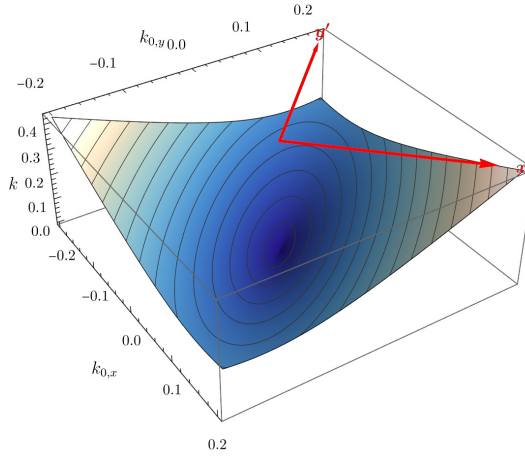
$$\varepsilon_{eff}^0 = \frac{n_r^2(1+f)^2 - f^2 + 1}{n_r^2 + 1 - f^2(n_r^2 - 1) + 2f\cos(2(\delta - \theta_0))}, \quad (6.59)$$



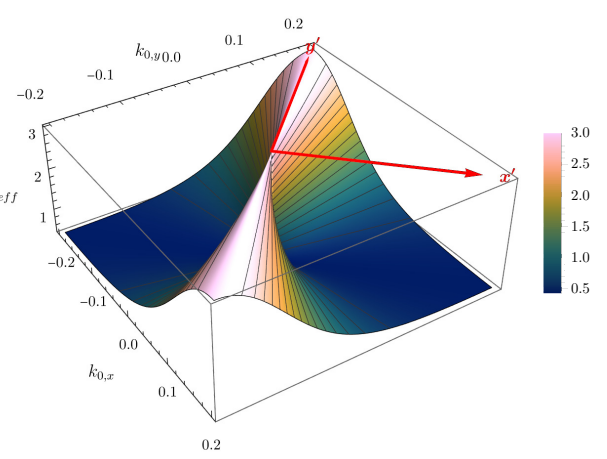
(a) $\delta = \frac{\pi}{2}$, $f = 0.5$, $n_r = 3$, $e = 0.471$



(b) $\delta = \frac{\pi}{2}$, $f = 0.5$, $n_r = 3$



(c) $\delta = \frac{\pi}{2}$, $f = 0.5$, $n_r = \frac{1}{3}$, $e = 0.926$



(d) $\delta = \frac{\pi}{2}$, $f = 0.5$, $n_r = \frac{1}{3}$

Figure 6.4: First dispersion surface $k = \alpha k_0$ and corresponding effective permittivity ε_{eff} for parameters $\delta = \pi/2$, $f = 0.5$ and (a, b) $n_r = 3$, (c, d) $n_r = 1/3$ in the portion of the Brillouin zone $(k_{0,x}, k_{0,y}) \in [-0.2, 0.2]$. The eccentricity e is given by (6.61). Principal axes labelled in red.

such that along the principal axes:

$$\varepsilon_{x'} = \frac{n_r^2(1+f)^2 - f^2 + 1}{n_r^2 + 1 - f^2(n_r^2 - 1) + 2f}, \quad (6.60a)$$

$$\varepsilon_{y'} = \frac{1+f}{1-f}. \quad (6.60b)$$

Eqs. (6.60) admit elliptical solutions of eccentricity:

$$e = \sqrt{\frac{4f}{(1+f)(n_r^2(1-f) + f + 1)}} \quad (6.61)$$

which trivially reduces to (6.56) when $n_r = 1$, as do Eqs. (6.58)-(6.60) reduce to their $n_r = 1$ counterparts. Note that due to the presence of n_r^2 in the denominator of (6.61) the eccentricity of the elliptical dispersion surfaces will fall for n_r increasing and rise for n_r decreasing. In other words, a lattice of large material contrast will tend to either the isotropic or anisotropic scattering of light depending on the composition of the interior material relative to that of the exterior. In fact, if we replace n_r^2 by:

$$n_r^2 = \frac{\tau + 1}{\tau - 1} \quad (6.62)$$

in (6.39), where $1/\tau$ represents the dielectric contrast across the interface between the interstitial dielectric and the exterior bulk, we arrive to:

$$\alpha_0 = \sqrt{\frac{\tau - f^2 + f(\tau - 1) \cos(2(\delta - \theta))}{(1+f)(f+\tau)}}. \quad (6.63)$$

Then along x' :

$$\varepsilon_{x'} = \frac{\tau + f}{\tau - f}, \quad (6.64)$$

and $\varepsilon_{y'} = (1+f)/(1-f)$ as before. Eq. (6.64) is of the form of the Lorentz-Lorenz or Clausius-Mossotti equation for an array of dielectric cylinders [13, 153] and obeys Keller's theorem [156]; by replacing τ with $-\tau$ we obtain $1/\varepsilon_{x'}$ along x' . Keller's theorem is not obeyed along any other direction due to the anisotropy induced by the plate-array, which is expressed through the $\cos(2(\delta - \theta))$ term at leading order.

The effects of a relatively small material contrast on the anisotropic dispersion of light is visualized in Fig. 6.4 for $\delta = \pi/2$ and $f = 0.5$ for normalised refractive index (a, b) $n_r = 3$ and (c, d) $n_r = 1/3$. Examining the dispersion surfaces Fig. 6.4(a, c) we note that the

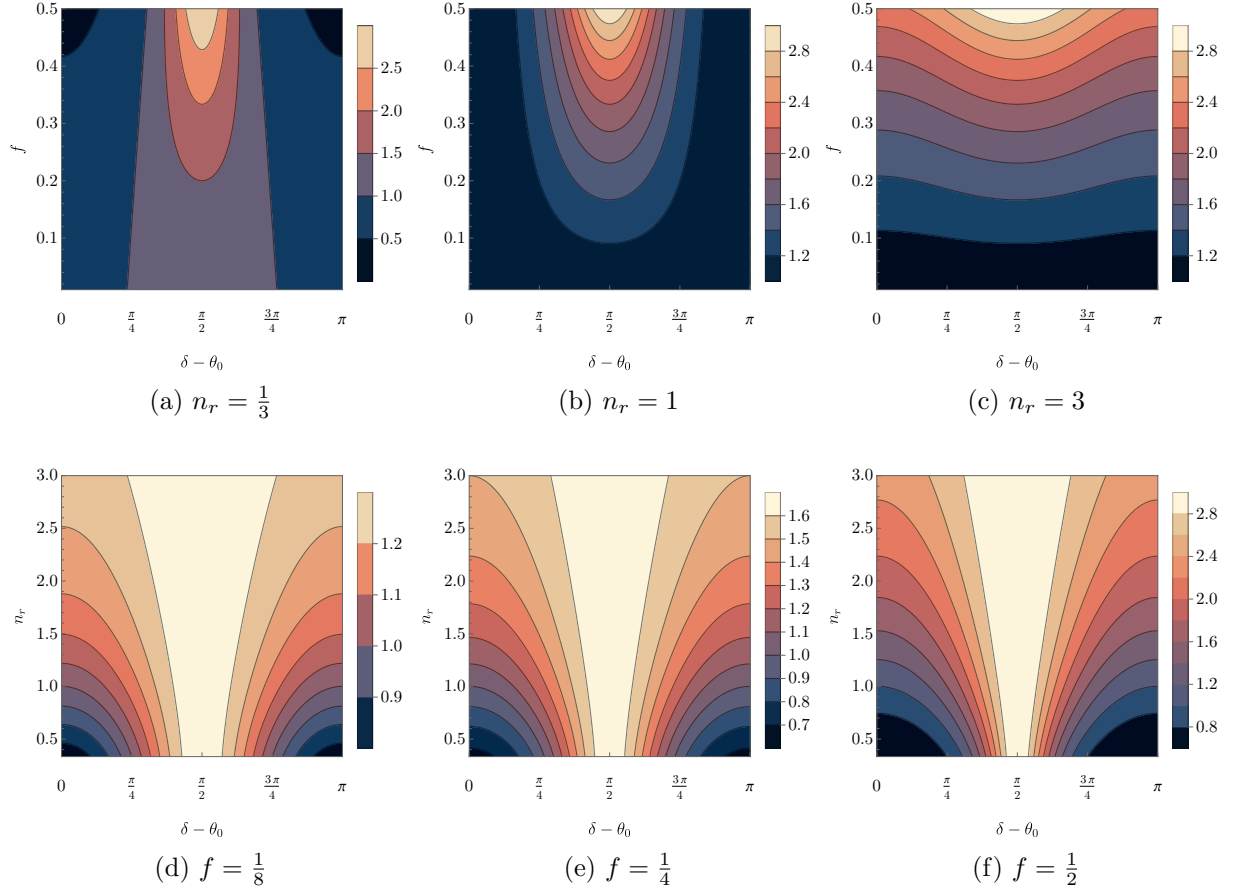


Figure 6.5: ε_{eff}^0 plotted as a function of (a-c) varying f and constant n_r (labelled) and (d-f) varying n_r and constant f (labelled). All solutions are symmetric by virtue of the $2 \cos(2(\delta - \theta_0))$ term in (6.59). Note the change in color-scale from panel to panel.

eccentricity has fallen in the case of $n_r = 3$ with respect to the result quoted in Fig. 6.3(a) under the same area fraction, and likewise increased with respect to the same result in the case of $n_r = 1/3$. The respective permittivity surfaces Fig. 6.4(b, d) illustrate the same effect, with the effective permittivity in Fig. 6.4(b) varying more smoothly between x' and y' than in Fig. 6.4(d). This parameter space is explored in Fig. 6.5 in which the effective permittivity, as approximated by the Maxwell Garnett equation (6.59), is plotted over the range of relative angle $\delta - \theta_0 \in [0, \pi]$ for varying (a-c) f and (d-f) n_r . These types of phase portraits are useful for visualising the steepness in the effective permittivity between the principal axes at $\delta - \theta_0 = 0$ and $\delta - \theta_0 = \pi/2$, and in this way illustrate the strength of the anisotropic scattering of light by the crystal. Panels Fig. 6.5(a-c) demonstrate how the eccentricity of the resulting elliptical dispersion surfaces falls as the relative refractive index is increased from $n_r = 1/3$ to $n_r = 3$, as the surface contours flatten and widen

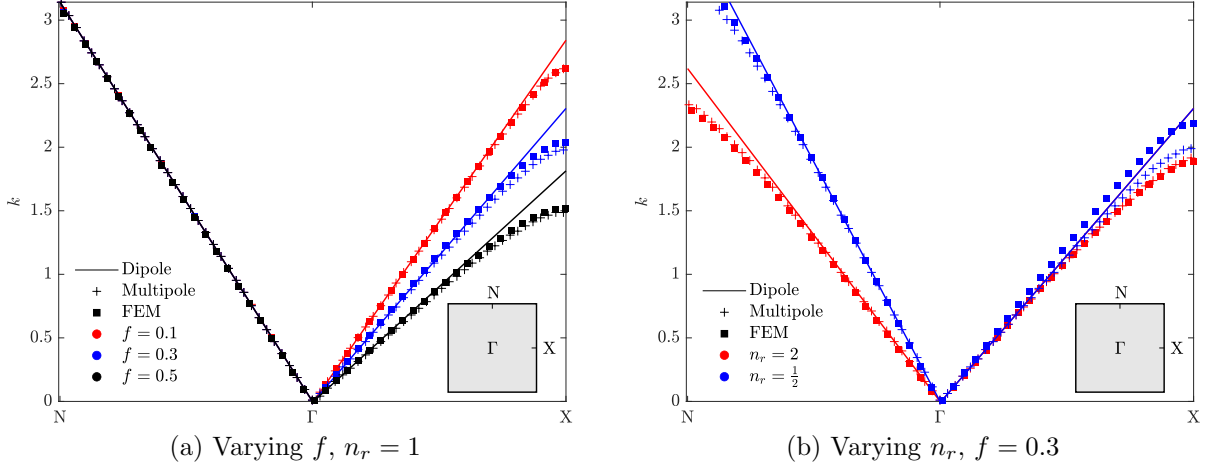


Figure 6.6: Acoustic bands for a plate-array cylinder of angle $\delta = \pi/2$. Shown are the linear Dipole approximations (6.52) and (6.58) (solid lines), the multipole system (6.37)-(6.38) (crosses) and FEM computations (squares).

across the angular range. Likewise in panels Fig. 6.5(d-f) an increase in the area fraction f gives rise to narrowing surface contours about $\delta - \theta_0 = \pi/2$.

6.4.3 Numerical Validation

In order to validate the leading order approximations (6.52), (6.58), we carry out a comparison between a numerical implementation of system (6.37)-(6.38) truncated at $M = 6$, and an FEM implementation in COMSOL Multiphysics [116]. Provided in Fig. 6.6a and 6.6b is the portion of the acoustic band along $N \rightarrow \Gamma \rightarrow X$ (see inset) for a plate-array cylinder aligned at angle $\delta = \pi/2$ such that the path within the Brillouin zone follows the principal crystalline axes. Panel (a) depicts the acoustic band as a function of f and panel (b) as a function of n_r . The FEM computations were carried out specifying a cylinder of 100 plates of plate thickness $w_p = a/100$ and inter-plate spacing $d_p = a/100$.

