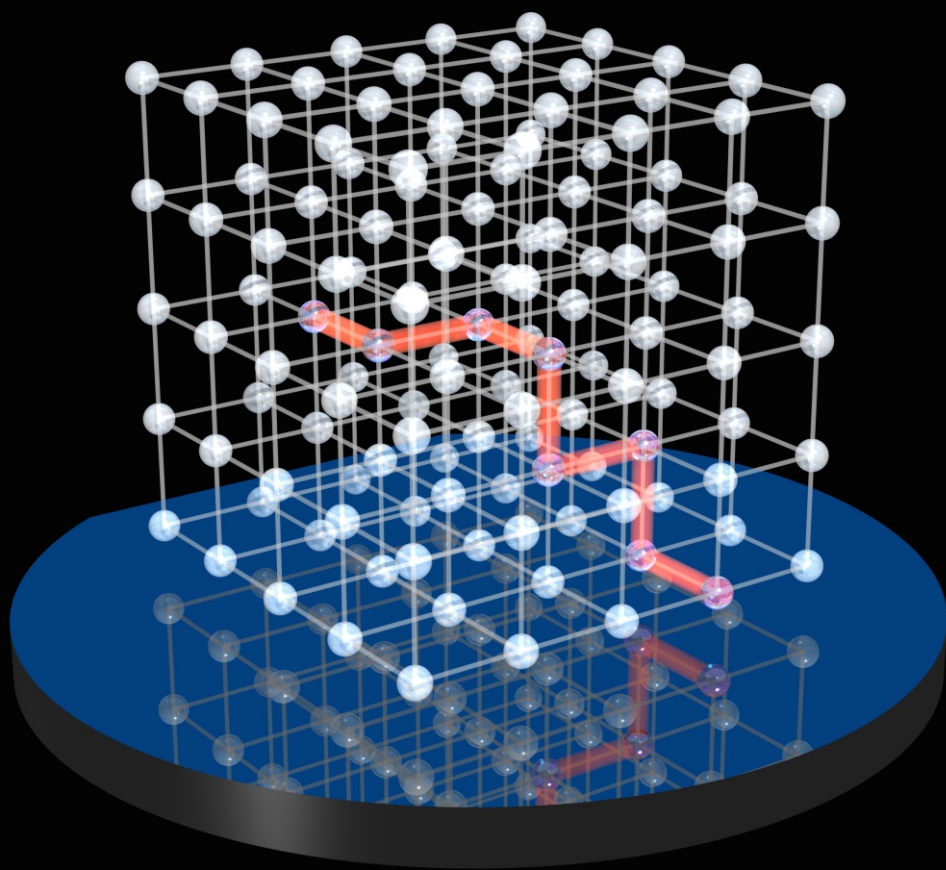


Computational Nanophotonics in 3D



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Computational Nanophotonics in 3D

Sjoerd Arthur Hack

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To my parents

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CHAPTER 1

Introduction

1.1 Optics

Ever since antiquity, the properties of light have fascinated humanity [1]. Indeed, the scientists of the ancient world were familiar with the rectilinear propagation of light as well as the law of reflection, and made fairly precise measurements of the angles of incidence and refraction in various media [2]. The first variational principle in physics was formulated by Hero of Alexandria in the first century AD, who stated that *the path taken by light in going from some point S to a point P via a reflecting surface is the shortest possible one*. Around 1000, Ibn al-Haytham [1] extended the theory of reflection and gave a detailed description of the human eye.

People have also long sought to manipulate light. Optical tools such as mirrors, magnifying and burning glasses have been excavated in such places as the workers' quarters near the pyramid of Sesostris and in Pompeii, and are widely alluded to in texts by ancient writers. Since spectacles were in wide use by the late Middle Ages, it is not surprising that the first patent on a telescope was applied for by a spectacle maker, the Dutchman Lippershey in 1608, although it is not clear who invented it. At the same time, telescopes and microscopes started to transform our vision of the world. Galilei observed the moons of Jupiter, and Van Leeuwenhoek observed life at microscopic length scales [3]. Kepler's descriptions of the human eye as a lens and of the workings of telescopes are widely considered to be the beginning of modern optics [4].

By the seventeenth century, scientists were developing mathematical theories of the nature of light and heavily debating them. The Dutchman Huygens derived the laws of reflection and refraction and even explained the double refraction of calcite employing his wave theory [5]. Newton discovered that white light actually consists of many colors of light [6], colors of the rainbow, and explained his results with a corpuscular theory of light [7]. Newton's main objection to the wave theory was the rectilinear propagation of light, which seemed daunting to explain with a wave theory, and for a time this determined the scientific consensus. The missing ingredient was the principle of wave interference, which was discovered by Young, and presented at meetings of the Royal Society in 1801-1803. He was able to explain the colored fringes of thin films using Newton's data. Maxwell developed a theory of electricity and magnetism and discovered that *light is an electromagnetic disturbance in the form of waves*. Some objections to the wave theory were not fully resolved until the discovery of relativity by Einstein in 1905.

In 1905, building on ideas by Planck [8], Einstein also proposed a theory of light based on the dual nature of light as an electromagnetic wave and as a particle [9]. While light behaves like a wave in the sense that it can form interference fringes, its energy is quantized in case of any interaction with matter, such as absorption or emission. Each quantum of energy $\mathcal{E} = \hbar\omega$, with ω the frequency and $\hbar$ Planck's constant, is called a *photon*. The particle nature of light can be made visible in a photomultiplier tube, where the arrival of a single photons can be seen as dots on a screen or as clicks on a loudspeaker. The quantum mechanical theory of light is crucial to understand how light is emitted and absorbed by atoms, for a pedagogical introduction see Ref. [10]. This theory underpins the understanding of lasers, which have deeply transformed technology in recent decades, and are used for reading videodisks at home, cutting steel in factories, scanning labels in supermarkets, performing surgery in hospitals, and for many many other applications that have influenced modern scientists [1].

1.2 Nanophotonics

Understanding the properties of light and the interaction of light with materials has been a topic of intense research for many years. Examples of light-matter interactions are lasing [11–13], Förster energy transfer [14–16], spontaneous emission [11, 12, 17] and absorption [17]. For low frequencies, such interactions are thoroughly scrambled by phonons. It is therefore necessary to consider optical wavelengths in the range of 10^2 THz for the study of light-matter interactions. Light has wavelengths of the order of 10^2 nm and controlling it requires nanoscale structures, such as random media, photonic crystals, plasmonic antennae, metamaterials, and cavity arrays that are studied in the field of nanophotonics [18–21].

A broad classification of nanophotonic structures distinguishes disordered nanophotonic structures, *i.e.*, a random arrangement of the constituent materials (for example silicon and air), from ordered nanophotonic structures, *i.e.*, a periodic arrangement of the constituent materials. Disordered nanophotonic structures [22, 23] are used as the textured optical sheets in solar cells [24], and phosphor plates in a white LED [25]. Light propagation in disordered nanostructures is not “out of control”, and it is possible to focus light through or in such structures by shaping the incident wavefronts [26, 27]. Ordered nanophotonic structures are employed for multi-emitter quantum electrodynamics [28], extreme field confinement in plasmonic systems [29], topologically-protected propagation [30], in which light propagates without backscattering, cloaks and metamaterials [31], and slow light [32].

The optical properties of photonic nanostructures can be totally unexpected even if one knows all about the constituent materials [33]. Frequently, these optical properties are first predicted by investigating analogies between the behavior of photons at the nanoscale, and the physics of electrons, spins, and phonons in condensed matter [34–39]. The underlying physics in either case is the multiple scattering of waves. Each inhomogeneity in the refractive index in a small region of space in a nanophotonic structure can loosely speaking be seen as a scattering

particle, which scatters an incident light wave in all possible directions.

1.3 Scattering of light

In photonic nanostructures, there are many inhomogeneities, with the result that light is repeatedly scattered.

For weakly-scattering random structures, the scattering of a light wave by the structure can be seen as a random walk. The transport mean free path length l gives the distance before the direction of light waves is fully randomized. This scattering is described by Ohm's law, similar to the diffusion of electrons through a resistor. The diffuse transmission, or conductance, is proportional to the ratio of the transport mean free path to the sample thickness (l/L) [34, 40]. Such scattering is also observed in clouds, sugar, toothpaste, paper, paint, and biological skin tissue.

In strongly-scattering random structures, there is interference between the many paths that the scattering can take. Waves passing a certain location in a structure return more easily to this location than that they travel away during multiple scatterings since the time-reversed versions of closed scattering paths constructively interfere. In the extreme case, this leads to Anderson localization of light, which is a peculiar state of light where the transport is completely halted due to interference between multiple scattering paths [17, 22, 40–43], in analogy to Anderson localization of spins [43]. Anderson localization of light may give enhanced absorption in a material [41]. For strongly scattering random samples, Anderson localization is predicted to occur when the mean free path l is on the order of the wavelength of light, λ [17, 22, 40–43]

$$2\pi l/\lambda \approx 1, \quad (1.1)$$

which is also known as the Ioffe-Regel criterion [40, 44]. The quest for Anderson localization of light continues to receive attention to date [22, 45, 46]. Another well-known interference phenomenon in strongly-scattering random structures is the weak localization or enhanced backscattering of light [47, 48], in analogy to that of electrons [49]

Three-dimensional photonic crystals are an important class of ordered nanophotonic structures [12, 17, 50]. In photonic crystals, the refractive index varies spatially with a periodicity on length scales comparable to the wavelength of light. Photonic crystals can be seen as an optical analogue of semiconductors [50]. Interference of waves diffracted by different lattice planes determines the optical modes and dispersion. The periodicity gives rise to Bragg diffractions, which are associated with frequency windows that are forbidden for propagation of light in a certain direction [51]. Such *stop gaps* have long been known to arise for light in one-dimensionally periodic structures, known as dielectric mirrors or Bragg stacks [52]. A stop gap is associated with propagation along a specific direction. In three-dimensional photonic crystals a stop gap for all directions simultaneously can be achieved, resulting in a so-called *photonic band gap* [12, 17, 50], in analogy to the electronic band gap in a semiconductor crystal

such as silicon or germanium [51].

The total absence of optical states in the frequency range of the 3D band gap has important ramifications for the interaction between light and matter. The inhibition of spontaneous emission in periodic structures was first predicted by Bykov in 1972 [11]: excited atoms inside a crystal with their transition frequencies tuned to the band gap cannot emit photons, which was experimentally demonstrated on quantum dots by Leistikow *et al.* [53]. Once a band gap is created, the physics can be further enriched by creating isolated defects that act as resonant cavities. Such defects are predicted to introduce single electromagnetic modes with a frequency in the band gap, confined to within a wavelength [54–56], also called a “cage for light”. It is important to realize that confinement by a band gap differs fundamentally from Anderson localization: a defect is surrounded by a spatial region that has no optical states for a certain frequency range and therefore acts as a mirror, whereas Anderson localized states occur throughout an entire spatial region and frequency range, but are not propagating. Such “cages for light” [57] provide a route to solid state cavity quantum electrodynamics [58].

During the past years, enormous progress has been made in the fabrication of high-quality three-dimensional (3D) photonic-band-gap crystals [59–72]. However, inevitable variations in the size and position of geometrical building blocks occur in any fabricated 3D crystal [73]. Light then scatters at the defects in the photonic crystal structure, which results in the extinction of a light beam into diffuse light [73]. Conversely, disorder leads to rich physics related to diffusion of light and Anderson localization of light [17, 22, 40–43, 73].

In photonic band gap crystals, the Ioffe-Regel criterion for Anderson localization is modified to $kl \approx 1/\sqrt{\rho_s}$, with k the wave vector and $\rho_s = N(\omega)/N_0(\omega)$ the modification of the photonic density of states (DOS) $N(\omega)$ relative to free-space $N_0(\omega)$ [17, 73–75]. The density of states $N(\omega)$ counts the number of electromagnetic modes $N(\omega)\Delta\omega$ in the frequency window from ω to $\omega + \Delta\omega$, and appears notably in Fermi’s golden rule for the spontaneous emission rate of an emitter [57]. At the edges of the band gap, the density of states is very low. Effectively, the reduction in the density of states in or near a gap corresponds to a reduction of the dimensionality of the phase space for light. Since a lower system dimension (*e.g.* 1D or 2D vs 3D) is known to be favorable for localization [40], the modified Ioffe-Regel criterion is predicted to be easily satisfied [17, 74, 75]. As a result, as the scattering disorder strength increases, the band gap is progressively filled with localized states, starting from the edges and proceeding inwards. This would be visible as a smoothening of the density of states at the edges of the band gap. Indeed, a numerical study by Conti and Fratalocchi of 3D inverse opal photonic crystals with strong disorder shows the progressive closing of the band gap, a non-exponential decay of transmission, and Anderson localization of light [76].

To obtain a full picture of localization in 3D photonic band gap crystals, it is necessary to know the density of states, which is effectively identified as the wave vector k in the product kl . In calculations with externally-incident light beams such as in Ref. [76], it is likely that we incompletely sample the DOS, and thus there is a systematic error in the measure of kl . Therefore, in Chapter 4, we perform a numerical study of the DOS in disordered photonic crystals with a

method that unambiguously samples all possible modes in the DOS.

The COPS research group [77] fabricates and experimentally studies a class of 3D photonic crystals called inverse woodpile photonic crystals. These structures have nearly the same symmetry as a diamond crystal of carbon atoms [78], yet thousandfold magnified, as illustrated in a youtube animation [79]. It is well-known experimentally that diamond structured photonic crystals have broad band gaps [58, 80, 81], which is important for obtaining a strong inhibition of spontaneous emission. The inverse woodpile crystal structure consists of two perpendicular 2D arrays of nanopores with radius r in a high-index medium such as silicon [78], as illustrated in Figure 1.1(a) and the fabricated crystal in Fig. 1.1(b). Each 2D pore array corresponds to a diamond $\{110\}$ crystal face. In view of the arrangement of the nanopores, it appears to be convenient to employ a tetragonal unit cell [82, 83] instead of the conventional cubic unit cell [51]. The tetragonal unit cell has lattice parameters c (in the x and z directions), and a (in the y direction) in a ratio $a/c = \sqrt{2}$ to ensure a cubic crystal structure.

Inverse woodpile photonic crystals possess a broad 3D photonic band gap, whose width strongly depends on the radius r of the pores [78, 82, 83]. For a normalized pore radius $r/a = 0.24$ a maximum relative bandwidth $\Delta\omega_{pbg}/\omega_c = 25.3\%$ occurs for $\epsilon = 12.1$ typical of silicon [82, 83], with $\Delta\omega_{pbg}$ the frequency width of the band gap, ω_c the band gap's center frequency, and ϵ the electric permittivity. Three-dimensional inverse woodpile crystal nanostructures have been fabricated from a number of different high-refractive index backbones [59–61, 84–86].

To create a resonant cavity in a inverse woodpile photonic crystal, Woldering *et al.* [87] proposed a design whereby two proximal perpendicular pores have a smaller radius ($r' < r$) than all other pores, as shown in Figure 1.1(a). Near the intersection region of the two smaller pores, light is confined in all three directions to within a mode volume as small as $V_{\text{mode}} = \lambda^3$, where λ is the free-space wavelength [87]. Supercell band structures revealed up to five resonances [88] within the band gap of the perfect crystal, depending on the defect pore radius r' [87]. These bands have quadrupolar symmetry and are the optical analogues of d-orbitals in solid-state-physics [51, 88].

1.4 Light in coupled cavities

Depending on the geometric structure of photonic crystals and the materials used, light propagation in photonic crystals can show very unusual behavior. An exciting research question is to investigate the light propagation in a 3D cavity superlattice embedded within a 3D photonic band gap crystal. The propagation of light in such a 3D cavity superlattice is analogous to electronic transport in an impurity band in a semiconductor [43, 51, 89]. The 3D cavity superlattice has superlattice Bloch modes where photons hop between cavities [90].

Since the resonances of the cavity have quadrupolar symmetry, one might naively expect neighbouring cavities to couple mostly in diagonal directions. For a 1D coupled-resonator optical waveguide (CROW), it is well-known that the

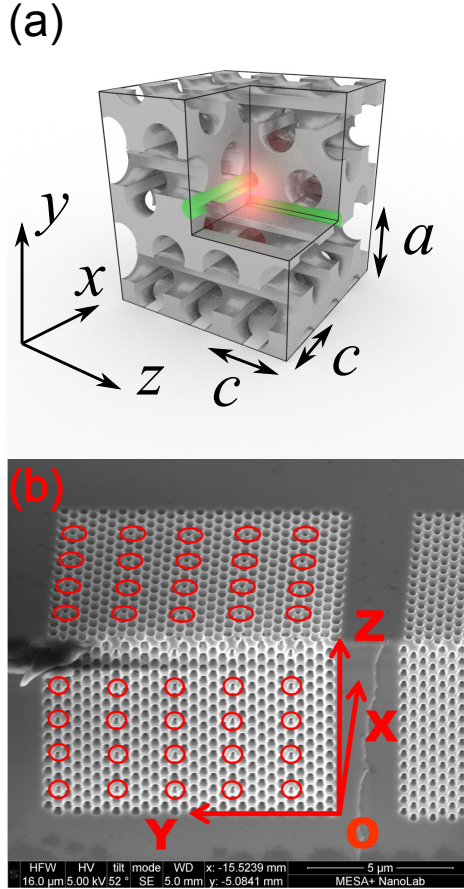


Figure 1.1: (a) Design of a single cavity in an inverse woodpile photonic band gap crystal shown in a cut-out of a $3 \times 3 \times 3$ supercell that is surrounded by boxed lines. The high-index backbone is shown in gray. Two proximal smaller defect pores are indicated in green, and the cavity region is highlighted as the bright region at the center. The tetragonal lattice parameters a and c are shown, as well as the x, y, z coordinate system. (b) SEM image of a superlattice of $5 \times 5 \times 5$ cavities in a 3D inverse woodpile photonic crystal fabricated in silicon. Smaller pores, which are marked with red circles, form cavities inside the structure. The scale bar is shown in the image. Image courtesy of Cock Harteveld.

coupling coefficient along the waveguide is proportional to the dispersion bandwidth [91]. A straightforward extension of this notion to a 3D cavity superlattice is to consider the dispersion bandwidth in various crystal directions. According to this 1D CROW-like argument, we might therefore expect the dispersion bandwidth to look like a quadrupolar radiation pattern. To understand the coupling between the cavities in a 3D cavity superlattice more fundamentally, it is necessary to derive the coupling coefficients from the dispersion relations using the tight-binding method [51, 91]. Therefore, in Chapter 2 we calculate for the first time the dispersion bandwidth as well as the coupling coefficients for the superlattice Bloch modes of the 3D cavity superlattice, and we see behavior that is remarkably different from the 1D CROW-like argument given above.

The superlattice Bloch modes do not give a full picture of light propagation in 3D cavity superlattices, since all the cavities are then excited simultaneously. Therefore, in Chapter 3, we calculate the time-resolved propagation for an ultrashort input pulse that initially excites only a single cavity, with frequencies within a single band of the superlattice.

A 3D cavity superlattice is the photonic analogue of the Nobel prize winning Anderson model for spins and electrons [43], albeit in the limit of zero disorder. We anticipate that the present study may form the basis for further exploration of the physics of the 3D Anderson model for nanophotonic cavity superlattices that will proceed by introducing controlled degrees of disorder in the cavity resonance frequencies.

1.5 Computational nanophotonics

New physics is often discovered by first investigating a theoretical model, see Ref. [43]. However, while the Maxwell equations have been known for a long time, they are rarely exactly solvable in nanophotonic media. Therefore, one often has to solve the equations numerically to find the phenomena predicted by the equations defining a theoretical model [50]. The theory and numerical solutions also often may give quantities that can be potentially observed in experiments, to verify if the experiment exhibits the physics predicted by the model or perhaps unexpected new phenomena. Thus, numerical simulations act as a bridge between theory and experiments. In this Section, we give a brief overview of methods that are frequently used for 3D photonic crystal computations. More extensive overviews of numerical methods for nanophotonic structures are given in Gallinet *et al.* [92] and in Appendix D of Ref. [50], and a quantitative comparison is presented in Ref. [93].

In the finite-difference time-domain (FDTD) method, both time and space are discretized, *i.e.*, all spatial and temporal derivatives in Maxwell's equations are replaced by finite difference quotients [94–96]. In order to ensure a stable numerical result, the time increment Δt should satisfy the Courant condition

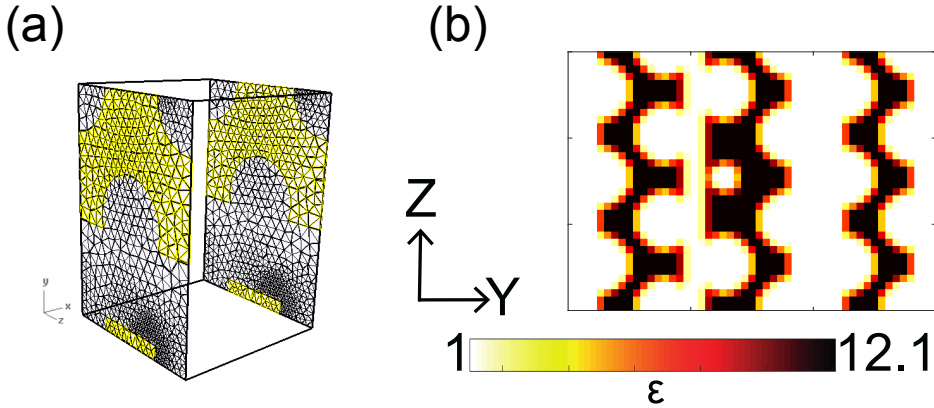


Figure 1.2: (a) Mesh for an inverse woodpile crystal employing tetrahedral elements, reproduced from Ref. [97]. While in Ref. [97] the mesh has been employed for discontinuous Galerkin finite element calculations, it could be used for conforming finite element calculations as well. (b) Cross section of the dielectric permittivity distribution $\epsilon(\mathbf{r})$ in the YZ plane of the $3 \times 3 \times 3$ supercell of a 3D inverse woodpile photonic crystal with point defect using the MPB plane-wave expansion (PWE) method with a grid resolution of $24 \times 34 \times 24$ [98]. The black color represents the high-index backbone and the white color represents free space. Two orthogonal defect pores result in a region with an excess of high-index backbone. In the MPB plane-wave expansion method, the curved material interfaces are represented with a staircase approximation together with a smoothing of the dielectric permittivity.

given by [95]

$$\Delta t \leq \frac{1}{c_0} \left(\sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}} \right)^{-1} = \frac{1}{c_0} \frac{1}{\sqrt{3}} \Delta x, \quad (1.2)$$

with c_0 the wave propagation speed, for $\Delta x = \Delta y = \Delta z$, *i.e.*, the time step should be smaller than a certain fraction of the spatial grid resolution. Therefore, the spatial resolution cannot be increased independently of the temporal resolution. The FDTD method is generally second-order accurate by nature of the central-difference approximation of the first-order spatial and temporal derivatives. Typically the spatial discretization error is dominant. However, when the position of a grid cell in the finite difference discretization does not follow the shape of material boundaries, this results in a staircase approximation for complex geometries and numerical inaccuracy, see Fig. 1.2(b). The spatial accuracy can be improved with nonhomogeneous grids [99] or the generalization of the Yee algorithm to irregular nonorthogonal unstructured grids [100]. Simply locally refining the grid is problematic since the time for a 3D FDTD simulation scales as resolution to the fourth power due to the Courant time step restriction [50].

A significant advantage of the FDTD, however, is that it scales only linearly with system size [101]. Also, the required computational memory scales only with

the volume of the computational domain, which makes FDTD efficient for large systems. Indeed, the finite-difference time-domain method has been employed by Conti and Fratalocchi to calculate Anderson localization of light in 3D inverse opal photonic crystals with strong disorder with as much as $8 \times 8 \times 8$ unit cells [76].

To perform accurate calculations of the electric field in and around complex structures, the conforming finite element method (FEM) is employed in the field of nanophotonics [102, 103]. The conforming FEM is efficient only in the frequency domain since at each time step one has to solve a linear system, even for explicit time integration methods, since the mass matrix is in general not diagonal [50, 104] or one has to use advanced mass lumping methods [105, 106]. The conforming FEM for the Maxwell equations generally employs Nédélec elements, which satisfy the DeRham complex, which is important to prevent spurious numerical oscillations since the mathematical structure of the Maxwell equations is better preserved, and allows for unstructured meshes [107–113] that can model accurately material boundaries, see Fig. 1.2(a). The conforming FEM is supported by an extensive mathematical theory, which gives it a solid theoretical basis [103, 114]. The conforming FEM requires, however, curl-conforming finite element spaces, which makes it rather difficult to use it for local *hp*-adaptation, where *h*-adaptation refers to local mesh refinement and *p*-adaptation to the local adjustment of the polynomial order. Another potential disadvantage of finite element methods for time-harmonic problems is that they require the solution of large systems of equations. Solving these equations directly would require $O(N^2)$ storage and $O(N^3)$ computing time with a direct (sparse) solver, where the number of degrees of freedom scales like $N \propto V$, where V is the volume of the system under consideration [50]. In principle, iterative methods would give linear scalings $O(N)$ for storage and $O(N)$ computing time [115]. The development of good iterative methods for time-harmonic Maxwell equations and the related Helmholtz equation is, however, still challenging and an active field of research [116–119]. In practice, finite element calculations of the Maxwell equations therefore often use a direct linear solver [88, 120, 121].

To calculate the band structure and eigenmodes of infinite periodic photonic crystals, the plane-wave expansion method is often employed [50, 98]. In this method, one solves for the Bloch envelope $\mathbf{u}_{\mathbf{k}}(\mathbf{r})$ of the magnetic field

$$\mathbf{H}_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} \mathbf{u}_{\mathbf{k}}(\mathbf{r}).$$

The Bloch envelope is expanded in a Fourier series

$$\mathbf{u}_{\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G}} \mathbf{c}_{\mathbf{G}}(\mathbf{k}) e^{i\mathbf{G} \cdot \mathbf{r}},$$

where the sum is taken over a discretization grid of reciprocal lattice vectors $\mathbf{G}$, and the Fourier coefficients are given by $\mathbf{c}_{\mathbf{G}} = \frac{1}{V} \int d^3\mathbf{r} e^{-i\mathbf{G} \cdot \mathbf{r}} \mathbf{u}_{\mathbf{k}}(\mathbf{r})$ with V the volume of the unit cell. To satisfy the divergence constraint $(\mathbf{k} + \mathbf{G}) \cdot \mathbf{c}_{\mathbf{G}} = 0$, the expansion coefficients are written in terms of two units vectors $\hat{\mathbf{e}}_{\mathbf{G}}^{(1)}$ and $\hat{\mathbf{e}}_{\mathbf{G}}^{(2)}$

that are themselves orthogonal to $\mathbf{k} + \mathbf{G}$, which gives

$$\mathbf{c}_{\mathbf{G}} = c_{\mathbf{G}}^{(1)} \hat{\mathbf{e}}_{\mathbf{G}}^{(1)} + c_{\mathbf{G}}^{(2)} \hat{\mathbf{e}}_{\mathbf{G}}^{(2)}.$$

The resulting eigenequations are solved by means of iterative methods, where the matrix-vector products are evaluated with of fast Fourier transforms, and that are accelerated with diagonal preconditioners [122]. For accurate results, it is important to use a sufficiently fine discretization grid of reciprocal lattice vectors. The convergence of the plane-wave expansion method is determined, however, by the rate of convergence of the Fourier expansion of the inverse dielectric function $\epsilon^{-1}(\mathbf{r}) = \sum_{\mathbf{G}} \epsilon_{\mathbf{G}}^{-1} e^{i\mathbf{G} \cdot \mathbf{r}}$, which is slow for structures with discontinuous material interfaces as a result of Gibbs oscillations. The rate of convergence can be improved with a smoothing of the dielectric function [122], but this will result in a significant loss of accuracy near singularities and material interfaces. An advantage of the plane-wave expansion method is that it unambiguously calculates all the modes in the DOS of a nanostructure, in contrast to methods that calculate the DOS by taking the Fourier transform of the field at a final time for a random field [101]. Hence, the DOS is strictly zero in a band gap. A concomitant disadvantage is that calculations of large crystals are expensive, since the number of modes scales with the volume of the structure as a result of band folding. In the present Thesis, we frequently employ the MIT Photonic Bands (MPB) package [98] implementation of the plane-wave expansion method.

The transfer matrix method in nanophotonics can be highly efficient for some applications [123–125], but it is also susceptible to instability [126], as is also our own experience.

1.6 Discontinuous Galerkin methods

The discontinuous Galerkin finite element method (DGFEM) [127–133] is mathematically proven to be much better suited for *hp*-adaptation than the conforming FEM. The DG method allows to accurately capture singularities at dielectric corners (that occur, for instance, in resonant cavities [87, 90]) by locally increasing the spatial resolution (*hp*-refinement). Moreover, the DG method treats elements individually due to the use of element-wise discontinuous basis functions and hence is ideally suited for adaptation and, since it results in a (block)-diagonal mass matrix, also for time-stepping [104].

Accurate eigenvalue computations, however, require that the DG discretization satisfies the divergence constraint in the time-harmonic Maxwell equations [129, 132, 134–138]. For the Maxwell eigenvalue problem, the neglect of the divergence condition leads to a large number of zero eigenvalues, which belong to the null space of the curl-curl operator. These zero-frequency eigenfunctions correspond to longitudinal fields [139]. Therefore, iterative eigenvalue solvers have difficulty to find the physical eigenvalues with the smallest frequencies due to the large spurious null space. An important advantage of the mixed DG method is that it provides a spectrum of electric field solutions that is (nearly) free of zero eigenvalues, and for some discretizations free of spurious (unphysical) modes [129,

132, 135–138].

In the present Thesis, we employ a mixed DG discretization with Brezzi-type numerical fluxes and element-wise curl-conforming elements [128, 129, 132, 135–138, 140]. The mixed method is based on the work by Houston *et al.* and Lu *et al.* [132, 135]. The advantage of using Brezzi-type numerical fluxes is that they allow a straightforward estimate of the penalty parameters that appear in the DG discretization [141]. In contrast, the stability of the interior penalty method depends on a careful selection of the penalty parameters dependent on the mesh resolution h , and suitable estimates have not yet been derived for the discretization described in Ref. [135]. We have implemented the mixed DG discretization using Brezzi-type numerical fluxes for the Maxwell equations with periodic boundary conditions in a fully parallelized code and tested it on 3D computations of photonic crystals [142]. The implementation uses a C++ software library for discontinuous Galerkin methods called hpGEM [143], and the PETSc linear solver [144] and SLEPc eigenvalue solver [145]. Further improvements in the efficient solution of the Maxwell eigenvalue problem are still subject of ongoing research [97, 142] and will not be presented in this thesis. The mixed DG method will, however, be presented in combination with a nonreflecting boundary condition suitable for the solution of scattering problems in finite structures, in Chapter 5.

1.7 Nonreflecting boundaries

There are many quantities in nanophotonics that relate to light propagation in finite structures. Examples are the power radiated by a source inside the structure, relevant to spontaneous emission experiments and cavity quantum electrodynamics (cQED), or the reflectivity for a wavefield impinging on a structure from the outside, for example a photonic crystal [88, 120]. It is well-known [103] that computations on finite structures frequently involve unbounded domains (in physics terms: a surrounding infinite vacuum) that do not fit into the computer memory. A well-known solution, which we employ in the mixed DG method, is to introduce an artificial boundary with a suitable boundary condition, as illustrated in Fig. 1.3. The boundary condition must absorb the radiated or scattered wavefield as good as possible and minimize unavoidable spurious reflections, that are required to be smaller than the level of the discretization error. Many boundary conditions for the Maxwell equations have been described in the scientific literature, such as the perfect electric conductor [147] or periodic boundary condition [148], but these are not suitable since they completely reflect the wavefield incident from the structure under study, and therefore perturb the desired wavefield, as shown in Fig. 1.3(a). Instead, one has to employ a nonreflecting boundary condition (Fig. 1.3(b)), see Refs. [149–151] for an overview of this topic.

Computations on structures that are finite in all three dimensions frequently employ the Silver-Müller boundary condition [103]. Here one employs the Silver-Müller radiation condition, which holds exactly at infinity, at the artificial bound-

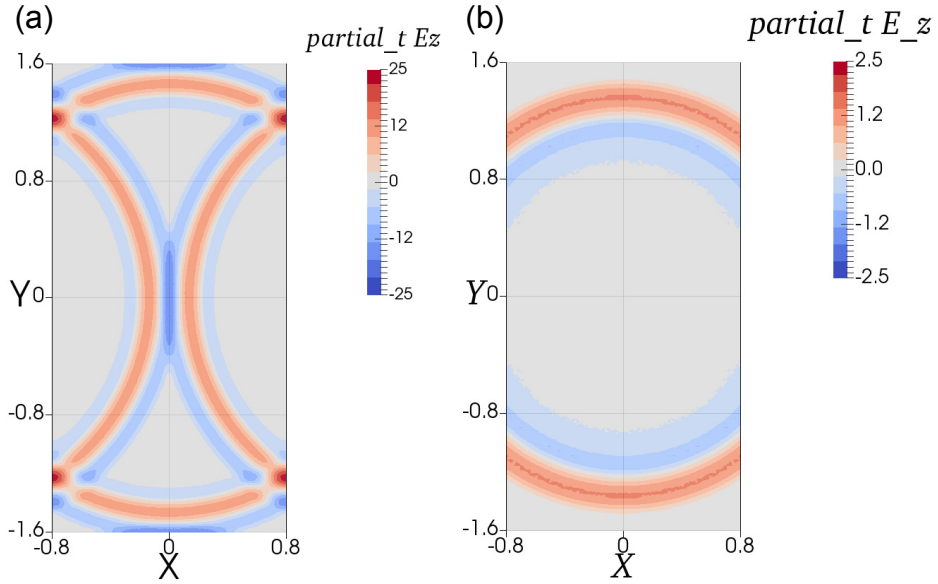


Figure 1.3: Time-derivative of the z -component of the electric field of a pulse calculated with a DG discretization of the 2D time-dependent Maxwell equations, with and without nonreflecting boundary conditions at the artificial boundaries. These time-dependent calculations are not otherwise presented in this Thesis. In (a) periodic boundary conditions are used and the incident pulse is spuriously reflected. In (b) the $P = 1$ Hagstrom-Warburton boundary condition [146] is used at the left and right artificial boundaries and the pulse passes through the boundary without distortions.

aries, that is, at a finite distance from the structure. Since, for structures that are finite in all three dimensions, the radiated or scattered wavefield satisfies the Silver-Müller radiation condition with progressively better accuracy as the distance from the scatterers increases, the spurious reflections can be made as small as desired by moving the artificial boundary away from the scatterers, but this becomes increasingly computationally expensive.

To compute the reflectivity of a wavefield impinging on a slab that is periodic in transverse directions, for example a 3D photonic crystal slab, one needs to employ a planar artificial boundary with periodic boundary conditions in the transverse directions [88, 120]. Here, the spurious reflections do not decay as the artificial boundary condition is placed further away from the structure, and it is therefore crucial to have a highly accurate nonreflecting boundary condition. A well-known nonreflecting boundary condition in electromagnetic engineering calculations that is suitable for planar boundaries is the perfectly matched layer proposed by Berenger [152]. Unfortunately, the accuracy of the perfectly matched layer depends on a smart choice of the decay parameter, which depends on the problem and the discretization used, and results in a lack of error estimates for the spurious reflection coefficient [153]. Alternatively, the Hagstrom-Warburton boundary condition has an a-priori error estimate for the spurious reflection coefficient and allows control over the error by adding an increasing number of wave directions that are exactly absorbed by the boundary condition [146]. We therefore in Chapter 5 adapt the Hagstrom-Warburton nonreflecting boundary condition to the mixed DG discretization of the Maxwell equations with element-wise curl-conforming basis functions.

1.8 Overview of this thesis

The key objectives for this thesis are

1. To theoretically and numerically investigate new features of light propagation in 3D photonic band gap crystals that provide new possibilities to tune the interaction between light and matter.
2. To develop highly accurate nonreflecting boundary conditions for a mixed DG discretization of the Maxwell equations on finite size computational domains.

The objectives outlined above will be addressed in the remaining chapters of this thesis.

In Chapter 2, we explore the propagation of light in a three-dimensional (3D) cavity superlattice embedded within a 3D photonic band-gap crystal. Using the plane-wave expansion method, we calculate the dispersion relations of a 3D cavity superlattice with the cubic inverse woodpile structure that reveal five coupled-cavity bands. These bands have quadrupolar symmetry and are the optical analogues of d-orbitals in solid-state physics. Therefore, one might naively expect neighbouring cavities to couple mostly in diagonal directions. To understand

the coupling between the cavities in the 3D cavity superlattice more fundamentally, we calculate the coupling coefficients from the dispersion relations using the tight-binding method. We compare the coupling coefficients with the dispersion bandwidth, and observe behavior that is unexpected from 1D CROW-like arguments.

In Chapter 3 we study the dynamics of light in a three-dimensional (3D) cavity superlattice embedded within a 3D photonic band gap crystal. The 3D cavity superlattice has Bloch modes where photons hop from one cavity to neighboring cavities. However, superlattice Bloch modes do not give a full picture of light propagation in 3D cavity superlattices, since all the cavities are excited simultaneously. Therefore, we calculate the time-resolved propagation for an ultrashort input pulse that initially excites only a single cavity, with frequencies within a single band of the superlattice.

In Chapter 4 we calculate the density of states of light in a 3D photonic band gap crystal with disorder, and we investigate the effects of progressive disorder on the band gap. We employ a method that unambiguously samples all possible modes in the DOS, in contrast to calculations with externally-incident light beams. We perform calculations over the entire physical range of disorder strengths where the structure retains its integrity. We investigate both the width of the band gap and shifts in the band edges. Our results provide guidance to ongoing experiments, and contribute to the study of the DOS during the localization transition.

In Chapter 5 we develop a nonreflecting boundary condition for a mixed DG discretization of the Maxwell equations. The boundary condition is obtained by applying the Hagstrom-Warburton boundary condition separately to each tangential component of the field. The auxiliary equations for the nonreflecting boundary condition are discretized with Bassi-Rebay type fluxes. This is the first time that the Hagstrom-Warburton boundary condition is adapted to a mixed DG discretization of the Maxwell equations with element-wise curl-conforming basis functions. The developed boundary condition successfully describes unboundedness with no spurious reflections. Accuracy is guaranteed by an estimate of the reflection coefficient, and will allow accurate computations of the behavior of light in nanophotonic structures.

In Chapter 6 we analyze the well posedness at the continuous level of a Hagstrom-Warburton type nonreflecting boundary condition for Maxwell's equations. We show that this boundary conditions satisfies a uniform Kreiss condition that is appropriate to nonreflecting boundary conditions [154, 155]. We also derive an estimate for the electric field in the interior in terms of the boundary data.

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CHAPTER 2

“Cartesian light”: unconventional propagation of light in a 3D superlattice of coupled cavities within a 3D photonic band gap

2.1 Introduction

Ever since the emergence of the field of nanophotonics, it is well-known that fruitful analogies can be drawn between the behavior of photons at the nanoscale on the one hand, and the physics of electrons, spins, and phonons in condensed matter on the other hand [1–6]. The seminal phenomenon considered in this respect was the three-dimensional (3D) Anderson localization of light [7, 8] - in analogy to Anderson localization of spins [9] - that continues to receive attention to date [10, 11]. Other well-known examples are the analogy between weak localization or enhanced backscattering of light [12, 13] and of electrons [14], and the analogy between a complete 3D photonic band gap in a 3D photonic crystal [15–17] and the electronic band gap in a semiconductor crystal such as silicon or germanium [18].

In this chapter, we explore the propagation of light in a 3D superlattice of coupled resonant cavities inside a 3D photonic band gap. The propagation of light in such a 3D cavity superlattice is analogous to electronic transport in an impurity band in a semiconductor [9, 18, 19]. Light hops from cavity to cavity throughout the 3D superlattice, which differs fundamentally from the conventional spatially-extended Bloch wave propagation outside the gap. Since the light hops predominantly in a few high-symmetry directions including the Cartesian (x, y, z) directions, we propose the name “Cartesian light” for the unusual propagation of light in the 3D superlattice of coupled cavities in a 3D photonic band gap.

In one dimension (1D), a chain of coupled resonant cavities is a well-known system that is known as a coupled resonator optical waveguide (CROW) [20]. The weak coupling between cavities in a CROW has been demonstrated at optical frequencies [21]. CROWs are widely studied for efficient nonlinear optical frequency conversion and for perfect transmission through bends, and for the one-dimensional (1D) localization of light [20, 22]. Two dimensional (2D) arrays of coupled cavities have been studied, notably for unusual discrete diffraction ef-

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fects [23], for intricate coupled nanolasers [24], for topologically-protected propagation [25], and for transverse localization [26, 27]. The coupling between the cavities at optical frequencies has been demonstrated to be significantly larger than the fabrication-induced disorder in the cavity frequencies [28]. In 3D resonator arrays without band gap, topologically-protected propagation was studied [29, 30], as well as the percolation of light through 3D lattices of coupled resonant microspheres [31], and dynamic localization of light [32]. In 3D photonic band gap crystals in the microwave regime, slow heavy-photon propagation was reported in a 1D array of weakly-coupled cavities [33–35]. Numerical calculations of a 2D array of cavities embedded in a 3D woodpile photonic crystal revealed ultraslow and negative group velocities [36]. To the best of our knowledge, 3D superlattices of coupled cavities with resonances in a 3D photonic band gap have not yet been studied before.

2.2 Methods

We study a 3D cavity superlattice that is embedded in a 3D photonic band gap crystal that has the inverse woodpile structure. This structure has nearly the same symmetry as a diamond crystal of carbon atoms [37], yet thousandfold magnified, as illustrated in a youtube animation [38]. The inverse woodpile crystal structure consists of two perpendicular 2D arrays of nanopores with radius r in a high-index medium such as silicon [37], as illustrated in Figure 2.1(a). Each 2D pore array corresponds to a diamond 110 crystal face. In view of the arrangement of the nanopores, it appears to be convenient to employ a tetragonal unit cell [39, 40] instead of the conventional cubic unit cell [18]. The tetragonal unit cell has lattice parameters c (in the x and z directions), and a (in the y direction) in a ratio $a/c = \sqrt{2}$ to ensure a cubic crystal structure. More details, notably on the Brillouin zone, are presented in Appendix 2.A.

Inverse woodpile photonic crystals possess a broad 3D photonic band gap, whose width strongly depends on the radius r of the pores [37, 39, 40]. For a normalized pore radius $r/a = 0.24$ - as considered here - a maximum relative bandwidth $\Delta\omega_{pbg}/\omega_c = 25.3\%$ occurs for $\epsilon = 12.1$ typical of silicon [39, 40], with $\Delta\omega_{pbg}$ the frequency width of the band gap, and ω_c the band gap’s center frequency. 3D inverse woodpile crystal nanostructures have been fabricated from a number of different high-refractive index backbones [41–46]. In nanophotonic experiments, the potential of silicon inverse woodpiles was demonstrated by the observation of a broad 3D photonic band gap for many angles [47], as well as a strong spontaneous emission inhibition of embedded quantum dots [48].

To create a resonant cavity in a inverse woodpile photonic crystal, Ref. [49] proposed a design whereby two proximal perpendicular pores have a smaller radius ($r' < r$) than all other pores, as shown in Figure 2.1(a). Near the intersection region of the two smaller pores, the light is confined in all three directions to within a mode volume as small as $V_{\text{mode}} \simeq \lambda^3$ where λ is the free-space wavelength [49]. Supercell band structures revealed up to five resonances within the band gap of the perfect crystal, depending on the defect pore radius r' [49], that

have quadrupolar symmetry [50]. The best confinement occurs for a defect radius $r'/r = 0.5$ that is also considered here.

Figure 2.1(b) shows a 3D superlattice of cavities as is studied here, where each sphere indicates one cavity, as shown in Fig. 2.1(a). The cavity superlattice has lattice parameters (c_s^x, a_s, c_s^z) in the (x, y, z) directions that are integer multiples of the underlying inverse woodpile lattice parameters: $c_s^x = M_x c$, $a_s = M_y a$, $c_s^z = M_z c$. Here, we study the $M_x M_y M_z = 3 \times 3 \times 3$ superlattice such that the cavities are repeated every three unit cells with lattice parameters $c_s^x = 3c$, $a_s = 3a$, $c_s^z = 3c$. Thus, the cavity superlattice is also cubic, similar to the underlying inverse woodpile structure (see section 2.4 for additional discussion).

We have calculated the band structure of the 3D cavity superlattice using the plane-wave expansion method [17, 18, 51]. Using the Richardson extrapolation method allows us to estimate the frequencies in the limit of infinite grid resolution [52, 53]. Details on the calculations and the convergence are given in Appendix 2.B. All calculations were performed on the “Serendipity” cluster in the MACS group at the MESA⁺ Institute [54]. Even on this powerful computer cluster the calculations took 210 hours.

2.3 Results

2.3.1 Band structure of coupled cavity resonances

In Fig. 2.2(a), the band structures are shown of a 3D cavity superlattice ($M_x M_y M_z = 3 \times 3 \times 3$) in an inverse woodpile photonic band gap crystal made of silicon. As a result of the intentional defect pores many bands appear in the band gap of the perfect crystal between reduced frequencies $\tilde{\omega} = \omega a / (2\pi c) = 0.492$ and 0.634 . The lowest five bands between $\tilde{\omega} = 0.5$ and 0.55 have a low dispersion and correspond to the five cavity resonances that are from now on labeled as $m = 1, \dots, 5$. The $m = 3, 4, 5$ bands are isolated in frequency, unlike the situation in solid state physics where the bands arising from d -orbitals are hybridized [18]. The dispersions of the bands in Fig. 2.2(a) agree well with those of Woldering *et al.* [49]. The dispersive bands in the top half of the gap (between $\tilde{\omega} = 0.55$ and 0.634) have unknown character, and may include waveguiding along the defect pores.

A closer inspection of the five dispersionless cavity bands in Fig. 2.2(b) reveals that these bands have nonzero bandwidths, indicating that cavity resonances in the $M_x M_y M_z = 3 \times 3 \times 3$ superlattice are coupled, as is investigated in this paper. Our results agree well with a simultaneous investigation of a single cavity in an inverse woodpile crystal with finite support, studied by other numerical methods [50]. Notably, Ref. [50] also reports that the first two bands are nearly degenerate. Based on the occurrence of five cavity bands, on degeneracies between bands, and on the field distribution (reported in Ref. [49]), it has been concluded that the resonances of the inverse woodpile cavity have quadrupolar symmetry and are the optical analogues of d -orbitals in solid-state physics [50]. Therefore, it is naively expected that neighboring cavities couple in diagonal directions.

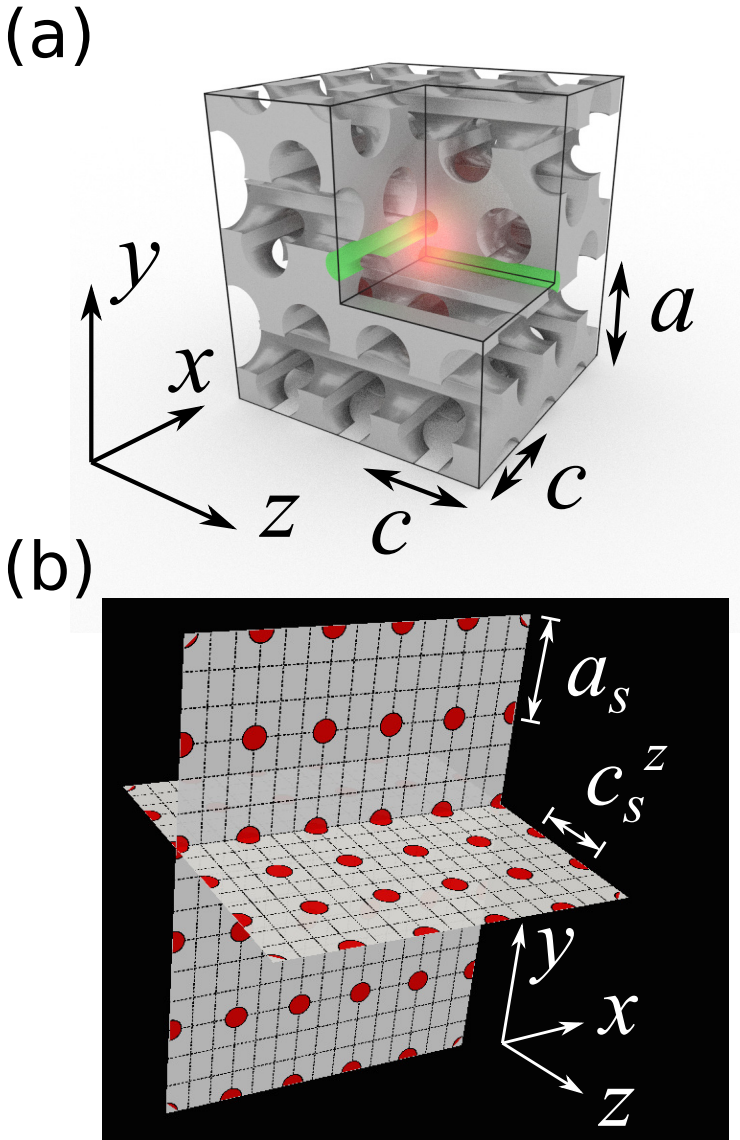


Figure 2.1: (a) Design of a single cavity in an inverse woodpile photonic band gap crystal shown in a cut-out of a $M_x M_y M_z = 3 \times 3 \times 3$ supercell that is surrounded by boxed lines. The high-index backbone is shown in gray. Two proximal smaller defect pores are indicated in green, and the cavity region is highlighted as the bright region at the center. The tetragonal lattice parameters a and c are shown, as well as the x, y, z coordinate system. (b) (x, z) and (x, y) cross sections through a 3D superlattice of resonant cavities, with red circles indicating cavities and dashed rectangles representing unit cells of the underlying inverse woodpile crystal structure (see (a)). The lattice parameters (c_s^x, a_s, c_s^z) of the superlattice are shown, as well as the x, y, z coordinate system.

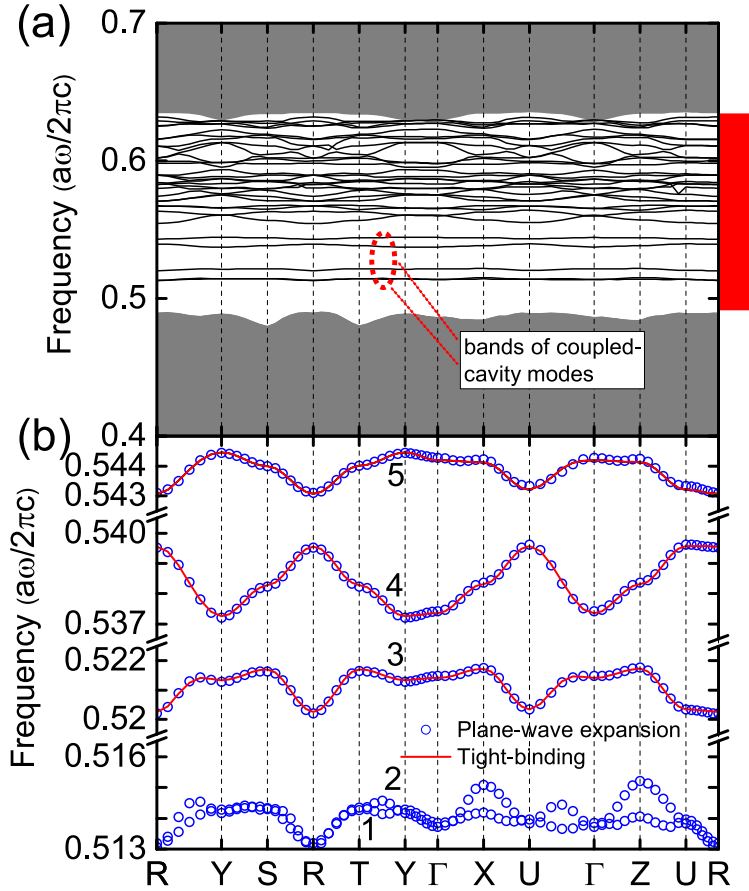


Figure 2.2: (a) Black curves are photonic bands of a 3D inverse woodpile photonic band gap crystal ($r/a = 0.24$, $\epsilon_{Si} = 12.1$) with two proximate defect pores ($r'/r = 0.5$). The abscissa indicates the wave vector between the high-symmetry points of the Brillouin zone (see Appendix 2.A). The 3D photonic band gap of the perfect crystal is shown as a red bar, and the range of allowed modes outside the band gap is shown in grey. The five bands of coupled-cavity modes are highlighted. (b) Zoom-in of the five coupled-cavity bands (blue circles), labeled $m = 1, \dots, 5$. The $m = 3, 4, 5$ bands are accurately described by the tight-binding model (red curves).

2.3.2 Dispersion bandwidths

For a 1D coupled-resonator optical waveguide (CROW), it is well-known that the coupling coefficient along the waveguide is proportional to the dispersion bandwidth [20, 35, 55]. A straightforward extension of this notion to a 3D cavity superlattice is to consider the dispersion bandwidth in various crystal directions, since this is straightforward to derive from photonic band structures as in Figure 2.2. For a given crystal direction characterized by wave vector $\mathbf{k}$, the dispersion bandwidth is defined as

$$\Delta\tilde{\omega} \equiv |\tilde{\omega}_{max} - \tilde{\omega}_{min}|_{\Gamma \rightarrow \mathbf{k}_{BZ}}, \quad (2.1)$$

in other words, the absolute value of the difference between the maximum and minimum frequencies on a trajectory in reciprocal space between the origin Γ and the edge of the Brillouin zone $\mathbf{k}_{BZ}$ in the direction of $\mathbf{k}$. As an example, for the $m = 3$ coupled-cavity band in Figure 2.2(b), between Γ and Z the minimum and maximum frequencies are nearly the same ($\tilde{\omega} = 0.521$) hence the bandwidth $\Delta\tilde{\omega}$ is nearly zero. Between Γ and U the minimum and maximum frequencies differ much more ($\tilde{\omega} = 0.520$ to 0.521) hence the dispersion bandwidth is much greater in the diagonal direction.

A polar plot of the dispersion bandwidth $\Delta\omega$ versus wave vector $\mathbf{k}$ in the (k_X, k_Z) plane is shown in Figure 2.3(a). From the band frequencies mentioned

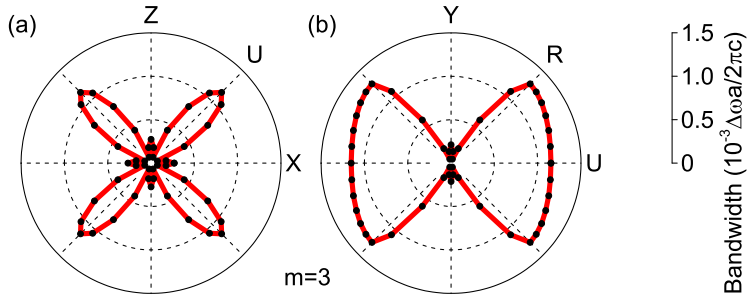


Figure 2.3: (a) Polar plot of the dispersion bandwidth for the $m = 3$ coupled-cavity band in the (k_X, k_Z) plane. The X , U , and Z high-symmetry points are shown. (b) Polar plot of the dispersion bandwidth for the $m = 3$ coupled-cavity band in the (k_Y, k_U) plane. The Y and U high-symmetry points are shown. The black circles indicate the plane-wave results (cf. Fig. 2.2), and the red lines are guides to the eye.

above, the dispersion bandwidth is very small in the real-space x and z -directions (corresponding to ΓX , ΓZ , respectively, in reciprocal space). In the diagonal directions that correspond to the ΓU high-symmetry trajectory the dispersion bandwidth is much greater. As seen from a given central cavity in real space, the wave vector $\mathbf{k}$ is then directed towards a second nearest neighboring cavity in the diagonal $1/\sqrt{2} \cdot (1, 0, 1)$ direction (see Appendix 2.A). The polar plot of the dispersion bandwidth for $m = 3$ therefore looks like a quadrupolar radiation pattern. Based on the 1D CROW-reasoning given above, one tentatively infers

that light is transported through the 3D cavity superlattice preferentially in the xz -diagonal (corresponding to ΓU) directions.

Figure 2.3(b) shows the dispersion bandwidth $\Delta\omega$ in the (k_Y, k_U) plane. The largest bandwidth occurs at about 45° off the (XUZ) plane, which corresponds to the ΓR high-symmetry direction. The bandwidth in the ΓY -direction is small, from which one tentatively infers that there is little light transport in the y -direction in real space.

The dispersion bandwidth for the $m = 4, 5$ bands is shown in Figures 2.4(a,b). For the $m = 4$ band, the dispersion bandwidth is large in the diagonal directions

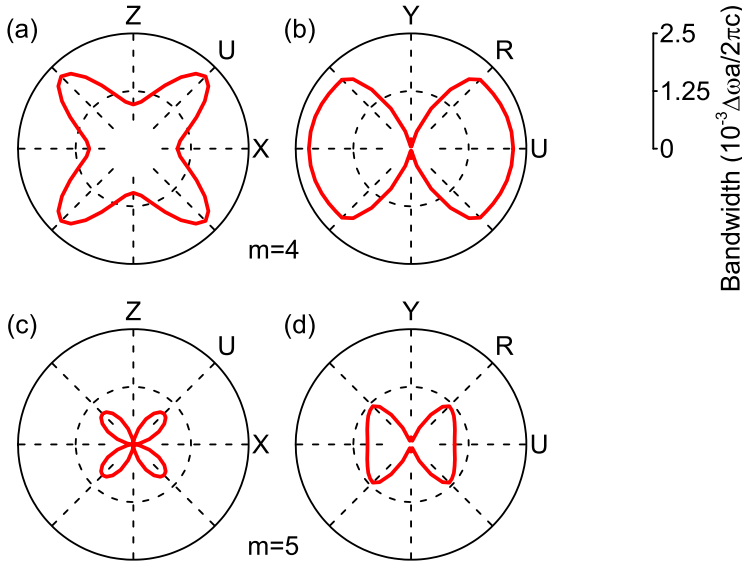


Figure 2.4: Polar plots of the dispersion bandwidth versus wave vector for the (a,b) $m = 4$ and (c,d) $m = 5$ coupled-cavity bands. Panels (a,c) are in the (k_X, k_Z) plane and (b,d) are in the (k_Y, k_U) plane.

that correspond to the ΓU high-symmetry directions, and it is smaller in the x and z -directions ($\Gamma X, \Gamma Z$, respectively). Compared to the $m = 3$ band, the dispersion bandwidth for the $m = 4$ band appears to be less strongly directional. To quantify the directionality, we consider a directionality D ratio between the maximum and the minimum bandwidths

$$D = \Delta\omega_{max} / \Delta\omega_{min} \quad (2.2)$$

in the (k_X, k_Z) plane, which yields a directionality of about $D = 4$ that is much lower than $D = 15$ for the $m = 3$ band.

For the $m = 5$ band in Figure 2.4(c), the polar plot of the dispersion bandwidth looks very much like a quadrupolar emission pattern. The bandwidth is small in the diagonal directions that correspond to the ΓU high-symmetry directions, about $2.5\times$ smaller than for the $m = 4$ band. The dispersion bandwidth is much

Table 2.1: Dimensionless coupling coefficients κ_i for 7 different high-symmetry directions i (x, y, z, xy, xz, yz, xyz), as defined in Eq. (2.24) in Appendix 2.C, for the cavity superlattice bands $m = 3, 4, 5$. We also list the parameter β that is defined in Eq. (2.23) in Appendix 2.C.

Coupling coefficients	$m = 3$	$m = 4$	$m = 5$
β	$-1.8 \cdot 10^{-10}$	$+3.3 \cdot 10^{-10}$	$-1.8 \cdot 10^{-10}$
κ_x	$+5.2 \cdot 10^{-4}$	$-1.0 \cdot 10^{-3}$	$+5.4 \cdot 10^{-4}$
κ_y	$+4.7 \cdot 10^{-5}$	$+4.3 \cdot 10^{-5}$	$+3.0 \cdot 10^{-5}$
κ_z	$+5.1 \cdot 10^{-4}$	$-1.1 \cdot 10^{-3}$	$+5.3 \cdot 10^{-4}$
κ_{xz} ($// \Gamma U$)	$-4.2 \cdot 10^{-4}$	$+6.6 \cdot 10^{-5}$	$-1.5 \cdot 10^{-4}$
κ_{xy} ($// \Gamma S$)	$-1.4 \cdot 10^{-6}$	$+9.7 \cdot 10^{-6}$	$-4.6 \cdot 10^{-5}$
κ_{yz} ($// \Gamma T$)	$-1.6 \cdot 10^{-6}$	$+1.0 \cdot 10^{-5}$	$-4.6 \cdot 10^{-5}$
κ_{xyz} ($// \Gamma R$)	$+7.4 \cdot 10^{-6}$	$+2.4 \cdot 10^{-6}$	$-2.2 \cdot 10^{-5}$

smaller in the x and z directions, corresponding to a large directionality $D = 26$.

2.3.3 Coupling coefficients

To understand the coupling between the cavities in a 3D cavity superlattice more fundamentally, we derive the coupling coefficients of light from the dispersion relations using the tight-binding method, see Appendix 2.C for details. Figure 2.2(b) shows that the $m = 3$ band is accurately described by the tight-binding model. It appears that only 7 independent coupling coefficients κ are needed in the tight-binding model, namely for the real-space directions x, y, z, xz – *diagonal* (corresponding to ΓU in reciprocal space), xy – *diagonal* (corresponding to ΓS), yz – *diagonal* (corresponding to ΓT), and xyz – *diagonal* (corresponding to ΓR). The reasons are as follows: since the inverse woodpile cavity has mirror symmetry with respect to the (y, z) and (x, y) planes, the coupling coefficients in the $+x$ and $+z$ directions are symmetry related to those in the $-x$ and $-z$ directions, respectively, and the coefficients in the xz – *diagonal* directions are symmetry related to each other. The coupling coefficients in the $+y$ and $-y$ directions are equal by reciprocity, see Appendix 2.D.

The coupling coefficients are given in Table 2.1 [57]. For the $m = 3$ band the coupling coefficients of light are overlaid on the cavity superlattice structure in Figure 2.5. In the x and z directions, the coupling coefficients are relatively large and positive, in the xz – *diagonal* directions the coupling coefficients are large and negative, in the y direction the coupling coefficient is about $10\times$ smaller, and in all other directions the coupling coefficients are vanishingly small (typically $100\times$ less).

Remarkably, the simultaneous occurrence of large coupling coefficients with near-vanishing dispersion bandwidths means that 1D CROW-like arguments *do not hold* for 3D cavity superlattices. In other words, the bandwidth in a particular crystal direction for a 3D cavity superlattice is not necessarily proportional to the coupling coefficient in the same direction in real space. The small difference between the x and z coefficients confirms that the x and z directions are

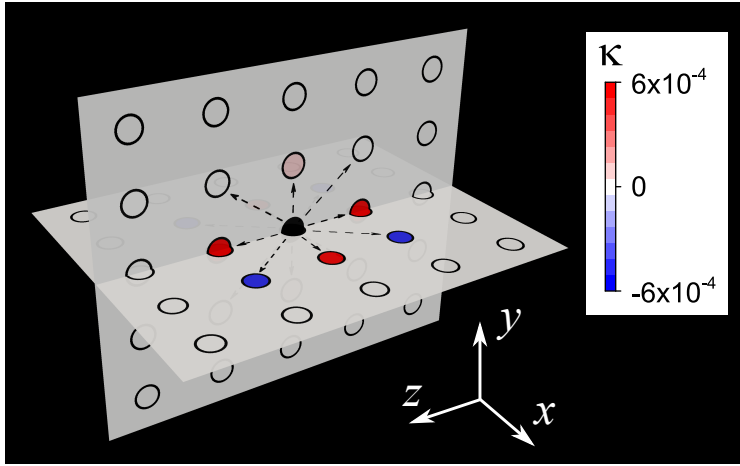


Figure 2.5: Coupling coefficients of light from a central cavity (black circle) to neighboring cavities (other circles) for the $m = 3$ coupled-cavity band, indicated with arrows. Nonzero coefficients only occur in the (x, y) and (x, z) planes. Blue and red indicate negative and positive coupling coefficients, respectively, as shown by the color bar. The x, y, z coordinate system is shown. This figure has been made using ParaView [56].

not symmetry related for the inverse-woodpile cavity, as opposed to the perfect inverse-woodpile structure [58].

According to an 1D CROW-like argument, the large coupling coefficient in the xz – *diagonal* directions agrees with the observation of a large dispersion bandwidth in the diagonal U direction, see Fig. 2.3. However, the negative sign disagrees with the fact that at the U point the band frequency is lower than at the Γ point, since the reverse is true for an 1D CROW, see Ref. [20].

The κ_y coupling coefficient in the y direction is small, in agreement with the band frequencies that are almost the same at Γ and Y . It is remarkable that the κ_y coupling coefficient is $10\times$ smaller than the coefficients for the x or z directions, while the nearest neighbor distance is only a $(\sqrt{2})$ greater than in the x or z directions, which would correspond to only a $(\exp(\sqrt{2}) \approx 4\times)$ smaller coefficient for cavities coupled by evanescent Bloch modes. We surmise that the quadrupolar field pattern of each cavity in the xz plane couples poorly to a neighboring cavity in a neighboring xz plane. Therefore, light mostly hops in 2D (x, z) -layers, which is analogous to 2D electron transport in graphite or graphene layers [59, 60]. Since the light propagates very unusually by hopping only in a few discrete directions, we propose the name “Cartesian light” for the propagation of light in a 3D cavity superlattice.

The coupling coefficients of light for the $m = 4, 5$ bands are shown in Fig. 2.6. For the $m = 4$ band, the nonzero coefficients are κ_x , and κ_z . The coupling coefficients to all other neighboring cavities vanish, including the coefficient κ_y in the y direction. In the hopping of the $m = 4$ band we find the ultimate Cartesian light: light hops only in the x - z directions. For the $m = 5$ band, the

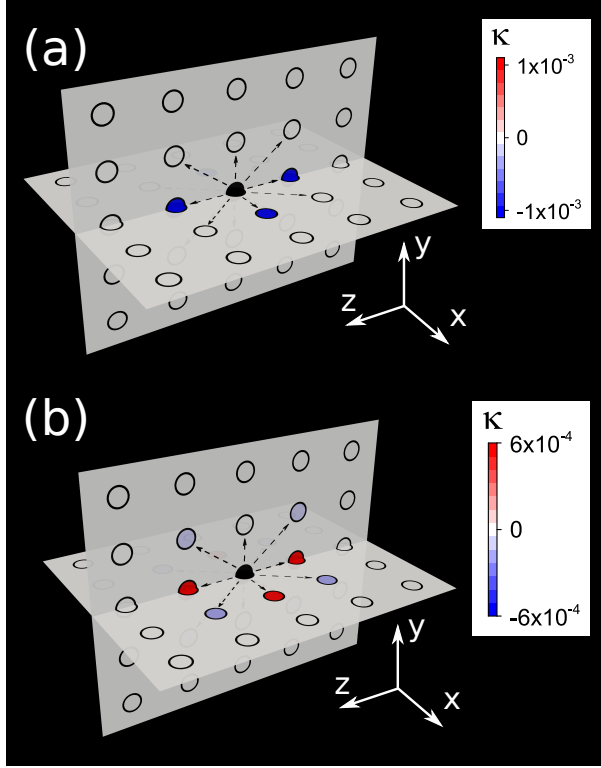


Figure 2.6: (a) Coupling coefficients of light from a central cavity (black circle) to neighboring cavities (other circles) for the $m = 4$ coupled-cavity band, indicated with arrows. Nonzero coefficients only occur in the (x, y) and (x, z) planes. Blue and red indicate negative/positive coupling coefficients, for which bonding/antibonding resonances of the two coupled cavities are energetically favorable. The x, y, z coordinate system is shown. (b) Coupling coefficients of light from a central cavity (black circle) to neighboring cavities (other circles) for the $m = 5$ coupled-cavity band.

nonzero coefficients are $\kappa_x, \kappa_y, \kappa_z, \kappa_{xz}, \kappa_{xy}, \kappa_{yz}$, and κ_{xyz} , that is, nonzero coupling coefficients to all neighboring cavities. In the (x, z) plane, there is a mix of positive x and z coupling coefficients, and negative xz – *diagonal* coupling coefficients, which is similar to the $m = 3$ band.

We have not analyzed the $m = 1, 2$ bands of coupled-cavity modes, since the band structures do not converge monotonically with increasing spatial resolution, as is elaborated in Appendix 2.B.

2.3.4 Propagation in 3D on the superlattice

We now discuss the propagation in real space, and why the dispersion bandwidth of the $m = 3$ band is much larger in the U direction than in the other directions in the (k_X, k_Z) plane in reciprocal space. We first discuss the dispersion bandwidth

in the xz – *diagonal* directions that are symmetry related to each other, and that correspond to the ΓU direction in reciprocal space.

Let us consider the relative phase of the resonating cavities for a wave vector at the U -point ($\mathbf{k} = \mathbf{k}_{BZ} = U$), as shown in Figure 2.7. Since this coupled resonance

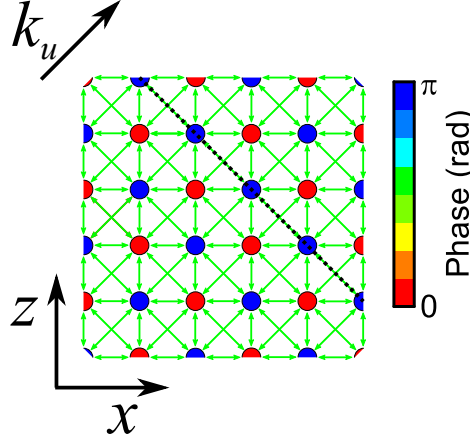


Figure 2.7: Relative phase of the resonating cavities for a coupled-cavity mode with a wave vector at the U high-symmetry point. As seen from a given cavity, the wave vector $\mathbf{k}$ is directed towards an xz diagonally neighboring cavity. The black dashed line indicates a wavefront of the Bloch wave. The blue and red cavities resonate out-of-phase with each other. The couplings are indicated with arrows, which are green if the corresponding cavities resonate with an energetically favorable relative phase, as is the case for all couplings.

eigenmode is a Bloch wave of the 3D superlattice (with a phase front as indicated in Fig. 2.7) it is clear that this collective oscillation differs fundamentally from waveguiding behavior in a 1D CROW; in other words, the superlattice Bloch modes differ from the ones in a CROW.

In Figure 2.7, neighboring cavities in the xz – *diagonal* direction resonate in-phase with each other. Neighboring cavities in the x , or z -direction resonate out-of-phase with each other. Hence, there is a checkerboard pattern of two sublattices of cavities that resonate out-of-phase with each other. The in-phase resonance of neighboring cavities in the xz -diagonal direction is energetically favorable for the negative coupling coefficient in the xz -diagonal directions, as can be understood from Eq. (2.24) in Appendix 2.C. The out-of-phase resonance of neighboring cavities in the x , or z -direction is energetically favorable for the positive coupling coefficient in the x , or z -direction. Hence, the checkerboard pattern of out-of-phase resonating cavities is energetically favorable for all coupling coefficients in the (x, z) -plane, and the band frequency is relatively low at the U high-symmetry point.