Overall there is good agreement between the leading order approximations and the multipole and FEM computations, particularly as $k, k_0 \rightarrow 0$. In the case of $n_r = 1$ (Fig. 6.6a) the approximation (6.52) is exact along $N \rightarrow \Gamma$ for which $\theta_0 = \delta$ and $\alpha_{x'} = 1$. On $\Gamma \rightarrow X$, $\theta_0 = \delta + \pi/2$ and $\alpha_{y'} \approx \sqrt{(1-f)/(1+f)}$. In this direction the divergence away from the linear increases as the area fraction approaches its maximum value of $f = 0.5$ (black line), for which the quasistatic approximation remains accurate until $k \approx 1$; even when the crystal is not dilute the quasistatic approximation remains a good estimation of the

acoustic band's gradient as $k_0 \rightarrow 0$.

In the case of $n_r \neq 1$ (Fig. 6.6b for which $f = 0.3$) the acoustic band along $N \rightarrow \Gamma$ is perturbed away from the light-line as the relative index is moved away from unity. The divergence between the linear and the multipole/FEM computations is also a function of the relative index, although in both cases shown the linear approximation remains accurate until $k \approx 2$. Along $\Gamma \rightarrow X$ the divergence between the quasistatic and multipole treatments can also be ascribed to the relative index, which plays a role exclusively in the higher order term α_2 along y' . In the case $n_r = 2$, although we approach the resonance at $k = 2.5416$, the acoustic band, as computed by the multipole method, converges to the FEM result at $M = 6$.

6.5 Remarks on Chapter 6

In this chapter we have presented a periodic medium of plate-array metacylinders which, in treating the plate-array as an effective medium, has been reduced to an elegant and computationally efficient semi-analytical formalism. The periodic structure comprises a mechanically tunable metamaterial wherein the principal axes' orientation is dictated by the uniform plate-array angle. A dipole system approximates the acoustic band as $k, k_0 \rightarrow 0$, for which a pair of leading order Maxwell Garnett equations describe the medium's principal effective permittivities in terms of the area fraction f and relative index n_r .

Although there is good agreement between the quasistatic approximations and multipole and FEM treatments, the leading order approximations fail to capture the wavenumber dependence of α . The higher order term α_2 is necessary to resolve the quadratic behaviour of the acoustic band at higher wavenumbers, as depicted in Fig. 6.6a and 6.6b. The determination of this higher order correction is left as an open problem.

7 Continuing Work

The work presented in this chapter constitutes several unfinished ideas that utilise topological concepts for actively tunable photonic phases. Some of the finer details have been omitted in favour of a broader overview of the necessary group theory and key unpublished results. A portion of this research was undertaken as part of a summer research project with student C Bou Dagher, whom was co-supervised by myself and my colleague R. Wiltshaw. R. Wiltshaw contributed to this work in performing the computations necessary for the bulk scattering simulations of Figs. 7.8 and 7.9. The code necessary for these results was written by R. Wiltshaw, M.P. Makwana and R.V. Craster.

7.1 Topological Photonics

Topological photonics is concerned with exotic phases of light in artificial electromagnetic media, the quintessential example being the photonic topological insulator [157, 158]. Topological insulators support topologically non-trivial edge modes; uni- or bi-directional modes that propagate along the boundary of the material, but are prevented from penetrating the interior. In artificial structured media these states of light may be conceived by means of replicating the spatial symmetry-breaking associated with graphene systems [159], so as to engineer valley-Hall insulators that preserve time-reversal symmetry (TRS) [160]. These include the breaking of spatial inversion (reflectional) symmetries in the fundamental cell [161, 162] so as to gap degeneracies in the photonic band structure. In hexagonal lattices these degeneracies are the guaranteed Dirac cones at the vertices K and K' of the Brillouin zone (BZ), whereas in square lattices the degeneracies occur accidentally along the edge of the square BZ. Gapping these degeneracies results in a topologically non-trivial band gap situated between a pair of local valleys, and these valleys harbour an associated nonzero valley Chern number [160, 163]. This quantity is defined as the integral of the Berry curvature [164] over the so-called ‘valley domains’ associated with each valley [165]. Topologically non-trivial band gaps are guaranteed

to host chiral edge modes when two media, of overlapping non-trivial band gaps and of opposite valley Chern number, are joined together. The interface between these media hosts the chiral edge modes, also known as topological confinement states [58]. These chiral edge states are topologically protected by virtue of the orbital behaviour of the time-averaged energy flux vortices appearing along the interface; see [58] Fig. 14 and [166] Fig. 4. Valley-Hall insulators of this type have been designed, theoretically and experimentally, for the purposes of guiding waves in photonic [160–162], acoustic [166–168], elastic [58, 169–171] and even water wave (dispersive) [172] systems. To understand how the breaking of spatial inversion symmetries guarantees the gapping of degeneracies and non-trivial edge modes, we rely on group theory. This group theoretic treatment of the spatial symmetries of photonic crystals was pioneered by Sakoda [173, 174] for isotropic crystals and by Alagappan *et al.* [19] for anisotropic crystals.

7.1.1 Group Theory

In two dimensions the spatial inversion symmetries of a lattice are the reflectional symmetries that leave the lattice structure invariant under transformation. The mirror reflection σ_x , for example, is the operation that transforms the point x to $-x$, and similarly σ_y is the operation that transforms y to $-y$. There are also the diagonal mirror reflections σ'_d , which transforms (x, y) to (y, x) and σ''_d , which transforms (x, y) to $(-y, -x)$ [†]. All of these mirror symmetries belong to the lattice depicted in Fig. 7.1a, which consists of four cylinders of some uniform nondescript boundary condition placed in a square formation. Stretching this structure vertically so as to form the rectangular lattice depicted in Fig. 7.1b breaks the diagonal mirror symmetries, but σ_x and σ_y are retained.

But the mirror reflections are not the only symmetries belonging to these lattices, as each geometry also remains invariant under appropriate rotation. We label these rotational symmetry operations as C_n , where n denotes the $2\pi/n$ radians through which a geometry can be rotated and retain its original structure. The lattice in Fig. 7.1a remains invariant under the operations C_4 , C_2 and C_4^{-1} , where the superscript denotes the inverse (clockwise) rotation. Successive rotations can also be written with superscript notation, for example $C_4^2 = C_2$, $C_4^3 = C_4^{-1}$, etc. The rectangular lattice in Fig. 7.1b has only one rotational symmetry, namely C_2 . The final symmetry belonging to any given two dimensional lattice structure is the identity operator, denoted E , which transforms the

*These are often referred to as σ_v (vertical) and σ_h (horizontal) mirror reflections, respectively, or collectively as σ_v reflections.

[†]These diagonal mirror reflections are often collectively written σ_d .

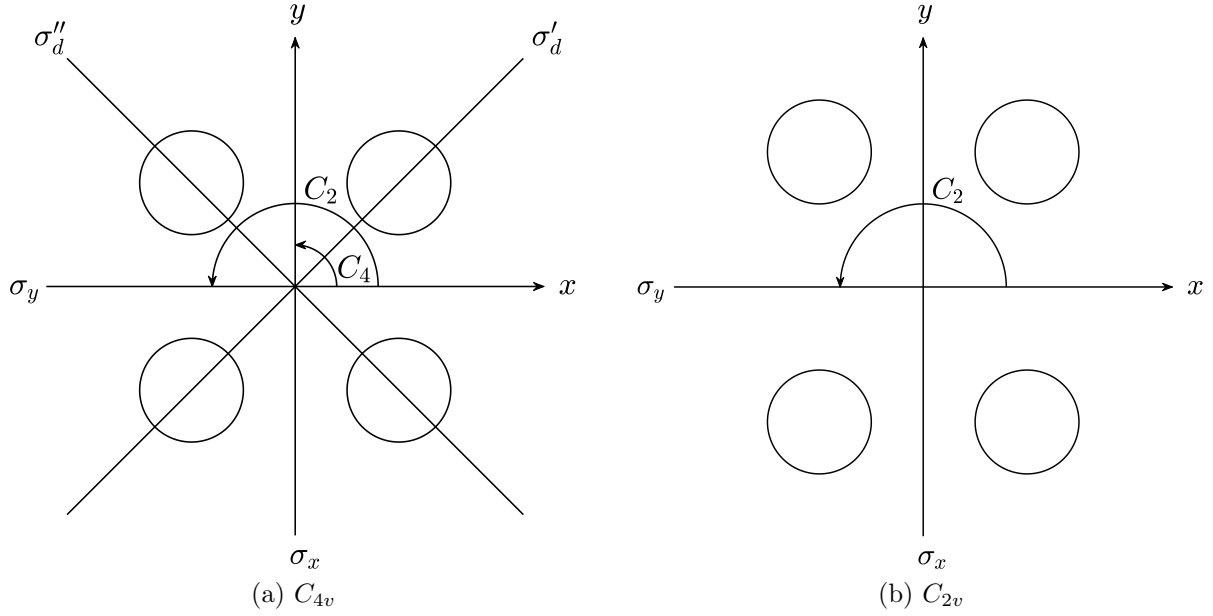


Figure 7.1: Square and rectangular lattices labelled by point group.

structure to itself.

Together the reflection, rotation and identity operators define the crystallographic point group; the total set of symmetry operations under which the lattice structure remains invariant. In Schoenflies notation the cyclic point groups are denoted C_{nv} , where n denotes the minimum permissible rotation operation and v the presence of mirror symmetries. The point group of the lattice of Fig. 7.1a is C_{4v} :

$$C_{4v} = \{E, C_4, C_4^2, C_4^3, \sigma_x, \sigma_y, \sigma'_d, \sigma''_d\}, \quad (7.1)$$

whereas that of Fig. 7.1b is C_{2v} :

$$C_{2v} = \{E, C_2, \sigma_x, \sigma_y\}. \quad (7.2)$$

In fact, any two successive symmetry operations in either of these groups are equivalent to a single symmetry operation in that group. Simple examples include $\sigma_x \sigma_y = C_2$ or $C_2^2 = E$. We also note that the inverse of any of these symmetry operations is also an operation belonging to each group. These types of successive symmetry operations are summarised in product tables, such as that of Table 3.1 of [174]. In relation to this is the conjugate relationship between symmetry operations and their matrix representations, but in the interest of brevity we refer the reader to [174] Eqs. (3.7)-(3.23).

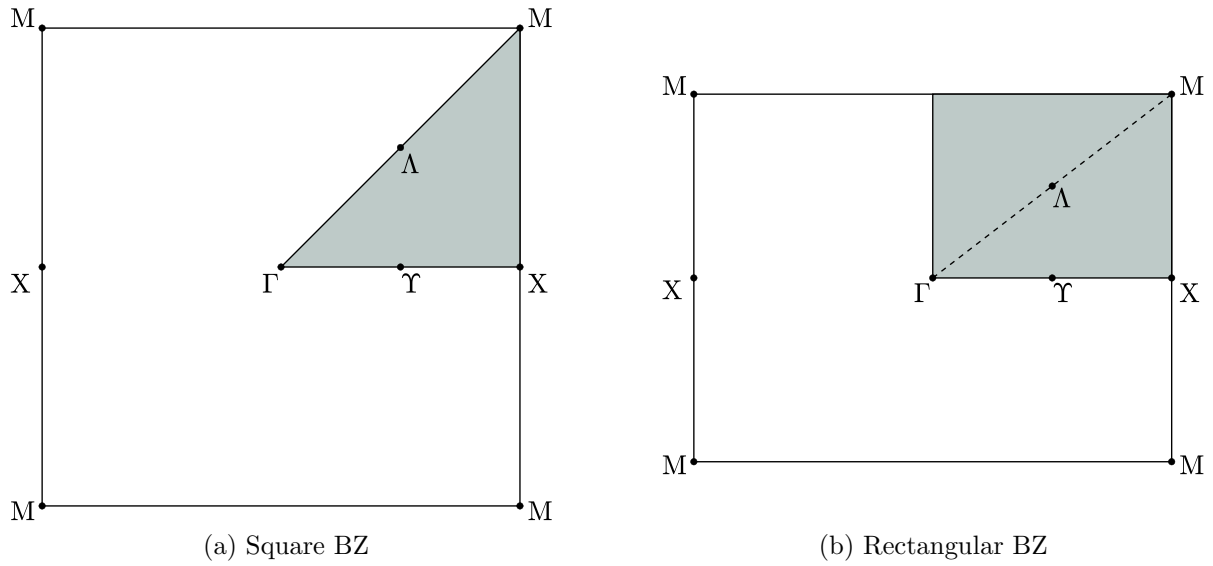


Figure 7.2: BZs labelled with high-symmetry points, IBZs highlighted in grey.