We now consider the superlattice Bloch mode at the $\mathbf{k} = \Gamma$ point (the origin in reciprocal space). All cavities resonate in-phase with each other, which is energetically favorable for the negative coupling coefficient in the xz -diagonal

direction. However, it is not energetically favorable for the positive coupling coefficients in the x , or z -direction. Hence, the band frequency is relatively high at the Γ point, and higher than at the U -point, in agreement with the observation of large dispersion bandwidth in Figure 2.2(b).

We now discuss the dispersion bandwidth in any direction in the (k_X, k_Z) plane other than the xz -diagonal direction. For example, the relative phase of the resonating cavities at the X high-symmetry point is shown in Fig. 2.8. Only the checkerboard pattern of out-of-phase resonating cavities at the U high-

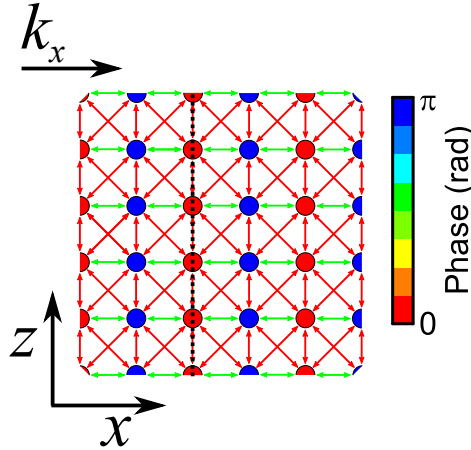


Figure 2.8: Relative phase of the resonating cavities for a coupled-cavity mode with a wave vector at the X high-symmetry point. As seen from a given cavity, the wave vector $\mathbf{k}$ is directed towards a nearest-neighboring cavity. The black dashed line indicates a wavefront of the Bloch wave. The blue and red cavities resonate out-of-phase with each other. The couplings are indicated with arrows, green arrows indicate an energetically favorable relative phase, and red arrows indicate an unfavorable phase.

symmetry point is energetically favorable for all coupling coefficients in the (x, z) plane. For any other point in the Brillouin zone, the relative phase of the resonating cavities is not energetically favorable for all coupling coefficients in the (x, z) plane. Hence, the dispersion bandwidth is small for directions other than the xz -diagonal direction, in agreement with the superlattice band structures in Figure 2.2(b).

2.4 Discussion

2.4.1 Differences with other forms of light transport

Cartesian light propagation on a 3D superlattice of cavities differs fundamentally from other known modes of propagation in periodic nanophotonic systems, notably from the conventional 3D spatially-extended Bloch wave propagation in crystals, from light tunneling through a band gap, from coupled-resonator optical waveguiding, and also from light diffusing at the edge of a gap.

(1) A characteristic feature of the 3D superlattice Bloch modes is that they are constructed from modes where the light field is hopping from lattice site to lattice site. In other words, the field pattern has its maxima on the lattice sites (i.e. the cavities) and decays exponentially in between lattice sites, since isolated cavities are tuned inside the photonic band gap where the wave vector is complex. In contrast, the Bloch modes outside the photonic band gap are constructed from purely real modes of propagation; there is no reason for field maxima to be located on preferred positions in the crystal.

(2) A second characteristic feature of the 3D superlattice Bloch modes is that they are genuine modes of propagation centred within the 3D photonic band gap. In this sense, they are distinguished from the modes in photonic crystals with finite support that were recently described in Ref. [61]. In that study, it was found that the finite extent of a photonic band gap crystal leads to the filling of the density of states (DOS) in the band gap by states that are centred outside the band gap, while extending into the band gap due to their substantial band width.

(3) The 3D Cartesian superlattice propagation differs fundamentally from the propagation in lower-dimensional 1D (a CROW) and 2D arrays of cavities. Firstly, in section 2.3.4 we have already discussed that the superlattice modes differ fundamentally from those of a CROW. In other words, a 3D superlattice does not seem to be a “3D CROW”. Secondly, if we perturb the frequency of one of the cavities in a superlattice, a bound state appears instantaneously in 1D and 2D, whereas a threshold frequency difference is required in 3D, see Ref. [62].

(4) The propagation of light in a 3D cavity superlattice in a photonic band gap differs fundamentally from directional diffusion that was identified for 3D photonic band gap crystals with a certain degree of disorder [63]. In the latter case, the modes of propagation are not waves but diffusive. Moreover, the typical frequencies are at the edge of the band gap, hence outside the gap, as opposed to the cavity superlattice modes that reside within the band gap, see Fig. 2.2.

2.4.2 Crystal structures of the cavity superlattice

If the magnification factors of the superlattice’s lattice parameters, compared to the underlying crystal structure’s lattice parameters, fulfill $M_i \neq (M_j, M_k)$ ($i, j, k = x, y, z$), the cavity superlattice is not cubic anymore - in contrast to the underlying inverse woodpile structure - but has become tetragonal. In the most general case with $M_x \neq M_y \neq M_z$ the superlattice has different cavity spacings in each direction (x, y, z); the superlattice has then become orthorhombic. Given that cavities in an inverse woodpile structure are necessarily located along the smaller-pore line defects, we currently doubt whether it is feasible to realize other 3D Bravais superlattices.

We have seen that for the $m = 3, 4, 5$ bands, the coupling coefficient in the y -direction is smaller than in the (x, z) plane, by typically $10\times$. To make the hopping of light more 3D, it is necessary to increase the coupling coefficient in the y -direction compared to the coefficients in the (x, z) -directions, which can be achieved by a closer cavity spacing in the y -direction, for example, in a

$M_x M_y M_z = 3 \times 2 \times 3$ supercell in case of $M_x = M_z = 3$ (as studied here) or in general for supercells with $M_y < (M_x, M_z)$.

Conversely, if it is desired to realize a superlattice with effectively 2D transport of light in (x, z) planes, the superlattice parameter in the y -direction should be made greater than the ones in the (x, z) -directions ($M_y \gg (M_x, M_z)$). In this situation, the 2D transport of light may hold analogies to that of charge carriers in graphite layers [59] or in high- T_c superconductors.

2.4.3 Disorder

We have studied the dispersion and hopping for superlattices without disorder. Let us briefly comment on the sensitivity of the results to a small degree of disorder, since we performed calculations for several grid resolutions in Appendix 2.B, and a change of the grid resolution implies a slight shift in the geometry. On the one hand, we observed that for all five bands of coupled-cavity modes, the center frequency is highly sensitive to the grid resolution and therefore to disorder. This is likely the result of the lightning rod effect of the cavity mode field pattern identified in Ref. [49], wherein the inverse woodpile cavity resonances have regions of high intensity at sharp corners in the dielectric material [64, 65]. If such sharp corners are slightly distorted, it is quite conceivable that the overlap with the field pattern changes, leading to a change in resonance frequency. On the other hand, we observe for bands $m = 3, 4, 5$ that the features of the dispersion bands remain the same while the grid resolution is increased. Therefore, we expect the coupling coefficients for the $m = 3, 4, 5$ bands to be robust to small degrees of disorder.

Commonly, in experimental nanophotonic studies one is not only concerned about the effects of disorder (however mild), but also about effects of weak absorption. Up to date, these two effects are treated on an equal footing as an effective extinction. Recent work, however, by Wolff, Busch, and Mortensen has pointed out that the describing absorption should be handled with care, as for instance apparent gaps in the DOS due to Lorentzian dispersion vanish when proper care is taken [66].

A 3D cavity superlattice is the photonic analogue of the Anderson model for spins and electrons [9], albeit in the limit of zero disorder. The 3D cavity superlattice also corresponds to the Hubbard model without interactions [67, 68]. We anticipate that the present study may form the basis for further exploration of the physics of the 3D Anderson model for nanophotonic cavity superlattices that will proceed by introducing controlled degrees of disorder in the cavity resonance frequencies.

2.4.4 Outlook

The 3D system of coupled photonic band gap cavities described here has a number of analogues in condensed matter physics, that may eventually be exploited to translate know-how garnered in the photonic system to the other systems. For instance, a feature that is readily available in optics is an input beam of light that

is both collimated (localized in wave vector space) and monochromatic (localized in frequency space.) Therefore, in a photonic system it will be very well feasible to study both the wave vector and the frequency responses of the coupled-cavity system. Hence, prospects are favorable to map out dispersion surfaces - as shown in, e.g., Figures 2.3(a,b) - that are predicted in this paper. Since the inverse woodpile cavities have a symmetry similar to a d-like atom, such detailed maps may offer - within the limitations of the electronic-photon analogy - relevant information for such solid-state crystals. Another condensed-matter system that could profit from the detailed photonic probing is a 3D superlattice of quantum dots with excitonic transport [69] that is challenging to resolve in k -space. An interesting avenue is to study 3D cavity superlattices where the lattice parameter in the y -direction is increased in order to further decrease the y -coupling. This situation could have potentially interesting ramifications for the 2D materials that are enjoying a fantastic scientific attention [59].

An attractive future line of research is opened by studying a 3D cavity superlattice where each cavity holds an active material, such as one (or more) two-level atoms. This hybrid combination allows one to explore light-matter interactions deep inside the band gap that are well shielded from any perturbing vacuum fluctuations by the surrounding 3D photonic band gap [70]. Indeed, recent parallel work has pointed out that with inverse woodpile cavities one can observe a substantially enhanced optical absorption at the cavity locations, which offers favorable opportunities for tiny optical sensors [50]. In presence of two-level Cs atoms, we anticipate hybrid dispersion effects much beyond those observed before in weakly-interacting opals [71]. In presence of disorder, the hybrid cavity-emitter superlattice may reveal intriguing quantum-optical spin glass behavior, as predicted by John and Quang [72]. In case the cavities are doped with diamond NV centra, a possible application would be a scalable and coherently linked network of NV-based registers that is pursued for quantum information processing, see Ref. [73]. In case each cavity and two-level emitter pair can be brought into the strong coupling regime of cavity quantum electrodynamics (cQED), the concomitant photon-blockade effect for each cavity-emitter pair will result in an intricate repulsion between excitations (photons) hopping through the superlattice. This physical situation is an example of the repulsive Bosonic system described by Fisher *et al.* that is predicted to reveal phase transitions to Boson localization and the superfluid-insulator transition, or even to a Bose glass [74]. There is surely no doubt that the prospect that photons could reveal any such phase transition would be truly exciting.

2.5 Summary

We present the first ever study of the propagation of photons in a 3D cavity superlattice within a 3D photonic band gap. Such a 3D cavity superlattice is the photonic analogue of the Anderson model in the limit of zero disorder. The light hops only in a few high-symmetry directions including the Cartesian (x, y, z) directions, therefore we propose the name “*Cartesian light*”. 3D Cartesian hopping

of light in a 3D band gap yields propagation as superlattice Bloch modes that differ fundamentally from the conventional 3D spatially-extended Bloch wave propagation in crystals, from light tunneling through a band gap, from coupled-resonator optical waveguiding, and also from light diffusing at the edge of a gap. The large coupling coefficients in the Cartesian directions occur simultaneously with a near vanishing dispersion bandwidth in this direction. This means that 1D CROW-like reasoning *does not* hold for 3D cavity superlattices. The unusually small dispersion bandwidth in the Cartesian directions is a result of interplay between positive and negative coupling coefficients in the Cartesian and diagonal directions.

2.A Brillouin zone and tetragonal unit cell

Figure 2.1(a) shows a tetragonal representation of the $M_x M_y M_z = 3 \times 3 \times 3$ supercell of the cubic inverse woodpile crystal structure including a pair of proximal defect nanopores that form a resonant cavity.

In terms of the unit vectors of the conventional cubic diamond structure[18], the tetragonal unit supercell has unit vectors $a_x = \frac{1}{\sqrt{2}}[M_x \ 0 \ M_x]$, $a_y = [0 \ M_y \ 0]$, and $a_z = \frac{1}{\sqrt{2}}[\bar{M}_z \ 0 \ M_z]$.

Figure 2.9 shows the first Brillouin zone of the inverse woodpile cavity superlattice with characteristic high-symmetry points. The main axes are given

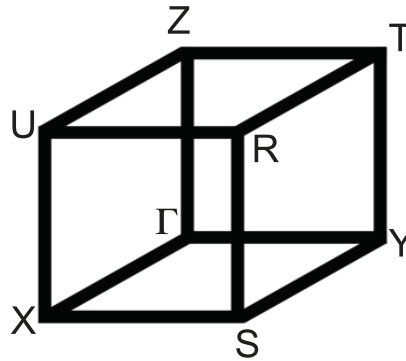


Figure 2.9: First Brillouin zone of the inverse woodpile crystal structure showing the high symmetry points X, Y, Z, S, R, T, U and the origin called Γ .

by $X = [\pi/c_s^x, 0, 0]$, $y = [0, \pi/a_s, 0]$, and $Z = [0, 0, \pi/c_s^z]$. The ΓX and ΓZ directions are notable as they correspond to waves propagating along each set of nanopores, while the diagonal ΓU direction lies in between. Due to the geometry of the cavity (composed of two proximal defect pores), the ΓX and ΓZ directions are not symmetry related, in contrast to the underlying inverse woodpile crystal structure [58].

2.B Calculations and convergence

We have calculated the band structure of 3D cavity superlattices using the plane-wave expansion method [17, 18], where we employed the well-known MIT PhotonicBands (MPB) package [51]. We performed calculations with increasing spatial grid resolutions of $12 \times 17 \times 12$, $24 \times 34 \times 24$, $48 \times 68 \times 48$, and $96 \times 136 \times 96$ per unit cell of the underlying inverse woodpile crystal. Although the $12 \times 17 \times 12$ calculation is a replication of Ref. [49], the results do not agree perfectly since the subpixel averaging has been updated in Version 1.5 of the MPB code that we use here. We verified that with an older version of MPB our calculations agree exactly with Ref. [49].

To study the convergence of the defect bands with increasing spatial resolution, we show in Figure 2.10(a,b) the $m = 1$ and $m = 3$ defect bands, respectively, for all resolutions considered. The general trend observed in the data - also seen

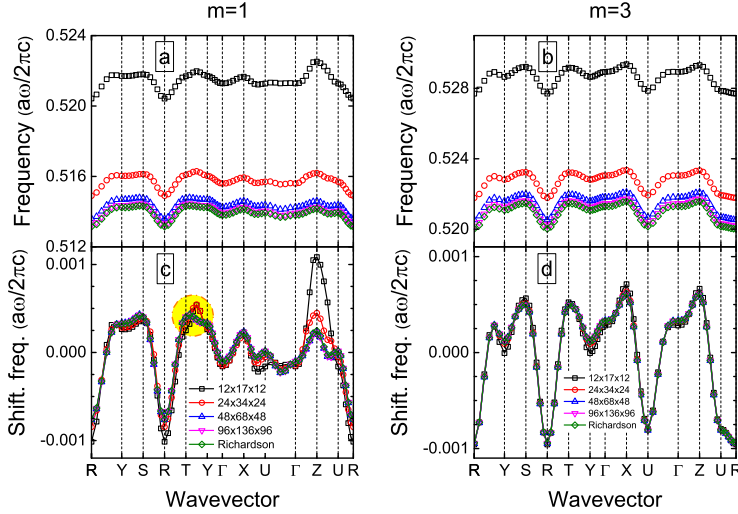


Figure 2.10: (a,b) Dispersion relations of the $m = 1, 3$ bands of coupled-cavity modes, respectively, for grid resolutions $12 \times 17 \times 12$ (black squares), $24 \times 34 \times 24$ (red circles), $48 \times 68 \times 48$ (blue upward triangles), and $96 \times 136 \times 96$ (magenta inverted triangles). The Richardson extrapolated data are shown as green diamonds. (c,d) Overlaid dispersion relations where the center frequency of each band is subtracted.

with the other three defect bands - is that the average frequency of the bands decreases with increasing resolution, where the initial decrease is fast, whereas for increasing resolution the decrease slows down, and the Richardson-extrapolated (or converged) band frequencies are reached at a resolution of $96 \times 136 \times 96$.

The initial refinement from $12 \times 17 \times 12$ to $24 \times 34 \times 24$ is remarkably large in comparison to the bandwidth of each defect band. We speculate that the shifts are related to the “lighting rod”-behavior of the field patterns of a cavity mode, whereby the high fields are concentrated at sharp corners [49, 64, 65]. A change in the grid resolution effectively corresponds to a change in the geometry. At

low resolution, the field pattern likely “misses” the sharp features of the high-index material, whereas with increased resolution the field pattern increasingly fits within the high-index material, causing a decrease of the field energy - in view of the variational principle [17] - as observed in Figure 2.10.

To quantify the rate of convergence, we calculate the convergence order following Ref. [52]. We assume that the grid spacing h is sufficiently refined for the error E to asymptotically approach zero as

$$E = \omega(h) - \omega_{\text{exact}} = Ch^p, \quad (2.3)$$

with $\omega(h)$ the frequency calculated for grid spacing h at a given wave vector, ω_{exact} the exact frequency at the same wave vector, C a constant. The convergence order p is obtained from a sequence of three resolutions as [52]

$$p = \ln \left(\frac{\omega(h) - \omega(\frac{h}{2})}{\omega(\frac{h}{2}) - \omega(\frac{h}{4})} \right) / \sqrt{2}, \quad (2.4)$$

where we used the $12 \times 17 \times 12$, $24 \times 34 \times 24$ and $48 \times 68 \times 48$ resolution results. From data as shown in Figure 2.10(a,b), we obtain $p = 1.85, 1.96, 2.24, 2.16, 2.10$ for $m = 1, 2, 3, 4, 5$, respectively, in close agreement with the convergence order $p = 2$ for the plane-wave expansion method [51]. We therefore conclude that the band frequencies are converging accurately, as expected.

Moreover, the convergence of the band frequencies allows us to use Richardson extrapolation to obtain the band frequency $\omega_{h=0}$ in the limit of infinite grid resolution ($h = 0$) [52, 53]. The frequency $\omega_{h=0}$ is estimated as

$$\omega_{h=0} = \omega\left(\frac{h}{4}\right) + \frac{\omega\left(\frac{h}{4}\right) - \omega\left(\frac{h}{2}\right)}{2^p - 1}. \quad (2.5)$$

The Richardson-extrapolated frequencies are shown in Fig. 2.10(a,b) as a function of wave vector for the $m = 1$ and $m = 3$ defect bands, respectively. The Richardson-extrapolated frequencies are slightly below the frequencies for the finest grid resolution ($96 \times 136 \times 96$) as expected in case of convergence [52].

Nevertheless, unexpected features were found in the dispersion relations as a function of spatial grid resolution. Figures 2.10(c,d) show the dispersion relations of the $m = 1$ and $m = 3$ defect bands that are overlaid for all grid resolutions by subtracting the average band frequencies from the data in Figures 2.10(a,b). For the $m = 1$ defect band, we observe that for resolutions $12 \times 17 \times 12$ and $24 \times 34 \times 24$, the band between the T and Y high-symmetry points has a maximum at the 4th symbol from the left, midway in between T and Y . For $48 \times 68 \times 48$ and $96 \times 136 \times 96$, the maximum has moved to the 1st symbol from the left, or one sixth of the way from T to Y . Thus, there is a qualitative change in the dispersion relations as the grid is refined. Similar observations were made on the $m = 2$ defect band. Therefore, we do not trust the $m = 1, 2$ defect bands sufficiently to derive coupling coefficients. In contrast, for the $m = 3$ defect band, the maximum in frequency is always at the T point, thus the shape is preserved,

and the band readily converges. Similar observations as for $m = 3$ were made on the $m = 4, 5$ defect bands. Therefore, we trust the convergence of the $m = 3, 4, 5$ bands sufficiently to warrant the extraction of coupling coefficients.

2.C Photonic tight-binding method

We employ the well-known tight-binding method to model the dispersion of the defect bands [18, 20]. In the tight-binding method we assume that the dielectric function of the cavity superlattice, ϵ , can be approximated in the vicinity of each lattice point by the dielectric function, ϵ_Ω , of a single cavity located at the lattice point. This assumption is valid for the inverse-woodpile cavity superlattice, since the superlattice dielectric function differs only from ϵ_Ω at the defect pores in the superlattice that do not form part of the cavity, all of which are at least a lattice constant away. We also assume that the modes of the cavity are confined to the cavity; i.e., if $\mathbf{E}_\Omega^m$ is a mode of a cavity at the origin,

$$\nabla \times \nabla \times \mathbf{E}_\Omega^m = \left(\frac{\Omega_m}{c}\right)^2 \epsilon_\Omega(\mathbf{r}) \mathbf{E}_\Omega^m, \quad (2.6)$$

with Ω_m the resonance frequency of the single cavity and c the speed of light, then we require that $\mathbf{E}_\Omega^m(\mathbf{r})$ be very small when r exceeds a distance of the order of the lattice constant, which we shall refer to as the “range” of $\mathbf{E}_\Omega^m$. Let us briefly verify this assumption: for the defect bands, the mode volume is about $V \approx \lambda^3$, with λ the free-space wavelength [49]. Hence, the electric field attenuates over a range of about $\lambda/2$ in a given direction. We model the cavity mode as an evanescent plane wave that attenuates by a factor of $1/e$ over this distance, which yields an imaginary part of the wave vector of $k'' = 2/\lambda$. The nearest neighbor distances are equal to the lattice parameters of the superlattice (c_s^x, a_s, c_s^z) that are multiples of the inverse woodpile lattice parameters (c_s^x, a_s, c_s^z) = $(3c, 3a, 3c)$ (with $c = a/\sqrt{2}$), and the reduced frequency $\omega' = a/\lambda$ of a cavity resonance is equal to $\omega' = 0.52\dots 0.54$ (for $m = 3, 4, 5$). For the directions x or z , this yields a product of the imaginary part of the wave vector k'' and the nearest neighbor distance Δr of

$$k'' \Delta r = \frac{2}{\lambda} \cdot c_s^{x,z} = \frac{2}{\omega'} \cdot 3c = 6 \frac{\omega'}{\sqrt{2}} \approx 2.2. \quad (2.7)$$

Thus the electric field intensity from one cavity has attenuated to as little as $\exp(-2.2) \approx 0.11$ at a nearest neighboring cavity in the directions x or z , and for the y -direction the decay is even greater, thereby readily fulfilling the requirements of the tight-binding method.

In the tight-binding method, we write the superlattice dielectric function ϵ as

$$\epsilon = \epsilon_\Omega + \Delta\epsilon(\mathbf{r}), \quad (2.8)$$

where $\Delta\epsilon(\mathbf{r})$ represents the perturbation to the cavity dielectric function required to produce the dielectric function of the superlattice. Since the product $\Delta\epsilon(\mathbf{r})\mathbf{E}_\Omega^m(\mathbf{r})$ is quite small, we expect the solution to the superlattice Maxwell

equations to be close to the cavity wave function $\mathbf{E}_\Omega^m(\mathbf{r})$, or to wave functions with which $\mathbf{E}_\Omega^m(\mathbf{r})$ is degenerate, for a cavity located at the origin. In the tight-binding approximation, we expand $\mathbf{E}(\mathbf{r})$ over a small number of cavity wave functions:

$$\mathbf{E}(\mathbf{r}) = \sum_{\mathbf{R}} e^{i\mathbf{k} \cdot \mathbf{R}} \sum_m b_m \mathbf{E}_\Omega^m(\mathbf{r} - \mathbf{R}). \quad (2.9)$$

The wave vector $\mathbf{k}$ describes the relative phase of the resonating cavities and ensures that $\mathbf{k}$ satisfies the Bloch theorem for the Brillouin zone of the superlattice of cavities.

We multiply the superlattice Maxwell equations

$$\nabla \times \nabla \times \mathbf{E}(\mathbf{r}) = \left(\frac{\omega}{c}\right)^2 [\epsilon_\Omega(\mathbf{r}) + \Delta\epsilon(\mathbf{r})] \mathbf{E}(\mathbf{r}) \quad (2.10)$$

by the cavity wave function $\mathbf{E}_\Omega^{n*}(\mathbf{r})$ where the star represents the complex conjugate, integrate over all $\mathbf{r}$, and use the fact that

$$\begin{aligned} & \int_{-\infty}^{\infty} \mathbf{E}_\Omega^{n*}(\mathbf{r}) \cdot \nabla \times \nabla \times \mathbf{E}(\mathbf{r}) d\mathbf{r} \\ &= \int_{-\infty}^{\infty} [\nabla \times \nabla \times \mathbf{E}_\Omega^n(\mathbf{r})]^* \cdot \mathbf{E}(\mathbf{r}) d\mathbf{r} \\ &= \left(\frac{\Omega_n}{c}\right)^2 \int_{-\infty}^{\infty} \epsilon_\Omega(\mathbf{r}) \mathbf{E}_\Omega^{n*}(\mathbf{r}) \cdot \mathbf{E}(\mathbf{r}) d\mathbf{r}, \end{aligned} \quad (2.11)$$

to find that

$$\begin{aligned} & \left[\left(\frac{\Omega_n}{c}\right)^2 - \left(\frac{\omega(\mathbf{k})}{c}\right)^2 \right] \int_{-\infty}^{\infty} \epsilon_\Omega(\mathbf{r}) \mathbf{E}_\Omega^{n*}(\mathbf{r}) \cdot \mathbf{E}(\mathbf{r}) d\mathbf{r} \\ &= \left(\frac{\omega(\mathbf{k})}{c}\right)^2 \int_{-\infty}^{\infty} \mathbf{E}_\Omega^{n*}(\mathbf{r}) \cdot \Delta\epsilon(\mathbf{r}) \mathbf{E}(\mathbf{r}) d\mathbf{r}. \end{aligned} \quad (2.12)$$

Inserting Eq. (2.9) into Eq. (2.12) and using the orthonormality of the cavity wave functions,

$$\int_{-\infty}^{\infty} \epsilon_\Omega(\mathbf{r}) \mathbf{E}_\Omega^{n*}(\mathbf{r}) \cdot \mathbf{E}_\Omega^m(\mathbf{r}) d\mathbf{r} = \delta_{mn}, \quad (2.13)$$

we arrive at an eigenvalue equation that determines the coefficients $b_m(\mathbf{k})$ and

the Bloch frequencies $(\omega(\mathbf{k})/c)^2$:

$$\begin{aligned}
 & \left[\left(\frac{\Omega_n}{c} \right)^2 - \left(\frac{\omega(\mathbf{k})}{c} \right)^2 \right] b_n \\
 &= - \left[\left(\frac{\Omega_n}{c} \right)^2 - \left(\frac{\omega(\mathbf{k})}{c} \right)^2 \right] \sum_m \\
 & \left(\sum_{\mathbf{R} \neq \mathbf{0}} \int_{-\infty}^{\infty} \mathbf{E}_{\Omega}^{n*}(\mathbf{r}) \cdot \epsilon_{\Omega}(\mathbf{r}) \mathbf{E}_{\Omega}^m(\mathbf{r} - \mathbf{R}) e^{i\mathbf{k} \cdot \mathbf{R}} d\mathbf{r} \right) b_m \\
 &+ \left(\frac{\omega(\mathbf{k})}{c} \right)^2 \sum_m \left(\int_{-\infty}^{\infty} \mathbf{E}_{\Omega}^{n*}(\mathbf{r}) \cdot \Delta \epsilon(\mathbf{r}) \mathbf{E}_{\Omega}^m(\mathbf{r}) d\mathbf{r} \right) b_m \\
 &+ \left(\frac{\omega(\mathbf{k})}{c} \right)^2 \sum_m \\
 & \left(\sum_{\mathbf{R} \neq \mathbf{0}} \int_{-\infty}^{\infty} \mathbf{E}_{\Omega}^{n*}(\mathbf{r}) \cdot \Delta \epsilon(\mathbf{r}) \mathbf{E}_{\Omega}^m(\mathbf{r} - \mathbf{R}) e^{i\mathbf{k} \cdot \mathbf{R}} d\mathbf{r} \right) b_m. \tag{2.14}
 \end{aligned}$$

The first term on the right of Eq. (2.14) contains integrals of the form

$$\int_{-\infty}^{\infty} d\mathbf{r} \mathbf{E}_{\Omega}^{n*}(\mathbf{r}) \cdot \epsilon_{\Omega}(\mathbf{r}) \mathbf{E}_{\Omega}^m(\mathbf{r} - \mathbf{R}). \tag{2.15}$$

Since we assumed the cavity modes to be confined to the cavity, the integral in Eq. (2.15) is small compared to unity. The integrals in the third term on the right of Eq. (2.14) are also small, since they also contain the product of two cavity wave functions centered at different sites. Finally, we the second term on the right of Eq. (2.14) is small because we assumed that the cavity wave functions are small at distances large enough for the superlattice dielectric function to deviate from the cavity one.

The right-hand side of (2.14) is therefore always small. Hence, $(\Omega_n/c)^2 - (\omega(\mathbf{k})/c)^2$ is small whenever b_n is not (and vice versa). This means that $(\omega(\mathbf{k})/c)^2$ must be close to a cavity mode, for example $(\Omega_0/c)^2$, and all the b_n except those going with that mode and modes degenerate with (or close to) it in frequency are small:

$$\begin{aligned}
 \left(\frac{\omega}{c} \right)^2(\mathbf{k}) &\approx \left(\frac{\Omega_0}{c} \right)^2, \quad b_n \approx 0 \text{ unless} \\
 \left(\frac{\Omega_n}{c} \right)^2 &\approx \left(\frac{\Omega_0}{c} \right)^2. \tag{2.16}
 \end{aligned}$$

If the cavity mode 0 is nondegenerate, i.e. an s -orbital like mode, then Eq. (2.14) reduces to a single equation giving an explicit expression for the frequency of the band arising from this s -orbital like mode (referred to as an “ s -orbital like band”)

$$\left(\frac{\omega(\mathbf{k})}{c} \right)^2 = \left(\frac{\Omega_s}{c} \right)^2 - \frac{\beta_k + \sum \gamma_k(\mathbf{R}) e^{i\mathbf{k} \cdot \mathbf{R}}}{1 + \sum \alpha(\mathbf{R}) e^{i\mathbf{k} \cdot \mathbf{R}}}, \tag{2.17}$$

where $(\Omega_s/c)^2$ is the frequency of the cavity s -orbital like mode, and

$$\beta_k \equiv \left(\frac{\omega(\mathbf{k})}{c}\right)^2 \int_{-\infty}^{\infty} d\mathbf{r} \mathbf{E}_{\Omega}^*(\mathbf{r}) \cdot \Delta\epsilon(\mathbf{r}) \mathbf{E}_{\Omega}(\mathbf{r}), \quad (2.18)$$

$$\alpha(\mathbf{R}) \equiv \int_{-\infty}^{\infty} d\mathbf{r} \mathbf{E}_{\Omega}^*(\mathbf{r}) \cdot \epsilon_{\Omega}(\mathbf{r}) \mathbf{E}_{\Omega}(\mathbf{r} - \mathbf{R}), \quad (2.19)$$

$$\gamma_k(\mathbf{R}) \equiv \left(\frac{\omega(\mathbf{k})}{c}\right)^2 \int_{-\infty}^{\infty} d\mathbf{r} \mathbf{E}_{\Omega}(\mathbf{r}) \cdot \Delta\epsilon(\mathbf{r}) \mathbf{E}_{\Omega}(\mathbf{r} - \mathbf{R}). \quad (2.20)$$

Here the $\gamma_k(\mathbf{R})$ coefficient is the optical analogue of the hopping integral known from the electronic case. In comparison to the tight-binding dispersion relation for Schrödinger waves (see Ref. [18] equation (10.15)), we note a remarkable difference, namely that the integral here is multiplied with the frequency. We infer that a physical reason for this difference is that electronic potentials can be arbitrarily high or low compared to kinetic energy, whereas the optical analogue “potential for light” is always below the photon energy level, see for illustration the 2nd Figure of Ref. [75].

We neglect the terms with α in the denominator of Eq. (2.17), since they give only small corrections to the numerator as we can see from a Taylor expansion. We assume that only nearest-neighbor separations give significant overlap integrals. Combining these assumptions, we simplify Eq. (2.17) to

$$\left(\frac{\omega(\mathbf{k})}{c}\right)^2 = \left(\frac{\Omega_s}{c}\right)^2 - \beta_k - \sum_{\text{n.n.}} \gamma_k(\mathbf{R}) e^{i\mathbf{k} \cdot \mathbf{R}}, \quad (2.21)$$

where the sum runs only over those $\mathbf{R}$ in the Bravais lattice that connect the origin to its nearest neighbors. An explicit expression for the frequency is

$$\left(\frac{\omega(\mathbf{k})}{c}\right)^2 = \left(\frac{\Omega_s}{c}\right)^2 \frac{1}{1 + \beta + \sum_{\text{n.n.}} \kappa(\mathbf{R}) e^{i\mathbf{k} \cdot \mathbf{R}}}, \quad (2.22)$$

with

$$\beta \equiv \int_{-\infty}^{\infty} d\mathbf{r} \mathbf{E}_{\Omega}^*(\mathbf{r}) \cdot \Delta\epsilon(\mathbf{r}) \mathbf{E}_{\Omega}(\mathbf{r}), \quad (2.23)$$

$$\kappa(\mathbf{R}) \equiv \int_{-\infty}^{\infty} d\mathbf{r} \mathbf{E}_{\Omega}^*(\mathbf{r}) \cdot \Delta\epsilon(\mathbf{r}) \mathbf{E}_{\Omega}(\mathbf{r} - \mathbf{R}). \quad (2.24)$$

The $\kappa(\mathbf{R})$ coefficients are referred to as the coupling coefficients of light in our paper, and are nondimensional. Since we verified that $\mathbf{E}_{\Omega}(\mathbf{r})$ is small at distances exceeding the lattice parameter of the superlattice, the coefficient in Eq. (2.23) is negligible. To obtain an expression for the frequency rather than the frequency squared, we take the square root, and we apply the first-order Taylor approximation $(1 + x)^{-\frac{1}{2}} = 1 - x/2 + O(|x|^2)$, which leads to the dispersion relation

$$\frac{\omega(\mathbf{k})}{c} = \frac{\Omega_s}{c} \left(1 - \frac{\beta}{2} - \frac{1}{2} \sum_{\mathbf{n}, \mathbf{n}'} \kappa(\mathbf{R}) e^{i\mathbf{k} \cdot \mathbf{R}} \right) \quad (2.25)$$

The coupling coefficients are extracted from the dispersion by means of a least-squares fit of the right-hand side of Eq. (2.25) to the dispersion throughout the whole first Brillouin zone. We represent the first Brillouin zone by a grid of $12 \times 12 \times 12$ cubes. We fit over the $\mathbf{k}$ vectors in the middle of the cubes. The results of the tight-binding calculations are discussed in Section 2.3. We note that for all nonzero coupling coefficients, the imaginary part is of the order of at most 10^{-6} , which is $100\times$ to $1000\times$ less than the real part (of the order of $\sim 10^{-4}$ for $m = 3, 5$ and $\sim 10^{-3}$ for $m = 4$). Therefore, we are confident that the coupling coefficients are physically significant. As expected, β is negligibly small, with a real part of the order of $\sim 10^{-10}$.