7.1.2 $\mathbf{k}$ -Groups

The eigenmodes of a lattice of associated point group $\mathcal{M}$ in direct space will be subject to the symmetry operations belonging to the $\mathbf{k}$ -group $\mathcal{M}_{\mathbf{k}}$ in reciprocal space. The $\mathbf{k}$ -group $\mathcal{M}_{\mathbf{k}}$ is the subgroup of the point group $\mathcal{M}$ under which the wavevector $\mathbf{k}$ remains invariant; this makes the $\mathbf{k}$ -group a function of position in the first Brillouin zone. Consider the BZs corresponding to the direct space lattices of Fig. 7.1a and 7.1b, depicted in Fig. 7.2a and 7.2b. In the square BZ Fig. 7.2a, the points Γ , X and M denote the coordinates $(0, 0)$, $(\pm\pi/d, 0)$ and $(\pm\pi/d, \pm\pi/d)$ respectively, where d is the dimension of the square cell. At the Γ point all symmetry operations in C_{4v} keep the point invariant, hence:

$$\mathcal{M}_{\Gamma} = C_{4v}. \quad (7.3)$$

Each X-point, and each M-point, are equivalent under translation by a linear combination of reciprocal lattice vectors; we consider a wavevector invariant under a symmetry transformation when this condition is met. Considering the point M first, all symmetry operations in C_{4v} keep the point invariant:

$$\mathcal{M}_{\text{M}} = C_{4v}. \quad (7.4)$$

On the other hand, the only operations in C_{4v} that do not keep the point X invariant are the diagonal mirror symmetries and the rotations through $\pi/4$ radians. Hence:

$$\mathcal{M}_X = \{E, C_2, \sigma_x, \sigma_y\} = C_{2v}. \quad (7.5)$$

Let us also consider the points Λ and Υ on the paths $\Gamma \rightarrow M$ and $\Gamma \rightarrow X$, respectively. These are not high-symmetry points, in that they do not lie at the centre, a vertex or a centre-face of the lattice structure, but they still retain invariance under select transforms. Examining Fig. 7.2a we readily observe:

$$\mathcal{M}_\Lambda = \{E, \sigma'_d\} = C_{1h}, \quad (7.6)$$

$$\mathcal{M}_\Upsilon = \{E, \sigma_y\} = C_{1h}. \quad (7.7)$$

As for the rectangular BZ Fig. 7.2b, each $\mathbf{k}$ -group is a subgroup of C_{2v} :

$$\mathcal{M}_\Gamma = C_{2v}, \quad (7.8)$$

$$\mathcal{M}_X = C_{2v}, \quad (7.9)$$

$$\mathcal{M}_M = C_{2v}, \quad (7.10)$$

$$\mathcal{M}_\Lambda = \{E\} = C_1, \quad (7.11)$$

$$\mathcal{M}_\Upsilon = \{E, \sigma_y\} = C_{1h}. \quad (7.12)$$

Note that the point group C_{1h} is commonly referred to as C_s or C_{1v} . It consists of the operations E and one mirror reflection σ .

7.1.3 Time-Reversal Symmetry

In classifying the $\mathbf{k}$ -groups as subgroups of the point group $\mathcal{M}$, we have only considered the spatial symmetries of the physical lattice. But there is an additional symmetry we have to take into account, that of time-reversal symmetry (TRS). TRS, which relates the point $\mathbf{k} \rightarrow -\mathbf{k}$, ensures that a photonic band structure has inversion symmetry even when the physical space lattice does not have inversion symmetry. If we solely consider TRS then we need only traverse half of the BZ for any given lattice shape; spatial (reflectional) symmetries can then be applied. Take for example the triangular arrangement of cylinders within a square cell depicted in Fig. 7.3a. In physical space the structure harbours only a single σ_x symmetry, and so according to our previous definition we would expect $\mathcal{M}_\Gamma = C_{1v}$, but this is not the case. The additional symmetry provided

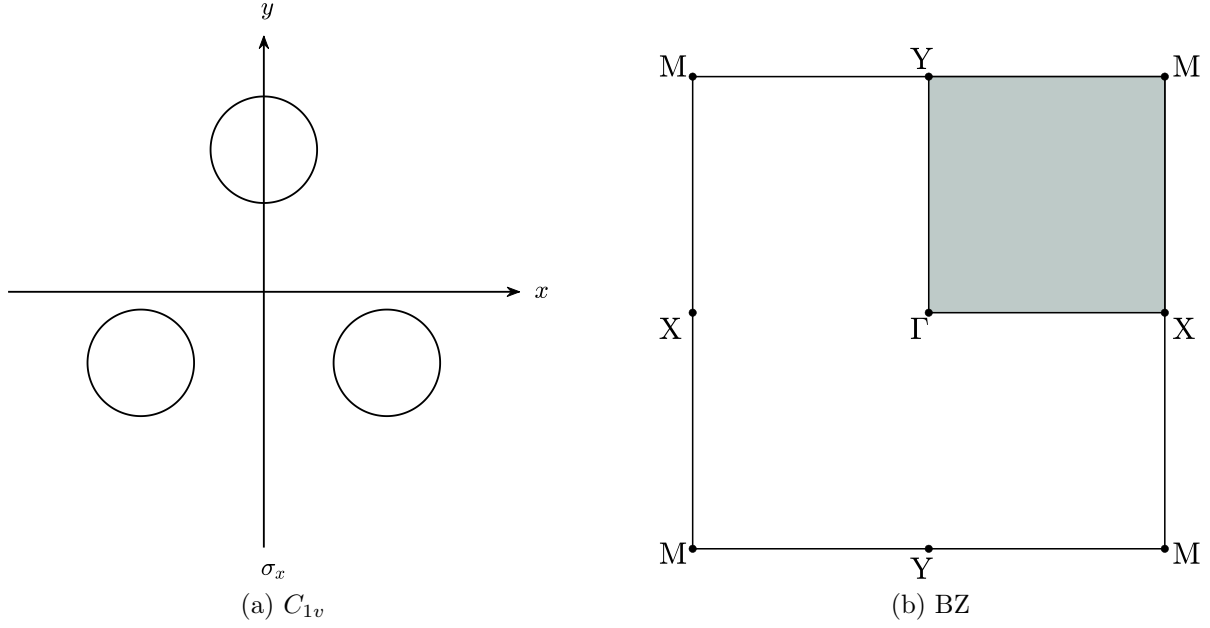


Figure 7.3: Triangular arrangement in a square lattice and corresponding BZ.

by TRS ensures that the point group at Γ is:

$$\mathcal{M}_{\Gamma} = \{E, C_2, \sigma_x, \sigma_y\} = C_{2v}, \quad (7.13)$$

where the additional mirror operation is present as the σ_x symmetry in physical space translates into a σ_y symmetry in Fourier space [171]*. This is also the point group at the corner $\mathcal{M}_M = C_{2v}$ and the centre-face $\mathcal{M}_X = C_{2v}$.

7.1.4 Irreducible Representations and Compatibility

The eigenmodes of the crystal, that is the electric or magnetic fields $E_z(\mathbf{k})$ or $H_z(\mathbf{k})$, at any point $\mathbf{k}$ in the BZ are the irreducible representations (IRs) of the group $\mathcal{M}_{\mathbf{k}}$. The point group C_{4v} , for example, has five IRs: A_1 , A_2 , B_1 , B_2 and E , where the former four IRs are referred to as one-dimensional and the final IR E is two-dimensional. This dimensionality indicates the degree of degeneracy of the eigenmode. Associated with each IR are a set of characters which delineate the behaviour of the IR under application of the symmetry operators of the point group. The characters of each IR of the group C_{4v} are listed in Tab. 7.1, where the number in front of the symmetry operator indicates that

*As any two successive operations in a point group must be equivalent to a single operation in that point group, the presence of both C_2 and one mirror reflection guarantees that the other mirror reflection will also be present: $C_2\sigma_x \equiv \sigma_y$.

C_{4v}	E	$2C_4$	C_2	$2\sigma_v$	$2\sigma_d$	Basis
A_1	+1	+1	+1	+1	+1	$x^2 + y^2$
A_2	+1	+1	+1	-1	-1	-
B_1	+1	-1	+1	+1	-1	$x^2 - y^2$
B_2	+1	-1	+1	-1	+1	xy
E	+2	0	-2	0	0	(xz, yz)

Table 7.1: Character table for the point group C_{4v} .

C_{2v}	E	C_2	σ_x	σ_y	Basis
A_1	+1	+1	+1	+1	x^2, y^2
A_2	+1	+1	-1	-1	xy
B_1	+1	-1	-1	+1	x, xy^2
B_2	+1	-1	+1	-1	y, x^2y

Table 7.2: Character table for the point group C_{2v} .

C_{1h}	E	σ	Basis
A	+1	+1	x^2, y^2
B	+1	-1	x, y

Table 7.3: Character table for the point group C_{1h} .

there are two such operations, conjugate to one-another, that have the same character. The conjugate mirror symmetries σ_x and σ_y are labelled σ_v and the conjugate diagonal mirror symmetries σ'_d and σ''_d are labelled σ_d . Sharing a character is not always guaranteed however, as in Tab. 7.2 for the C_{2v} point group.

The character of an IR associated with a symmetry operation dictates how the eigenmode will appear under that operation; a character of -1 under σ_x ensures that the field appears inverted through the y -axis. Each IR can equally be described by a basis function f_{IR} which is subject to the same characters as the eigenmode. For example, the C_{2v} IR A_1 has character $+1$ under every operation with basis $f_{A_1} = x^2, y^2$, which remain positive when $(x, y) \rightarrow (-x, -y)$. IR A_2 is has character -1 under σ_x and σ_y but $+1$ under C_2 , and is therefore appropriately described by the basis $f_{A_2} = xy$. Tabs. 7.1 to 7.3 include basis functions for each IR, although these entries are not exhaustive; see [175].

So far we have only addressed IRs occurring at high-symmetry points, but it is possible

Γ -point IR	Υ	Λ
A_1	A	A
A_2	B	B
B_1	B	A
B_2	A	B
E	$A + B$	$A + B$

Table 7.4: Compatibility relations between the Γ -point IRs and the points Υ and Λ in the case of the square lattice.

to relate these to IRs at nearby points in the BZ by way of compatibility relations. Take the points Γ and Υ in the square BZ of Fig. 7.2b, which have respective point groups C_{4v} and C_{1h} . The operations E and σ_d are shared between these point groups, and in comparing the character tables between these point groups the IRs A_1 and B_2 of C_{4v} share characters under these operations with the IR A of C_{1h} . Similarly, the IRs A_2 and B_1 share characters with the IR B . The IRs between these points are connected by the formula:

$$N_{A,\Upsilon} = \frac{\sum_{S \in C_{1h}} \chi_{A_1}(S) \chi_A(S)}{\text{ord}(C_{1h})} \quad (7.14)$$

where S denotes any symmetry operator, $\chi_{\text{IR}}(S)$ denotes the character under operation S for a given IR, and $\text{ord}(G)$ denotes the number of elements of the group G . The formula (7.14) informs us as to the number of the A IR at the Υ point due to the A_1 IR at the Γ -point. For one-dimensional IRs this is trivial; A_1 and B_2 will provide one A at Υ , and likewise A_2 and B_1 will provide one B at Υ . For the two-dimensional IR E this is not the case, and in applying the formula (7.14) we find that the degenerate E representation has split into two bands at the Υ -point, one of IR A and the other of IR B . Tab. 7.4 summarises the compatibility relations between Γ and the Υ - and Λ -points for the square lattice of Fig. 7.1a, and this can be extended to the other high-symmetry points as in [174] Tab. 3.5. See the band diagrams in [173] Figs. 1 and 2, [174] Fig. 3.4 and [171] Fig. 4 for examples of the evolution in irreducible representations across a band structure.

Lastly, these compatibility relations can be extended to consider other high-symmetry points in an extended zone scheme in reciprocal space, so as to further deduce the symmetries belonging to the eigenmodes of the crystal. This is discussed in detail in [173, 174].

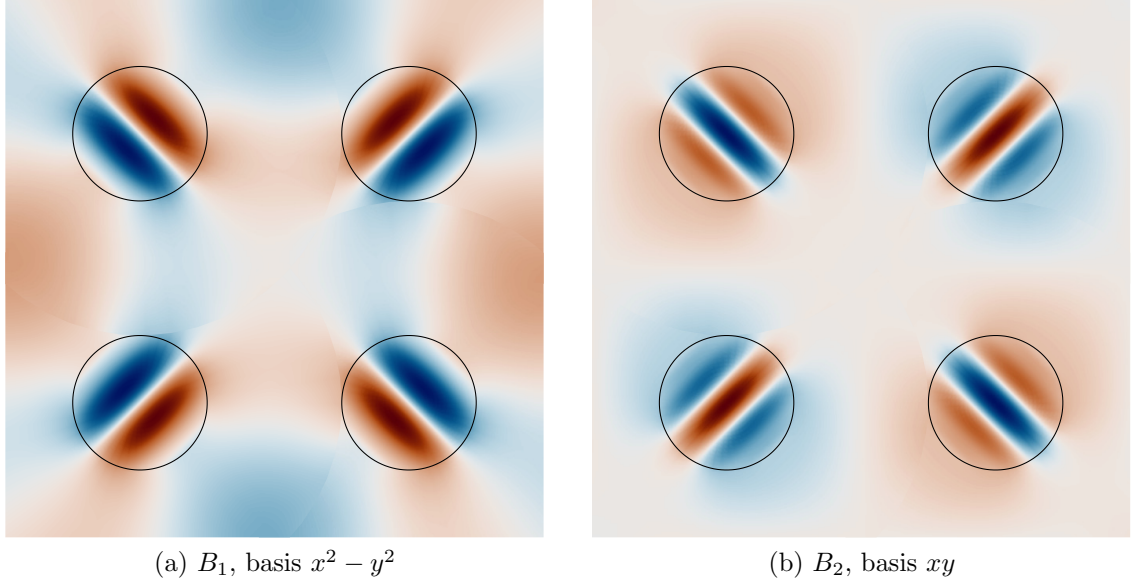


Figure 7.4: Eigenmodes of the square lattice of metacylinders at the Γ -point, labelled with irreducible representation and basis function.

7.1.5 Eigenmodes of the Square Lattice of Metacylinders

We can use our newly acquired knowledge of the symmetries of the lattice to classify its eigenmodes. Let's assert that the cylinders depicted in Fig. 7.1a are plate-array metacylinders, each of which is oriented such that the plate-array is parallel with the diagonals of the square cell. This preserves the mirror reflections $2\sigma_d$ so as to ensure that the point group of the lattice is C_{4v} in physical space. The system of equations for this supercell of metacylinders is a simple extension of the system of equations (6.37) and (6.38) to include multiple scatterers in the fundamental cell. This involves deducing so-called 'relative lattice sums' as in [90, 144]*. For brevity we omit the system of equations here, but its full multipole implementation was used to compute the provided eigenmodes. As the physical space lattice is C_{4v} so too is the group $\mathcal{M}_\Gamma = C_{4v}$. In Fig. 7.4 we provide two eigenmodes at the Γ -point, for which Fig. 7.4a corresponds to the B_1 IR and Fig. 7.4b corresponds to the B_2 IR.

In elucidating the symmetries of photonic crystals and their properties, it was the intention of the author to break these symmetries in an active sense. The plate-array metacylinders provide a geometric tunability to the photonic crystal at the cell-level,

*These relative lattice sums can be straightforwardly expressed in terms of ordinary lattice sums via application of Graf's addition theorem.

whereby uniform rotation through a small perturbative angle causes the cells of Fig. 7.4 to retain their rotational symmetries, but lose their mirror lines. As is explained in the following section, the breaking of symmetries in this fashion cracks open degeneracies that may lie along high-symmetry lines or high-symmetry points of the Brillouin zone, to which a pair of local valleys are formed. These valleys harbor a non-zero valley-Chern number that is indicative of topologically protected edge modes [161, 162], which propagate along interfaces between cells of opposite symmetry-breaking perturbation. The aim then was the breaking open of degeneracies belonging to photonic crystals not unlike that of Fig. 7.4, and in doing so, the realisation of edge modes along *virtually any direction* within the photonic crystal of metacylinders. There were, however, numerical impracticalities in this approach, not least because the method of deducing the dispersion curves of these plate-array crystals involved finding the zeros of the matrix determinant (which itself was a numerically unstable quantity) of matrices of size $N(4M + 4)$, where N was the number of metacylinders in a fundamental cell. This in turn required vast sweeps over Bloch wavenumber-space with a fine grid, necessitating parallelisation of the codes and taking days of computational time. Unfortunately, this work remains unfinished. In the following sections, symmetry breaking is instead leveraged so as to realise edge modes between media of equal symmetry-breaking perturbation, but opposite boundary condition, and a discussion of tunability is provided in the concluding remarks.

7.1.6 Symmetry Breaking

Just as spatial symmetries guarantee certain characteristics to a photonic band structure, the breaking of these symmetries guarantee their loss. Degeneracies, whether they occur accidentally along high-symmetry lines or by decree at high-symmetry points, are the first to fall victim. The term ‘accidental’ applies not to the two-dimensional IRs of a $\mathbf{k}$ -group, but rather to the incidental crossing of bands of opposite symmetry. Related to this is the notion of band repulsion, wherein two bands of a shared symmetry repulse one-another rather than become degenerate [176]. The symmetry of a band is denoted by the character of its IR under a symmetry operation, meaning that two bands of the same IR are symmetry repelled. Accidental crossings occur away from the high-symmetry points by virtue of the reduction in the IRs across the BZ, as in Tab. 7.4*. It is for this reason

*Neighbouring bands of representations (A_1, B_1) at the Γ -point will, by compatibility, evolve into the pair (A, B) at Υ and (A, A) at Λ . The pair (A, B) can be made, through appropriate parametric tuning [171], to cross along the high-symmetry line $\Gamma \rightarrow M$, whereas the pair (A, A) are symmetry repelled along the diagonal $\Gamma \rightarrow X$.

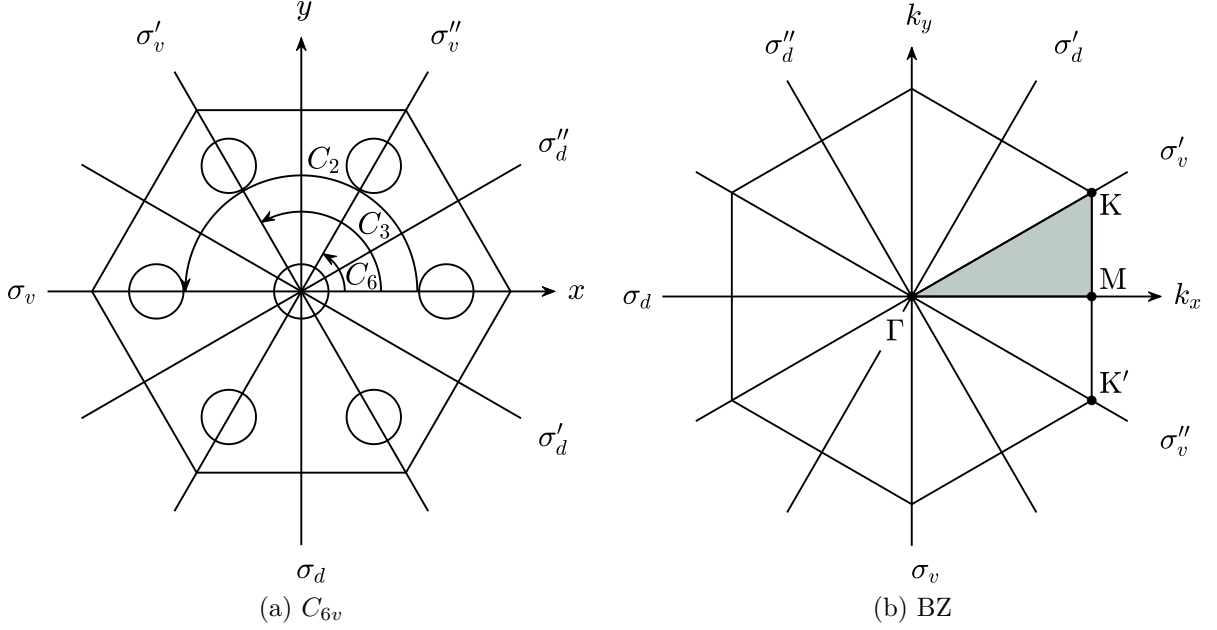


Figure 7.5: Hexagonal lattice in (a) direct space and (b) reciprocal space. Note that the hexagonal BZ is rotated $\pi/2$ radians w.r.t. the physical cell. Hence, $\{\sigma_d\}$ mirrors in direct space guarantee $\{\sigma_v\}$ symmetries in reciprocal space and vice versa.

that such degeneracies are referred to as being *symmetry protected* under σ , where σ is the mirror operation shared along the high-symmetry line. Naturally then, the breaking of this symmetry cracks open the degeneracy, as the IRs of both bands hybridize and symmetry repel [168].

But unlike the square lattice and its accidental crossings along high-symmetry lines, lattices of a hexagonal construction can guarantee degeneracies at the K/K' vertices of the BZ. These Dirac cones exist when the $\mathbf{k}$ -groups of the high-symmetry points $\{\mathcal{M}_\Gamma, \mathcal{M}_{K/K'}\} = \{C_{6v}, C_{3v}\}, \{C_{3v}, C_{3v}\}, \{C_6, C_3\}$ [169]. No amount of parametric tuning can remove them as long as these symmetry pairs are retained. The point group of the hexagonal lattice of Fig. 7.5a is C_{6v} , which consists of five rotational symmetries, six mirror reflections and the identity operator. The mirror operations are collectively labelled $\{\sigma_v\}$ and $\{\sigma_d\}$, where the vertical mirrors bisect the vertices of the cell and the *dihedral* mirrors bisect the C_2 rotations of the cylinder array. In reciprocal space the high-symmetry points labelled in Fig. 7.5b have symmetry groups:

$$\mathcal{M}_\Gamma = \{E, 2C_6, 2C_3, C_2, 3\sigma_v, 3\sigma_d\} = C_{6v}, \quad (7.15)$$

$$\mathcal{M}_{K/K'} = \{E, 2C_3, 3\sigma_v\} = C_{3v}. \quad (7.16)$$

C_{6v}	E	$2C_6$	$2C_3$	C_2	$3\sigma_d$	$3\sigma_v$
A_1	+1	+1	+1	+1	+1	+1
A_2	+1	+1	+1	+1	-1	-1
B_1	+1	-1	+1	-1	-1	+1
B_2	+1	-1	+1	-1	+1	-1
E_1	+2	+1	-1	-2	0	0
E_2	+2	-1	-1	+2	0	0

Table 7.5: Character table for the point group C_{6v} .

C_{3v}	E	$2C_3$	$3\sigma_v$
A_1	+1	+1	+1
A_2	+1	+1	-1
E	+2	-1	0

Table 7.6: Character table for the point group C_{3v} .

C_3	E	C_3	C_3^2
A	+1	+1	+1
E	+1	ω	ω^2
	+1	ω^2	ω

Table 7.7: Character table for the point group C_3 , $\omega = e^{2\pi i/3}$.

The characters of these operations are summarised in Tabs. 7.5 and 7.6. The two-dimensional E representation of C_{3v} is responsible for the guaranteed Dirac cones of this lattice. A perturbation of the array of cylinders, such as a uniform rotation through a small angle [162], breaks the mirror reflections but retains the rotational symmetries, such that $\{\mathcal{M}_\Gamma, \mathcal{M}_{K/K'}\}$ change from $\{C_{6v}, C_{3v}\}$ to $\{C_6, C_3\}$. However, this is not enough to gap the Dirac cones. The point group C_3 supports a Dirac cone *if and only if* $\mathcal{M}_\Gamma = C_6$, as in this case the two complex valued one-dimensional representations labelled collectively under E in Tab. 7.7 stick together [169]. This is due to TRS, which can introduce additional degeneracies that are detected by way of Herring's criterion [169, 177, 178]. Herein we omit the proof and refer the reader to [169] Eqs. (18)-(19), which demonstrates that this additional degeneracy is present when $\mathcal{M}_\Gamma = C_6$. Breaking the $2\pi/6$ rotational symmetries, via translational perturbations of the cylinders or otherwise, reduces the $\mathbf{k}$ -groups of the lattice to $\{C_3, C_3\}$ and gaps the Dirac cones.

The gapped degeneracies are transformed into pairs of locally quadratic valleys, each imbued with a non-zero valley Chern number [179, 180]. The valley Chern number at the vertices K/K' is defined as [165]:

$$C_{K/K'} = \frac{1}{2\pi} \int_{\mathcal{S}_{K/K'}} \mathcal{F}(\mathbf{k}) d^2\mathbf{k}, \quad (7.17)$$

where:

$$\mathcal{F}(\mathbf{k}) = \nabla_{\mathbf{k}} \times i\langle u_{\mathbf{k}} | \nabla_{\mathbf{k}} | u_{\mathbf{k}} \rangle, \quad (7.18)$$

is the Berry curvature [164]. The quantity $u_{\mathbf{k}}$ is our electric or magnetic field of Bloch wavevector $\mathbf{k}$ and $\mathcal{S}_{K/K'}$ is the so-called ‘valley domain’ in Fourier space; it is the triangular surface local to the K/K' vertex that forms one half of the reciprocal primitive unit cell*. This is illustrated in [165] Fig. 2. The band gap between these valleys is topologically non-trivial by virtue of the non-zero valley Chern number belonging to each valley, which are of equal magnitude but opposite sign on either side of the gap. Similarly, valleys pertaining to the same band at neighbouring K and K' vertices harbour valley Chern numbers of opposite sign. Oppositely perturbing the medium of Fig. 7.6a, such as via a rotation through $\pi/3$ radians, ensures that the sign of $C_{K/K'}$ is swapped at each vertex. Cf. [169] Fig. 8 or [161] Fig. 5. An interface is defined when the perturbed medium of Fig. 7.6a and its counter-rotated twin are joined, and as long as the vertices of associated opposite valley Chern numbers are made to overlap, the interface will host edge modes.