2.D Coupling coefficients in the y -direction

The coupling coefficients in the $+y$ and $-y$ -directions are equal by reciprocity which we derive in the following. We start with the definition of the coupling coefficient

$$\kappa(\mathbf{R}) = \int d\mathbf{r} \mathbf{E}_{\Omega}^*(\mathbf{r}) \cdot \Delta \epsilon(\mathbf{r}) \mathbf{E}_{\Omega}(\mathbf{r} - \mathbf{R}). \quad (2.26)$$

By definition

$$= \int d\mathbf{r} \mathbf{E}_{\Omega}^*(\mathbf{r}) \cdot [\epsilon(\mathbf{r}) - \epsilon_{\Omega}(\mathbf{r})] \mathbf{E}_{\Omega}(\mathbf{r} - \mathbf{R}). \quad (2.27)$$

Translating the coordinate system

$$= \int d\mathbf{r} \mathbf{E}_{\Omega}^*(\mathbf{r} + \mathbf{R}) \cdot [\epsilon(\mathbf{r} + \mathbf{R}) - \epsilon_{\Omega}(\mathbf{r} + \mathbf{R})] \mathbf{E}_{\Omega}(\mathbf{r}). \quad (2.28)$$

By Maxwell's equations for the individual cavity

$$= \int d\mathbf{r} \mathbf{E}_{\Omega}^*(\mathbf{r}) \cdot \epsilon(\mathbf{r}) \mathbf{E}_{\Omega}(\mathbf{r} + \mathbf{R}) \quad (2.29)$$

$$- \frac{1}{\left(\frac{\Omega_s}{c}\right)^2} \int d\mathbf{r} \nabla \times \nabla \times \mathbf{E}_{\Omega}^*(\mathbf{r} + \mathbf{R}) \cdot \mathbf{E}_{\Omega}(\mathbf{r}). \quad (2.30)$$

Performing integration by parts

$$= \int d\mathbf{r} \mathbf{E}_{\Omega}^*(\mathbf{r}) \cdot \epsilon(\mathbf{r}) \mathbf{E}_{\Omega}(\mathbf{r} + \mathbf{R}) \quad (2.31)$$

$$- \frac{1}{\left(\frac{\Omega_s}{c}\right)^2} \int d\mathbf{r} \mathbf{E}_{\Omega}^*(\mathbf{r} + \mathbf{R}) \cdot \nabla \times \nabla \times \mathbf{E}_{\Omega}(\mathbf{r}) d\mathbf{r}. \quad (2.32)$$

By Maxwell’s equations for the individual cavity

$$= \int d\mathbf{r} \mathbf{E}_{\Omega}^*(\mathbf{r}) \cdot \epsilon(\mathbf{r}) \mathbf{E}_{\Omega}(\mathbf{r} + \mathbf{R}) \tag{2.33}$$

$$- d\mathbf{r} \mathbf{E}_{\Omega}^*(\mathbf{r}) \epsilon_{\Omega}(\mathbf{r}) \mathbf{E}_{\Omega}(\mathbf{r} + \mathbf{R}) \tag{2.34}$$

$$= \kappa(-\mathbf{R}). \tag{2.35}$$

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CHAPTER 3

Time-dependent propagation of Cartesian light in a 3D cavity superlattice

3.1 Introduction

In the field of waves interacting with multiple resonances, a one-dimensional (1D) chain of coupled resonant cavities is a well-known system that is known as a coupled-resonator optical waveguide (CROW) [1]. Since light resonates for a long time before hopping between the consecutive cavities, such a system is expected to reveal slow light behaviour [2, 3]. Indeed, ultraslow propagation of optical pulses with group velocities well below $0.01c$ has been experimentally demonstrated in CROWs [4]. A proposal to employ optical pulses in CROWs for holographic storage was therefore made by Mookherjea and Yariv [5]. Also, arrays of cavities coupled with quantum systems, such as two-level systems, are predicted to show rich physics in the time-domain including a localization-delocalization transition [6], which has been demonstrated experimentally in a superconducting circuit setup [7]. The propagation of light through 1D CROWs is well-understood theoretically: the propagation distance Δz of an optical pulse after time Δt is proportional to the dispersion bandwidth $\Delta\omega$,

$$\Delta z/\Delta t \simeq \Delta\omega, \quad (3.1)$$

and the dispersion bandwidth is in turn proportional to the coupling coefficient [8].

For the propagation of light through a 2D lattice of coupled waveguides, the out-of-plane propagation direction is analogous to a time dimension in the Schrödinger equation, which has been used to achieve transverse localization of light by introducing disorder in the transverse directions [9, 10]. Two-dimensional (2D) networks of waveguides show peculiar discrete diffraction effects [11–13]. For example, in waveguide lattices where a narrow input beam excites a single site, most of the output light is distributed in two distinct outer lobes, as seen in experiments [11]. Discrete solitons in such structures travel along preassigned paths, including bends, and can be routed to any destination port by blockers, in the time-domain [11]. By modulating the refractive index periodically in time in periodic 2D cavity superlattices, a synthetic third dimension can be created and topologically-protected propagation, *i.e.* without backscattering, is observed in calculations [14, 15]. Two-dimensional (2D) multicore fibers enable large data

transmission rates, but suffer from optical crosstalk between fibers [16–18]. A deep understanding of light propagation in 2D lattices may enable optimized designs that minimize crosstalk.

3D cavity superlattices have been studied in the time-domain for the dynamic localization of light [19]. In 3D photonic band gap crystals in the microwave regime, extremely small group velocities and long photon lifetimes have been observed in a 1D array of weakly-coupled cavities as expected from CROW considerations [20, 21].

3D cavity superlattices show markedly different light propagation compared with 1D CROWs, as the dispersion bandwidth is not necessarily proportional to the coupling coefficient, see Chapter 2. This is likely a result of the interference between the many hopping paths that contribute to 3D propagation [22]. The dispersion bandwidth does not, however, give a full picture of propagation in 3D cavity superlattices, as it is a property that pertains to delocalized Bloch modes where many or all cavities are excited simultaneously. It would therefore also be of great interest to understand the propagation of an input pulse that initially excites only a single or a few cavities. Such propagation can be calculated in the time-domain [23]. The time-dependent propagation in 3D superlattices is also interesting in its own right, since the dynamics is likely to be significantly different from 1D. Therefore, in this Chapter, we explore the time-dependent propagation of light in a superlattice of cavities embedded in a 3D photonic band gap crystal.

3.2 Structures

3.2.1 Inverse woodpile cavity superlattices

We explore the time-dependent propagation of light in a superlattice of cavities in an inverse woodpile photonic crystal with pore radius $r/a = 0.24$. The defect pore radius that defines the cavities has a radius of $r'/r = 0.5$ [24, 25]. The cavity superlattice has lattice parameters (c_s^x, a_s, c_s^z) in the (x, y, z) directions that are integer multiples of the underlying inverse woodpile lattice parameters: $c_s^x = M_x c$, $a_s = M_y a$, $c_s^z = M_z c$, with M_x, M_y, M_z integers. In Fig. 3.1(a), the band structure is shown for a $M_x M_y M_z = 3 \times 3 \times 3$ cavity superlattice in an inverse woodpile photonic band gap crystal made of silicon, where the cavities are repeated every three unit cells with lattice parameters $c_s^x = 3c$, $a_s = 3a$, $c_s^z = 3c$ with $a/c = \sqrt{2}$ in the underlying inverse woodpile crystal for cubic symmetry. As a result of the intentional defect pores many bands appear in the band gap of the perfect crystal between reduced frequencies $\tilde{\omega} = \omega a / (2\pi c) = 0.492$ and 0.634 . The lowest five bands between $\tilde{\omega} = 0.5$ and 0.55 have a low dispersion and correspond to five cavity resonances that are from now on labeled as $m = 1, \dots, 5$. The $m = 3, 4, 5$ bands are isolated in frequency. A closer inspection of the five dispersionless cavity bands in Fig. 3.1(b) reveals that these bands have nonzero bandwidths, indicating that cavity resonances in the $M_x M_y M_z = 3 \times 3 \times 3$ superlattice are coupled, since, in a tight-binding model, a dispersion bandwidth corresponds to nonzero coupling coefficients.

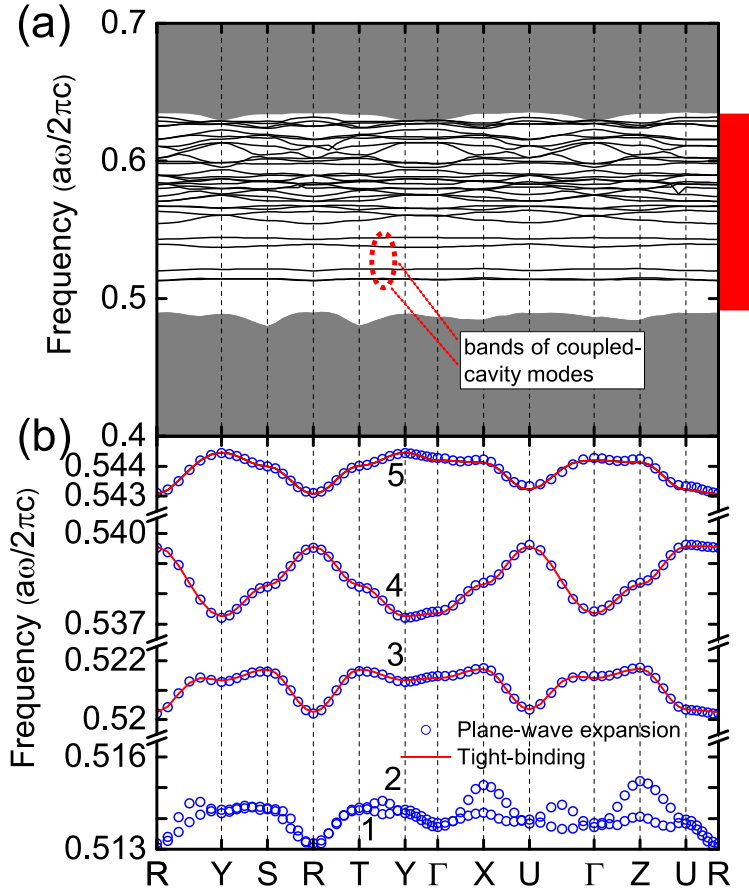


Figure 3.1: (a) Black curves are photonic bands of a 3D inverse woodpile photonic band gap crystal ($r/a = 0.24$, $\epsilon_{Si} = 12.1$) with a $M_x M_y M_z = 3 \times 3 \times 3$ superlattice with defect pores as shown in Fig. 2.1 and of radius $r'/r = 0.5$. Figure also shown as Fig. 2.2(a) in Chapter 2. The frequencies are given in reduced units $\tilde{\omega} = \omega a / (2\pi c)$, where c is the speed of light. The abscissa indicates the wave vector between the high-symmetry points of the Brillouin zone (see Appendix 2.A). The 3D photonic band gap of the perfect crystal is shown as a red bar, and the range of allowed modes outside the band gap is shown in grey. The five bands of coupled-cavity modes are highlighted. (b) Zoom-in on the five coupled-cavity bands (blue circles), labeled $m = 1, \dots, 5$. The $m = 3, 4, 5$ bands are accurately described by the tight-binding model, see Chapter 2 (red curves).

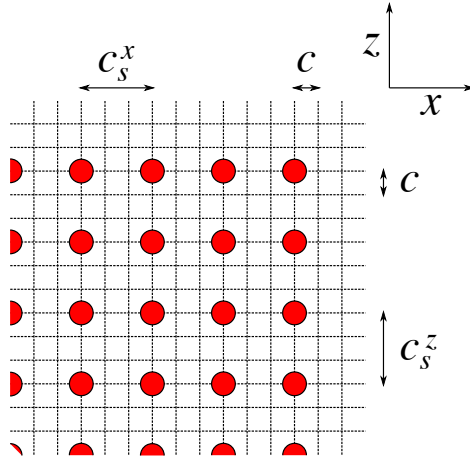


Figure 3.2: schematic of the $(+x, +z)$ corner of the finite cavity superlattice, with red circles indicating cavities and dashed rectangles representing unit cells of the underlying inverse woodpile crystal structure. The lattice parameters (c_s^x, c_s^z) of the superlattice are shown, as well as the x, y, z coordinate system. The cavity superlattice is embedded in an infinitely extended inverse woodpile photonic crystal.

3.2.2 Finite superlattice

In order to investigate the behavior of light in a superlattice of cavities we calculate the time-resolved hopping of light within three coupled-cavity bands in a 2D $n_x \times n_z = 101 \times 101$ superlattice of 3D inverse woodpile cavities. In the superlattice, the cavities are repeated every three unit cells with lattice parameters $c_s^x = 3c$, $c_s^z = 3c$. We consider only a single $x - z$ plane of cavities, since the coupling coefficient in the y -direction was found to be smaller by typically $10\times$ than in the (x, z) plane for the inverse woodpile 3D cavity superlattice with $M_x M_y M_z = 3 \times 3 \times 3$, see Chapter 2. The cavity superlattice is illustrated in Fig. 3.2. Due to the surrounding band gap, light is strictly confined to the superlattice, as opposed to, for instance, 1D and 2D systems where light readily leaks out. The finite extent of the superlattice simplifies the calculations since we only need to expand the field over a finite set of superlattice modes. On the other hand, the finite extent does not limit the dynamics, since we consider times where the energy has not propagated to the edge of the superlattice.

3.2.3 Cavity superlattice mode frequencies

The Maxwell eigenvalue problem for the electric field $\mathbf{E}_\Omega(\mathbf{r})$ in a single cavity in a photonic band gap is equal to

$$\nabla \times \nabla \times \mathbf{E}_\Omega^m(\mathbf{r}) = \left(\frac{\tilde{\Omega}_m}{c} \right)^2 \epsilon_\Omega(\mathbf{r}) \mathbf{E}_\Omega^m(\mathbf{r}), \quad (3.2)$$

with $\tilde{\Omega}_m = \Omega_m a / (2\pi c)$ the resonance frequency of the single cavity in reduced units, c the speed of light, and $\epsilon_\Omega(\mathbf{r})$ the spatial permittivity distribution of the single cavity in the 3D band gap crystal. We take the field of the single cavity to be normalized as

$$\int_{-\infty}^{\infty} \epsilon_\Omega(\mathbf{r}) |\mathbf{E}_\Omega^m|^2 d\mathbf{r} = 1. \quad (3.3)$$

We expand the field $\mathbf{E}^m(\mathbf{r})$ for the full superlattice in terms of the eigenmodes of the single cavities obtained from Eq. (3.2) resulting in

$$\mathbf{E}^m(\mathbf{r}) = \sum_{\mathbf{R}} a_{\mathbf{R}}^m \mathbf{E}_\Omega^m(\mathbf{r} - \mathbf{R}), \quad (3.4)$$

where $\mathbf{R}$ is the displacement of each cavity in the superlattice and $a_{\mathbf{R}}$ is the amplitude at cavity $\mathbf{R}$, and the summation is over all cavities in the finite superlattice [26]. The Maxwell eigenvalue problem for the superlattice field $\mathbf{E}^m(\mathbf{r})$ is equal to

$$\nabla \times \nabla \times \mathbf{E}^m(\mathbf{r}) = \left(\frac{\tilde{\omega}}{c} \right)^2 \epsilon(\mathbf{r}) \mathbf{E}^m(\mathbf{r}), \quad (3.5)$$

with $\epsilon(\mathbf{r})$ the permittivity distribution of the superlattice and $\tilde{\omega}_m = (a\omega_m/2\pi c)$ the frequency of the mode of the superlattice in reduced units. To solve the superlattice Maxwell wave equation (3.5) for the superlattice field and frequencies, we multiply with the single cavity wave eigenfunction $\mathbf{E}_\Omega^{m*}(\mathbf{r} - \mathbf{R}')$ and integrate over all space

$$\int_{-\infty}^{\infty} \mathbf{E}_\Omega^{m*}(\mathbf{r} - \mathbf{R}') \cdot \nabla \times \nabla \times \mathbf{E}^m(\mathbf{r}) d\mathbf{r} \quad (3.6)$$

$$= \left(\frac{\tilde{\omega}}{c} \right)^2 \int_{-\infty}^{\infty} \epsilon(\mathbf{r}) \mathbf{E}_\Omega^{m*}(\mathbf{r} - \mathbf{R}') \cdot \mathbf{E}^m(\mathbf{r}) d\mathbf{r}. \quad (3.7)$$

We use the fact that the curl-curl operator is Hermitian to find that the left-hand side of Eq. (3.6) equals

$$\int_{-\infty}^{\infty} \mathbf{E}_\Omega^{m*}(\mathbf{r} - \mathbf{R}') \cdot \nabla \times \nabla \times \mathbf{E}^m(\mathbf{r}) d\mathbf{r} \quad (3.8)$$

$$= \int_{-\infty}^{\infty} [\nabla \times \nabla \times \mathbf{E}_\Omega^m(\mathbf{r} - \mathbf{R}')]^* \cdot \mathbf{E}^m(\mathbf{r}) d\mathbf{r} \quad (3.9)$$

$$= \left(\frac{\tilde{\Omega}_m}{c} \right)^2 \int_{-\infty}^{\infty} \epsilon_\Omega(\mathbf{r} - \mathbf{R}') \mathbf{E}_\Omega^m(\mathbf{r} - \mathbf{R}') \cdot \mathbf{E}^m(\mathbf{r}) d\mathbf{r}, \quad (3.10)$$

where in the last line Eq. (3.2) was inserted. Since we integrate over all space, in the integration by parts two times from Eq. (3.8) to Eq. (3.9) we do not need to consider boundary terms. Substituting Eq. (3.4) and Eq. (3.10) in Eq. (3.6),

we find the generalized eigenvalue problem for the superlattice frequency $\tilde{\omega}_m$

$$\tilde{\Omega}_m^2 \sum_{\mathbf{R}} A_{\mathbf{R}'\mathbf{R}}^m a_{\mathbf{R}}^m = \tilde{\omega}_m^2 \sum_{\mathbf{R}} B_{\mathbf{R}'\mathbf{R}}^m a_{\mathbf{R}}^m, \quad (3.11)$$

with the summation $\mathbf{R}$ over the cavities in the superlattice, and with coefficients

$$A_{\mathbf{R}'\mathbf{R}}^m = \int_{-\infty}^{\infty} \epsilon_{\Omega}(\mathbf{r} - \mathbf{R}') \mathbf{E}_{\Omega}^m(\mathbf{r} - \mathbf{R}') \cdot \mathbf{E}_{\Omega}^m(\mathbf{r} - \mathbf{R}) d\mathbf{r},$$

$$B_{\mathbf{R}'\mathbf{R}}^m = \int_{-\infty}^{\infty} \epsilon(\mathbf{r}) \mathbf{E}_{\Omega}^m(\mathbf{r} - \mathbf{R}') \cdot \mathbf{E}_{\Omega}^m(\mathbf{r} - \mathbf{R}) d\mathbf{r},$$

that effectively describe the electromagnetic interaction between the cavities. We separate the right-hand side of Eq. (3.11) in a term with the same cavity ($\Omega' = \Omega$) and all others ($\Omega' \neq \Omega$)

$$\tilde{\omega}_m^2 \sum_{\mathbf{R}} B_{\mathbf{R}'\mathbf{R}}^m a_{\mathbf{R}}^m = \tilde{\omega}_m^2 B_{\mathbf{R}'\mathbf{R}'}^m a_{\mathbf{R}'}^m + \tilde{\omega}_m^2 \sum_{\mathbf{R} \neq \mathbf{R}'} B_{\mathbf{R}'\mathbf{R}}^m a_{\mathbf{R}}^m. \quad (3.12)$$

Next, we define the perturbation coefficient

$$\beta^m \equiv \int_{-\infty}^{\infty} d\mathbf{r} \Delta\epsilon(\mathbf{r} - \mathbf{R}') \mathbf{E}_{\Omega}^m(\mathbf{r} - \mathbf{R}') \cdot \mathbf{E}_{\Omega}^m(\mathbf{r} - \mathbf{R}'), \quad (3.13)$$

with $\Delta\epsilon(\mathbf{r}) = \epsilon(\mathbf{r}) - \epsilon_{\Omega}(\mathbf{r})$ as the difference between the dielectric function of the whole superlattice with the lattice with only one cavity. We note that the coefficient β^m in Eq. (3.13) is the same as the β from Eq. (2.23) by a change of variables $\mathbf{r} - \mathbf{R}' \rightarrow \mathbf{r}$. We express Eq. (3.12) now in terms of the coefficient β^m defined in Eq. (3.13):

$$\tilde{\omega}_m^2 \sum_{\mathbf{R}} B_{\mathbf{R}'\mathbf{R}}^m a_{\mathbf{R}}^m = \tilde{\omega}_m^2 (1 + \beta^m) a_{\mathbf{R}'}^m + \tilde{\omega}_m^2 \sum_{\mathbf{R} \neq \mathbf{R}'} B_{\mathbf{R}'\mathbf{R}}^m a_{\mathbf{R}}^m. \quad (3.14)$$

Next, we write the frequency in the second term in Eq. (3.14) as a perturbation to the single cavity frequency:

$$\begin{aligned} \tilde{\omega}_m^2 \sum_{\mathbf{R}} B_{\mathbf{R}'\mathbf{R}}^m a_{\mathbf{R}}^m &= \tilde{\omega}_m^2 a_{\mathbf{R}'}^m + \tilde{\omega}_m^2 (\beta^m a_{\mathbf{R}'}^m + \sum_{\mathbf{R} \neq \mathbf{R}'} B_{\mathbf{R}'\mathbf{R}}^m a_{\mathbf{R}}^m) \\ &= \tilde{\omega}_m^2 a_{\mathbf{R}'}^m + (\tilde{\Omega}_m^2 + (\tilde{\omega}_m^2 - \tilde{\Omega}_m^2)) (\beta^m a_{\mathbf{R}'}^m + \sum_{\mathbf{R} \neq \mathbf{R}'} B_{\mathbf{R}'\mathbf{R}}^m a_{\mathbf{R}}^m), \end{aligned} \quad (3.15)$$

where in the first line we rearranged the brackets from Eq. (3.14) and in the second line we used the equality $\tilde{\omega}_m^2 = \tilde{\Omega}_m^2 + (\tilde{\omega}_m^2 - \tilde{\Omega}_m^2)$. The assumption of tight-binding gives us a number of inequalities that we can use. First, it is reasonable to assume that the difference between the superlattice band $\tilde{\omega}_m$ and the single cavity resonance $\tilde{\Omega}_m$ is much smaller than the superlattice band frequency, hence $\tilde{\omega}_m^2 -$

$\tilde{\Omega}_m^2 \ll \tilde{\omega}_m^2$. Second, in the coefficient (3.13) the perturbation in the permittivity $\Delta\epsilon(\mathbf{r}-\mathbf{R}')$ is nonzero only at the cavities away from $\mathbf{R}'$ where the field $\mathbf{E}_\Omega^m(\mathbf{r}-\mathbf{R}')$ is small, hence $\beta^m \ll 1$. Third, since $B_{\mathbf{R}'\mathbf{R}}^m$ for $\mathbf{R}' \neq \mathbf{R}$ describes the overlap of two wave functions that are evanescently coupled as is assumed in a tight-binding model, it is reasonable to assume that $B_{\mathbf{R}'\mathbf{R}} \ll 1$. With these three ingredients we now find the following approximation for the right-hand side of Eq. (3.15):

$$\tilde{\omega}_m^2 \sum_{\mathbf{R}} B_{\mathbf{R}'\mathbf{R}}^m a_{\mathbf{R}}^m \approx \tilde{\omega}_m^2 a_{\mathbf{R}'}^m + \tilde{\Omega}_m^2 (\beta^m a_{\mathbf{R}'}^m + \sum_{\mathbf{R} \neq \mathbf{R}'} B_{\mathbf{R}'\mathbf{R}}^m a_{\mathbf{R}}^m). \quad (3.16)$$

For the left hand side of Eq. (3.11) we find using the normalization defined in Eq. (3.3), and by separating the summation in a term with $\mathbf{R}'$ and all others, that

$$\tilde{\Omega}_m^2 \sum_{\mathbf{R}} A_{\mathbf{R}'\mathbf{R}}^m a_{\mathbf{R}}^m = \tilde{\Omega}_m^2 (a_{\mathbf{R}'}^m + \sum_{\mathbf{R} \neq \mathbf{R}'} A_{\mathbf{R}'\mathbf{R}}^m a_{\mathbf{R}}^m) \quad (3.17)$$

Using Eq. (3.11) and the expressions (3.16)-(3.17) we find that the standard eigenvalue problem can be simplified into

$$\tilde{\omega}_m^2 a_{\mathbf{R}'}^m = \tilde{\Omega}_m^2 (1 - \beta^m) a_{\mathbf{R}'}^m + \tilde{\Omega}_m^2 \sum_{\mathbf{R} \neq \mathbf{R}'} C_{\mathbf{R}'\mathbf{R}}^m a_{\mathbf{R}}^m, \quad (3.18)$$

where

$$C_{\mathbf{R}'\mathbf{R}}^m \equiv A_{\mathbf{R}'\mathbf{R}}^m - B_{\mathbf{R}'\mathbf{R}}^m \quad (3.19)$$

are the hopping coefficients defined in Eq. (2.24). The coefficients $A_{\mathbf{R}'\mathbf{R}}^m$ and $B_{\mathbf{R}'\mathbf{R}}^m$ in the generalized eigenvalue problem (3.11) are unknown and may be difficult to calculate. The coefficients (3.19) in the standard eigenvalue problem (3.18), on the other hand, were calculated in Appendix 2.C in Chapter 2.

The single cavity resonance frequency $\tilde{\Omega}_m$ in Eq. (3.18) was also calculated in Chapter 2 based on the band structure of an infinite $M_x M_y M_z = 3 \times 3 \times 3$ cavity superlattice. There, we represented the first Brillouin zone of the infinite 3D cavity superlattice by a grid of $12 \times 12 \times 12$ rectangles, and calculated the frequencies at the wave vectors $\mathbf{k}_i$ in the middle of the rectangles. We then estimated the isolated cavity resonance frequency $\tilde{\Omega}_m$ as the arithmetic mean of the frequencies over these k -vectors

$$\tilde{\Omega}_m = (1/N_k) \sum_{i=1}^{N_k} \tilde{\omega}_m(\mathbf{k}_i),$$

where $\tilde{\omega}_m(\mathbf{k}_i)$ is the frequency of the m th coupled-cavity band at wave vector $\mathbf{k}_i$, and N_k the total number of $\mathbf{k}$ vectors. The isolated cavity resonance (angular) frequencies for the $m = 3, 4, 5$ coupled-cavity bands are $\tilde{\Omega}_3, \tilde{\Omega}_4, \tilde{\Omega}_5 = 0.5213, 0.5384, 0.5439(a/2\pi c)$. To obtain the frequency in physical units, we take a lattice parameter $a = 677\text{nm}$, which was shown in Devashish et al. [28] to give the best match between the center frequencies of reflectivity peaks in finite-element calculations and in experiments. For crystals with a lattice parameter

$a = 677\text{nm}$, the (non-angular) frequency of the third mode in physical units is $\tilde{\Omega}_3 = 2.3 \cdot 10^2 \text{THz}$. The oscillation period is $2\pi/\tilde{\Omega}_3 = 4.3\text{fs}$.

3.2.4 Finite superlattice dynamics

We consider a superlattice with number of cavities $N = n_x \cdot n_z$. After solving the eigenvalue problem (3.18) we obtain a matrix of eigenvectors $V = [e_1, \dots, e_N]$, with $e_1, \dots, e_N$ the eigenvectors, and eigenvalues $\tilde{\omega}_1^2, \dots, \tilde{\omega}_N^2$ in units of $\left(\frac{2\pi c}{a}\right)^2$, which we take to be ordered from the lowest eigenfrequency to the highest eigenfrequency. We verified that the eigenfrequencies are all within the bandwidth of the coupled-cavity band of the infinite superlattice. Let l denote the index of the eigenmode of the finite superlattice. In Fig. 3.3 we show as an example the energy distribution $|a_{\mathbf{R}}|^2$ for the $l = 1$ and $l = 10201$ modes of the superlattice. We observe that the $l = 1$ mode has a single peak typical of a low wave vector and the $l = 10201$ mode has many peaks and nodes typical of a high wave vector.

Let (i, j) denote the $(i\text{th}, j\text{th})$ cavity. At initial time we excite the central cavity $(i, j) = (0, 0)$. The vector of amplitudes is then

$$a_{\mathbf{R}}^{\text{initial}} = \begin{cases} 1 & \text{if } \mathbf{R} = \mathbf{0} \\ 0 & \text{if } \mathbf{R} \neq \mathbf{0}. \end{cases}$$

In the eigenvector basis, the expansion coefficients are then

$$c = \begin{bmatrix} c_1 \\ \vdots \\ c_N \end{bmatrix} = V^{-1} a^{\text{initial}}.$$

Next, we calculate the field distribution in time. The amplitudes at time t are then

$$a(t) = \sum_{i=1}^N c_i e_i e^{i\omega_i t}.$$

The amplitudes can be evaluated at any desired time without time-stepping. As reported in Chapter 2, the coupling coefficients (3.19) ((2.24) in Chapter 2) have been calculated on the powerful ‘‘Serendipity’’ cluster in the MACS group at the MESA⁺ Institute [27], where the calculations took 210h. The eigenvalue problem (3.18) has been solved on a MacBookPro11,5, where the calculations took about ten minutes.

3.3 Results

Before presenting the results, we define a number of spatial regions to simplify the discussion, see Fig. 3.4(a) and Fig. 3.8(a). We denote the cavities in a square about the center with the following notation

$$D_{\text{center}} = (-10 \leq i \leq 10, -10 \leq j \leq 10).$$

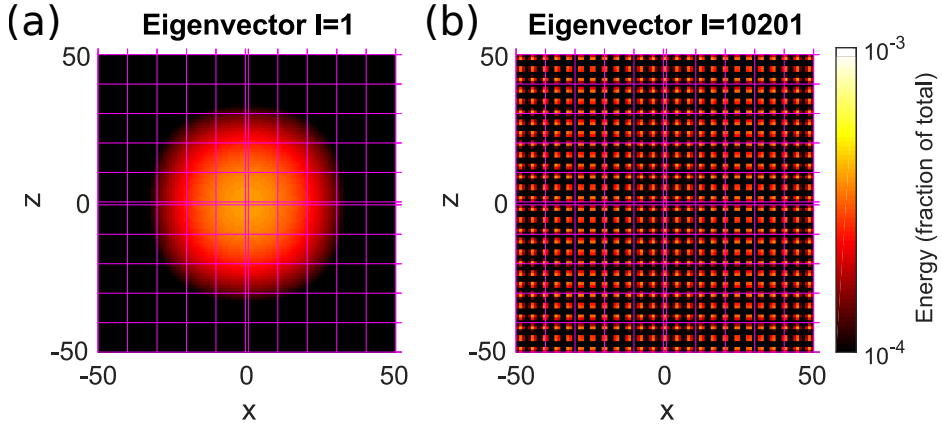


Figure 3.3: Energy distribution for the light hopping in the $l = 1$ and $l = 10201$ superlattice modes. The coordinates x, z indicate the i, j indices of the cavities. The magenta grid lines are repeated every 10 cavities, except for the central row and column of cavities which have been separately indicated.

We define the following notation for the cavities in the (x, z) Cartesian directions

$$D_{\text{Cartesian}} = (-50 \leq i \leq -11, -10 \leq j \leq 10) \cup \\ (11 \leq i \leq 50, -10 \leq j \leq 10) \cup \\ (-10 \leq i \leq 10, 11 \leq j \leq 50) \cup \\ (-10 \leq i \leq 10, -50 \leq j \leq -11).$$

We define the following notation for the cavities in the diagonal directions

$$D_{\text{xz-diag}} = (11 \leq i \leq 50, 11 \leq j \leq 50) \cup \\ (-50 \leq i \leq -11, 11 \leq j \leq 50) \cup \\ (11 \leq i \leq 50, -50 \leq j \leq -11) \cup \\ (-50 \leq i \leq -11, -50 \leq j \leq -11).$$

We define the following region where strong peaks occur for the $m = 4$ resonance

$$D_{\text{peaks}} = (-40 \leq i \leq -31, -40 \leq j \leq -31) \cup \\ (31 \leq i \leq 40, -40 \leq j \leq -31) \cup \\ (-40 \leq i \leq -31, 31 \leq j \leq 40) \cup \\ (31 \leq i \leq 40, 31 \leq j \leq 40).$$

3.3.1 $m = 3$ resonance

In Fig. 3.4 we show the energy distribution at times $t = 0, 250, 2000, 5500(2\pi/\tilde{\Omega}_3) = 0, 1.1, 8.7, 23.8ps$. At the initial time $t = 0(2\pi/\tilde{\Omega}_3)$

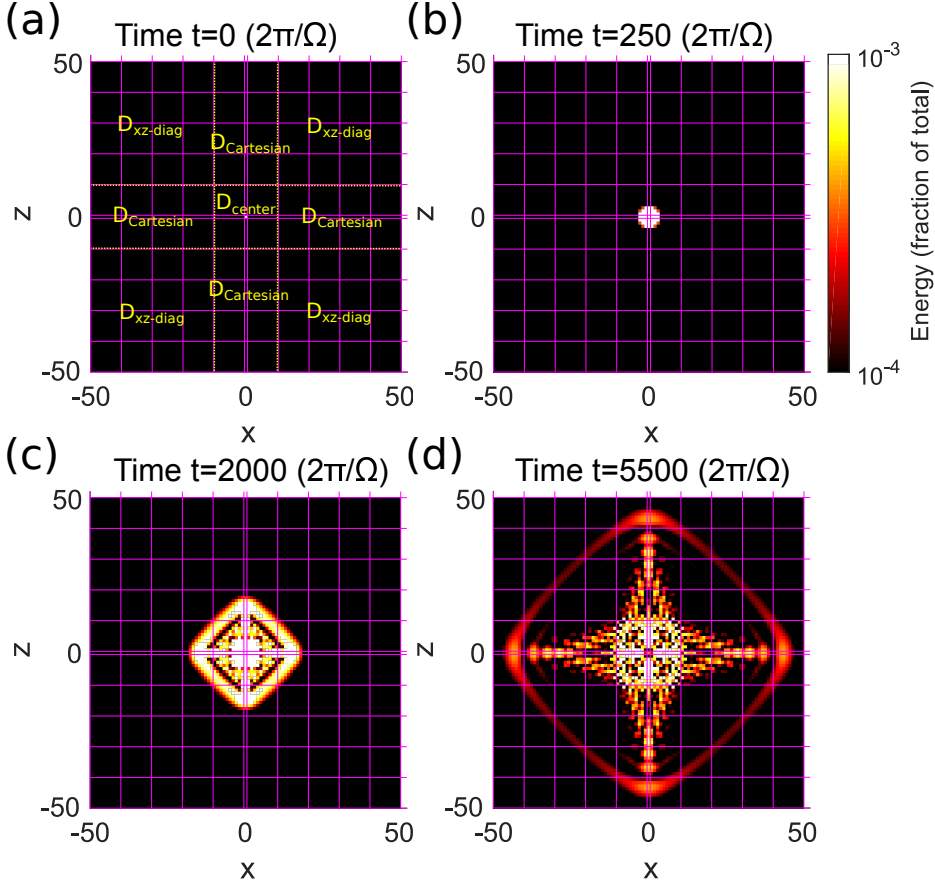


Figure 3.4: Energy distribution for light hopping in the $m = 3$ coupled-cavity band for times (a) $t = 0(2\pi/\tilde{\Omega}_3)$, (b) $t = 250(2\pi/\tilde{\Omega}_3)$, (c) $t = 2000(2\pi/\tilde{\Omega}_3)$ and (d) $t = 5500(2\pi/\tilde{\Omega}_3)$. The magenta grid lines are repeated every 10 cavities, except for the central row and column of cavities, which have been separately indicated.

only the central cavity is excited. At $t = 250(2\pi/\tilde{\Omega}_3)$ (Fig. 3.4(b)) the energy density is high in the central 7×7 cavities, including the central cavity. From Fig. 3.4(b) the distribution appears to be more-or-less radially symmetric, that is, the energy appears to depend only on the distance to the central cavity and not on x and z separately. At $t = 2000(2\pi/\tilde{\Omega}_3)$ (Fig. 3.4(c)) the energy distribution is high in the central 9×9 cavities, including the central cavity, as well as in four beams along the $\pm x$ and $\pm z$ axes. In the diagonal $(\pm x, \pm z)$ directions we appear to see a single wavefront. Behind this wavefront closer to the central cavity, but outside the central 9×9 cavities, we see a speckle pattern with a considerable average energy density. At $t = 5500(2\pi/\tilde{\Omega}_3)$ (Fig. 3.4(d)) the central cavity has a low energy density. Within the central 21×21 (D_{center}) cavities, we see a speckled pattern of cavities with high ($> 0.1\%$) or low ($< 0.1\%$) energies, so it appears that there are high wave vector $|\mathbf{k}|$ superlattice Bloch modes that do not travel fast. Overall the central region D_{center} appears very bright in Fig. 3.4(d). We see four beams with a sequence of high-energy peaks along the Cartesian $\pm x$ and $\pm z$ axes ($D_{\text{Cartesian}}$). From a snapshot in time it is not clear whether the peaks are the maxima of a standing wave, or pulses propagating outward. In the diagonal $(\pm x, \pm z)$ directions ($D_{\text{xz-diag}}$) we clearly see one wavefront, and two or three additional wavefronts appear to be barely visible closer to the central cavity. From Fig. 3.4 it naively appears that a remarkable amount of energy remains in D_{center} even for long times, while the energy in the central cavity is not always large, and that the light propagates mostly in four beams in the Cartesian directions.