7.1.7 Topologically Non-Trivial Complete Photonic Band-Gaps

We perform the symmetry breaking perturbations indicated in Fig. 7.6a for the purposes of generating a non-trivial complete photonic band gap (CPBG)[†]. CPBGs occur when light of TE and TM polarizations share an overlapping band gap, which ensures that wave propagation is prohibited no matter the polarization of the incident field. The symmetry broken arrangement in Fig. 7.6a has guaranteed crackings open of Dirac degeneracies regardless of the material composition of the scatterers, which herein are considered to be perfect electrical conductors. They are therefore of Neumann (Dirichlet) boundary

* $C_{K/K'}$ is not a quantised topological invariant as $\mathcal{S}_{K/K'}$ is not a closed surface. The integral of the Berry curvature over the whole reciprocal primitive unit cell (a rhombus) equates to zero. Naturally, integrating over half of this surface we arrive to a quantity that is *locally* non-trivial (non-zero), but *globally* trivial.

[†]Although we perform this symmetry breaking in an idealised two-dimensional photonic crystal, the same topological arguments apply in three dimensions [181].

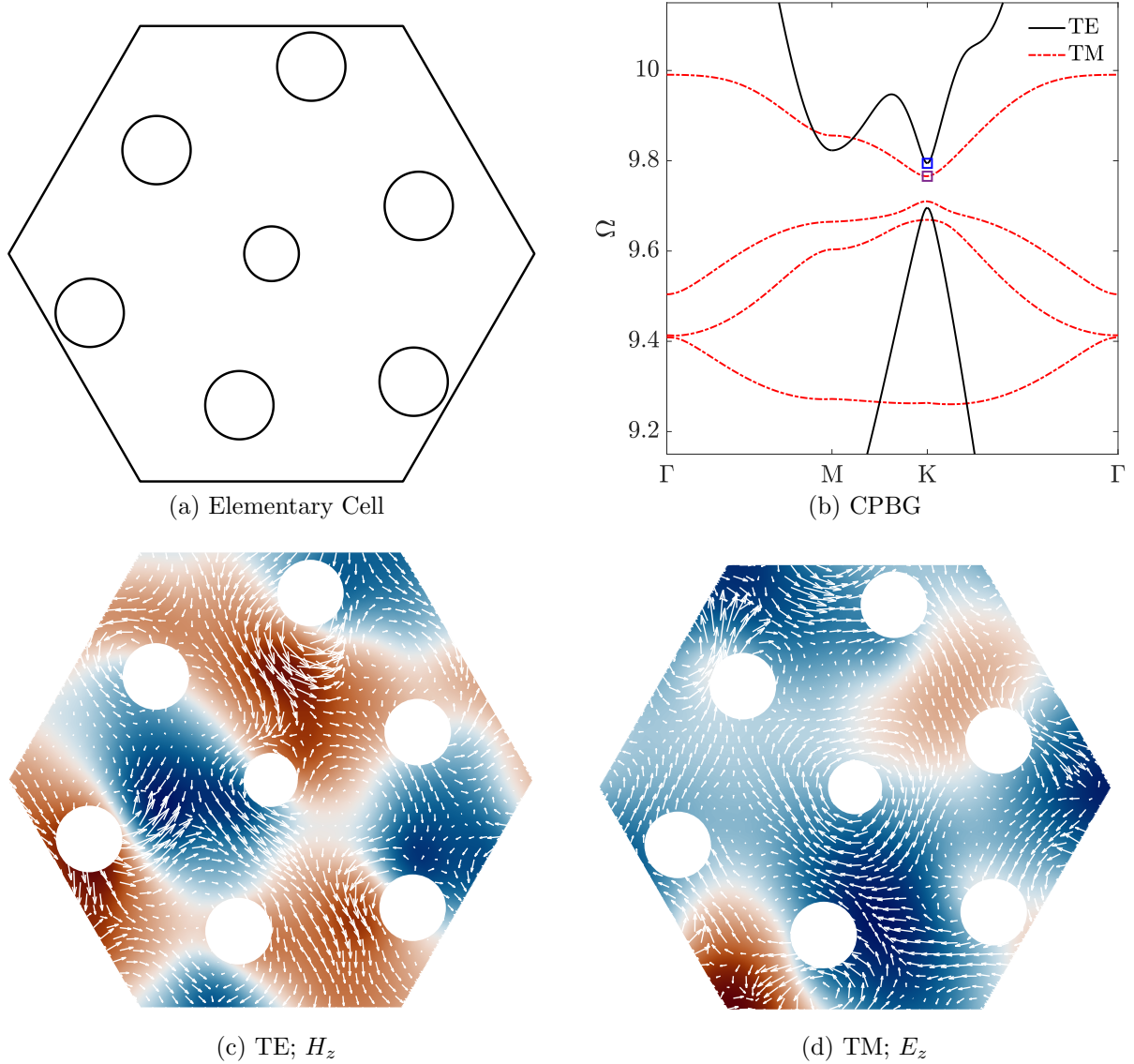


Figure 7.6: Symmetry broken hexagonal lattice harbouring a topologically non-trivial CPBG. The elementary cell depicted in (a) has lost its mirror reflectional and $\pi/6$ rotational symmetries due to the rotational and translational perturbations of the cylinders. The CPBG engendered by this symmetry breaking is depicted in (b), wherein parametric tuning of the cylinder radii was performed to maximise the overlap of the non-trivial band gaps. The eigenmodes correspond to the upper valleys at the blue and purple squares for (c) TE, $\Omega = 9.7943$ and (d) TM, $\Omega = 9.7657$, respectively. The white arrows depict the opposite vorticity in the Poynting vector fields.

condition for light of TE (TM) polarization. The topologically non-trivial band gaps that arise due to this symmetry breaking will occur for both polarizations of light, although not necessarily over the same range of frequencies. These non-trivial band gaps have

been made to overlap through appropriate parametric tuning of the cylinder radii and positions (preserving the $\{C_3, C_3\}$ pairing). Our computations have been carried out using a numerical implementation of the matched-asymptotic schemes of Craster, Schnitzer, Wiltshaw and Makwana [167, 182], which apply in the limit of vanishing radius*. These codes were written by Makwana, Wiltshaw and Craster.

The CPBG belonging to this symmetry broken arrangement is shown in Fig. 7.6b, and is made obvious by the overlapping of the photonic band structures for each polarization. The CPBG lies between the frequencies $\Omega = 9.7101$ and $\Omega = 9.7657$, which mark the lower and upper valleys of the TM polarized waves. The blue and purple squares at the basins of the upper valleys delineate the frequencies Ω of the eigenmodes of Figs. 7.6c and 7.6d, which depict, respectively, the longitudinal field components H_z (TE) and E_z (TM). Each upper valley, as well as each lower valley, are imbued with a non-zero valley Chern number, and it is the case that these valley Chern numbers are of opposite sign for each polarization. This difference in sign manifests in the opposite chirality of the Poynting vector fields in prescribed regions of the physical cell, as shown by the overlayed white arrows in Figs. 7.6c and 7.6d. It is this chirality in the Poynting vector fields that provides the topological protection to the edge states [165]. Another way of visualizing this difference in sign is provided by the Berry curvature plotted over the primitive Fourier rhombus for each polarization, as shown in Fig. 7.7. The Berry phase is given by:

$$\theta = \iint_S \mathcal{F}(\mathbf{k}) d\mathbf{k}, \quad (7.19)$$

where S is a small triangular surface element of the discretised Fourier rhombus. The numerical computation of the Berry phase is carried out using a finite differences scheme found in [170] Eqs. (19)-(23). The Berry curvature is then just $\theta/\mathcal{A}$, where $\mathcal{A}$ is the area of the triangular element. The valley Chern number (7.17) is then simply the sum of the Berry curvatures over the the surface $\mathcal{S}_{K/K'}$, normalised by 2π . Fig. 7.7 depicts the Berry curvature over the primitive rhombus for light of TE 7.7a and TM 7.7b polarizations. From the colour inversion at the K/K' vertices it is immediately obvious that the sign of the valley Chern number at each vertex is swapped when the polarization is swapped. The non-zero Berry curvature at each vertex also ensures that the non-trivial band gap will foster edge modes when two such media, of opposite rotational perturbations, are joined. Oppositely perturbing the medium of Fig. 7.6a inverts the colours at the K/K' vertices of Figs. 7.7a and 7.7b (not shown).

*This implementation is advantageous over multipole computations, as the Bloch states are solved for via a simple eigenvalue problem rather than as the zeros of a complex matrix determinant.

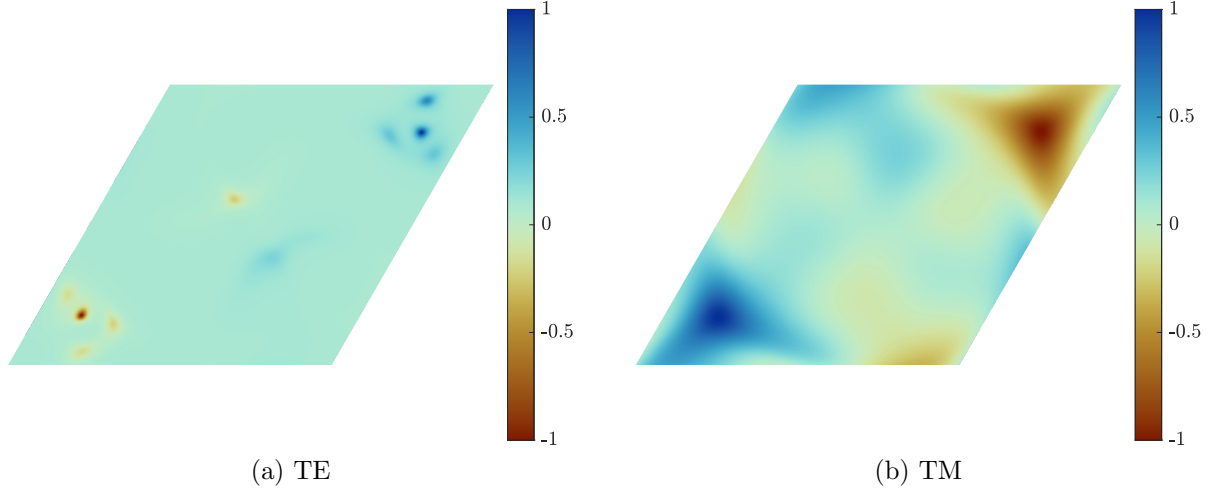
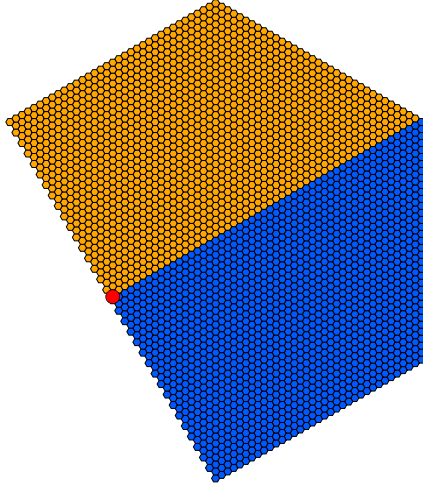


Figure 7.7: Normalized Berry curvatures of the upper bands of Fig. 7.6b over the primitive Fourier rhombus for light of (a) TE and (b) TM polarization.

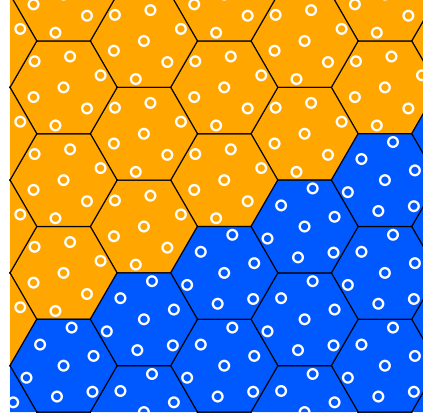
7.1.8 Edge Modes

Fig. 7.8 depicts the realisation of edge modes in propagation along the interface between two media of oppositely perturbed elementary cells. Each side of the medium is said to have a positive or negative chirality, which corresponds to a clockwise or anticlockwise symmetry breaking rotation. A point-source marked in red is placed at the left end of the interface, and emits a wave of frequency $\Omega = 9.7224$, which sits within the CPBG of Fig. 7.6b. The medium on either side of the interface is insulating to the radiation for both TE (Fig. 7.8c) and TM (Fig. 7.8d) polarizations in its bulk, but acts as a conductor along the interface. Note that the color scale is matched for both TE and TM polarizations, and that the intensity of the edge mode under TE polarization is visibly less than that under TM polarization. In general, Neumann inclusions have a weaker scattering response than Dirichlet inclusions.

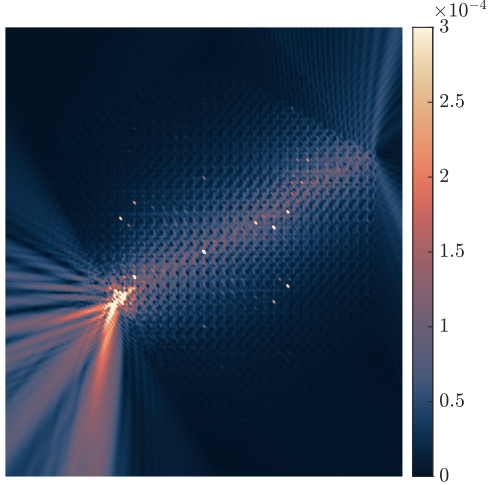
The overlapping of band gaps for both polarizations simultaneously has made it possible to excite edge modes between two media of the same chiral perturbation, but opposite boundary condition. Inverting the boundary condition from Neumann to Dirichlet inverts the sign of the Berry curvatures at the K/K' vertices, as shown in Fig. 7.7. This inverts the sign of the associated valley-Chern number at each vertex, which ensures that an interface between two such media will host edge modes. We excite these along such an interface in Fig. 7.9, for which the upper medium is of Neumann boundary condition, and the lower of Dirichlet boundary condition. This corresponds to perfect electric/magnetic



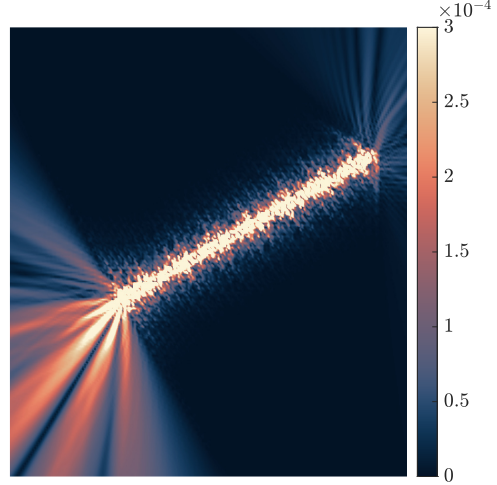
(a) Adjoined Media



(b) Opposite Chirality, Same BC



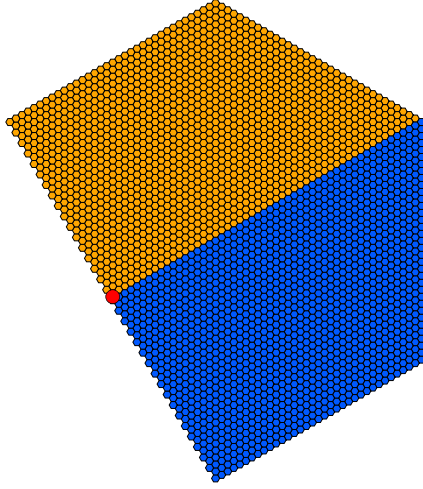
(c) TE; $|H_z|$



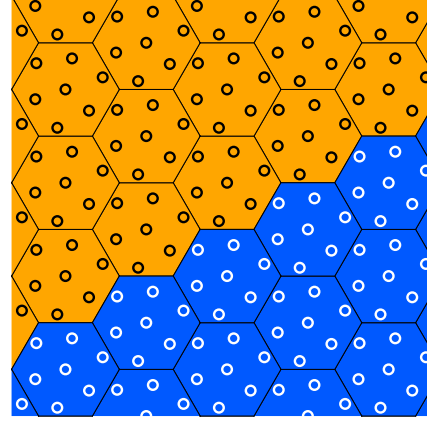
(d) TM; $|E_z|$

Figure 7.8: The interface between oppositely perturbed media supports edge modes for both polarizations of light simultaneously. The adjoined media in (a) have opposite chirality in their symmetry breaking perturbation (b). Edge modes for both polarizations of light occur simultaneously at frequency $\Omega = 9.7224$ (c) and (d).

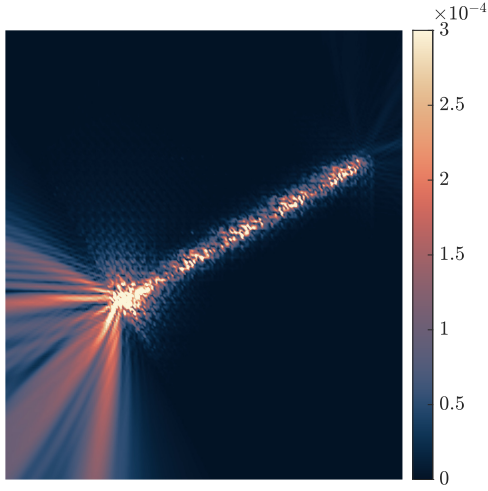
conductors in the upper half and perfect magnetic/electric conductors in the lower half, for light of TE/TM polarization. The edge mode depicted in Fig. 7.9c occurs at the same frequency of those of Fig. 7.8 i.e. at a frequency within the CPBG. Both media are insulating in their bulk and conducting at their surface. In Fig. 7.9d we have excited a mode of frequency $\Omega = 9.7878$, which lies within the TE band gap, but outside of the TM band gap. Thus, propagation into the bulk is visible in the bottom half of the adjoined medium, but not the upper half, which remains a conductor along the interface.



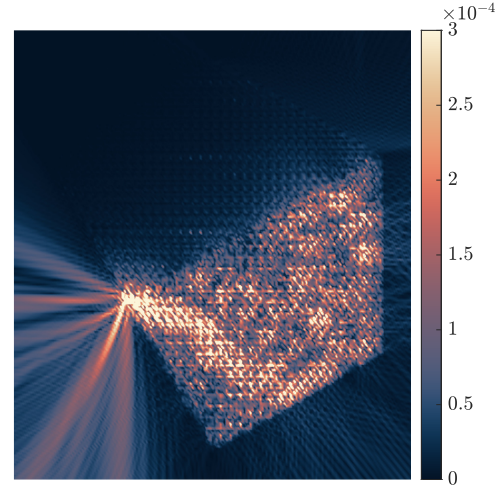
(a) Adjoined Media



(b) Same Chirality, Opposite BC



(c) $\Omega = 9.7224$



(d) $\Omega = 9.7878$

Figure 7.9: Edge modes in propagation between two media of the same perturbation (a), but opposite boundary condition (b). An edge mode (c) occurring at frequency $\Omega = 9.7224$ (within the CPBG), and a partial edge mode (d) occurring at frequency $\Omega = 9.7878$, which lies between the upper valleys in Fig.7.6b

7.2 Remarks on Chapter 7

By analysing the symmorphic symmetries of 2D photonic crystals in the language of group theory, we have seen how the topology of a crystal guarantees certain characteristics to its photonic band structure. These symmetries are reflected in the crystal's eigenmodes, which are classified by their parity under symmetry operations as the irreducible represen-

tations of the crystal's point group. Symmetry breaking has been leveraged to crack open degeneracies in the photonic band structure, enabling a topologically non-trivial complete photonic band gap in a hexagonal lattice of symmetry pairing $\{\mathcal{M}_\Gamma, \mathcal{M}_{K/K'}\} = \{C_3, C_3\}$. This in turn guarantees the valley-Hall insulator phase of light when two such media, of opposite chirality, are conjoined to form an interface. However, the motivation for generating edge modes between media of opposite boundary condition, as in Fig. 7.9, is not immediately obvious. After all, how can one engineer a perfect magnetic conductor? Moreover, what would be the means to transform a material from a perfect electric to perfect magnetic conductor?

In reality, the two boundary conditions we have considered should be thought of as extremes, rather than as realistic parameters, although similar edge modes could be generated in structured media that possess tunable material parameters. As long as a medium is shown to host a topologically non-trivial band gap, reconfiguring the medium parametrically could allow for edge modes to be sent in any chosen direction. Hence, total control over wave motion within the structure is feasible. The popular method of adjoining two oppositely perturbed geometries is certainly effective [171], but does not represent an actively tunable mechanism; once fabricated, the geometry of a given cell cannot be altered. The road to active tunability must come from geometrical or parametric tuning of the constituent scatterers, and this avenue of research is at the forefront of photonics, acoustics and platronics. The methods by which this can be achieved are provided in the concluding remarks, including very recent publications.

8 Conclusions

In this thesis we have employed methods in homogenization for the purposes of analysing a plate-array metamaterial occupying a cylindrical geometry. Reducing the plate-array to an effective medium description has facilitated a semi-analytical formalism, in the language of cylindrical harmonics, to describe the medium's interaction with light under normal incidence and TE polarization. The method naturally lends itself to large-scale numerical computations thanks to the rapid convergence of the multipole field expansions, allowing us to simulate the scattering of light by hundreds of metacylinders simultaneously. Periodically arranging these metacylinders along one or two axes has engendered macroscopic media, of a hierarchical structuration, that possess a tunable electromagnetic response. This tunable response has been demonstrated in number of fashions, including: in the quality factor of structured ring resonators, plane-wave scattering by a diffraction grating, the dispersion of Rayleigh-Bloch modes, and in the effective permittivity of a 2D metasurface. The topology of photonic crystals has also been explored for the purposes of realising 2D photonic phases in reconfigurable media. For this work, the rapid semi-analytical solver of Craster, Wiltshaw and Schnitzer [166, 167, 182] was employed for the purposes of simulating edge modes in chiral media. Via appropriate parametric tuning, a complete photonic band gap was shown to host edge modes for both TE and TM polarizations simultaneously. This enabled the first example of edge modes excited between two media of the same symmetry breaking perturbation, but opposite boundary condition.

There are a number of results facilitated by the plate-array homogenization of chapter 4 that warrant discussion. In particular, the plate-array metasurface considered in chapter 6 is a promising structure. The rotational degree of freedom of the metacylinders provides the surface with a geometrical tunability, and this tunability could be leveraged for the purposes of controlling wave propagation. Take for example the geometry depicted in Fig. 7.4, which consists of four metacylinders of a plate-array angle parallel with the diagonals of the square lattice. Uniformly rotating the metacylinders clockwise through

a small angle, about their respective axes, breaks the σ_v and σ_d symmetries of the square lattice, and reduces the $\mathbf{k}$ -groups $\{\mathcal{M}_M, \mathcal{M}_X\}$ from $\{C_{4v}, C_{2v}\}$ to $\{C_4, C_2\}$. This invariably alters the irreducible representations available at these high-symmetry points and along the high-symmetry line $X \rightarrow M$. If an accidental crossing of bands of opposite parity occurred along this line before the symmetry breaking perturbation was applied, this degeneracy will be cracked open to yield a non-trivial gap as in [168, 171]. This is the mechanism by which control over wave propagation could be achieved, as any given cell edge could be made a conducting interface for edge modes. This approach was attempted for various unit cell geometries, and symmetry breaking perturbations were successfully found to have opened a band gap in a square lattice of metacylinders. However, the computational cost of multipole simulations akin to those of Fig. 7.8 were too great. For such computations, the dimensions of the scattering matrix were of $\mathcal{O}(10^4)$, which blighted its numerical stability. There are techniques to improve this numerical behaviour, but unfortunately the implementation of these techniques remains unattempted.

A natural extension to the metasurface problem would be the scattering of waves under conical incidence i.e. $k_{\parallel} \neq 0$. This approach is motivated by the ability of a metasurface to act as a thin layer, or film, through which a conically propagating field would interact. The idea would be to demonstrate the dynamic reconfiguration of the metasurface in response to a photonic beam for the purposes of influencing the transmitted field. However, this proposed extension to conical incidence is not incremental, as the continuity of the tangential field components results in non-zero cross-coupling terms within the scattering matrix. In other words, both the electric and magnetic fields must be computed simultaneously in one large system of equations, and this facilitates a multipole description of the electric field to match that of the magnetic field. This is known as the Rayleigh system for dielectric cylinders [149], and relies on the distinction between multipole moments of the form b_m^H and b_m^E . Likewise, we require an expression for the longitudinal electric field in the interior domain E_z^i , and this necessitates an effective medium description akin to that of (4.11). We expect that given the Dirichlet condition on the channel walls, the electric field will be written as a sum over standing waves. The homogenization should follow the method set out in chapter 4 i.e. solving for the field $E_{m,z}^i$ and assuming a power series expansion of the form (4.8). What remains is a closure of the problem by application of the Dirichlet condition, and in this we may find that the effective PDE involves mixed orders in the x' and y' terms. Naturally, this would also involve treating the cylinders with a finite depth, and integrating over their depth modes as in [99].