To study quantitatively the energy remaining in D_{center} and the central cavity, we show the fraction of energy versus time for the duration $t = 0 \dots 5500(2\pi/\tilde{\Omega}_3)$, in Fig. 3.5. We observe (Fig. 3.5(a)) that a large fraction of energy remains within the central 21×21 cavities (D_{center}) for the duration $t = 0 \dots 5500(2\pi/\tilde{\Omega}_3)$, decreasing from 100% at $t = 0(2\pi/\tilde{\Omega}_3)$ to 65% at $t = 2000(2\pi/\tilde{\Omega}_3)$ and as much as 31% at $t = 5500(2\pi/\tilde{\Omega}_3)$. In the limit $t \rightarrow \infty$, we might expect to see a speckle pattern where the energy is more-or-less equally distributed in space (since the cavity superlattice is surrounded by a 3D photonic band gap that reflects light). The area of the cavities D_{center} is about 4.3% of the complete superlattice, so we would expect that about 4.3% of the energy remains in D_{center} as $t \rightarrow \infty$, which is $7 \times$ less than 31% at $t = 5500(2\pi/\tilde{\Omega}_3)$. The rate of decrease of the total energy in D_{center} decreases on the log-scale as can be seen in Fig. 3.5(a), which may be reasonable since only cavities at the edge of D_{center} contribute to the decay. For large times $t > 2500(2\pi/\tilde{\Omega}_3)$ the rate is approximately constant.

For the central cavity (Fig. 3.5(b)), the fraction of remaining energy decreases quickly from 100% at $t = 0(2\pi/\tilde{\Omega}_3)$ to 37% at $t = 250(2\pi/\tilde{\Omega}_3)$, to 2.2% at $t = 2000(2\pi/\tilde{\Omega}_3)$, and to 0.04% at $t = 5500(2\pi/\tilde{\Omega}_3)$. We would expect the fraction of remaining energy to be $\frac{1}{N} = 0.01\%$ as $t \rightarrow \infty$, which is about $4 \times$ smaller than the observed energy fraction at $t = 5500(2\pi/\tilde{\Omega}_3)$ confirming that $t = 5500(2\pi/\tilde{\Omega}_3)$ is not yet in steady state. For small t where the fraction of energy in the central cavity is much larger than in its neighbours, we would expect the decay to be exponential. This is most explicitly visible in a coupled-mode theory, see Joannopoulos et al. [29]. Initially, the energy is very large in

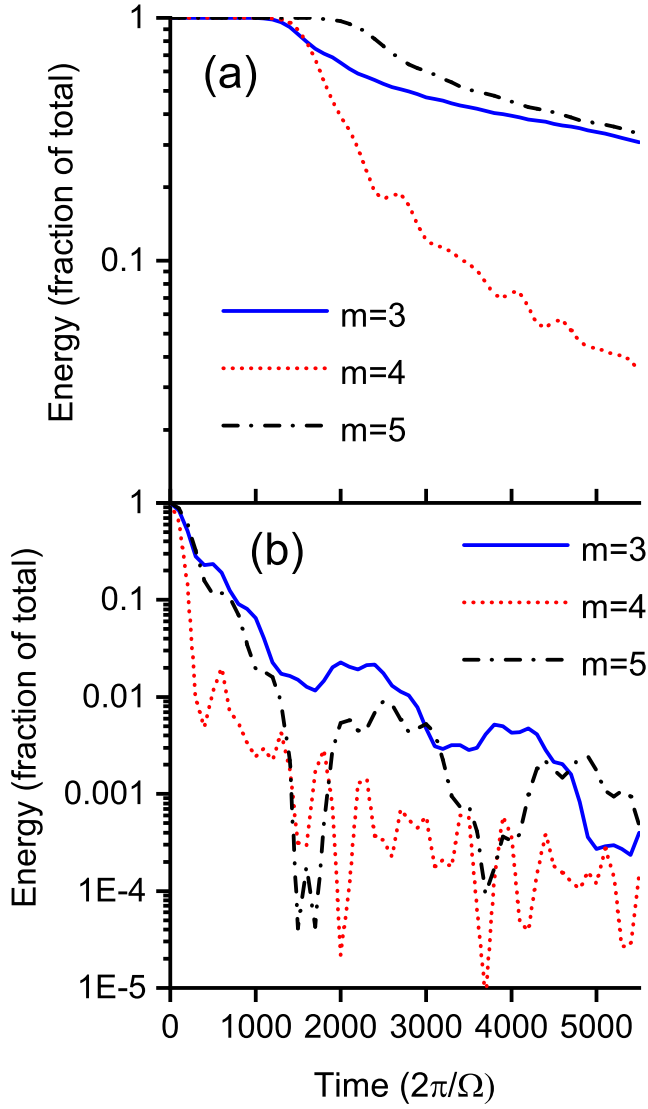


Figure 3.5: Energy versus time in (a) the cavities D_{center} and (b) the central cavity $(i, j) = (0, 0)$ for the $m = 3, 4, 5$ resonances. The time axis is given in reduced units of time, with Ω the resonance frequency of a single cavity for modes $m = 3, 4, 5$, which is slightly different for the three modes: $\tilde{\Omega}_3, \tilde{\Omega}_4, \tilde{\Omega}_5 = 0.5213, 0.5384, 0.5439(a/2\pi c)$.

the central cavity and very small in the neighbouring cavities, and the transfer of energy from the neighbouring cavities to the central cavity can be neglected. The transfer of energy from the central cavity to the neighbouring cavities is, on the other hand, significant. In the coupled-mode theory, the mode amplitude of the central cavity then decays exponentially over time. In Fig. 3.5(b) it appears that the time-dependence of the energy at early times can be fitted with a linear curve in the log-plot, giving a decay of $\sim e^{-0.0017t}$.

To study quantitatively the four beams in the Cartesian directions, we list the energy in several regions at $t = 5500(2\pi/\tilde{\Omega}_3)$. The fraction of energy in $D_{\text{Cartesian}}$ is 47.5% and $D_{\text{xz-diag}}$ is 13% (we do not show the time-dependence for these regions). We see that Cartesian hopping light in the time-domain for mode $m = 3$ propagates $3.7\times$ more energy in the x and z directions than in the diagonal directions, while the hopping coefficients are large, both in the diagonal directions as well as the x and z directions (see Table 2.1). We observe that the predominant propagation directions are not readily inferred from the coupling coefficients. We also consider the dispersion bandwidth that was defined in Eq. (2.1) in Chapter 2 as the difference between the maximum and minimum frequencies in the band m of the infinite $M_x M_y M_z = 3 \times 3 \times 3$ cavity superlattice. The energy also propagates in different directions from what would be naively expected from the dispersion bandwidth for $m = 3$, which is large in the diagonal directions with a directionality of $D = 15$, see Chapter 2. These phenomena reflect the interference between multiple hopping paths in 2D [22].

We study next how the speed of propagation in the Cartesian directions compares with a CROW. In the x -direction at $t = 5500(2\pi/\tilde{\Omega}_3)$, the energy has travelled on average $L = 17.3$ unit cells, according to the formula

$$L = \frac{\sum_{i=0,\dots,50} i |a_{(ic_s \hat{x}, \mathbf{0})}|^2}{\sum_{i=0,\dots,50} |a_{(ic_s \hat{x}, \mathbf{0})}|^2},$$

that is, the arithmetic mean of the distance travelled by the energy from the origin along a line on the x -axis. We check now whether this makes sense according to a CROW-like argument. In Yariv et al. [1] the following expression is derived for the group velocity in a 1D coupled-resonator optical waveguide:

$$v_g(k) = -\tilde{\Omega}_3 c_s^x \kappa \sin(k c_s^x),$$

with k the wave vector and κ the coupling coefficient. The group velocity in units of the lattice parameter per oscillation period of the single cavity is

$$\frac{v_g}{(c_s^x/(2\pi/\tilde{\Omega}_3))} = -2\pi\kappa \sin(k c_s^x).$$

The maximum of the modulus in the Brillouin zone equals

$$\frac{|v_g|}{(c_s^x/(2\pi/\tilde{\Omega}_3))} = 2\pi|\kappa|.$$

From the coupling coefficients in Table 2.1 we find for the $m = 3$ resonance band

that the coupling parameter with the largest modulus is $\kappa_x = 5.2 \cdot 10^{-4}$. Over $t = 5500(2\pi/\tilde{\Omega}_3)$ oscillations we expect the energy to cover a distance of

$$L = 5500 \left| \frac{v_g \left(\frac{2\pi}{\tilde{\Omega}_3} \right)}{c_s^x} \right| = 5500 \cdot 2\pi \cdot 5.2 \cdot 10^{-4} \approx 18.0 \text{ unit cells.}$$

This is in remarkably good agreement with the observed 17.3 unit cells, while the steady-state physics of propagation is very different in 3D from 1D, see Chapter 2.

We next assess whether the various wavefronts that we have naively identified in the preceding paragraphs really have a constant phase. In Fig. 3.6 we show the real part of the field at $t = 0, 250, 2000, 5500(2\pi/\tilde{\Omega}_3)$. At $t = 250(2\pi/\tilde{\Omega}_3)$ (Fig. 3.6(b)), we see phase fronts that, in comparison to a radially-symmetric wave, are sharply distorted along the Cartesian $\pm x, \pm z$ directions, so that the phase fronts look like stars. The observed phase distribution is consistent with waves travelling predominantly in the diagonal directions, but not with a cylindrical wave. We remark that the energy distribution did appear radially-symmetric. At $t = 2000(2\pi/\tilde{\Omega}_3)$ (Fig. 3.6(c)), we see that in the region D_{center} there is a complicated phase pattern of multiple resonating cavities, but there are groups of neighbouring cavities that are resonating at the same phase. In this region, we cannot identify a travelling wave with a flat wavefront. In the diagonal $(\pm x, \pm z)$ directions we count five nearly-flat wavefronts running in the diagonal directions. For example at the cavity $(i, j) = (25, 25)$ the phase front is normal to $\frac{1}{\sqrt{2}}(1, 1)$. The predominant wavelength is two cavities, i.e., the wavelength is

$$\lambda = 2\sqrt{c_s^{x2} + c_s^{z2}} = 2\sqrt{2}c_s^x = 6\sqrt{2}c,$$

where c is the lattice parameter of the underlying inverse woodpile photonic crystal, and the predominant wave vector is

$$\mathbf{k} = \left(\frac{\pi}{2c_s^x}, 0, \frac{\pi}{2c_s^z} \right),$$

which is in the direction of the U -high-symmetry point in the Brillouin zone of the periodic 3D superlattice, see Chapter 2. We found there that the U -point is energetically favorable, which results in a large dispersion bandwidth in the diagonal directions, with a directionality of $D = 15$, defined in Eq. (2.2) in Section 2.3.2. At $t = 5500(2\pi/\tilde{\Omega}_3)$ (Fig. 3.6(c)) we see that in the region D_{center} there are groups of cavities resonating in-phase, in a more-or-less radially-symmetric pattern. We observe nearly-flat wavefronts running in the diagonal $(\pm x, \pm z)$ directions. The predominant wave vector also is $\mathbf{k} = (\frac{\pi}{2c_s^x}, 0, \frac{\pi}{2c_s^z})$ at the exemplary cavity. In the vicinity of the x -axis in Fig. 3.6, we see an alternating pattern in j (corresponding to z) of out-of-phase resonating cavities. The “beams” in the Cartesian directions are therefore not in the form of a traveling wave.

At $t = 5500(2\pi/\tilde{\Omega}_3)$, for individual j , we see wave-like profiles in the x -direction, as shown for $j = 0$ in the x -direction in Fig. 3.7(a). In the diagonal direction in Fig. 3.7(b) we see that the amplitude is small at a distance of 30

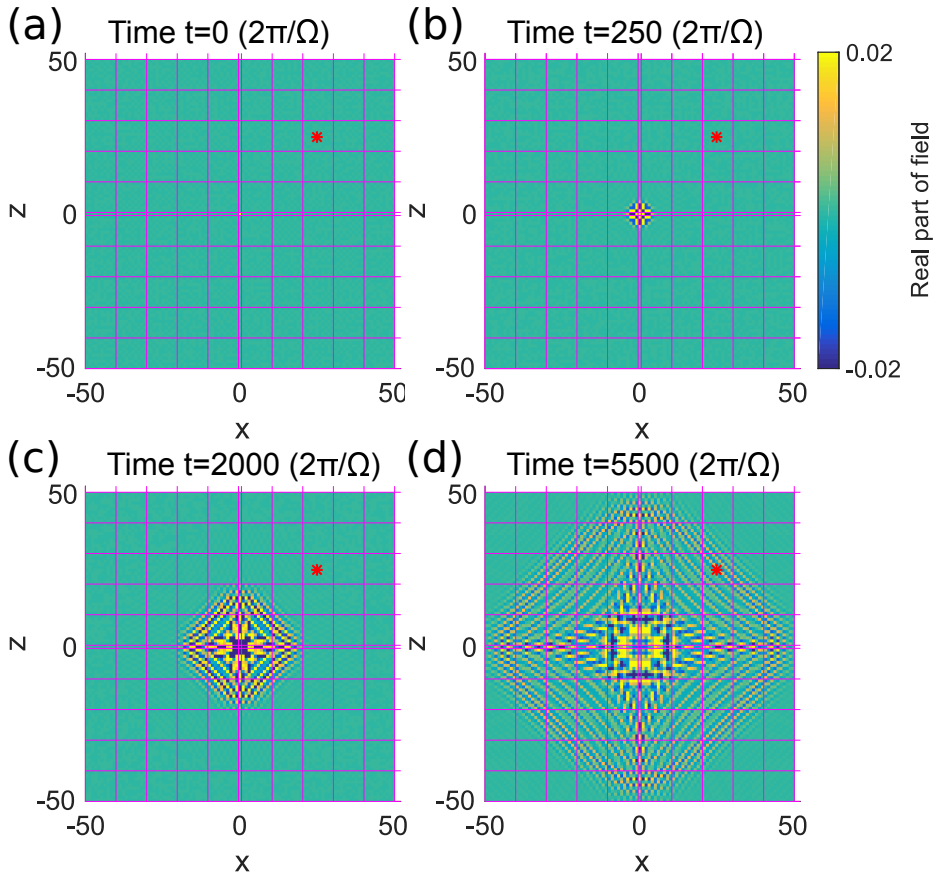


Figure 3.6: Real part of the field for the light hopping in the $m = 3$ coupled-cavity band for times (a) $t = 0(2\pi/\Omega_3)$, (b) $t = 250(2\pi/\Omega_3)$, (c) $t = 2000(2\pi/\Omega_3)$ and (d) $t = 5500(2\pi/\Omega_3)$. The field has been normalized so that the integrated energy equals one. The red star symbol indicates an exemplary cavity at $(i, j) = (25, 25)$.

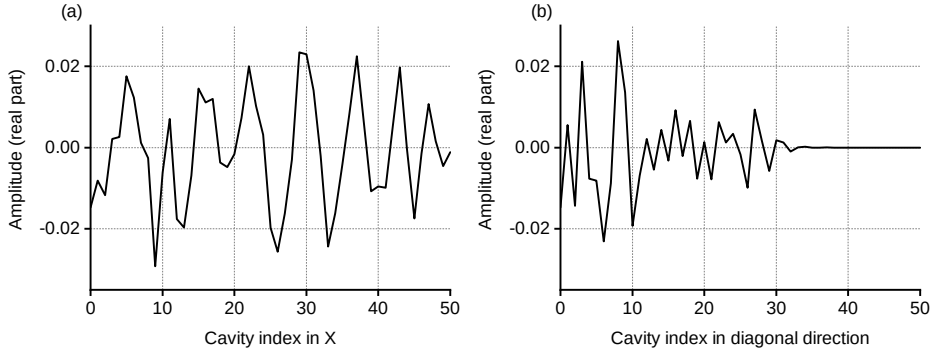


Figure 3.7: Amplitude versus the cavity index at $t = 5500(2\pi/\tilde{\Omega}_3)$ in the (a) x -direction along the cavities $(i, 0)$ and (b) diagonal direction. In (b), the index i denotes the cavity (i, i) .

cavities or further away from the central cavity.

3.3.2 $m = 4$ resonance

The $m = 4$ resonance has nonzero coupling coefficients in the x and z directions only, and the directionality $D = 4$ of the dispersion bandwidth is much lower than for the $m = 3$ resonance, which has $D = 15$. We therefore expect that the dynamics is markedly different as well.

In Fig. 3.8 we show the energy distribution at times $t = 0, 250, 2000, 5500(2\pi/\tilde{\Omega}_4)$. At the initial time $t = 0(2\pi/\tilde{\Omega}_4)$ only the central cavity is excited. At $t = 250(2\pi/\tilde{\Omega}_4)$ we see that the energy is within the central 7×7 cavities, with high energy densities. The energy distribution appears to be roughly radially-symmetric. At $t = 2000(2\pi/\tilde{\Omega}_4)$ the energy has propagated to a nearly square region of about 30×30 cavities wide. There are areas with high intensities at the corners of the rectangle, and along the entire front of the rectangle. Inside the rectangle, there are a number of cavities that are not excited. In particular, there is low energy density within the central cavity. In fact, there is little energy within a sequence of cavities in the x and z directions. At $t = 5500(2\pi/\tilde{\Omega}_4)$ the energy distribution is still nearly square, with bright field intensities at the corners as well as an additional series of peaks along the edges of the rectangle. Inside the square, there is a periodic pattern of peaks and troughs that is reminiscent of Fig. 3.3, with low intensities. The energy distribution is similar to the transverse mode pattern for a Hermite-gaussian mode of high-order [30]. There is a small amount of energy left in the central cavity.

It appears naively that little energy remains within the central region D_{center} for large times. In Fig. 3.5 we plot the energy within D_{center} versus time and within the central cavity versus time. For D_{center} (Fig. 3.5(a)), the energy decreases quickly from 100% at $t = 0$ to 39.3% at $t = 2000(2\pi/\tilde{\Omega}_4)$ and 3.5% at

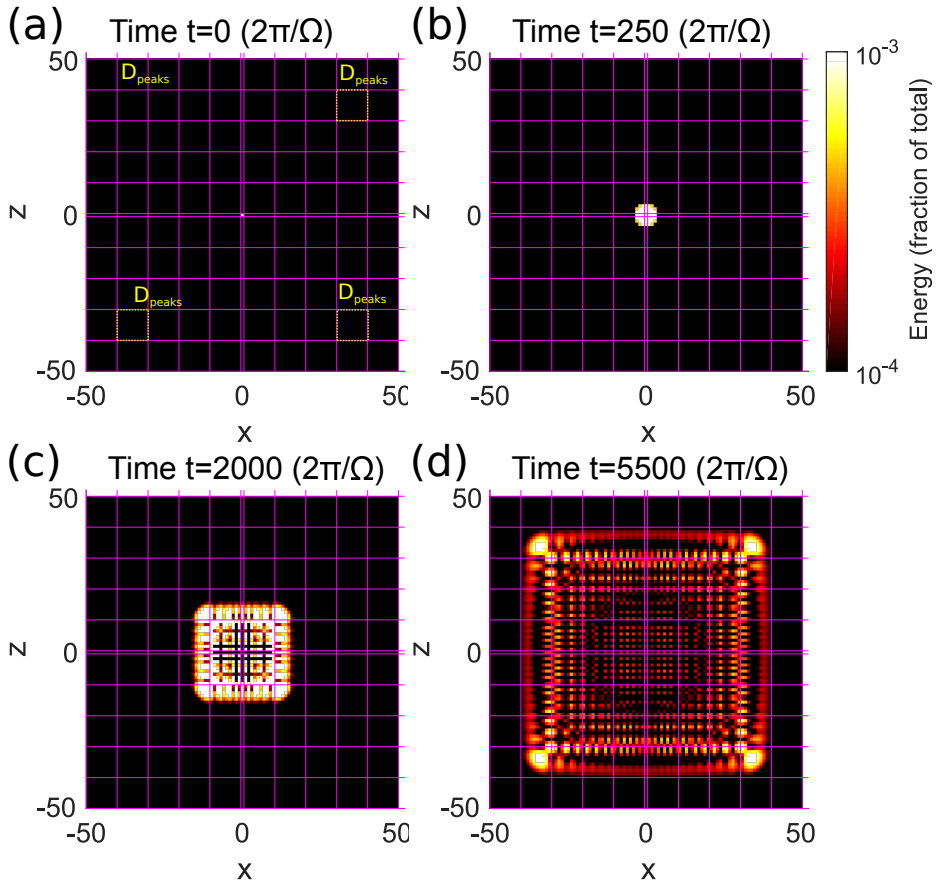


Figure 3.8: Energy distribution for light hopping in the $m = 4$ coupled-cavity band at times (a) $t = 0(2\pi/\tilde{\Omega}_4)$, (b) $t = 250(2\pi/\tilde{\Omega}_4)$, (c) $t = 2000(2\pi/\tilde{\Omega}_4)$ and (d) $t = 5500(2\pi/\tilde{\Omega}_4)$.

$t = 5500(2\pi/\tilde{\Omega}_4)$. In the limit $t \rightarrow \infty$ we expect about 4.3% of the energy to be within D_{center} , which is only slightly more than the observed 3.5% so apparently we are close to steady state. Like the $m = 3$ resonance, the rate of decay decreases over time exponentially as $e^{-\gamma t}$. It is conceivable that there is a transition between two regimes, one in the time-range from $t = 1500(2\pi/\tilde{\Omega}_4)$ to $t = 2500(2\pi/\tilde{\Omega}_4)$ with a large and constant rate $\gamma = 0.0016$, and another from $t = 2500(2\pi/\tilde{\Omega}_4)$ to $5500(2\pi/\tilde{\Omega}_4)$ with a rate that is about $4\times$ smaller, $\gamma = 0.0004$, with some variations. The decay on a logarithmic scale in the first regime is almost as fast as the decay of the single central cavity for $m = 3$, which is $\gamma = 0.0017$. For the central cavity, the energy decreases quickly from 100% at $t = 0(2\pi/\tilde{\Omega}_4)$ to 3.8% at $t = 250(2\pi/\tilde{\Omega}_4)$. After that, in the time-range from $t = 250(2\pi/\tilde{\Omega}_4)$ to $t = 5500(2\pi/\tilde{\Omega}_4)$ there are large variations in the energy, with an overall decrease. At $t = 2000(2\pi/\tilde{\Omega}_4)$ the energy is 0.002% and at $t = 5500(2\pi/\tilde{\Omega}_4)$ the energy is 0.01%. The increase in energy at $t = 5500(2\pi/\tilde{\Omega}_4)$ reflects energy incoupling from adjacent cavities. In the limit $t \rightarrow \infty$ we expect the energy to be about equally distributed over all cavities, about 0.01% which is the same as the observed energy conforming again the tentative conclusion that $t = 5500(2\pi/\tilde{\Omega}_4)$ is close to steady-state. We see that the rate of decrease on the log-scale decreases over time. It is conceivable that there are two regimes, one in the time-range from $t = 0$ to $t = 250(2\pi/\tilde{\Omega}_4)$ with a large rate of decrease $\gamma = 0.01$, and another from $t = 250(2\pi/\tilde{\Omega}_4)$ till $t = 5500(2\pi/\tilde{\Omega}_4)$ with a small rate of decrease $\gamma = 0.0004$ and large variations. The initial decay is about $5.9\times$ higher than for $m = 3$. It makes sense that initially the energy decreases exponentially, since almost all the energy is in the central cavity. When there is a significant fraction of energy in the adjacent cavities, it starts to leak back in significant amounts to the central cavity, and the exponential decrease of the central cavity slows down.

It appears that there are high intensities at the corners in Fig. 3.8 at $t = 5500(2\pi/\tilde{\Omega}_4)$. Nevertheless, in Fig. 3.8 a wide range of intensity values corresponds to the upper edge of the color scale. We therefore give the energy in several regions. While the energy in D_{peaks} in Fig. 3.8 appears very bright, only 13.4% of the total energy is in this region. In the Cartesian directions $D_{\text{Cartesian}}$ the total energy is 30.5%. In the diagonal directions $D_{\text{xz-diag}}$ the total energy is 66%. For the $m = 4$ resonance, about $66\%/30.5\% \approx 2.2\times$ as much energy travels in the diagonal directions than in the Cartesian directions. This is consistent with the smaller directionality $D = 4$ of the dispersion bandwidth for the $m = 4$ band. Similar to the $m = 3$ band, the significant energy transport in the diagonal directions is not obvious from the coupling parameters, which are about $100\times$ larger in the x and z directions than in the diagonal directions and therefore strongly directional.

We verify that the highest intensities indeed occur at the corners. In Fig. 3.9(b), we show the energy versus cavity index for the diagonal direction at $t = 5500(2\pi/\tilde{\Omega}_4)$. We see that the peak energy density occurs for $i = 34$. For comparison, we also plot the energy versus the x -direction in Fig. 3.9(a). The energy appears equally distributed over x , with peaks and valleys.

To investigate the phase patterns we show the real part of the field in Fig. 3.10

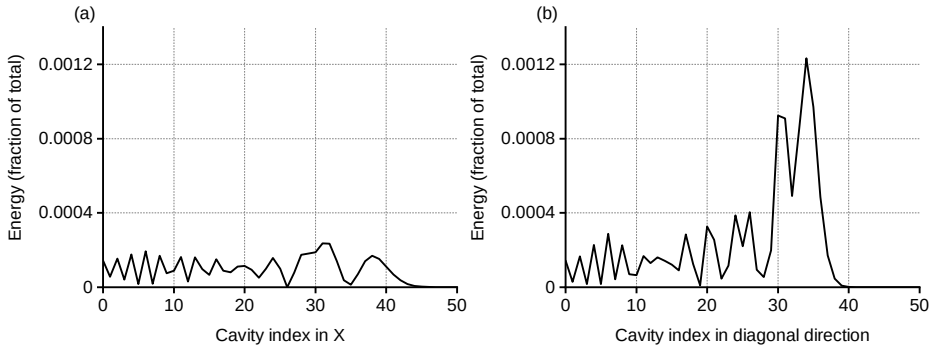


Figure 3.9: Energy versus the cavity index in the (a) x -direction and (b) diagonal direction at $t = 5500(2\pi/\tilde{\Omega}_4)$. In (b), the index i denotes the cavity (i, i) .

at times $t = 0(2\pi/\tilde{\Omega}_4)$, $t = 250(2\pi/\tilde{\Omega}_4)$, $t = 2000(2\pi/\tilde{\Omega}_4)$ and $t = 5500(2\pi/\tilde{\Omega}_4)$. At $t = 250(2\pi/\tilde{\Omega}_4)$ we see a wavefront that is nearly flat in the diagonal directions, with corners on the x and z axes. At the central cavity another wavefront appears to be forming. The predominant wave vector appears to be $\mathbf{k} = (\frac{\pi}{2c_s^x}, 0, \frac{\pi}{2c_s^z})$, which we determine by visual inspection. At $t = 2000(2\pi/\tilde{\Omega}_4)$, the field has propagated outward. At the outer edge of the field in the diagonal directions, for instance at $(i, j) = (12, 12)$, we see a series of wavefronts with $\mathbf{k} = (\frac{\pi}{2c_s^x}, 0, \frac{\pi}{2c_s^z})$. In between these wavefronts, close to the x and z axes, for instance at $(i, j) = (14, 0)$, we see a checkerboard pattern of out-of-phase resonating cavities, albeit with a modulation in the intensity along the axes. In the region D_{center} we see a cylindrical pulse. At $t = 5500(2\pi/\tilde{\Omega}_5)$, the field has propagated even further. In the regions D_{peaks} we see a series of wavefronts with $\mathbf{k} = U$. At the propagation front, in between D_{peaks} , for instance at $(i, j) = (40, 0)$, we see a checkerboard pattern of out-of-phase resonating cavities, albeit with a modulation in the intensity along the axes. In the central $(-30 \leq i \leq 30, -30 \leq j \leq 30)$ cavities, we see four or five wavefronts of a cylindrical wave.

3.3.3 $m = 5$ resonance

We briefly describe the energy distribution for the $m = 5$ band. The coupling parameters are similar to $m = 3$, except that the diagonal couplings are smaller, see Table 2.1. In view of the coupling parameters we expect similar behavior as for $m = 3$. In Fig. 3.8 we show the energy distribution at times $t = 0, 250, 2000, 9000(2\pi/\tilde{\Omega}_5)$, where the last time is different from what we considered before, since, as we will see, the propagation is slower than for the other bands. At initial time $t = 0(2\pi/\tilde{\Omega}_5)$ only the central cavity is excited. At $t = 250(2\pi/\tilde{\Omega}_5)$ we see an approximately radially-symmetric distribution of energy in the central 7×7 cavities. At $t = 2000(2\pi/\tilde{\Omega}_5)$ the energy has propagated outward to the central 21×21 cavities. The front of the propagation is remarkably radially-symmetric. Within the distribution, a quadrupolar pattern

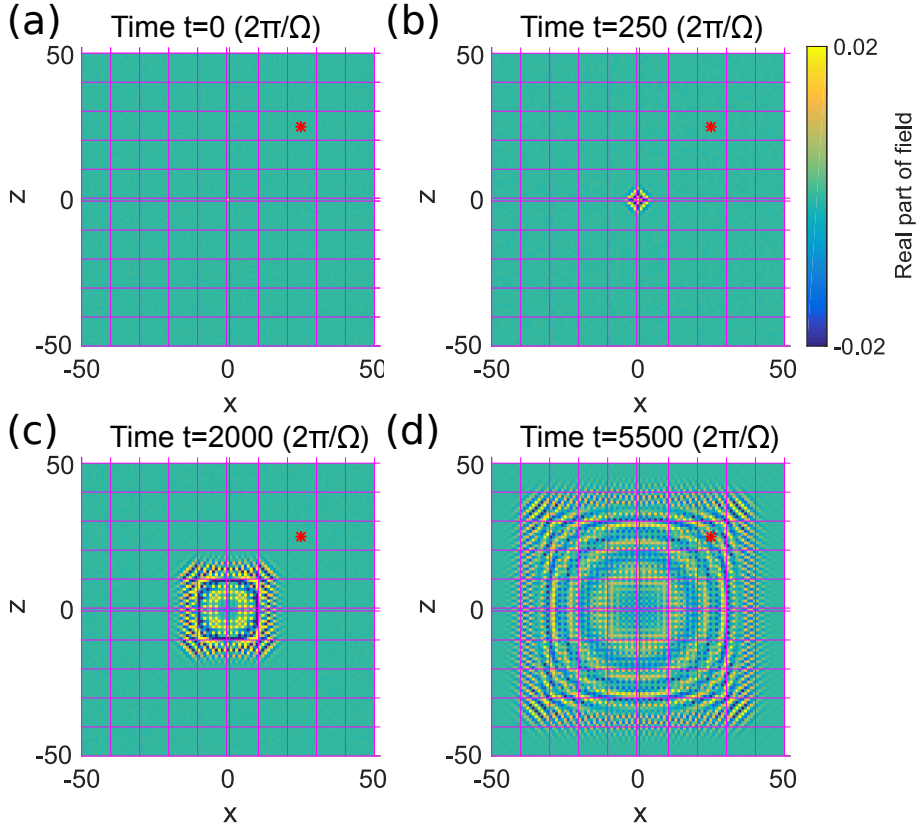


Figure 3.10: Real part of the field for the light hopping in the $m = 4$ coupled-cavity band at times (a) $t = 0(2\pi/\tilde{\Omega}_4)$, (b) $t = 250(2\pi/\tilde{\Omega}_4)$, (c) $t = 2000(2\pi/\tilde{\Omega}_4)$ and (d) $t = 5500(2\pi/\tilde{\Omega}_4)$.

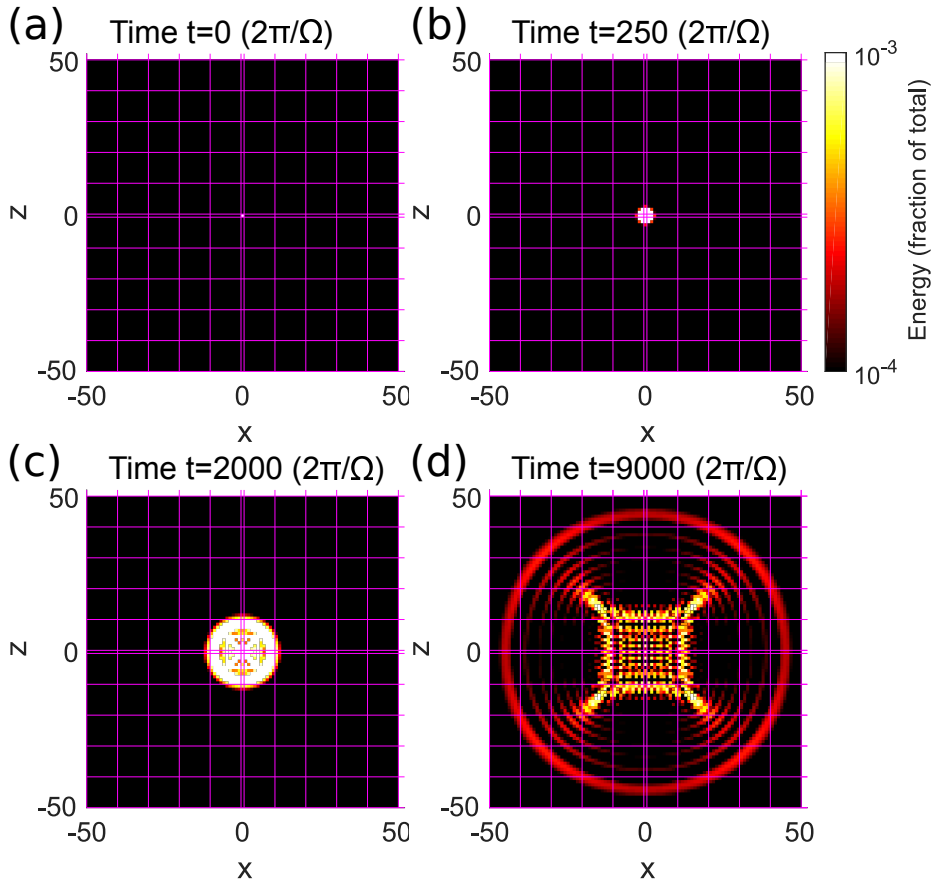


Figure 3.11: Energy distribution for light hopping in the $m = 5$ coupled-cavity band at times (a) $t = 0(2\pi/\Omega_5)$, (b) $t = 250(2\pi/\Omega_5)$, (c) $t = 2000(2\pi/\Omega_5)$ and (d) $t = 9000(2\pi/\Omega_5)$.

appears to be forming. At $t = 5500(2\pi/\tilde{\Omega}_5)$ (not shown) the energy has propagated less far than for the $m = 3, 4$ resonances, and occupies only about the central 61×61 cavities. This is consistent with the smaller dispersion bandwidth for $m = 5$ than for $m = 3, 4$, see Fig. 2.3 and Fig. 2.4, and must be the result of the smaller diagonal couplings. At $t = 9000(2\pi/\tilde{\Omega}_5)$, the outer edge of propagation appears like a cylindrical wave, and several more wavefronts are visible. In the diagonal directions, for example in the vicinity of $(i, j) = (20, 20)$, we see a high-intensity pulses. We do not show $t = 9000(2\pi/\tilde{\Omega}_i)$ for the other resonances $i = 3, 4$ since they have reflected from the superlattice edge by that time. Near the central 30×30 cavities, we see a pattern of peaks and valleys that is similar to the $m = 4$ resonance. Surprisingly, the smaller diagonal couplings lead to a completely different energy transport from the $m = 3$ resonance.

3.4 Discussion

A first question we address is how much the finite extent of the superlattice will affect the observed dynamics. The energy cannot propagate out of the superlattice, either from the sides or from the top or bottom, since we consider a superlattice that is surrounded by an infinite 3D photonic band gap crystal on all sides. At very long times (which we do not consider here), after the light has propagated to the side walls, it will be reflected back into the cavity superlattice. We expect only a very slight (machine precision) perturbation in the results if the cavities at the edge are periodically connected to cavities on the other side of the cavity superlattice.

For the $m = 3$ resonance, about $3.7\times$ as much energy travels in the Cartesian directions as in the diagonal directions. This observation is at variance with the dispersion bandwidth, which is large in the diagonal directions, with a directionality of $D = 15$. Since, for a 1D CROW, the group velocity v_g is proportional to the dispersion bandwidth [1],

$$v_g \simeq \Delta\omega,$$

we expect the superlattice Bloch modes to have large group velocities for $\mathbf{k}$ in the diagonal directions. Continuing the 1D CROW-like argument, the propagation distance Δz after time Δt for an optical pulse is proportional to the group velocity [8]

$$\Delta z / \Delta t \simeq \Delta\omega \simeq v_g,$$

and we would expect the pulse to propagate farthest in the diagonal directions, which is clearly not what we see. The issue with this argument is that in 3D the group velocity is the normal to the dispersion surface

$$\mathbf{v}_g = \nabla_{\mathbf{k}}\omega.$$

We expect that for most of the wave vectors, the group velocity points mostly in the Cartesian directions. The propagation in the Cartesian directions is also not obvious from the coupling parameters, which are large in the Cartesian directions as well as the diagonal directions.

For the $m = 4$ resonance, about $2.2\times$ as much energy travels in the diagonal directions as in the Cartesian directions. This is consistent with the smaller directionality $D = 4$ of the dispersion bandwidth for the $m = 4$ bandwidth as this suggests smaller disparities between the directions of $\mathbf{k}$ and $\mathbf{v}_g = \nabla_{\mathbf{k}}\omega$. The significant energy transport in the diagonal directions is not obvious from the coupling parameters, which are about $100\times$ larger in the x and z directions than in the diagonal directions and therefore strongly directional.

To explain the puzzling contrast between the hopping directions and the propagation directions, we note that the propagation in 3D superlattices can be seen as a summations over many interfering hopping paths [22]. For the $m = 3$ resonance there are likely many more contributing paths than for $m = 4$, since the photons can also jump along the diagonal directions. We speculate that the propagation has a stronger contribution from the interference between different paths. This would be consistent with the larger directionality of the bandwidth for $m = 3$ versus $m = 4$. For $m = 5$, the diagonal couplings are nonzero, but about $0.3\times$ the magnitude of the x and z couplings. The dispersion bandwidth is highly directional, with $D = 26$, and the energy transport is mostly in the diagonal directions. Due to the interference, the predominant propagation directions are not readily inferred from the coupling coefficients, as we have seen.

Some of our observations have similarities with earlier 1D waveguide lattices [11]. In waveguide lattices where a narrow input beam excites a single site, most of the output light is distributed in two distinct outer lobes, called *discrete diffraction* [11]. For the $m = 4$ resonance, we also see highest-energy peaks at the corners of the wavefront.

In the future the findings discussed in this chapter will be further investigated experimentally. The COPS group has fabricated $5 \times 5 \times 5$ superlattices in inverse woodpile crystals in silicon [31]. The superlattices are fabricated on the edge of a wafer, with the y -direction aligned with the edge. By etching away silicon on the sides of the superlattice, it would be possible to uncover a $5 \times 5(x, z)$ superlattice to air: $(-2 \leq i \leq 2, -2 \leq j \leq 2)$. One could excite any of the cavities by an input pulse, for example by wavefront shaping [32, 33]. By exciting a cavity with different distances to the two side facets of the cavity, for example $(1, 0)$, we should obtain the output signal at different times t_1 and t_2 . From the difference $\Delta t = |t_1 - t_2|$ we would expect to extract the speed of propagation of the modes

$$v = \Delta t / \Delta z = \Delta t / c_s,$$

which is different for the modes $m = 3, 4, 5$. As seen in Fig. 3.5, the decay to 2% of the original energy of the central cavity occurs after about 272 and 1272 oscillations respectively for the $m = 4, 3$ modes. In physical units this is 1.1ps and 5.5ps. The difference in these arrival times would be measurable with available technology.

3.5 Summary

We explore for the first time ever the time-dependent propagation of light in a superlattice of cavities in a 3D photonic band gap. For the $m = 3$ resonance of the inverse-woodpile cavity, we observe that the energy propagates mostly along the Cartesian $x - z$ directions, while the coupling coefficients are large along the diagonal directions as well, and the dispersion bandwidth is large only along the diagonal directions. This differs markedly from a 1D CROW, where all these quantities are proportional. For the $m = 4$ resonance, we see that the light propagates outward in a rectangular pattern, which is similar to a Hermite-gaussian mode of high-order, while the coupling coefficients are large only along the $x - z$ directions, and the dispersion bandwidth has no pronounced directionality. For $m = 5$ we see highly directional propagation in the diagonal directions. All observations, both the sensible and puzzling ones, can be rationalized by 3D hopping arguments. Propagation in 3D can be seen as a summation over many interfering hopping paths, and the predominant propagation directions are not readily inferred from the coupling coefficients.

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CHAPTER 4

Effects of disorder on the three-dimensional (3D) photonic band gap in inverse woodpile crystals

4.1 Introduction

Enormous progress has been made in the fabrication of high-quality three-dimensional (3D) photonic-band-gap crystals [1–14]. However, inevitable variations in the size and position of geometrical building blocks occur in any 3D crystal [15]. Light then scatters at the defects in the photonic crystal structure, which results in the extinction of a light beam into diffuse light [15]. Conversely, disorder leads to rich physics related to diffusion of light and Anderson localization of light [15–21].

Anderson localization is a peculiar state of light where the transport is completely halted [16–21]. For strongly scattering random samples, it is predicted to occur when the mean free path l is on the order of the wavelength of light λ [16–21]

$$2\pi l/\lambda \approx 1,$$

which is also known as the Ioffe-Regel criterion [20, 22]. The quest for Anderson localization of light continues to receive attention to date [21, 23, 24]. A little explored pathway to Anderson localization is to consider 3D photonic band gap materials [19, 25]. In photonic band gap materials, the Ioffe-Regel criterion is modified to $kl \approx 1/\sqrt{\rho_s}$, with ρ_s the modification of the photonic density of states (DOS) relative to free space [19, 25, 26]. At the edges of the band gap, the density of states is very low. Effectively, the lowering of the density of states corresponds to a reduction of the dimensionality of the phase space for light. Since a lower system dimension is known to be favorable for localization [20], the modified Ioffe-Regel criterion is predicted to be easily satisfied [19, 25, 26]. As a result, as the scattering disorder strength increases, the band gap is progressively filled with localized states, starting from the edges and proceeding inwards. This would be visible as a smoothening of the density of states at the edges of the band gap. Indeed, a numerical study by Conti and Fratalocchi of 3D inverse opal photonic crystals with strong disorder [27] shows the progressive closing of the band gap, non-exponential decay of transmission, and Anderson localization of light.

To obtain a full picture of localization in 3D photonic band gap crystals, it is necessary to know the density of states, which is effectively identified as the wave

vector k in the product kl [28]. In calculations with externally-incident light beams such as in Ref. [27], it is likely that we incompletely sample the DOS, and thus there is systematic error in the measure of kl . Therefore, we study in this Chapter the density of states of light in a 3D photonic band gap crystal with disorder, and we investigate the effects of progressive disorder on the band gap. Our results provide guidance to ongoing experiments, and contribute to the study of the DOS during the localization transition.

Previously, Woldering *et al.* [29] studied the effect of fabrication imperfections on the band gap of inverse woodpile crystals. The band gap is found to be robust to systematic deviations that relate to the radii, positions, and angular alignment of pores, but sensitive to the possible tapering of the pores. The results in the present Chapter complement and extend the results from Ref. [29] by considering random variations instead of systematic variations, and providing the density of states rather than the band structure at the high-symmetry points.

It appears that there is not *a priori* a clear relation between structural disorder and the DOS, and it is not obvious that a gap closes with increasing disorder [22]. For instance, in the electronic case, there is the well-known case of amorphous and crystalline silicon [30]. In amorphous silicon, there is still a band gap, albeit somewhat smaller than in c-Si. This remarkable fact is in some variance to the scattering argument above and notably related to the atomic level subtleties of Si [30]. Edagawa *et al.* [31] found that “photonic amorphous diamond” structures exhibit a 3D photonic band gap of 18% relative bandwidth in the DOS, which is only slightly smaller than the 26% for photonic crystalline diamond. Liew *et al.* [32] studied the DOS in 3D photonic amorphous structures, and found that interconnected topologies, uniform scatterers, reduced fluctuations in the refractive index, high index contrast, and optimal volume fraction of high index material contribute to photonic band gap formation. In two-dimensional (2D) crystals of dielectric cylinders, the band gap for *s*-polarized light closes as the disorder strength is increased [33], as is also seen in microwave transmission experiments [34]. These studies calculate the DOS by taking the Fourier transform of the field at a final time for a random input field, and it is not obvious that the resulting spectral intensities equal the exact DOS. In fact, in these studies the calculated DOS is nowhere strictly zero in the frequency range identified as the band gap. Therefore, we perform a study of the DOS in disordered photonic crystals with a method that unambiguously samples all possible modes in the DOS.

4.2 Structures

We investigate 3D photonic band gap crystals that have the inverse woodpile structure. This structure has nearly the same symmetry as a diamond crystal of carbon atoms [35], as illustrated in a youtube animation [36], yet the lattice parameter is a thousandfold magnified. The inverse woodpile crystal structure consists of two perpendicular 2D arrays of nanopores with radius r_0 in a high-index medium such as silicon [35], as illustrated in Figure 2.1(a). Each 2D pore

array corresponds to a diamond $\{110\}$ crystal face. In view of the arrangement of the nanopores, it appears to be convenient to employ a tetragonal unit cell [29, 37] instead of the conventional cubic unit cell [38]. The tetragonal unit cell has lattice parameters c^{iw} (in the x and z directions), and a^{iw} (in the y direction) in a ratio $a^{iw}/c^{iw} = \sqrt{2}$ to ensure a cubic crystal structure. More details, notably on the Brillouin zone, are presented in Appendix 2.A.

Inverse woodpile photonic crystals possess a broad 3D photonic band gap, whose width strongly depends on the radius r of the pores [29, 35, 37]. For a normalized pore radius $r_0/a^{iw} = 0.24$ - as considered here in the limit of zero disorder - a maximum relative bandwidth $\Delta\omega_{pbg}/\omega_c = 25.3\%$ occurs for $\epsilon = 12.1$, as is typical of silicon [29, 37], with $\Delta\omega_{pbg}$ the frequency width of the band gap, and ω_c the band gap's center frequency.

It is known that in photonic crystals made by top-down methods the dominant form of disorder is the size variation of the building blocks. Moreover, Koenderink *et al.* [15] showed that size variations have twice greater effect than position variations. Therefore, we study here only size variations. For each pore separately, we introduce a perturbation of the pore radius given by

$$r = r_0(1 + \gamma\xi),$$

with γ the disorder strength, and ξ a realization from the uniform distribution on the interval $[-1 \dots 1]$. Fig. 4.1(a)(c) show (x, y) and (x, z) views of the supercell with disorder $\gamma = 0.25$. While the underlying structure of pore axes is still periodic, the silicon walls between the pores are randomly distributed and thick and thin. At some points the walls are so thin that they might collapse. We therefore take $\gamma = 0 \dots 0.25$ as the range of physical disorder strengths [39]. In Fig. 4.1(b)(d) we show the permittivity distribution in the (x, y) plane for the 3D structure for several disorder strengths. For $\gamma = 0$ the dielectric is clearly periodic and connected. For a large disorder $\gamma = 0.25$ we clearly see the parental inverse woodpile structure. At some positions (*e.g.*, (0.25c, 1.8a)) the walls are very thin and in view of the permittivity smoothing in the computations it is an open question whether the structure retains integrity [40]. The volume fraction of silicon has a non-monotonic dependence on the disorder strength: for $\gamma = 0$ the volume fraction is 21.3%, it increases to 21.5% at $\gamma = 0.05$, and then decreases to 20.4% at $\gamma = 0.25$.

We employ supercells with wavevector-shifted periodic boundary conditions [41] where the disordered crystal has lattice parameters (c_d^x, a_d, c_d^z) in the (x, y, z) directions that are integer multiples of the underlying inverse woodpile lattice parameters: $c_d^x = M_x c^{iw}$, $a_d = M_y a^{iw}$, $c_d^z = M_z c^{iw}$. Here, we employ a $M_x M_y M_z = 3 \times 3 \times 3$ supercell such that the disorder is repeated every three unit cells with lattice parameters $c_d^x = 3c^{iw}$, $a_d = 3a^{iw}$, $c_d^z = 3c^{iw}$. Thus, the disordered crystal is also cubic, similar to the underlying inverse woodpile structure. For each disorder strength $N_r = 10$ realizations are calculated. The ensemble average of the DOS converges as the number of realizations is increased, and the value of $N_r = 10$ is comparable to the values in literature [27, 32, 33]. In the limit of zero disorder, the band gap occurs between the 4th and 5th band

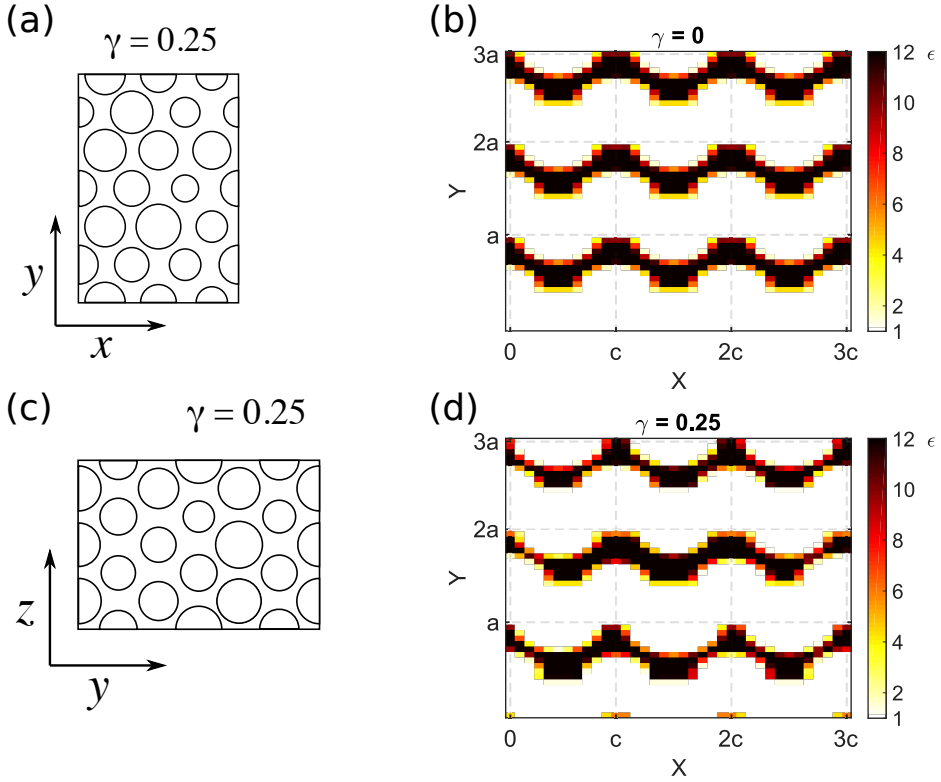


Figure 4.1: Design pattern in (a) the (x, y) plane and (c) the (y, z) plane for $\gamma = 0.25$ as well as the permittivity distribution in the (x, y) plane for (b) $\gamma = 0$ and (d) $\gamma = 0.25$ as taken in the planewave computational code MPB.

between frequencies $\tilde{\omega} \equiv \omega a / 2\pi c = 0.50 \dots 0.64$. Since in the supercell each band is folded $M_x \times M_y \times M_z = 3 \times 3 \times 3 = 27$ times, we therefore calculate the first 135 bands - equivalent to the first five bands in the inverse woodpile crystal - to investigate the effects of the disorder on the band gap.

We have calculated the band structure of the disordered photonic crystals using the plane-wave expansion method [38, 40, 41]. We employ the recent version 1.5 of the MIT photonic bands (MPB) code [40]. We perform calculations with grid resolutions of $12 \times 17 \times 12$ per unit cell of the underlying crystal. In Chapter 2.B we performed a grid convergence study for the challenging case of a defect consisting of two touching single defect pores, and we found the order of convergence $p \simeq 2$ in close agreement with the convergence order $p = 2$ for the plane-wave expansion method [40]. All calculations were performed on the “Serendipity” cluster in the MACS group at the MESA⁺ Institute [42], and the calculations took several days altogether.

We represent the first Brillouin zone by a grid of $n_k \times n_k \times n_k$ points, where we choose $n_k = 7$, and we calculate the modes at the $\mathbf{k}$ vectors in the middle of the rectangles. The frequency resolution of the density of states is $\Delta\omega = |\nabla_{\mathbf{k}}\omega|\Delta k = c\Delta k$, where c is the speed of light (see Ref. [43]) and we assume a plane-wave dispersion relation. This estimate of the frequency resolution is pessimistic, since for photonic crystals $|\nabla_{\mathbf{k}}\omega|$ is typically much smaller than c . In our calculations, $c = 1$, $\Delta k = 0.14$ and we have a reduced frequency resolution of better than

$$\Delta\tilde{\omega} = 0.14, \quad (4.1)$$

which is sufficient to resolve the unperturbed band gap width $\Delta\tilde{\omega}_{bg} = 0.139$ as well as narrower gaps, as we will see below.

The density of states $N(\tilde{\omega})$ at reduced frequency $\tilde{\omega}$ is defined as [38]

$$N(\tilde{\omega}) = \lim_{\Delta\tilde{\omega} \rightarrow 0} \frac{Q(\tilde{\omega})}{\Delta\tilde{\omega}}, \quad (4.2)$$

where $Q(\tilde{\omega})$ is the number of states with frequencies $\tilde{\omega}_n(\mathbf{k})$ in the frequency interval $[\tilde{\omega}, \tilde{\omega} + \Delta\tilde{\omega}]$ divided by the volume of a superlattice with N_s superlattice unit cells in each direction and periodic boundary conditions, as $N_s \rightarrow \infty$. The number of states is equal to

$$Q(\tilde{\omega}) = \lim_{N_s \rightarrow \infty} \frac{1}{N_s^3 c_s^2 a_s} \sum_{n,\mathbf{k}} \begin{cases} 1, & \tilde{\omega} \leq \tilde{\omega}_n(\mathbf{k}) \leq \tilde{\omega} + \Delta\tilde{\omega} \\ 0, & \text{otherwise} \end{cases},$$

where the summation is over the allowed $\mathbf{k}$ vectors in the reciprocal space of a single superlattice unit cell, consistent with the periodic boundary conditions after N_s superlattice unit cells in each direction. The total number of allowed $\mathbf{k}$ vectors is N_s^3 . We define the indicator function

$$\mathbb{I}(\tilde{\omega}_n(\mathbf{k})) = \begin{cases} 1, & \tilde{\omega} \leq \tilde{\omega}_n(\mathbf{k}) \leq \tilde{\omega} + \Delta\tilde{\omega} \\ 0, & \text{otherwise} \end{cases}.$$

We replace the sum with an integral

$$\begin{aligned}
 Q(\tilde{\omega}) &= \lim_{N_s \rightarrow \infty} \frac{1}{N_s^3 c_s^2 a_s} \sum_{n, \mathbf{k}} \mathbb{I}(\tilde{\omega}_n(\mathbf{k})) \\
 &= \lim_{N_s \rightarrow \infty} \frac{1}{N_s^3 c_s^2 a_s} \int_0^{2\pi/c_s} \int_0^{2\pi/a_s} \int_0^{2\pi/c_s} \frac{1}{\left(\frac{8\pi^3}{c_s^2 a_s N_s^3}\right)} \mathbb{I}(\tilde{\omega}_n(\mathbf{k})) dk_x dk_y dk_z \\
 &= \frac{1}{8\pi^3} \int_0^{2\pi/c_s} \int_0^{2\pi/a_s} \int_0^{2\pi/c_s} \mathbb{I}(\tilde{\omega}_n(\mathbf{k})) dk_x dk_y dk_z.
 \end{aligned}$$

We discretize the superlattice Brillouin zone with n_k grid cells in each direction, which gives a k -grid spacing $(\Delta k_x, \Delta k_y, \Delta k_z) = (\frac{2\pi}{c_s n_k}, \frac{2\pi}{a_s n_k}, \frac{2\pi}{c_s n_k})$. We then discretize the integral with the root-sampling method [44] to obtain,

$$\begin{aligned}
 Q(\tilde{\omega}) &= \frac{1}{8\pi^3} \int_0^{2\pi/c_s} \int_0^{2\pi/a_s} \int_0^{2\pi/c_s} \mathbb{I}(\tilde{\omega}_n(\mathbf{k})) dk_x dk_y dk_z \\
 &= \frac{1}{8\pi^3} \sum_{n, \mathbf{k}} \mathbb{I}(\tilde{\omega}_n(\mathbf{k})) \frac{8\pi^3}{c_s^2 a_s n_k^3} \\
 &= \frac{1}{n_k^3 c_s^2 a_s} \sum_{n, \mathbf{k}} \mathbb{I}(\tilde{\omega}_n(\mathbf{k})).
 \end{aligned}$$

If the frequency bins are small enough, we then find the DOS

$$N(\tilde{\omega}) \simeq \frac{Q(\tilde{\omega})}{\Delta \tilde{\omega}} = \frac{1}{c_s^2 a_s \Delta \tilde{\omega} n_k^3} \sum_{n, \mathbf{k}} \begin{cases} 1, & \tilde{\omega} \leq \tilde{\omega}_n(\mathbf{k}) \leq \tilde{\omega} + \Delta \tilde{\omega} \\ 0, & \text{otherwise} \end{cases}. \quad (4.3)$$

The density of states in Eq. (4.3) is reported in units of $(c_s^2 a_s \frac{2\pi c}{a})^{-1} = (\frac{m^3}{s})^{-1}$. To conform with the literature [43, 45], we from now on report the density of states in reduced units of $\frac{\omega_a^2}{\pi^2 c}$, with $\omega_a = \frac{2\pi c}{a}$, that we simplify to $\frac{\omega_a^2}{\pi^2 c} = \frac{4}{a^2 c}$. In this Chapter we will show density of states histograms computed with Eq. (4.3) with a step size $\Delta \tilde{\omega} = 0.02$ rather than the continuous density of states (4.2). The width of the frequency bins $\Delta \tilde{\omega} = 0.02$ is much finer than the frequency resolution $\Delta \tilde{\omega} = 0.14$ in Eq. (4.1). We expect the results to be reasonably accurate since the estimate in Eq. (4.1) pertains to a plane-wave dispersion relation in free space, whereas the bands in the photonic crystal have a much lower group velocity. Nevertheless, some of the variations in the results may be the result of binning noise.

4.3 Results

In Fig. 4.2 we show the density of states versus frequency for silicon inverse woodpile photonic crystals with increasing disorder for $\gamma = 0$, $\gamma = 0.08$ and $\gamma = 0.15$, averaged over the realizations. It is relevant to realize that the DOS

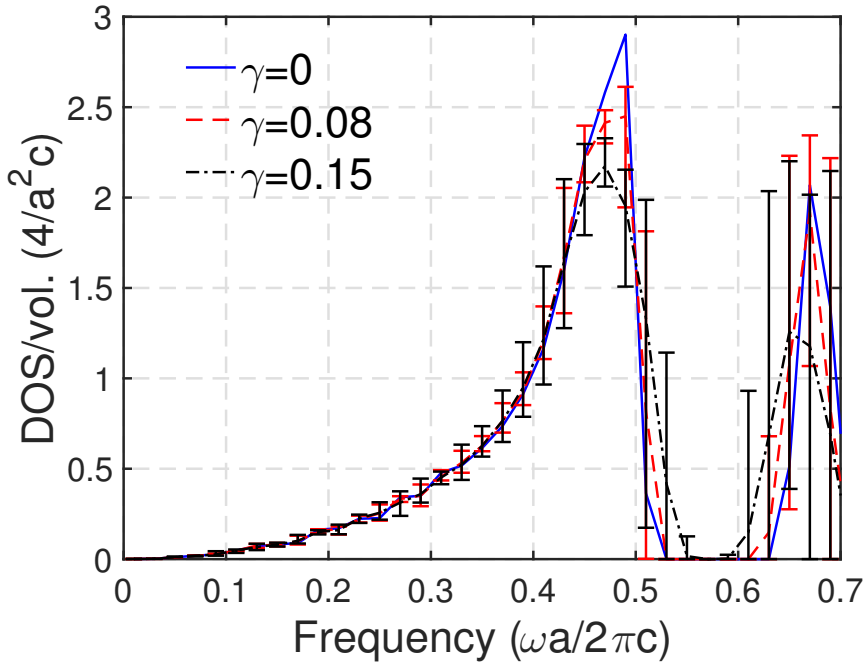


Figure 4.2: Density of states versus frequency for silicon inverse woodpile photonic crystals with increasing amounts of disorder $\gamma = 0$, $\gamma = 0.08$ and $\gamma = 0.15$. The width of the frequency bins is $\Delta\tilde{\omega} = 0.02$. The data are averaged over the realizations. For $\gamma = 0.08$ and $\gamma = 0.15$, we show the range of DOS values over the realizations as vertical bars.

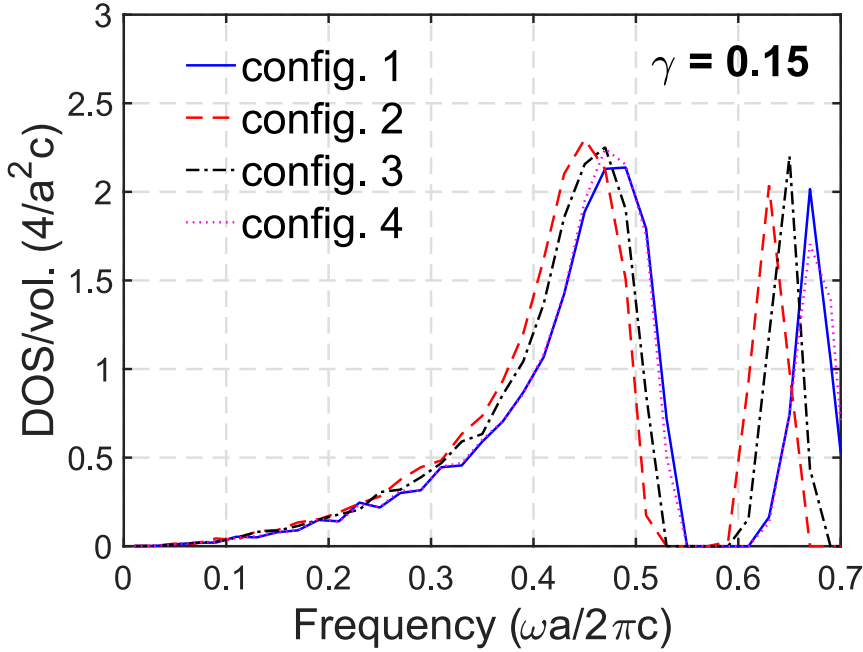


Figure 4.3: DOS for four different configurations for $\gamma = 0.15$.

at constant frequency varies markedly from realization to realization as shown in Fig. 4.3. This is mostly the result of frequency shifts of the DOS curves between each different realization, rather than radically different curve shapes. In other words, the DOS spectra between each different realization can readily be overlaid on one another. For the different realizations at $\gamma = 0.15$, the volume fractions are quite different: 20.0%, 23.5%, 22.1%, 20.2% for configurations 1, 2, 3, 4. These volume fractions correspond to lower band edges at $\tilde{\omega} = 0.51$, $\tilde{\omega} = 0.48$, $\tilde{\omega} = 0.49$, $\tilde{\omega} = 0.51$, which agrees well with the observed band edges in Fig. 4.3. It is clear in Fig. 4.3 that the maximum differences between different realizations are especially large in the spectral ranges where the slope is steep. For $\gamma = 0.15$, the maximum variation at constant frequency $\tilde{\omega} \geq 0.51$ is at least as large as the DOS itself, as shown by the extremes in Fig. 4.2. For $\gamma = 0.08$ the maximum variation is unexpectedly slightly larger than for $\gamma = 0.15$ at frequencies $\tilde{\omega} = 0.49$ and $\tilde{\omega} = 0.65$ in the vicinity of the band gap. Similar variations also occur for larger γ , but we will not plot the variations to make the figures more easily readable.

In Fig. 4.2 we see that all average DOS spectra reveal a clear band gap. We observe that the band gap narrows from two sides as γ increases from 0 to 0.15. This is naively reasonable, since it is also seen in the literature for dielectric cylinders with 2D *s*-polarized waves [33]. For the different configurations in Fig. 4.3 at $\gamma = 0.15$ all four configurations have a smooth DOS tail at the upper band

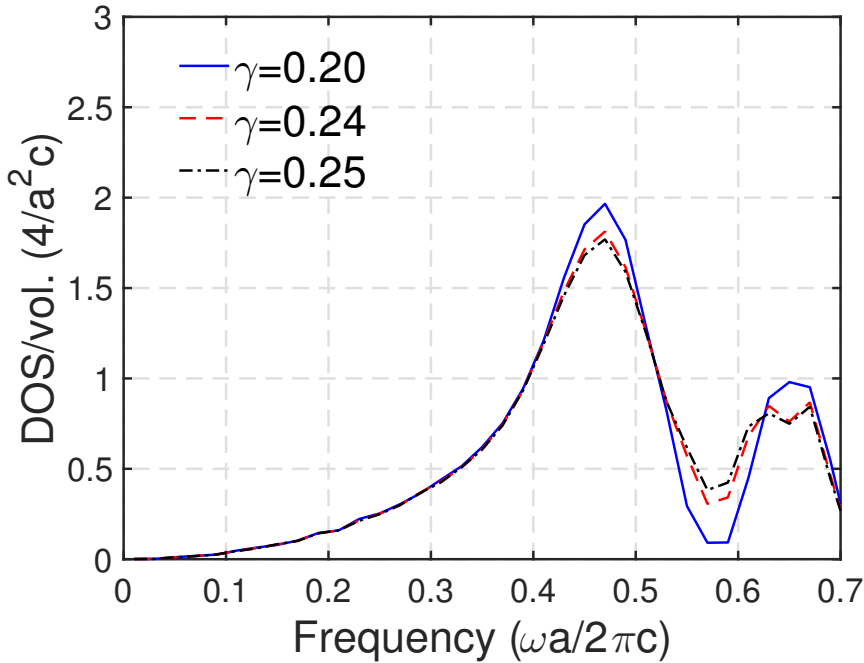


Figure 4.4: Density of states versus frequency for $\gamma = 0.20$, $\gamma = 0.24$ and $\gamma = 0.25$. The width of the frequency bins is $\Delta\tilde{\omega} = 0.02$.

edge, whereas three out of four configurations 1, 3, and 4 have a sharp lower band edge. The smooth tail at the upper band edge may be a Lifshitz tail of localized states [46, 47]. The sharp lower band edge cannot be simply represented as the upwards shift by $\Delta\tilde{\omega} = 0.025$ due to decreasing volume fraction, as has been observed for the DOS in Ref. [32]. For decreasing volume fractions from 21.3% at $\gamma = 0$ to 21.1% at $\gamma = 0.15$, the relative shift in the pore radii for systematic variations is about 0.2%, which corresponds to a frequency shift of $\Delta\tilde{\omega} = 0.01$, which is insufficient to explain the frequency shift of about $\Delta\tilde{\omega} = 0.025$ of the lower band edge [29]. We therefore explain the upward shift of the lower band edge by the filling of the band gap as well. Indeed, in previous work [48] as well as parallel calculations [49], it has been observed that single defect pores induce new states in the band gap, predominantly in the upper half.

In Fig. 4.4 we show the density of states histogram versus frequency for strong disorder $\gamma = 0.20$, $\gamma = 0.24$ and $\gamma = 0.25$. At disorder strength $\gamma = 0.25$ there is a single realization where the band gap is closed. It is remarkable that the band gap continues to exist over the entire physical range of disorder strengths studied here. We observe that as γ increases from 0.20 to 0.25, the configuration-averaged band gap is increasingly filled with states, and the gap is smoothened. Even at the maximum physical disorder strength $\gamma = 0.25$ there is still a strong

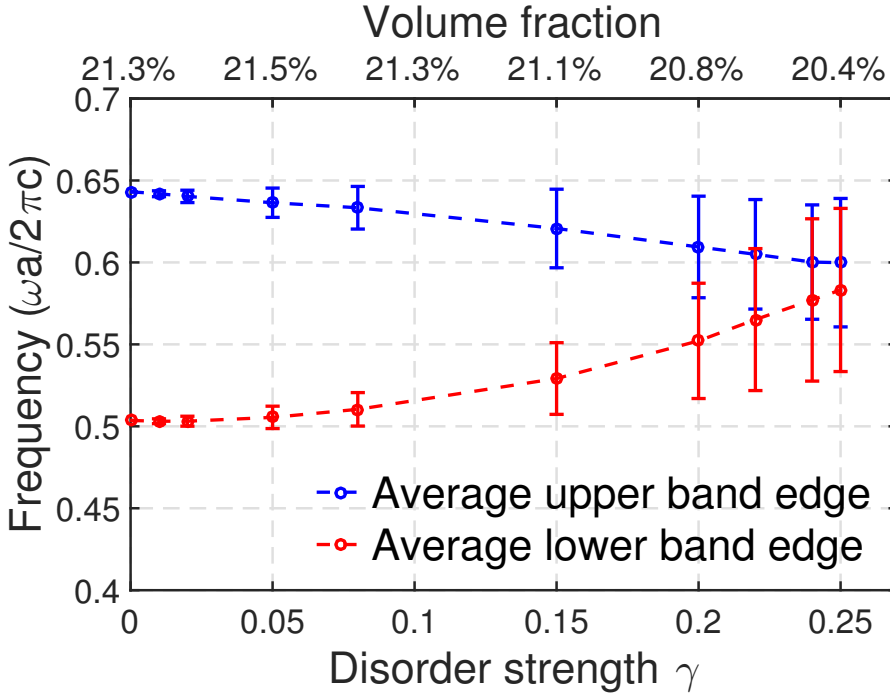


Figure 4.5: Band gap edges versus disorder strength γ . The circles give the average band gap edges, with the minimum and maximum edges from all realizations shown by error bars. The dashed lines connect the data. For $\gamma = 0.25$ only 9 data points with nonzero band gap width are taken into account.

inhibition in the average DOS by at least a factor $2\times$ in the frequency range of the unperturbed band gap that occurs between $\tilde{\omega} = 0.50$ and 0.64 . Thus, even strongly disordered inverse woodpile crystals retain a substantial functionality, notably regarding spontaneous emission control [50].