In a different research direction, the plate-array medium serves as a good candidate

material for the absorption of incident radiation. We have already seen in chapter 5 how the plate-array material can be implemented so as to tune the reflection and transmission of incident plane-waves, so it is foreseeable how this model could be extended to include an absorption parameter. What is more promising however would be the absorption of the plate-array medium in the form of a continuous slab, or block, as in [101], so as to ensure that there are no gaps in the medium through which a wave could propagate unattenuated. The absorption could be modelled as a function of the difference in angle between the plate-array and incident plane-wave, and would be brought about by a negative imaginary component to the interstitial refractive index (which, additionally, will dampen out the channel resonances as in chapter 4). Placing one side of the slab on a hard surface would be the sensible approach to maximising the absorption, as the hard surface would act to reflect the incident field back through damped dielectric channels. This structure may also lend itself well to experiments, as the dynamic reconfiguration of the plate-array could be achieved by mechanically deforming its underlying substrate.

Another extension to this work would be the analysis of symmetries belonging to 3D photonic crystals, and the breaking of both the spatial and temporal symmetries to realise topological photonic phases in three-dimensions. As mentioned in chapter 1, the very first 3D Chern insulator was realised just over 12 months ago in a photonic crystal [16], and the first topologically non-trivial 3D photonic valley-Hall insulator not long before that [181]. In the latter publication, the authors break a σ_z symmetry in a double-layered hexagonal lattice to achieve their complete photonic band gap. There is however much more to be explored with regards to symmetry breaking in 3D photonic crystals, particularly with regards to the accidental degeneracies of the square-faced cell. In addition, TRS broken 3D topological phases lie at the forefront of photonics research [183], and involve two novel methods to bring about the temporal symmetry breaking. The first involves the implementation of gyroid metamaterials to the lattice sites as in [16, 183], before applying an external magnetic field. This introduces vortices to the Poynting vector field that favour wave propagation in a unidirectional sense. The second approach involves applying a helical twist down a cylindrical inclusion and writing the propagation in time as a function of the longitudinal coordinate z [184]. This results in TRS broken Floquet topological insulators which host non-trivial photonic phases in the (x, y) plane. In this, it could be of interest to develop upon the dynamic multipole method of chapter 3 for the scattering by helical inclusions, as a function of the twist radius and length.

Gyroid metamaterials could also be implemented in the elastic line and ring structures of chapter 2 so as to bring about unidirectional propagation of guided waves. They have

recently been modelled as embedded inclusions on a thin-elastic plate [185], and engender a new class of elastic waveform: the chiral flexural wave. Periodically structuring these plate gyroids into coupled ring-array circuits, like those of Figs. 2.10 and 2.11, would ensure that wave motion through the circuit is unidirectional. It would be of interest to examine the quality factor of the gyroid ring resonator quasi-modes, as one can imagine that the vorticity in the flexural energy flux may prevent leakage from the ring. What's more, placing two 2D lattices of opposite gyroscopic spin side-by-side ensures that modes propagating along the interface can do so in only the favoured direction, and it is likely that these modes are robust to disorder in the platonic structure. This is a very promising development, as it will allow for TRS broken elastic phases on 2D plates.

Finally, we ought to discuss the means by which active tunability could be achieved in photonic crystals, particularly for an operating range in the infrared or near-visible regimes where the meta-atoms are of a nanometre scale. Many of the cited examples herein concern photonic crystals that are static [161, 162]; their configurations are determined in design/fabrication such that their electromagnetic response cannot be altered. An idealised photonic crystal would harbour programmability at the pixel-level [130], with each meta-atom possessing a mechanical or material reconfigurability. The meta-cylinder of chapters 4-6 is a representative example of the former case, at least in the microwave regime for which the assumption of perfectly conducting plates holds true. The long-range uniformity in plate-array angle is the chief factor in determining the electromagnetic response of the metagrating of chapter 5 and 2D metasurface of chapter 6. If a mechanism were to be conceived to adjust the plate-array angle of each metacylinder, such as via tangential forcing via motorised actuators at the base of each cylinder, this would enable the user to arrange symmetry-broken supercells possessing non-trivial band gaps.

One recent metasurface that has a demonstrably impressive dynamic tunability is that of Abdollahramezani *et al.* [186]. This optical metasurface is based on the phase-change material germanium-antimony-tellurium (GST) incorporated into meta-atoms of a metal-dielectric composition. GST is capable of changing phases between amorphous (a-GST) and crystalline (c-GST) states due to heating, which makes it an excellent material for the purposes of rapidly changing the optical response of a metasurface. Under thermal-based conversion between a-GST and c-GST, the dynamic tunability of the metasurfaces considered in [186] is demonstrated in the amplitude and phase of reflected light as a function of wavelength in Fig. 1b(ii),c(ii). It is this kind of reprogrammability that we have in mind for the adjoined media of identical chiral perturbations in Fig. 7.9,

as the continuum of crystallisation levels offered by GST provides the medium with a smooth transition in its photonic band structure. Taking the extremes of 0% and 100% crystallisation (a-GST and c-GST), the method would involve parametric tuning of the crystalline geometry so as to ensure that the amorphous and crystalline states share an overlapping band gap as in Fig. 7.6b (a CPBG for both GST phases, rather than both polarizations of light). As in chapter 7, this would enable the medium to host edge modes at the interface between the a-GST and c-GST cells, and the locations of these cells would be determined by thermal control.

In summary, this body of work has demonstrated that homogenization techniques can be employed to great effect in the modelling of microstructured media. The semi-analytical formalism developed in this manner is an attractive alternative to finite element methods, as it provides us with an unrivalled mathematical insight to the problem at hand. Consider the line array of masses embedded in a thin-elastic plate, as in Fig. 2.3, for which the application of HFH revealed the beat wavelength of the energy carrying envelope. In turn, the bending of the line array into a ring revealed that the whispering-Bloch modes of the ring corresponded to integer numbers of the beat wavelengths circumnavigating the structure, as in Fig. 2.8. Finite element methods may well have been used to deduce this result empirically, but not in a fashion as elegant, nor as convincing, as that given here. Additionally, semi-analytical techniques are generally far less computationally costly in both machine time and memory usage than their FEM counterparts. The latter relies on vast frequency sweeps to deduce the eigenmodes of a medium, whereas those of a homogenized medium can be deduced quickly as the solutions to a simple eigenvalue problem or as the zeros of a scattering matrix. This is not to say that finite elements methods are not useful, but rather that in certain cases where the geometry of a problem is amenable, the benefits of a homogenized description are numerous.

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A Useful Formulae in Cylindrical Geometries

A.1 Bessel Functions

We define $\mathcal{S}_m(x)$ as denoting $J_m(x)$, $Y_m(x)$, $H_m^{(1)}(x)$, $H_m^{(2)}(x)$ or any other linear combination of these functions.

CONNECTION FORMULAE

$$\mathcal{S}_{-m}(x) = (-1)^m \mathcal{S}_m(x), \quad (\text{A.1})$$

$$H_m^{(1)}(x) = J_m(x) + iY_m(x), \quad (\text{A.2})$$

$$H_m^{(2)}(x) = J_m(x) - iY_m(x), \quad (\text{A.3})$$

$$H_0^{(2)}(x) = -H_0^{(1)}(-x), \quad (\text{A.4})$$

RECURRENCE RELATIONS

$$\frac{1}{2}(\mathcal{S}_{m-1}(x) - \mathcal{S}_{m+1}(x)) = \mathcal{S}'_m(x), \quad (\text{A.5})$$

$$\frac{x}{2m}(\mathcal{S}_{m-1}(x) + \mathcal{S}_{m+1}(x)) = \mathcal{S}_m(x), \quad (\text{A.6})$$

JACOBI-ANGER IDENTITY

$$e^{ikr \cos(\theta)} = \sum_{n \in \mathbb{Z}} i^n J_n(kr) e^{in\theta}. \quad (\text{A.7})$$

ASYMPTOTIC FORMULAE

$$\lim_{x \rightarrow 0} J_0(x) = 1, \quad (\text{A.8})$$

$$\lim_{x \rightarrow 0} J_m(x) \sim \frac{1}{\Gamma(m+1)} \left(\frac{x}{2}\right)^m, \quad m > 0, \quad (\text{A.9})$$

$$\lim_{x \rightarrow \infty} J_m(x) \sim \sqrt{\frac{2}{\pi x}} \cos\left(x - \frac{m\pi}{2} - \frac{\pi}{4}\right), \quad \forall m. \quad (\text{A.10})$$

$$\lim_{x \rightarrow 0} Y_0(x) \sim \frac{2}{\pi} \ln(x), \quad (\text{A.11})$$

$$\lim_{x \rightarrow 0} Y_m(x) \sim -\frac{\Gamma(m)}{\pi} \left(\frac{2}{x}\right)^m, \quad m > 0, \quad (\text{A.12})$$

$$\lim_{x \rightarrow \infty} Y_m(x) \sim \sqrt{\frac{2}{\pi x}} \sin\left(x - \frac{m\pi}{2} - \frac{\pi}{4}\right), \quad \forall m. \quad (\text{A.13})$$

$$\lim_{x \rightarrow \infty} H_m^{(1)}(x) \sim \sqrt{\frac{2}{\pi x}} e^{i(x - \frac{m\pi}{2} - \frac{\pi}{4})}, \quad \forall m, \quad (\text{A.14})$$

$$\lim_{x \rightarrow \infty} H_m^{(2)}(x) \sim \sqrt{\frac{2}{\pi x}} e^{-i(x - \frac{m\pi}{2} - \frac{\pi}{4})}, \quad \forall m. \quad (\text{A.15})$$

INTEGRALS

$$\int_0^\eta \xi^{l+1} J_l(k\xi) d\xi = \eta^{l+1} \frac{J_{l+1}(k\eta)}{k}, \quad (\text{A.16})$$

$$\int_0^\eta \xi^{l+1} Y_l(k\xi) d\xi = \eta^{l+1} \frac{Y_{l+1}(k\eta)}{k} + \frac{2^{l+1} l!}{\pi k^{l+2}}. \quad (\text{A.17})$$

A.2 Operators

CURL OF CURL IDENTITY

$$\nabla \times (\nabla \times \mathbf{V}) = \nabla(\nabla \cdot \mathbf{V}) - \nabla^2 \mathbf{V} \quad (\text{A.18})$$

BIHARMONIC OPERATOR IN POLAR COORDINATES

$$\nabla^4 u = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} \left(\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial u}{\partial r} \right) \right) \right) + \frac{2}{r^2} \frac{\partial^4 u}{\partial \theta^2 \partial r^2} + \frac{1}{r^4} \frac{\partial^4 u}{\partial \theta^4} - \frac{2}{r^3} \frac{\partial^3 u}{\partial \theta^2 \partial r} + \frac{4}{r^4} \frac{\partial^2 u}{\partial \theta^4} \quad (\text{A.19})$$

A.3 Addition Theorems

POISSON SUMMATION FORMULA

$$\sum_{n \in \mathbb{Z}} \int_{-\infty}^{\infty} e^{\pm i n u} F(u) du = 2\pi \sum_{n \in \mathbb{Z}} F(2\pi n) \quad (\text{A.20})$$

$$\sum_{n \in \mathbb{Z}} e^{i n u} = 2\pi \sum_{n \in \mathbb{Z}} \delta(2\pi n + u) \quad (\text{A.21})$$

GRAF'S ADDITION THEOREM

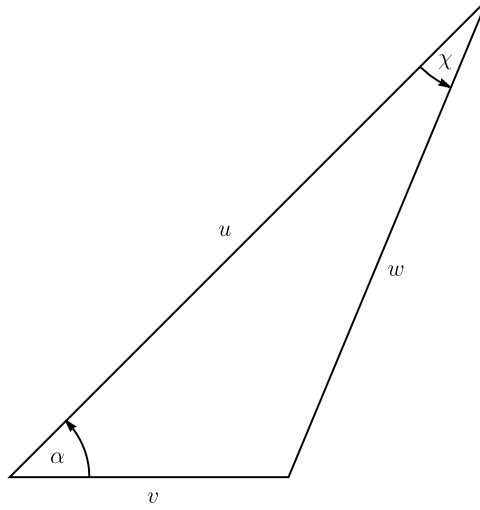


Figure A.1: Graf's addition theorem.

$$\mathcal{S}_m(w) e^{i m \chi} = \sum_{q \in \mathbb{Z}} \mathcal{S}_{m+q}(u) J_q(v) e^{i q \alpha}, \text{ for } v < u \quad (\text{A.22})$$

B Asymptotic Formulae for Lattice Homogenization

B.1 Approximations of Boundary Coefficients

The boundary coefficients (6.40a) are approximated as the following series expansions in small k for $p \in [0, 1, 2]$:

$$M_0 = \frac{2\gamma}{\pi} + \frac{2}{\pi} \log \left(\frac{ka}{2} \right), \quad (\text{B.1a})$$

$$M_1 = -\frac{4}{\pi(ka)^2} + \frac{-3 + 4\gamma}{2\pi} + \frac{2}{\pi} \log \left(\frac{ka}{2} \right), \quad (\text{B.1b})$$

$$M_2 = -\frac{32}{\pi(ka)^4} - \frac{32}{3\pi(ka)^2} + \frac{-83 + 72\gamma}{36\pi} + \frac{2}{\pi} \log \left(\frac{ka}{2} \right), \quad (\text{B.1c})$$

and

$$M'_0 = -\frac{4}{\pi(ka)^2} + \frac{-3 + 4\gamma}{2\pi} + \frac{2}{\pi} \log \left(\frac{ka}{2} \right), \quad (\text{B.2a})$$

$$M'_1 = \frac{4}{\pi(ka)^2} + \frac{5 + 4\gamma}{2\pi} + \frac{2}{\pi} \log \left(\frac{ka}{2} \right), \quad (\text{B.2b})$$

$$M'_2 = \frac{32}{\pi(ka)^4} + \frac{16}{3\pi(ka)^2} + \frac{5 + 72\gamma}{36\pi} + \frac{2}{\pi} \log \left(\frac{ka}{2} \right). \quad (\text{B.2c})$$

All approximations (B.1), (B.2) have been truncated so as to exclude all terms of $\mathcal{O}(ka)^2$.