In Fig. 4.5 the band gap edges are shown versus the disorder strength. We see that the band gap narrows as the disorder strength increases. We observe the band gap at $\tilde{\omega} = 0.58 \dots 0.60$ at $\gamma = 0.25$. The volume fraction of 20.4% at $\gamma = 0.25$ gives a band gap $\tilde{\omega} = 0.51 \dots 0.64$ for systematic variations [29]. The volume fraction therefore only explains a minor amount of the band gap narrowing. It appears that the lower band edge shifts $1.8\times$ as much in frequency as the upper band edge. This agrees with observations on single pore defects that for many combinations of pore radii r_0 and defect pore radii r' it is predominantly the upper half of the band gap that is filled with states [48, 49]. In simultaneous experiments, the lower band edge is remarkably constant over many realizations and the upper band edge shows a large variation.

In Fig. 4.6 the band gap width is shown versus the disorder strength. We see that the band gap width decreases as the disorder strength decreases. For

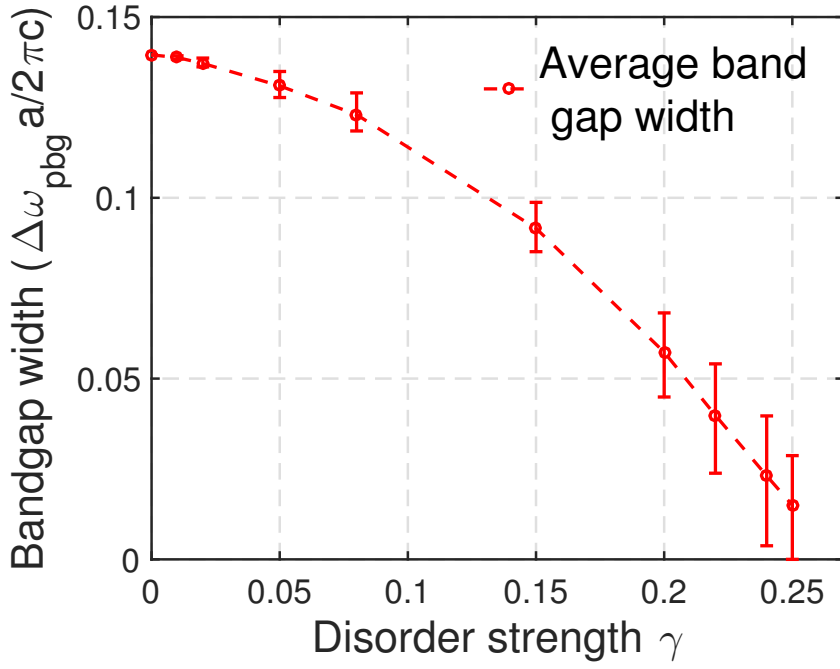


Figure 4.6: Band gap width versus disorder strength γ . The circles give the average band gap width over the realizations, with the minimum and maximum widths shown by error bars. The dashed lines are guides to the eye.

the range $\gamma = 0 \dots 0.2$ the variations the band gap width are smaller than the band gap width itself, whereas the maximum variation at constant frequency in the DOS is at least as large as the DOS itself for some frequencies, as we have seen before in Fig. 4.2. We see that even for $\gamma = 0.2$ each realization has a band gap with about $1/3 \times$ the width of the unperturbed band gap $\tilde{\omega} = 0.50$ and $\tilde{\omega} = 0.64$, whereas the average DOS shows states throughout the entire range of the unperturbed band gap frequencies, see Fig. 4.4. Therefore, we see again that even strongly disordered inverse woodpile crystals retain a substantial functionality, confirming their robustness.

4.4 Discussion

Silicon can have a large electronic band gap for amorphous structures [31]. Such gaps are also seen for photonic amorphous structures with zero long-range order. For instance, Edagawa *et al.* [31] calculated the DOS for photonic crystalline diamond and photonic amorphous diamond. For photonic crystalline diamond, they find a trough in the DOS of 26% relative bandwidth, corresponding to the photonic band gap [51]. For photonic amorphous diamond, they find a trough in the DOS of 18% relative bandwidth, smaller than for photonic crystalline diamond. In contrast, in the inverse woodpile crystals we observe that the photonic band gap becomes much more narrow or even closes as the disorder strength is increased to $\gamma = 0.25$. To explain this difference with amorphous diamond, we note that even at $\gamma = 0.25$ there is still visibly long-range order in Fig. 4.1. We tentatively infer that the presence of long-range order prevents the formation of a large photonic band gap in strongly disordered inverse woodpile crystals, and that inverse woodpile crystals should not be seen as a photonic analog of a-Si.

In Ref. [31], the DOS inhibition is nearly the same for photonic amorphous diamond as for photonic crystalline diamond, indicating no appreciable localized-state formations in the gap for photonic amorphous diamond. We observe that the band gap of the inverse woodpile crystal is progressively filled with states as the disorder strength becomes larger than $\gamma = 0.20$. These states may be localized, which requires further work.

Another example of a photonic amorphous structure is the tetrahedral dielectric network investigated by Liew *et al.* [32]. In this structure, the DOS inhibition in the band gap does not decrease monotonically with positional disorder, *i.e.*, the inhibition reaches a maximum for a certain non-zero disorder strength [32]. We do not see this for inverse woodpile crystals, where the DOS inhibition in the band gap decreases monotonically with disorder. To explain the nonmonotonicity of the DOS inhibition, Liew *et al.* [32] employ the tetrahedral bond order as a variable. This variable does not pertain to inverse woodpile crystals, which is consistent with the observed monotonicity of the DOS inhibition. The monotonicity of the DOS inhibition agrees with our previous conclusion that inverse woodpile photonic crystals with strong disorder cannot be seen as a photonic analog of a-Si.

For *s*-polarized waves in 2D, the 2D band gaps in the DOS become narrower

Table 4.1: Edge shifts for several crystals in literature. The shifts are reported as a fraction of the unperturbed band gap width. We have obtained these values ourselves from the figures in the cited papers.

crystal type	2D/3D	disorder	lower edge shift	upper edge shift
inverse woodpile	3D	radius	$+0.5\times$	$-0.3\times$
tetrahedral [32]	3D	positional	$< 0.1\times$	$< 0.1\times$
PAD [31]	3D	positional	$< 0.1\times$	$-0.3\times$
diel. cyl. [33]	2D	radius	$< 0.1\times$ (first) $+0.4\times$ (second)	$< 0.1\times$ (first) $-0.2\times$ (second)
inv. opal [27]	3D	radius	$+0.8\times$	$+0.4\times$

about the center frequency with increasing disorder up to $d_r = 0.2$ [33], see also Table 4.1. As reported in Ref. [33] the first 2D band gap narrows. However, we see only a small change in the band gap width in Fig. 6 from Ref. [33]. For the second 2D band gap, we see that the lower edge shifts upwards $2\times$ as much as the upper band edge shifts downwards in the figure. This is similar to the $1.8\times$ difference that we see for inverse woodpile crystals. In the disorder model by Sigalas *et al.* [33] with uniform deviations in the radius of dielectric spheres, we would expect the volume fraction to increase as the disorder strength increases. The upper band edge would then shift downwards because of the increased volume fraction. For defects with smaller radius than the background pore radius $r = 0.2a$, with a the lattice constant, an acceptorlike resonance appears in the 2D system near $r = 0.15a$ that splits off from the lower band edge [52], and which we propose may contribute to the shift of the lower band edge to higher frequency as the disorder strength increases. However, it is not completely clear if $r = 0.2a$ is indeed the background radius that is used in Ref. [33] and the dielectric index is somewhat different ($n = 3.2$ in Ref. [33] versus $n = 3.4$ in Ref. [52]). For the inverse woodpile crystal, the volume fraction decreases slightly as the disorder strength increases from $\gamma = 0$ to $\gamma = 0.25$. This agrees with the observed upward frequency shift of the lower band edge, but it is only a minor contribution. We therefore explain the upward shift of the lower band edge primarily by the filling of the band gap. Indeed, in previous work [48] as well as parallel calculations [49], it has been observed that single defect pores induce new states in the band gap, predominantly in the upper half, but also in the lower half. Since there is a large number of new states in the upper half of the band gap, we attribute the downward shift of the upper band edge to the appearance of these new states. Comparing the arguments we made for the 2D system and the 3D inverse woodpile crystal, we conclude that they are at least qualitatively consistent.

In the calculations by Conti *et al.* [27], we see that both the lower and upper band edges shift upwards with frequency, which makes sense in terms of the reduced volume fraction for inverted opals with uniform perturbations on the pores radius. In Ref. [27] the band gap closes for a few percent of randomness in the pore radii, which is smaller than the $\gamma = 0.25$ (where we found the first

realization with a closed band gap), which makes sense since the band gap is much narrower in an inverse opal crystal ($\frac{\Delta\omega_{pbg}}{\omega_c} = 4.25\%$ [53]) than in an inverse woodpile crystal ($\frac{\Delta\omega_{pbg}}{\omega_c} = 25.3\%$ [29, 37]).

4.5 Summary

In this Chapter we have investigated the density of states in 3D photonic band gap crystals with disorder, notably the band gap. We observe that the band gap becomes narrower as the disorder strength increases from 0% to 25% of the pore radius. At a disorder strength of 25%, the band gap closes for one realization out of ten. However, at this disorder strength the structure is so thin that the real structure may collapse. The band gap is therefore remarkably robust over the entire physical range of disorder strengths. Interestingly, we observe a larger frequency shift of the lower band edge than the upper band edge, which agrees with separate observations of states appearing in the upper half of the band gap for many parameters of defect pores used in the design of cavities [48, 49].

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$$\rho(\omega, \mathbf{r}, \mathbf{r}) = \text{Im}G(\omega, \mathbf{r}, \mathbf{r}).$$

Physically the Green's function of light gives the electric field at position $\mathbf{r}$ in response to a point source at position $\mathbf{r}'$:

$$G(\omega, \mathbf{r}, \mathbf{r}') = \frac{i \sin(k|\mathbf{r} - \mathbf{r}'|)}{k|\mathbf{r} - \mathbf{r}'|} + \cos(k|\mathbf{r} - \mathbf{r}'|).$$

Taking the limit to find the LDOS, we obtain

$$\rho(\omega, \mathbf{r}, \mathbf{r}) = \lim_{\mathbf{r} \rightarrow \mathbf{r}'} \text{Im}G(\omega, \mathbf{r}, \mathbf{r}') = k.$$

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CHAPTER 5

Nonreflecting boundary conditions for a mixed discontinuous Galerkin discretization of the Maxwell equations

5.1 Introduction

Mixed discontinuous Galerkin (DG) finite element methods are well suited to solve the Maxwell equations in complex structures, as they allow to efficiently capture singularities at dielectric corners and interfaces and also provide a spectrum of electric field solutions that is free of spurious modes [1–6]. In this Chapter, we combine such a mixed DG discretization with a nonreflecting boundary condition. The resulting method allows the computation of light propagation in finite structures. Examples are the calculation of the power radiated by a source inside the structure, or the calculation of the reflectivity of a wavefield impinging on a structure from outside.

It is well-known [7] that computations on finite structures frequently involve unbounded domains that do not fit into the computer memory. A well-known solution, which we employ here, is to introduce an artificial boundary with a suitable boundary condition. The boundary condition must absorb the radiated or scattered wavefield as good as possible and minimize unavoidable spurious reflections that are required to be smaller than the level of the discretization error. Many boundary conditions for the Maxwell equations have been described in the scientific literature, such as the perfect electric conductor [8] or periodic boundary conditions [9], but these are not suitable since they completely reflect the wavefield incident from the structure under study, and therefore perturb the desired wavefield. Instead, one has to employ a nonreflecting boundary condition, see Refs. [10–12] for an overview of this topic.

Computations on structures that are finite in all three dimensions frequently employ the Silver-Müller boundary condition [7, 13]. In this approach one employs the Silver-Müller radiation condition, which holds exactly at infinity, at artificial boundaries, that is, at a finite distance from the structure. For structures that are finite in all three dimensions, the radiated or scattered wavefield satisfies the Silver-Müller radiation condition with progressively better accuracy as the distance from the scatterers increases. The spurious reflections can therefore be made as small as desired by moving the artificial boundary away from the scatterers. In practice, it is, however, desirable to have a more accurate nonre-

flecting boundary condition that can be placed closer to the structure, reducing computing time and memory use. Such nonreflecting boundary conditions have been developed for spherical boundaries, and can be incorporated in a variational formulation. For instance, Webb and Kanellopoulos [14] developed a second-order nonreflecting boundary condition, that is, it eliminates two terms in the Wilcox expansion of outgoing waves [7]. Nonreflecting boundary conditions for spherical boundaries with arbitrarily high order have been derived by Grote [15].

In this Chapter we develop a nonreflecting boundary condition for a planar artificial boundary in combination with a mixed DG discretization of the Maxwell equations. Such a nonreflecting boundary condition can be used, for example, to compute the reflectivity of a wavefield impinging on a slab that is periodic in the transverse directions. Here, the spurious reflections do not decay as the artificial boundary condition is placed further away from the structure, and it is therefore crucial to have a highly accurate nonreflecting boundary condition.

A well-known nonreflecting boundary condition in electromagnetic engineering calculations that is suitable for planar boundaries is the perfectly matched layer proposed by Berenger [16]. Unfortunately, the accuracy of the perfectly matched layer depends on a smart choice of the decay parameter, which depends on the problem and the discretization used, and results in a lack of error estimates for the reflection coefficient [17]. The perfectly matched layer is subject to ongoing research and recently Chern [18] developed a discretization that is reflectionless at the discrete level, but it may be nontrivial to extend this approach to finite element discretizations. Collino and Joly [19] have proposed nonreflecting boundary conditions for a variational formulation of the second order Maxwell equations at a plane boundary, but numerical results of this boundary condition did not appear in literature. In Hall and Kabakian [20] a sequence of absorbing boundary conditions is derived for the Maxwell equations, but the formulation is in terms of both $\mathbf{E}$ and $\mathbf{B}$, instead of only the electric field. In Assous and Sonnendrücker [21] the Joly-Mercier nonreflecting boundary condition [22], which is of second-order, is applied in a mixed finite-element formulation of the Maxwell equations, but a boundary condition with a higher order of accuracy is desirable for computations of wave phenomena.

We therefore consider a class of high-order local nonreflecting boundary conditions at a planar boundary, that are known to have good estimates for the spurious reflection coefficient [12, 17], and that can make the spurious reflections as small as desired, in particular smaller than the discretization error. For scalar waves in one dimension (1D) it is straightforward to absorb the incident wavefield exactly. Let us assume that the incident wavefield propagates from left to right. At the right boundary one imposes the advection equation, which is consistent with right-moving (outgoing) waves and inconsistent with left-moving (incoming waves). In three dimensions such a boundary condition is called the first-order Engquist-Majda nonreflecting boundary condition [23, 24]. While the absorption is perfect for normally incident waves, the spurious reflection coefficient increases strongly for oblique incident waves, reaching unity for tangential waves, which is not desirable in computations.

By solving the dispersion relation for the normal component of the wave vector,

one can derive a dispersion relation for outgoing waves. This dispersion relation is the starting point for deriving boundary conditions based on boundary integrals, which are exact, but also are computationally expensive [11, 25]. Higher-order Engquist-Majda boundary conditions are derived as rational approximations to this dispersion relation [23, 24]. Higdon reformulated the high-order Engquist-Majda boundary conditions in terms of only normal derivatives [26]. In the Higdon nonreflecting boundary condition, we have control over the error with a parameter here labelled P , which can be set arbitrarily (typically $P = 1, \dots, 5$). At the incidence angles $\theta_1, \dots, \theta_P$, that can be chosen arbitrarily, the waves are absorbed exactly. At other angles, the spurious reflection amplitude is estimated to be small, and decays exponentially with P . Unfortunately, the Higdon boundary condition is impractical, since it contains high derivatives up to order P . Therefore the Givoli-Neta boundary condition reformulates the Higdon boundary condition by introducing auxiliary variables on the boundary and eliminating the high derivatives beyond second-order [27]. In this work, we employ, however, the Hagstrom-Warburton boundary condition [28], which has the advantage with respect to the Givoli-Neta boundary condition that the auxiliary variables satisfy a symmetrizable system of second-order wave equations at the boundary.

For the Maxwell equations, the Hagstrom-Warburton boundary condition has been applied to a discretization with nodal discontinuous elements [11, 28, 29], which is often used for time-domain calculations [30]. This discretization, however, can suffer from spurious modes in the frequency-domain due to the artificial damping in the upwind fluxes [30], although this issue can be alleviated or even eliminated with a suitable modification of the fluxes [31]. In this discretization, error estimates are given for the combined fields $\mathbf{q} = (\mathbf{E}, \mathbf{B})^T$ and the Hagstrom-Warburton boundary condition is applied to characteristic variables that are combinations of these fields. The mixed DG method [6] employed in the present Chapter has a spurious-free spectrum, and uses Nédélec elements [32]. In the discretization, the electric field has one order higher accuracy than the magnetic field, and it is desirable to formulate the Hagstrom-Warburton condition in terms of only the electric field. This is the first time that the Hagstrom-Warburton boundary condition is adapted to a mixed DG discretization of the Maxwell equations. In our approach, we exploit the fact that each field component separately satisfies the Helmholtz equation, as observed by Mur [33]. It is stated by Monk [7] that from the Stratton-Chu formula [34] we can see that each field component also satisfies the radiation condition appropriate for the Helmholtz equation. Hence, it is possible to use nonreflecting boundary conditions appropriate for the Helmholtz equation on each component of the scattered field. In fact, we apply the Hagstrom-Warburton boundary condition only to the tangential components of the electric field.

The outline of this Chapter is as follows. In Section 5.2 we give an extended introduction to nonreflecting boundary conditions. In Section 5.3 we describe the Hagstrom-Warburton nonreflecting boundary conditions for the Maxwell equations. In Section 5.4 we summarize the mixed discontinuous Galerkin finite element discretization of the Maxwell equations, which is based on Brezzi numerical fluxes, a detailed derivation of the mixed DG discretization is given in Appendix

5.A. In Section 5.5 we present the vector-valued nonreflecting boundary condition and discuss the implementation in the DG formulation, followed by a presentation of results for a plane-wave test case in Section 5.6. We finish with conclusions in Section 5.7.

5.2 Introduction to nonreflecting boundaries

In this section we will give an overview of the basic approaches used in the construction of nonreflecting boundary conditions. In one dimension (1D) it is straightforward to develop a nonreflecting boundary condition. Consider a domain $x < 0$ and a boundary at $x = 0$. We start by introducing boundary conditions for the scalar wave equation. Throughout the present Chapter we will work in the frequency domain. We factorize the 1D Helmholtz operator into an advection operator for a right-moving wave and an advection operator for a left-moving wave:

$$(\omega^2 + c^2 \partial_x^2)u = 0, \quad (5.1)$$

$$\underbrace{(i\omega - c\partial_x)}_{\text{left}} \underbrace{(i\omega + c\partial_x)}_{\text{right}} u = 0, \quad (5.2)$$

with u the wave amplitude, ω the frequency, c the speed of light, and where the underlining indicates the advection operator for the left- and right-moving waves. We obtain a nonreflecting boundary condition by imposing the advection equation for the right-moving wave at the boundary:

$$(i\omega + c\partial_x)u|_{x=0} = 0. \quad (5.3)$$

Boundary condition (5.3) is satisfied by outgoing (right-moving) waves and inconsistent with incoming (left-moving) waves. It is therefore perfectly absorbing in 1D. In literature boundary condition (5.3) is called the Sommerfeld boundary condition [35, 36].

In three dimensions (3D) the Sommerfeld boundary condition is only perfectly absorbing for normally-incident waves. Typically, there will also be oblique waves incident on the boundary, of which part will be spuriously reflected. In 3D, for scatterers bounded in space, the waves will be overwhelmingly normal when the boundary is placed at a large distance from the scatterers, and the Sommerfeld operator on a sphere scales like

$$(i\omega + c\partial_r)u \sim O(1/r^{(d-1)/2}), \quad (5.4)$$

when the radius $r = |\mathbf{x}| \rightarrow \infty$, with $d = 3$ the spatial dimension, and the spurious reflections decay in magnitude. However, many computations concern a wavefield impinging on a slab that is periodic in the transverse directions. Here, the scatterers are unbounded, and there is no decay in spurious reflections as the distance between the boundary and the scatterers increases. Indeed, for a wave with a 45° angle of incidence the boundary condition (5.3) reflects waves with an

amplitude that is 17% of the amplitude of the incident wave [23], which is undesirable in calculations. For the Maxwell equations, the Silver-Müller operator [7] has the same scaling as the Sommerfeld operator (5.4).

The idea underlying the Sommerfeld boundary condition can be generalized to construct an accurate nonreflecting boundary condition in higher dimensions, which we will now do for three dimensions (3D). We start from the three-dimensional Helmholtz equation

$$(\omega^2 + c^2 \partial_x^2 + c^2 \nabla_t^2)u = 0, \quad x < 0, \quad (5.5)$$

with the tangential derivatives $\nabla_t^2 = \partial_y^2 + \partial_z^2$. We take a Fourier transform of Eq. (5.5) in the tangential variables (y, z) :

$$(-\omega^2 - c^2 \partial_x^2 + c^2 k_y^2 + c^2 k_z^2)\hat{u} = 0.$$

We find, as in 1D, a factorization into left and right propagating advection equations

$$\underbrace{(i\omega \sqrt{1 - (ck_y/\omega)^2 - (ck_z/\omega)^2} - c\partial_x)}_{\text{left}} \underbrace{(i\omega \sqrt{1 - (ck_y/\omega)^2 - (ck_z/\omega)^2} + c\partial_x)}_{\text{right}} \hat{u} = 0,$$

where we have underlined the advection operator for the left-moving and right-moving waves with phase velocity $c/\sqrt{1 - (ck_y/\omega)^2 - (ck_z/\omega)^2}$. We then impose the advection operator for the right-moving wave at the boundary

$$(i\omega \sqrt{1 - (ck_y/\omega)^2 - (ck_z/\omega)^2} + c\partial_x)\hat{u}|_{x=0} = 0. \quad (5.6)$$

The boundary condition (5.6) holds for all propagating waves with $k_x \geq 0$, that is, waves moving out of the domain, and it is inconsistent with all incoming waves [25]. Therefore, boundary condition (5.6) constitutes an exact boundary condition. Transforming boundary condition (5.6) to real space yields

$$\left(c\partial_x u(x, y, z) + \int_{-\infty}^{\infty} e^{i(k_y y + k_z z)} i\omega \sqrt{1 - (ck_y/\omega)^2 - (ck_z/\omega)^2} \hat{u}(x, k_y, k_z) dy dz \right) |_{x=0} = 0, \quad (5.7)$$

where we integrate over the entire planar boundary $y = -\infty \dots \infty, z = -\infty \dots \infty$. We see that evaluating the exact boundary condition (5.7) at any point y, z on the boundary involves calculating a Fourier transform, applying an operator, and calculating the inverse Fourier transform. This results in a non-local boundary condition and is very expensive to compute in 3D.

As an alternative, Engquist and Majda [23, 24] have developed approximations to boundary condition (5.6) that can be evaluated more efficiently in real space.

The square root factor in Eq. (5.6) is approximated by a finite continued fraction expansion

$$\sqrt{1 - x^2} \simeq \mathcal{P}_P(x) + O(|x|^{2(P+1)}),$$

with $x = \sqrt{(ck_y/\omega)^2 + (ck_z/\omega)^2}$ and $P \geq 0$ the order that can be chosen arbitrarily [24]. The finite continued fraction expansion is given recursively by

$$\begin{aligned} \mathcal{P}_0 &\equiv 1, \\ \mathcal{P}_1 &\equiv 1 - \frac{x^2}{2}, \\ &\vdots \\ \mathcal{P}_P &\equiv 1 - \frac{x^2}{1 + \mathcal{P}_{P-1}}. \end{aligned}$$

Note that any finite continued fraction expansion can be written as a rational function. Indeed, the approximations of order $P = 0, 1, 2$ are [23]

$$\begin{aligned} \mathcal{P}_0 &= 1, \\ \mathcal{P}_1 &= \frac{2 - x^2}{2}, \end{aligned} \tag{5.8}$$

$$\mathcal{P}_2 = \frac{2 - (3x^2/2)}{2 - (x^2/2)}, \tag{5.9}$$

and high-order approximations can also be written as rational functions. Engquist & Majda [24] show that the corresponding boundary conditions are

$$\mathcal{B}_0 u|_{x=0} \equiv (i\omega + c\partial_x)u|_{x=0} = 0, \tag{5.10}$$

$$\mathcal{B}_1 u|_{x=0} \equiv (-\omega^2 + i\omega c\partial_x - \frac{1}{2}\nabla_t^2)u|_{x=0} = 0, \tag{5.11}$$

$$\vdots \tag{5.12}$$

$$\mathcal{B}_P u|_{x=0} \equiv (i\omega\mathcal{B}_{P-1}(u) - \frac{1}{4}\nabla_t^2\mathcal{B}_{P-2}(u))|_{x=0} = 0, \tag{5.13}$$

see Footnote [37] for a derivation of the second boundary condition (5.11). By employing the wave equation to eliminate the tangential derivatives, Higdon [26] has shown that the boundary condition for order P can be written as

$$\mathcal{B}_P u|_{x=0} = (i\omega + c\partial_x)^{P+1}u|_{x=0} = 0.$$

See Footnote [38] for a proof. An extension by Higdon [26] is to replace, for each factor separately, the c with the phase velocity in the x -direction, $c/\cos(\theta_p)$, for

waves propagating with an incidence angle θ_p :

$$\prod_{p=0}^P (\cos(\theta_p)i\omega + c\partial_x)u = 0, \quad (5.14)$$

with $-\pi/2 \leq \theta_p \leq \pi/2$. In the Higdon boundary condition (5.14), one can choose the order P arbitrarily, together with a set of P incidence angles θ_p such that the waves in these directions are exactly absorbed in addition to the normal incident wave. The Higdon boundary condition has a reflection coefficient giving the amplitude of spuriously reflected waves as a fraction of the amplitude of the incident waves, which is equal to [26]

$$R(\theta) = - \prod_{p=0}^P \left(\frac{\cos(\theta_p) - \cos(\theta)}{\cos(\theta_p) + \cos(\theta)} \right) \quad \text{for } -\pi/2 \leq \theta \leq \pi/2. \quad (5.15)$$

For $\theta = \theta_p$ one can verify that the reflection (5.15) is indeed equal to zero. For $\theta \neq \theta_p$ the spurious reflection is nonzero, but decays exponentially with P .

The Higdon boundary condition (5.14) has high-order spatial derivatives that are not straightforward to implement in a finite-difference or finite-element method [27]. Therefore, in the Givoli-Neta boundary condition [27], auxiliary functions are employed to eliminate the high-order derivatives. In their derivation, the auxiliary functions ϕ_i are defined in an open set D containing the artificial boundary and the exterior domain:

$$(\cos(\theta_0)i\omega + c\partial_x)u = \phi_1, \quad (5.16)$$

$$(\cos(\theta_1)i\omega + c\partial_x)\phi_1 = \phi_2, \quad (5.17)$$

$$\vdots \quad (5.18)$$

$$(\cos(\theta_P)i\omega + c\partial_x)\phi_P = 0 \quad (x, y, z) \in D. \quad (5.19)$$

The open set is employed to make the normal derivatives well defined. Givoli and Neta then eliminate the normal derivatives in Eqns. (5.16)–(5.19) using the wave equation [27] and impose the resulting equations at the boundary only, resulting in a nonreflecting boundary condition. The reflection coefficient of the Givoli-Neta boundary condition equals that of the Higdon boundary condition (5.15) [27].

Hagstrom and Warburton [28] proposed a modification of the Givoli-Neta boundary condition that uses same-order differential operators on both sides of the equations to define the auxiliary variables. We will employ the Hagstrom-Warburton boundary condition, since it has better stability as shown by Givoli et al. [39]. The Hagstrom-Warburton boundary condition employs a recursion [28] that is defined in the open set D containing the artificial boundary and the

exterior domain

$$(\cos(\theta_0)i\omega + c\partial_x)u = a_0i\omega\phi_1, \quad (5.20)$$

$$(\cos(\theta_1)i\omega + c\partial_x)\phi_1 = (\cos(\theta_1)i\omega - c\partial_x)\phi_2,$$

$$\vdots$$

$$(\cos(\theta_p)i\omega + c\partial_x)\phi_p = (\cos(\theta_p)i\omega - c\partial_x)\phi_{p+1}, \quad (5.21)$$

$$\vdots$$

$$(\cos(\theta_P)i\omega + c\partial_x)\phi_P = 0 \quad (x, y, z) \in D. \quad (5.22)$$

In Eq. (5.20) we have placed the factor a_0 in front of the frequency on the right hand side following Ref. [40], which is essential for extending the method to inhomogeneous media (but we will not pursue this in the present Chapter where $a_0 = 1$). To rewrite the boundary condition in terms of tangential derivatives, we use a slightly different derivation than in Ref. [28], where Hagstrom and Warburton first define an infinite sequence for the auxiliary variables instead of the finite one in Eq. (5.22). We use the following Lemma [28]:

Lemma 1. *The variables ϕ_p , $p = 1, \dots, P$, satisfy:*

$$(\omega^2 + c^2\nabla^2)\phi_p \equiv \square\phi_p = 0 \quad (x, y, z) \in D. \quad (5.23)$$

Proof. Applying the Helmholtz operator $\square$ to the first equation in the Hagstrom-Warburton recursion (5.20) results in

$$i\omega\square\phi_1 = (\cos(\theta_0)i\omega + c\partial_x)\square u = 0.$$

Let us assume that the Lemma holds for ϕ_p

$$\square\phi_p = 0.$$

We then apply the Helmholtz operator $\square$ to the auxiliary equation for ϕ_{p+1} (5.21), yielding

$$(\cos(\theta_p)i\omega - c\partial_x)\square\phi_{p+1} = (\cos(\theta_p)i\omega + c\partial_x)\square\phi_p = 0. \quad (5.24)$$

Since the right hand side vanishes by assumption, so does the left hand side. Since the region D is source-free, the left side of Eq. (5.24) can be integrated along characteristics $x + ct/\cos(\theta_p)$ to find that

$$\square\phi_{p+1} = 0.$$

□

Let us define $a_p \equiv \cos(\theta_p)$. We multiply Eq. (5.21) with $a_p i\omega + c\partial_x$ and Eq. (5.21) for $p - 1$ with $a_{p-1} i\omega - c\partial_x$ and use the wave equation for the auxiliary

variables (5.23) to eliminate ∂_x^2 to obtain (see Footnote [41])

$$\begin{aligned} &(-(a_p^2 + 1)\omega^2 + 2a_p i\omega c\partial_x - c^2\nabla_t^2)\phi_p = (-(a_p^2 - 1)\omega^2 + c^2\nabla_t^2)\phi_{p+1} \\ &(-(a_{p-1}^2 + 1)\omega^2 - 2a_{p-1} i\omega c\partial_x - c^2\nabla_t^2)\phi_p = (-(a_{p-1}^2 - 1)\omega^2 + c^2\nabla_t^2)\phi_{p-1}. \end{aligned}$$

Multiplying the first equation by a_{p-1} , the second equation by a_p , and adding the results, we finally obtain for $p = 2, \dots, P-1$:

$$\begin{aligned} &-l_{p,p-1}\omega^2\phi_{p-1} - l_{pp}\omega^2\phi_p - l_{p,p+1}\omega^2\phi_{p+1} = c^2(a_p\nabla_t^2\phi_{p-1} \\ &+ (a_p + a_{p-1})\nabla_t^2\phi_p + a_{p-1}\nabla_t^2\phi_{p+1}) \quad p = 1, \dots, P-1, \end{aligned}$$

where

$$\begin{aligned} l_{p,p-1} &= a_p(1 - a_{p-1}^2), \quad l_{p,p+1} = a_{p-1}(1 - a_p^2), \\ l_{pp} &= a_p(1 + a_{p-1}^2) + a_{p-1}(1 + a_p^2). \end{aligned} \quad (5.25)$$

A similar calculation applied to the first equation of the Hagstrom-Warburton boundary condition (5.20) yields:

$$-2a_1(1 - a_0^2)\omega^2 u - l_{11}\omega^2\phi_1 - l_{12}\omega^2\phi_2 = c^2(2a_1\nabla_t^2 u + a_0\nabla_t^2\phi_1 + a_0\nabla_t^2\phi_2),$$

where

$$l_{11} = a_0(1 + a_1^2 + 2a_1a_0), \quad l_{12} = a_0(1 - a_1^2). \quad (5.26)$$

Finally, when the procedure is applied to the last equation of the Hagstrom-Warburton boundary condition (5.22) we obtain

$$-l_{P,P-1}\omega^2\phi_{P-1} - l_{PP}\omega^2\phi_P = c^2(a_P\nabla_t^2\phi_{P-1} + (a_P + a_{P-1})\nabla_t^2\phi_P),$$

with

$$l_{P,P-1} = a_P(1 - a_{P-1}^2), \quad l_{PP} = a_P(1 + a_{P-1}^2) + a_{P-1}(1 + a_P^2). \quad (5.27)$$

Now that the recursion of the Hagstrom-Warburton boundary condition is formulated in tangential derivatives, it is imposed only at the boundary, resulting in the boundary conditions

$$(a_0 i\omega + c\partial_x)u = a_0 i\omega\phi_1, \quad (5.28)$$

$$-l_{1,0}\omega^2 u - l_{11}\omega^2\phi_1 - l_{12}\omega^2\phi_2 = c^2(m_{1,0}\nabla_t^2 u + m_{11}\nabla_t^2\phi_1 + m_{1,2}\nabla_t^2\phi_2), \quad (5.29)$$

$$\begin{aligned} &-l_{p,p-1}\omega^2\phi_{p-1} - l_{pp}\omega^2\phi_p - l_{p,p+1}\omega^2\phi_{p+1} = c^2(m_{p,p-1}\nabla_t^2\phi_{p-1} \\ &+ m_{pp}\nabla_t^2\phi_p + m_{p,p+1}\nabla_t^2\phi_{p+1}), \quad p = 2, \dots, P-1, \end{aligned}$$

$$-l_{P,P-1}\omega^2\phi_{P-1} - l_{PP}\omega^2\phi_P = c^2(m_{P,P-1}\nabla_t^2\phi_{P-1} + m_{PP}\nabla_t^2\phi_P),$$

with l_{11} and l_{12} defined in Eq. (5.26), $l_{p,p-1}$ and $l_{p,p+1}$ in Eq. (5.25), $l_{P,P-1}$ and

l_{PP} in Eq. (5.27), and

$$l_{1,0} = 2a_1(1 - a_0^2), \quad m_{1,0} = 2a_1, \quad m_{11} = a_0, \quad m_{1,2} = a_0, \\ m_{p,p-1} = a_p, \quad m_{pp} = a_p + a_{p-1}, \quad m_{p,p+1} = a_{p-1}.$$

The reflection coefficient giving the amplitude of spuriously reflected waves in terms of the amplitude of the incident wave is [28]

$$R(\theta) = -\frac{\cos(\theta_0) - \cos(\theta)}{\cos(\theta_0) + \cos(\theta)} \prod_{p=1}^P \left(\frac{\cos(\theta_p) - \cos(\theta)}{\cos(\theta_p) + \cos(\theta)} \right)^2. \quad (5.30)$$

Comparing the reflection coefficient (5.30) of the Hagstrom-Warburton boundary condition with that of the Higdon boundary condition (5.15) [26] or Givoli-Neta boundary condition [27], it is seen that the factors for $p = 1, \dots, P$ in the product are squared, which is another advantage of using the Hagstrom-Warburton boundary condition. In the Hagstrom-Warburton boundary condition, the order P can be set arbitrarily, and P incidence angles θ_p can be chosen that are absorbed exactly. Estimate (5.30) is insensitive to the problem parameters (for example the frequency) and to the discretization, unlike perfectly matched layers [17].