B.2 Approximations of Interior Coefficients

The interior coefficients (6.40b) and (6.40c) are approximated as the following series expansions in small k for $p \in [-2, \dots, 1]$, $n \in [0, 1]$:

$$\{C_{-2,0}, D_{-2,0}\} = e^{2i\delta} n_r^2 \left(1 - \frac{1}{12} (ka)^2 (n_r^2 - 1) \right), \quad (\text{B.3a})$$

$$\{C_{-2,1}, D_{-2,1}\} = e^{2i\delta} n_r \left(\pm \frac{2}{ka} \mp \frac{1}{6} (ka) (n_r^2 - 1) \right), \quad (\text{B.3b})$$

$$\{C_{-1,0}, D_{-1,0}\} = ie^{i\delta} n_r \left(\pm 1 \mp \frac{1}{8} (ka)^2 (n_r^2 - 1) \right), \quad (\text{B.3c})$$

$$\{C_{-1,1}, D_{-1,1}\} = ie^{i\delta} \left(\frac{1}{ka} - \frac{1}{8} (ka) (n_r^2 - 1) \right), \quad (\text{B.3d})$$

$$\{C_{0,0}, D_{0,0}\} = -1 + \frac{1}{4} (ka)^2 (n_r^2 - 1), \quad (\text{B.3e})$$

$$\{C_{0,1}, D_{0,1}\} = 0, \quad (\text{B.3f})$$

$$\{C_{1,0}, D_{1,0}\} = ie^{-i\delta} n_r \left(\mp 1 \pm \frac{1}{8} (ka)^2 (n_r^2 - 1) \right), \quad (\text{B.3g})$$

$$\{C_{1,1}, D_{1,1}\} = ie^{-i\delta} \left(\frac{1}{ka} - \frac{1}{8} (ka) (n_r^2 - 1) \right), \quad (\text{B.3h})$$

and

$$\{C'_{-2,0}, D'_{-2,0}\} = e^{2i\delta} n_r \left(1 - \frac{1}{6} (ka)^2 (n_r^2 - 1) \right), \quad (\text{B.4a})$$

$$\{C'_{-2,1}, D'_{-2,1}\} = e^{2i\delta} n_r \left(\pm \frac{1}{ka} \mp \frac{1}{12} (ka) (3n_r^2 - 2) \right), \quad (\text{B.4b})$$

$$\{C'_{-1,0}, D'_{-1,0}\} = ie^{i\delta} \left(\pm 1 \mp \frac{3}{8} (ka)^2 (n_r^2 - 1) \right), \quad (\text{B.4c})$$

$$\{C'_{-1,1}, D'_{-1,1}\} = -ie^{i\delta} \frac{1}{4} (ka) n_r, \quad (\text{B.4d})$$

$$\{C'_{0,0}, D'_{0,0}\} = n_r \left(-1 + \frac{1}{8} (ka)^2 (n_r^2 - 1) \right), \quad (\text{B.4e})$$

$$\{C'_{0,1}, D'_{0,1}\} = 0, \quad (\text{B.4f})$$

$$\{C'_{1,0}, D'_{1,0}\} = ie^{-i\delta} \left(\mp 1 \pm \frac{3}{8} (ka)^2 (n_r^2 - 1) \right), \quad (\text{B.4g})$$

$$\{C'_{1,1}, D'_{1,1}\} = -ie^{-i\delta} \frac{3}{8} (ka) n_r. \quad (\text{B.4h})$$

All approximations (B.3), (B.4) have been truncated so as to exclude all terms of $\mathcal{O}(ka)^3$.

B.3 Approximations of Lattice Sums

The following method for approximating the dynamic lattice sums:

$$S_l^Y(k, \mathbf{k}_0) J_l(k\xi) = -Y_0(k\xi) \delta_{l,0} - \frac{4}{A} i^l \sum_h \frac{J_l(Qh\xi)}{Q_h^2 - k^2} e^{il\theta_h}. \quad (\text{B.5})$$

follows that set out by Poulton [143]. In homogenizing the plate-array crystal, we require the series expansion of (B.5) correct to $\mathcal{O}(k^0)$. By separating the $h = 0$ and $h \neq 0$ terms and making use of Graf's addition theorem on the latter summation, we arrive to the expression:

$$\begin{aligned} S_l^Y = & -\frac{Y_0(k\xi)}{J_0(k\xi)} \delta_{l,0} - i^l \frac{4}{d^2} \frac{e^{il\theta_0}}{k_0^2 - k^2} \frac{J_l(k_0\xi)}{J_l(k\xi)} \\ & - \frac{i^l}{J_l(k\xi)} \frac{4}{d^2} \sum_{h \neq 0} \sum_{m \in \mathbb{Z}} \frac{(-1)^m J_{l+m}(K_h\xi) J_m(k_0\xi) e^{i(l+m)\psi_h - im\theta_0}}{Q_h^2 - k^2}, \end{aligned} \quad (\text{B.6})$$

where $\mathbf{K}_h = (K_h, \psi_h)$. The denominators $(Q_h^2 - k^2)^{-1}$ are approximated to $\mathcal{O}(k^2)$:

$$\begin{aligned} (Q_h^2 - k^2)^{-1} & \approx K_h^{-2} \left(1 + 2 \frac{k_0}{K_h} \cos(\psi_h - \theta_0) + \frac{k_0^2 - k^2}{K_h^2} \right)^{-1} \\ & = K_h^{-2} \left(1 - 2 \frac{k_0}{K_h} \cos(\psi_h - \theta_0) + 2 \frac{k_0^2}{K_h^2} \cos(2(\psi_h - \theta_0)) + \frac{k_0^2 + k^2}{K_h^2} \right), \end{aligned} \quad (\text{B.7})$$

for which it was assumed $k, k_0 < K_h, \forall h \neq 0$. By combining (B.6) and (B.7) we obtain the approximation formulae for the dynamic lattice sums of all requisite orders 0-3. Orders 0-2 are available in chapter 4 of [143], and are repeated here to $\mathcal{O}(k^0)$:

$$S_0^Y = -\frac{4}{d^2(k_0^2 - k^2)} - \left(\frac{2\gamma}{\pi} + 4\gamma_0 \right) - \frac{2}{\pi} \log(kd) + \mathcal{O}(k_0d), \quad (\text{B.8})$$

$$S_1^Y = -\frac{4ie^{i\theta_0}}{d^2} \frac{k_0}{k} \left(\frac{1}{k_0^2 - k^2} - \frac{d^2}{4\pi} \right) + \mathcal{O}(k_0d), \quad (\text{B.9})$$

$$S_2^Y = \frac{4}{d^2} \frac{k_0^2}{k^2} \left\{ \left(\frac{1}{k_0^2 - k^2} - \frac{d^2}{8\pi} \right) e^{2i\theta_0} + \frac{d^2}{4\pi^2} \tilde{\sigma}_2^{(4)} e^{-2i\theta_0} \right\} + \mathcal{O}(k_0d), \quad (\text{B.10})$$

where γ is the Euler constant, $\gamma_0 = -0.318895593319827$ is a constant and $\tilde{\sigma}_2^{(4)} = 4.0784511611614 - \pi/2$. This latter quantity, defined in chapter 3 of [143] and in [13], is a type of static lattice sum. These static lattice sums are prevalent in electrostatic or elastostatic problems i.e. fields subject to Laplace's equation. The quoted highly accurate numerical value of the static lattice sum was evaluated in [187, 188]. Order 3 of (B.5) is approximated as:

$$\begin{aligned}
S_3^Y \approx & \frac{4ie^{3i\theta_0}}{d^2} \left\{ \frac{1}{k_0^2 - k^2} \frac{J_3(k_0\xi)}{J_3(k\xi)} - k_0 d^3 S_{1,0,3} \frac{J_2(k_0\xi)}{J_3(k\xi)} + k_0^2 d^4 S_{2,0,4} \frac{J_1(k_0\xi)}{J_3(k\xi)} \right\} \\
& + \frac{4ie^{-i\theta_0}}{d^2} \left\{ \left(k_0^2 d^4 S_{2,4,4} - d^2 S_{4,4,2} - (k_0^2 + k^2) d^4 S_{4,4,4} \right) \frac{J_1(k_0\xi)}{J_3(k\xi)} \right. \\
& \left. - k_0 d^3 S_{3,4,3} \frac{J_0(k_0\xi)}{J_3(k\xi)} - k_0 d^3 S_{5,4,3} \frac{J_2(k_0\xi)}{J_3(k\xi)} \right\}
\end{aligned} \tag{B.11}$$

where:

$$S_{l,m,n}(\xi) = \sum_{h \neq 0} \frac{J_l(K_h \xi) e^{im\psi_h}}{(K_h d)^n}, \tag{B.12}$$

is another type of lattice sum. Expressions for sums of the form (B.12) are found using the lattice sum recurrence relations found in chapter 3 of [143]. The remaining sums not found in [143] are of the form:

$$S_{4,4,4} = \frac{\tilde{\sigma}_2^{(4)}}{12\pi} \left(\frac{\xi}{2d} \right)^4 - \frac{\sigma_4^{(4)}}{5\pi} \left(\frac{\xi}{2d} \right)^6, \tag{B.13a}$$

$$S_{5,4,3} = \frac{\sigma_4^{(4)}}{5\pi} \left(\frac{\xi}{2d} \right)^5, \tag{B.13b}$$

where $\sigma_4^{(4)} = 3.1512120021539$ [187], Table 2. Combining (B.11), (B.13) and the remaining sums found in [143], and making use of the following series expansions:

$$\begin{aligned} \frac{J_0(k_0\xi)}{J_3(k\xi)} &= \frac{48}{k^3\xi^3} + \left(\frac{3k_0}{k} - \frac{12k_0^3}{k^3}\right) \frac{1}{k_0\xi} + \frac{3}{4} \left(\frac{k_0^3}{k^3} - \frac{k_0}{k}\right) k_0\xi \\ &\quad + \left(\frac{3k_0^3}{64k} - \frac{k_0^3}{48k^3}\right) k_0^3\xi^3 + \mathcal{O}(k_0\xi)^5, \end{aligned} \quad (\text{B.14})$$

$$\frac{J_1(k_0\xi)}{J_3(k\xi)} = \frac{24k_0}{k^3\xi^2} + 3 \left(\frac{k_0}{2k} - \frac{k_0^3}{k^3}\right) + \left(\frac{k_0^3}{8k^3} - \frac{3k_0}{16k}\right) k_0^2\xi^2 + \mathcal{O}(k_0\xi)^4, \quad (\text{B.15})$$

$$\begin{aligned} \frac{J_2(k_0\xi)}{J_3(k\xi)} &= \frac{6k_0^2}{k^3\xi} + \left(\frac{3k_0}{8k} - \frac{k_0^3}{2k^3}\right) k_0\xi + \left(\frac{k_0^3}{64k^3} - \frac{k_0}{32k}\right) k_0^3\xi^3 \\ &\quad + \mathcal{O}(k_0\xi)^5, \end{aligned} \quad (\text{B.16})$$

$$\frac{J_3(k_0\xi)}{J_3(k\xi)} = \frac{k_0^3}{k^3} + \left(\frac{k_0}{16k} - \frac{k_0^3}{16k^3}\right) k_0^2\xi^2 + \mathcal{O}(k_0\xi)^4, \quad (\text{B.17})$$

we obtain:

$$S_3^Y = \frac{4i}{d^2} \frac{k_0^3}{k^3} \left\{ e^{3i\theta_0} \left(\frac{1}{k_0^2 - k^2} + \frac{3d^2}{8\pi} \right) + e^{-i\theta_0} \left(\frac{3d^2 \tilde{\sigma}_2^{(4)}}{4\pi^2} - \frac{2\tilde{\sigma}_2^{(4)}}{\pi k_0^2} \right) \right\} + \mathcal{O}(k_0 d). \quad (\text{B.18})$$

Note that the variable ξ is not present in (B.18) as the lattice sum S_l^Y is independent of ξ , as per (B.5). The approximation (B.18) has undergone validation by numerical comparison with the accelerated summation (6.31) for which the number of successive integrations p was set to $p = 5$.