In this Chapter we employ the following procedure for choosing the angles θ_p . For the $P = 0$ boundary condition, we set $\theta_0 = 0$. For the $P = 1$ boundary condition, we set $\theta_0 = 0$, and choose θ_1 as the minimizer of the maximum of $|R(\theta)|$ over $-\pi/4 \leq \theta \leq \pi/4$, which results in $\theta_1 = 0.22\pi$. We performed the minimization numerically by iterating over all values, with grid spacings $\Delta\theta_1 = \pi/200$ and $\Delta\theta = \pi/200$. In this Chapter we will only implement the $P = 0$ and $P = 1$ boundary conditions, but one could continue this procedure to make the reflection coefficient even smaller. For the $P = 2$ boundary condition, we set $\theta_0 = 0$, $\theta_1 = 0.22\pi$, and add 50% of the remaining interval to the minimization interval, $-3\pi/8 \leq \theta \leq 3\pi/8$, which results in $\theta_2 = 0.36\pi$. This procedure for choosing angles has the advantage that the modulus of the reflection coefficient always decreases monotonically with increasing P , and highly-oblique waves are progressively better absorbed with increasing P .

In Fig. 5.1 the spurious reflection coefficient (5.30) is shown versus the angle of incidence for these values of θ_0 , θ_1 and θ_2 . Setting $P = 0$ and $\theta_0 = 0$ so that normally incident waves are exactly absorbed, the spurious reflection coefficient is indeed zero for θ_0 . As the incidence angle increases, the modulus of the spurious reflection coefficient increases, until at tangential incidence $\theta = \pi/2$, the waves propagate along the boundary surface with a spurious reflection coefficient $R = 1$. Due to the exponential decay in the modulus of the spurious reflection coefficient (5.30) with order P , it can be made significantly smaller even for a small value of P . For $P = 1$ with $\theta_1 = 0.22\pi = 39.6^\circ$ the modulus of the spurious reflection coefficient is significantly smaller than for $P = 0$ for $\theta < \pi/2$. In the vicinity of $\theta = \pi/2$ it rises steeply to $R = 1$. The modulus of the reflection coefficient no longer increases monotonically with incidence angle as a result of our choice to exactly absorb certain oblique angles. For the $P = 2$ boundary condition, we

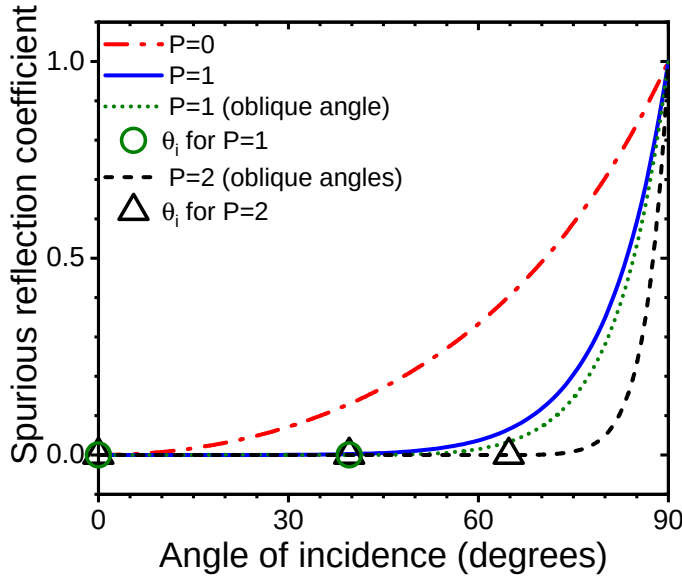


Figure 5.1: Modulus of the estimate (5.30) for the spurious reflection coefficient versus angle of incidence for the $P = 0, 1, 2$ Hagstrom-Warburton boundary conditions. The $P = 0$ boundary condition corresponds to the Sommerfeld boundary condition without auxiliary variables. For the $P = 1$ boundary condition, we present results for $\theta_1 = 0$ (blue curve) and $\theta_1 = 0.22\pi$ (green dotted curve). For the $P = 2$ boundary condition, two angles $\theta_1 = 0.22\pi = 39.6^\circ$ and $\theta_2 = 0.36\pi = 64.8^\circ$ have been chosen to be exactly absorbed.

have chosen the angles $\theta_1 = 0.22\pi = 39.6^\circ$ and $\theta_2 = 0.36\pi = 64.8^\circ$ to be exactly absorbed. In Fig. 5.1 we indeed see $R = 0$ for these angles. In the vicinity of $\theta = \pi/2$ the reflection coefficient rises steeply to $R = 1$. However, the modulus of the spurious reflection coefficient for $P = 2$ is very small for most angles, with $|R| = 1.95 \cdot 10^{-5}$ for $\theta = 45^\circ$, as we can also see in Fig. 5.1. This is much smaller than the $R = 0.17$ for the Sommerfeld boundary condition [23].

5.3 Nonreflecting boundary condition for Maxwell's equations

Let Ω be the computational domain and $\partial\Omega$ the computational domain boundary. Applying the Hagstrom-Warburton boundary condition to all sides of a rectangular, or more generally, polyhedral domain, requires the development and discretization of special corner conditions in terms of only the electric field [28]. In the present Chapter we will assume that there are two planar boundaries, as shown in Fig. 5.2. At the left ($x = x_{left}$) and right ($x = x_{right}$) boundaries ($\partial\Omega_{NRBC}$) the Hagstrom-Warburton boundary condition of order $P = 1$

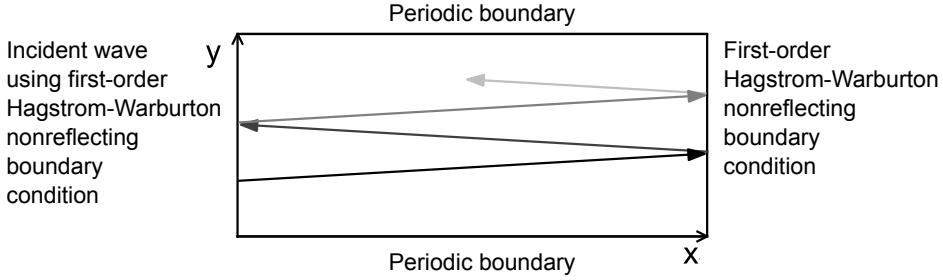


Figure 5.2: Computational domain. The x and y axes are indicated. At the left and right boundaries in the x -direction the first-order Hagstrom-Warburton nonreflecting boundary condition is imposed. The Hagstrom-Warburton condition at the left boundary generates the incident wave. At the top and bottom boundaries in the y -direction the periodic boundary condition is imposed. The propagation direction of the incident wave is indicated with a black arrow. Several spuriously reflected waves are indicated with gray arrows.

is imposed. The Hagstrom-Warburton boundary condition at the left boundary also generates the incident wave, that will be described later. At the top ($y = y_{top}$) and bottom ($y = y_{bottom}$) boundaries ($\partial\Omega_{periodic}$) periodic boundary conditions are imposed. More details about the dimensions of the domain will be given later. We solve the time-harmonic Maxwell equations with nonreflecting boundary conditions

$$\nabla \times \mu^{-1} \nabla \times \mathbf{E} - \omega^2 \epsilon \mathbf{E} = 0 \quad \text{in } \Omega, \quad (5.31)$$

$$\nabla \cdot (\epsilon \mathbf{E}) = 0 \quad \text{in } \Omega, \quad (5.32)$$

$$\text{H-W condition for } \mathbf{E}^s \quad \text{at } \partial\Omega_{NRBC},$$

$$\text{periodic boundary conditions} \quad \text{at } \partial\Omega_{periodic},$$

with $\mathbf{E}$ the electric field, ω the frequency, μ the magnetic permeability that we set to unity, $\mu = 1$, since it is close to constant for most optical problems. Note, $\mathbf{E}^s = \mathbf{E} - \mathbf{E}^{inc}$ corresponds to the scattered field in the total-field/scattered-field formulation and the boundary condition can be employed to generate an incident wave [7]. We further assume that the electric permittivity equals unity, $\epsilon = 1$, in the vicinity of the computational boundary. We also assume that the interior forcing $\mathbf{j} = 0$, since the application of the Hagstrom-Warburton boundary condition to problems with light sources inside the domain would require a modification for evanescent waves [40], which we will not pursue here. We denote the unit vectors in the x, y, z direction, respectively, as $\hat{\mathbf{x}}, \hat{\mathbf{y}}, \hat{\mathbf{z}}$. The right boundary has outward unit normal vector $\hat{\mathbf{n}} = \hat{\mathbf{x}}$, and the left boundary $\hat{\mathbf{n}} = -\hat{\mathbf{x}}$. Let $E_x = \hat{\mathbf{x}} \cdot \mathbf{E}$, $E_y = \hat{\mathbf{y}} \cdot \mathbf{E}$, $E_z = \hat{\mathbf{z}} \cdot \mathbf{E}$ denote the electric field components in the Cartesian coordinate directions. To solve the time-harmonic Maxwell equations (5.31)-(5.32) in the interior of the domain, we employ a mixed DG discretization with Brezzi-type numerical fluxes and element-wise curl-conforming elements [6, 42], that will be

elaborated in the following Section.

The mixed formulation employs a Lagrange parameter p to enforce a discrete divergence free field. The mixed formulation has a spurious-free spectrum and there is a straightforward estimate for the penalty parameters [43]. In this mixed formulation we solve the time-harmonic Maxwell equations with a Lagrange multiplier term and nonreflecting boundary conditions:

$$\begin{aligned}
 \nabla \times \nabla \times \mathbf{E} - \omega^2 \epsilon \mathbf{E} - \epsilon \nabla p &= 0 & \text{in } \Omega, \\
 \nabla \cdot (\epsilon \mathbf{E}) &= 0 & \text{in } \Omega, \\
 \text{H-W condition for } \mathbf{E}^s & & \text{at } \partial\Omega_{NRBC}, \\
 p &= 0 & \text{at } \partial\Omega_{NRBC}, \\
 \text{periodic boundary conditions} & & \text{at } \partial\Omega_{periodic}.
 \end{aligned} \tag{5.33}$$

We will describe the Hagstrom-Warburton (H-W) boundary condition for Maxwell's equations in the following paragraphs.

To develop a nonreflecting boundary condition for the mixed problem (5.33), we use the fact that each field component E_x, E_y, E_z separately satisfies the scalar wave equation [33]

$$(\omega^2 + c^2 \partial_x^2 + c^2 \nabla_t^2) E_{x,y,z} = 0 \quad \text{in } \Omega.$$

In the present Chapter we develop the Hagstrom-Warburton boundary condition for order $P = 1$, where we choose $\theta_0 = 0$ and $\theta_1 = 0$ to reduce the number of tunable parameters in our calculations. In fact, we apply the Hagstrom-Warburton boundary condition only to the tangential components, as is done for the perfect electric conductor condition [8], but not for the Silver-Müller boundary condition [7]. We denote the first auxiliary variables (ϕ_1 in the Hagstrom-Warburton boundary condition (5.28)) corresponding to E_y, E_z with g_y, g_z . The Hagstrom-Warburton boundary condition equations (5.28) and (5.29) then give

$$\begin{aligned}
 (a_0 i \omega + c \partial_n) E_i^s &= i \omega g_i & \text{at } \partial\Omega, \quad i = y, z, \\
 -l_{1,0} \omega^2 E_i^s - l_{1,1} \omega^2 g_i &= c^2 (m_{1,0} \nabla_t^2 E_i^s + m_{1,1} \nabla_t^2 g_i) & \text{at } \partial\Omega, \quad i = y, z,
 \end{aligned} \tag{5.34}$$

with $\partial_n = \hat{\mathbf{n}} \cdot \nabla$ the normal derivative. Next, we will develop a DG discretization for the auxiliary equations (5.34) that is based on Bassi-Rebay type numerical fluxes [42]. We then obtain the following formulation of the time-harmonic Maxwell equations

$$\nabla \times \nabla \times \mathbf{E} - \omega^2 \epsilon \mathbf{E} - \epsilon \nabla p = 0, \quad \text{in } \Omega, \tag{5.35}$$

$$\nabla \cdot (\epsilon \mathbf{E}) = 0, \quad \text{in } \Omega, \tag{5.36}$$

with Hagstrom-Warburton nonreflecting boundary conditions for $i = y, z$

$$(a_0 i\omega + \partial_n)E_i^s = i\omega g_i, \quad \text{at } \partial\Omega_{NRBC}, \quad (5.37)$$

$$\begin{aligned} -l_{1,0}\omega^2 E_i^s - l_{1,1}\omega^2 g_i &= c^2(m_{1,0}\partial_y \lambda^{i,y} + m_{1,0}\partial_z \lambda^{i,z} \\ &+ m_{1,1}\partial_y \sigma^{i,y} + m_{1,1}\partial_z \sigma^{i,z}), \quad \text{at } \partial\Omega_{NRBC}, \end{aligned} \quad (5.38)$$

$$p = 0, \quad \text{at } \partial\Omega_{NRBC}, \quad (5.39)$$

$$\text{periodic boundary conditions} \quad \text{at } \partial\Omega_{\text{periodic}}, \quad (5.40)$$

and auxiliary variables

$$\sigma^{i,y} = \partial_y g_i, \quad \text{at } \partial\Omega_{NRBC}, \quad (5.41)$$

$$\sigma^{i,z} = \partial_z g_i, \quad \text{at } \partial\Omega_{NRBC}, \quad (5.42)$$

$$\lambda^{i,y} = \partial_y E_i^s, \quad \text{at } \partial\Omega_{NRBC}, \quad (5.43)$$

$$\lambda^{i,z} = \partial_z E_i^s, \quad \text{at } \partial\Omega_{NRBC}. \quad (5.44)$$

In the next section we will discuss the numerical discretization of these equations using a mixed discontinuous Galerkin discretization.

5.4 Mixed discontinuous Galerkin discretization using Brezzi-type numerical fluxes

In this Section we will summarize the mixed DG discretization for Eqns. (5.35)-(5.36) using Brezzi-type numerical fluxes and element-wise curl-conforming elements [2, 6, 42] in the interior of the domain. The mixed DG method is based on the work by Houston *et al.* [2] and Lu *et al.* [6], but we use Brezzi-type numerical fluxes instead of interior penalty fluxes [42]. The advantage of using Brezzi-type numerical fluxes is that they allow a straightforward estimate of the penalty parameters that appear in the DG discretization [43]. In contrast, the stability of the interior penalty method in [2, 6] depends on a careful selection of the penalty parameters that is dependent on the mesh resolution h , and suitable estimates have not yet been derived [6]. We have implemented the mixed DG discretization with Brezzi-type numerical fluxes with periodic and perfectly conducting boundary conditions in a parallel implementation and tested it on 3D computations of photonic crystals [44]. In the mixed discretization with Hagstrom-Warburton boundary conditions, we employ numerical fluxes that are suitable for a natural boundary condition [42]. The combination of the mixed DG discretization with the Hagstrom-Warburton boundary condition (5.37) will be discussed in Section 5.5. For the discretization, we use a mesh with tetrahedral elements.

Let $\mathcal{T}_h$ denote the set of elements in the computational domain. The mesh size is defined as $h = \max_{T \in \mathcal{T}_h} h_T$, where h_T is the radius of the element $T \in \mathcal{T}_h$. We will employ element-wise curl-conforming elements for the electric field $\mathbf{E}$ in the discretization. Let $K \in \mathcal{T}_h$ denote an element. Let $P_l(K)$ be the set of local polynomials of degree less than or equal to l on K . We denote the space of

elementwise Nédélec basis functions [32] of the first kind of order l by $\mathbf{V}_h^l$ by

$$\mathbf{V}_h^l \equiv \{\mathbf{v} \in L^2(\Omega)^3 : \mathbf{v}|_K \in \mathbf{S}^l(K), \forall K \in \mathcal{T}_h\}.$$

The functions in $\mathbf{S}^l(K)$ have the form $\mathbf{a}(\mathbf{x}) + \mathbf{b}(\mathbf{x}) \times \mathbf{x}$ with $\mathbf{a}, \mathbf{b} \in (P_l(K))^3$. In our 3D computations these basis functions have been implemented using the procedure proposed by Gopalakrishnan *et al.* [45], and in our 2D computations following Rapetti and Bossavit [46].

For the Lagrange parameter p we use nodal Lagrangian elements. We define the space of elementwise polynomial functions of order less than or equal to l as $Q_{h,d}^l$, and the space of polynomial functions of order less than or equal to l on the boundary faces as $Q_{h,d-1}^l$

$$\begin{aligned} Q_{h,d}^l &\equiv \{q \in L^2(\Omega) : q|_K \in P^l(K), \forall K \in \mathcal{T}_h\}, \\ Q_{h,d-1}^l &\equiv \{q \in L^2(\partial\Omega) : q|_F \in P^l(F), \forall F \in \mathcal{F}_h^b\}, \end{aligned}$$

with $d = \dim(\Omega)$ the dimension. The space $Q_{h,d-1}^l$ will be employed in the next section for the discretization of the Hagstrom-Warburton nonreflecting boundary condition.

We next introduce some DG notation. Let $\mathcal{F}_h$ denote the set of all faces in the domain, $\mathcal{F}_h^i$ the set of interior faces, and $\mathcal{F}_h^b$ the set of boundary faces. To account for multi-valued traces in the DG formulation at element faces of two neighbouring elements $T^L, T^R \in \mathcal{T}_h$ we use the standard jump and average operators. To define these let $\hat{\mathbf{n}}^{L,R}$ be the outward pointing unit normal to the elements $T^{L,R}$, let $\mathbf{v}$ and q , respectively, be a vector valued and scalar function with the traces at $T^{L,R}$ denoted as $\mathbf{v}^{L,R}$ and $q^{L,R}$. Then we define the following jumps and averages

$$\begin{aligned} \llbracket \mathbf{v} \rrbracket_T &= \hat{\mathbf{n}}^L \times \mathbf{v}^L + \hat{\mathbf{n}}^R \times \mathbf{v}^R, & F \in \mathcal{F}_h^i, \\ \llbracket \mathbf{v} \rrbracket_N &= \hat{\mathbf{n}}^L \cdot \mathbf{v}^L + \hat{\mathbf{n}}^R \cdot \mathbf{v}^R, & F \in \mathcal{F}_h^i, \end{aligned} \quad (5.45)$$

$$\llbracket q \rrbracket = q^L \hat{\mathbf{n}}^L + q^R \hat{\mathbf{n}}^R, \quad F \in \mathcal{F}_h^i, \quad (5.46)$$

$$\{\!\!\{ \mathbf{v} \}\!\!\} = \frac{1}{2}(\mathbf{v}^L + \mathbf{v}^R), \quad F \in \mathcal{F}_h^i, \quad (5.47)$$

$$\{\!\!\{ q \}\!\!\} = \frac{1}{2}(q^L + q^R), \quad F \in \mathcal{F}_h^i,$$

while for boundary faces, where $\mathbf{v}$ and q are single valued, they are defined as

$$\begin{aligned} \llbracket \mathbf{v} \rrbracket_T &= \hat{\mathbf{n}}^L \times \mathbf{v}^L, & F \in \mathcal{F}_h^b, \\ \llbracket \mathbf{v} \rrbracket_N &= \hat{\mathbf{n}}^L \cdot \mathbf{v}^L, & F \in \mathcal{F}_h^b, \end{aligned} \quad (5.48)$$

$$\llbracket q \rrbracket = q^L \hat{\mathbf{n}}^L, \quad F \in \mathcal{F}_h^b, \quad (5.49)$$

$$\{\!\!\{ \mathbf{v} \}\!\!\} = \mathbf{v}^L, \quad F \in \mathcal{F}_h^b, \quad (5.50)$$

$$\{\!\!\{ q \}\!\!\} = q^L, \quad F \in \mathcal{F}_h^b.$$

A detailed derivation of the mixed DG method of Lu *et al.* [6] for the time-harmonic Maxwell equations using the interior penalty numerical flux is given in the thesis by Devashish [47]. The derivation of the mixed DG method using Brezzi-type numerical fluxes will be given in Appendix 5.A. The DG discretization requires the definition of lifting operators. Let $(\cdot, \cdot)_\Omega$ denote the L^2 -inner product over the domain Ω

$$(\mathbf{u}, \mathbf{v})_\Omega = \int_\Omega \mathbf{u} \cdot \mathbf{v} dV.$$

We define the global lifting operators $\mathcal{L} : [L^2(\mathcal{F}_h^i)]^3 \rightarrow \mathbf{V}_h^l$, $\mathcal{R} : [L^2(\mathcal{F}_h)]^3 \rightarrow \mathbf{V}_h^l$, and the local lifting operators $\mathcal{R}_F : [L^2(F)]^3 \rightarrow \mathbf{V}_h^l$ and $\mathcal{S}_F : L^2(F) \rightarrow Q_{h,d}^l$ for a single face $F \in \mathcal{F}_h$ by

$$(\mathcal{L}(\mathbf{u}), \mathbf{w})_\Omega = \sum_{F \in \mathcal{F}_h^i} \int_F \mathbf{u} \cdot \llbracket \mathbf{w} \rrbracket_T dS \quad \forall \mathbf{w} \in \mathbf{V}_h^l, \quad (5.51)$$

$$(\mathcal{R}(\mathbf{u}), \mathbf{w})_\Omega = \sum_{F \in \mathcal{F}_h} \int_F \mathbf{u} \cdot \{\!\!\{ \mathbf{w} \}\!\!\} dS \quad \forall \mathbf{w} \in \mathbf{V}_h^l, \quad (5.52)$$

$$(\mathcal{R}_F(\mathbf{u}), \mathbf{v})_\Omega = \int_F \mathbf{u} \cdot \{\!\!\{ \mathbf{v} \}\!\!\} dS \quad \forall \mathbf{v} \in \mathbf{V}_h^l, \quad (5.53)$$

$$(\mathcal{S}_F(p), q)_\Omega = \int_F p \{\!\!\{ q \}\!\!\} dS \quad \forall q \in Q_{h,d}^l.$$

We now give the weak formulation of the mixed Maxwell equations (5.35), (5.36), and (5.40). Note, the weak formulation is still incompletely specified since the Hagstrom-Warburton boundary condition is not included yet. Define the following bilinear forms: $a_h : \mathbf{V}_h^l \times \mathbf{V}_h^l$, $b_h : \mathbf{V}_h^l \times Q_{h,d}^l$, and $c_h : Q_{h,d}^l \times Q_{h,d}^l$ as:

$$\begin{aligned} a_h(\mathbf{E}_h, \mathbf{v}) &= (\nabla_h \times \mathbf{E}_h, \nabla_h \times \mathbf{v})_\Omega \\ &\quad - \sum_{F \in \mathcal{F}_h^i} \int_F \llbracket \mathbf{E}_h \rrbracket_T \cdot \{\!\!\{ \nabla_h \times \mathbf{v} \}\!\!\} dS \\ &\quad - \sum_{F \in \mathcal{F}_h} \int_F \{\!\!\{ \nabla_h \times \mathbf{E}_h \}\!\!\} \cdot \llbracket \mathbf{v} \rrbracket_T dS \\ &\quad + \sum_{F \in \mathcal{F}_h^i} \sum_{T \in \mathcal{T}_h} (\alpha_F + n_T) (\mathcal{R}_F(\llbracket \mathbf{E}_h \rrbracket_T), \mathcal{R}_F(\llbracket \mathbf{v} \rrbracket_T))_T \\ &\quad + \sum_{F \in \mathcal{F}_h^i} \beta_F (\mathcal{S}_F(\llbracket \epsilon \mathbf{E}_h \rrbracket_N), \mathcal{S}_F(\llbracket \epsilon \mathbf{v} \rrbracket_N))_\Omega, \\ b_h(\mathbf{v}, p_h) &= -(\nabla_h p_h, \epsilon \mathbf{v})_\Omega \\ &\quad + \sum_{F \in \mathcal{F}_h} \int_F \llbracket p_h \rrbracket_T \cdot \{\!\!\{ \epsilon \mathbf{v} \}\!\!\} dS, \end{aligned} \quad (5.54)$$

$$c_h(p_h, q) = \sum_{F \in \mathcal{F}_h} \int_{\Omega} \gamma_F \mathcal{R}_F(\llbracket q \rrbracket_T) \cdot \mathcal{R}_F(\llbracket p_h \rrbracket_T) d\Omega.$$

The mixed DG formulation for the time-harmonic Maxwell equations (except for the Hagstrom-Warburton boundary condition) is then: find $(\mathbf{E}_h, p_h) \in \mathbf{V}_h^l \times Q_{h,d}^l$ such that

$$\begin{aligned} a_h(\mathbf{E}_h, \mathbf{v}_h) - \omega^2(\epsilon \mathbf{E}_h, \mathbf{v}_h)_{\Omega} + b_h(\mathbf{v}_h, p_h) &= (\mathbf{j}, \mathbf{v}_h)_{\Omega} \\ b_h(\mathbf{E}_h, q_h) - c_h(p_h, q_h) &= 0, \end{aligned} \quad (5.55)$$

for all $(\mathbf{v}_h, q_h) \in \mathbf{V}_h^l \times Q_{h,d}^l$. The bilinear form a_h corresponds to a Brezzi-type discretization of the curl-curl operator with an additional normal jump penalization using a lifting operator. The bilinear form b_h discretizes the divergence constraint in the mixed Maxwell equations using a discontinuous Galerkin scheme. The bilinear form c_h is a stabilization term, which penalizes jumps in the Lagrange parameter p by means of lifting operators. The parameters $\alpha_F, \beta_F, \gamma_F$ are nonnegative penalty parameters, which potentially depend on the mesh size and polynomial order.

To determine suitable penalty parameters, we consider the fact that an interior penalty DG discretization [6] can be obtained from Eq. (5.54) by replacing $\mathcal{R}_F$ and $\mathcal{S}_F$ with the identity operator. In analogy with the corresponding IP parameters [6], a constraint on the penalty parameters is then $\alpha_F > 0, \beta_F > 0, \gamma_F > 0$, sufficiently large. For a suitable choice of function spaces, this can be relaxed to $\alpha_F > 0, \beta_F = 0, \gamma_F > 0$ [3]. For the Brezzi numerical flux it is known that α should be strictly larger than n_T , $n_T = 4$ in 3D [48], where n_T is the number of faces of an element. We have therefore used the following penalty parameters in all calculations: $\alpha_F = 5, \beta_F = 0$, and $\gamma_F = 5$. In the next section we will derive a DG discretization of the Hagstrom-Warburton boundary condition in combination with the mixed DG discretization discussed in this Section.

5.5 Discretization of Hagstrom-Warburton boundary condition

In this Section we combine the mixed DG formulation (5.54) with the Hagstrom-Warburton boundary condition (5.37)-(5.44). We will develop a DG discretization of the auxiliary equations (5.34)-(5.44) that is based on Bassi-Rebay type numerical fluxes [42]. In this discretization, we employ nodal elements for the

auxiliary variables for $i = y, z$

$$\begin{aligned} g_i &\rightarrow g_{i,h} \in Q_{h,d-1}^l, \\ \sigma^{i,y} &\rightarrow \sigma_h^{i,y} \in Q_{h,d-1}^l, \\ \sigma^{i,z} &\rightarrow \sigma_h^{i,z} \in Q_{h,d-1}^l, \\ \lambda^{i,y} &\rightarrow \lambda_h^{i,y} \in Q_{h,d-1}^l, \\ \lambda^{i,z} &\rightarrow \lambda_h^{i,z} \in Q_{h,d-1}^l. \end{aligned}$$

In the variational formulation, we employ corresponding test functions

$$\psi_h^i, \xi_h^{i,y}, \xi_h^{i,z}, \zeta_h^{i,y}, \zeta_h^{i,z} \in Q_{h,d-1}^l \quad i = y, z. \quad (5.56)$$

The auxiliary variables are coupled with the mixed DG discretization (5.55) by means of the Hagstrom-Warburton equation (5.37). Since we will be working with vector expressions, we rewrite Eq. (5.37) here in vector form

$$(\partial_n + i\omega)((\hat{\mathbf{n}} \times \mathbf{E}) \times \hat{\mathbf{n}}) = i\omega g_y \hat{\mathbf{y}} + i\omega g_z \hat{\mathbf{z}}, \quad (5.57)$$

where we assumed $\mathbf{E}^{inc} = 0$. The discretization for a nonzero incident field is similar and will not be given here. The Hagstrom-Warburton boundary condition (5.57) will be applied to the boundary part of the integral (5.54) in the mixed DG discretization. This will be our starting point and we simplify this expression into

$$- \sum_{F \in \mathcal{F}_h^b} \int_F \{\{\nabla_h \times \mathbf{E}_h\}\} \cdot \llbracket \mathbf{v} \rrbracket_T dS = \sum_{F \in \mathcal{F}_h^b} \int_F (\hat{\mathbf{n}} \times \nabla_h \times \mathbf{E}_h) \cdot \mathbf{v}_h dS. \quad (5.58)$$

5.5.1 Discretization of first two equations

The derivations in this Section are for a planar boundary $x = \text{constant}$. The relations for computational boundaries $y = \text{constant}$ or $z = \text{constant}$ can be obtained analogously. Since boundary condition (5.57) is applied to the tangential components of the field, it is beneficial to use such a decomposition of the electric field. It is well-known that we can decompose a vector field into a normal and a tangential component using the vector triple product

$$\mathbf{E}_h = (\mathbf{E}_h \cdot \hat{\mathbf{n}})\hat{\mathbf{n}} + (\hat{\mathbf{n}} \times \mathbf{E}_h) \times \hat{\mathbf{n}}. \quad (5.59)$$

We substitute decomposition (5.59) into an expression for the cross product of the unit normal vector and the field appearing in Eq. (5.58), resulting in

$$\hat{\mathbf{n}} \times \nabla_h \times \mathbf{E}_h = \hat{\mathbf{n}} \times \nabla_h \times ((\mathbf{E}_h \cdot \hat{\mathbf{n}})\hat{\mathbf{n}} + (\hat{\mathbf{n}} \times \mathbf{E}_h) \times \hat{\mathbf{n}}). \quad (5.60)$$

For the first term on the right-hand side of Eq. (5.60) we apply the vector calculus identity

$$\nabla_h \times ((\mathbf{E}_h \cdot \hat{\mathbf{n}})\hat{\mathbf{n}}) = (\mathbf{E}_h \cdot \hat{\mathbf{n}})(\nabla_h \times \hat{\mathbf{n}}) + (\nabla_h(\mathbf{E}_h \cdot \hat{\mathbf{n}})) \times \hat{\mathbf{n}},$$

where the first term on the right hand side is zero since $\hat{\mathbf{n}}$ is constant at the boundary $x = \text{constant}$. The first term on the right-hand side of Eq. (5.60) then becomes

$$\hat{\mathbf{n}} \times \nabla_h \times ((\mathbf{E}_h \cdot \hat{\mathbf{n}})\hat{\mathbf{n}}) = (\hat{\mathbf{n}} \times \nabla_h(\mathbf{E}_h \cdot \hat{\mathbf{n}})) \times \hat{\mathbf{n}}, \quad (5.61)$$

where we used the anticommutativity of the inner product twice. For the second term on the right-hand side of Eq. (5.60) we use the identity

$$\begin{aligned} \nabla_h \times ((\hat{\mathbf{n}} \times \mathbf{E}_h) \times \hat{\mathbf{n}}) &= (\hat{\mathbf{n}} \times \mathbf{E}_h)(\nabla_h \cdot \hat{\mathbf{n}}) - \hat{\mathbf{n}}(\nabla_h \cdot (\hat{\mathbf{n}} \times \mathbf{E}_h)) \\ &\quad + (\hat{\mathbf{n}} \cdot \nabla_h)(\hat{\mathbf{n}} \times \mathbf{E}_h) - ((\hat{\mathbf{n}} \times \mathbf{E}_h) \cdot \nabla_h)\hat{\mathbf{n}} \\ &= -\hat{\mathbf{n}}(\nabla_h \cdot (\hat{\mathbf{n}} \times \mathbf{E}_h)) + (\hat{\mathbf{n}} \cdot \nabla_h)(\hat{\mathbf{n}} \times \mathbf{E}_h). \end{aligned} \quad (5.62)$$

Taking the cross product of the unit normal vector with Eq. (5.62) we find for the second term on the right-hand side of Eq. (5.60)

$$\hat{\mathbf{n}} \times \nabla_h \times ((\hat{\mathbf{n}} \times \mathbf{E}_h) \times \hat{\mathbf{n}}) = -(\hat{\mathbf{n}} \cdot \nabla_h)((\hat{\mathbf{n}} \times \mathbf{E}_h) \times \hat{\mathbf{n}}). \quad (5.63)$$

Substituting Eq. (5.61) and Eq. (5.63) into the right-hand side of Eq. (5.60) we obtain an expression for the cross product of the unit normal vector with the curl of the field at a planar computational boundary $x = \text{constant}$

$$\hat{\mathbf{n}} \times \nabla_h \times \mathbf{E}_h = (\hat{\mathbf{n}} \times \nabla_h(\mathbf{E}_h \cdot \hat{\mathbf{n}})) \times \hat{\mathbf{n}} - (\hat{\mathbf{n}} \cdot \nabla_h)((\hat{\mathbf{n}} \times \mathbf{E}_h) \times \hat{\mathbf{n}}) \quad (5.64)$$

Now that we have a suitable decomposition of the field we can apply the Hagstrom-Warburton boundary condition. Applying boundary condition (5.57) to the second term on the right-hand side of Eq. (5.64) we find

$$\begin{aligned} \hat{\mathbf{n}} \times \nabla_h \times \mathbf{E}_h &= (\hat{\mathbf{n}} \times \nabla_h(\mathbf{E}_h \cdot \hat{\mathbf{n}})) \times \hat{\mathbf{n}} \\ &\quad + i\omega(\hat{\mathbf{n}} \times \mathbf{E}_h) \times \hat{\mathbf{n}} - i\omega g_{y,h}\hat{\mathbf{y}} - i\omega g_{z,h}\hat{\mathbf{z}}. \end{aligned}$$

Denote $v_{h,y}$ and $v_{h,z}$ the y - and z -components of $\mathbf{v}_h$. We then obtain for the boundary term in Eq. (5.58) that

$$\begin{aligned} \sum_{F \in \mathcal{F}_h^b} \int_F (\hat{\mathbf{n}} \times (\nabla_h \times \mathbf{E}_h)) \cdot \mathbf{v}_h dS &= \sum_{F \in \mathcal{F}_h^b} \int_F ((\hat{\mathbf{n}} \times \nabla_h(\mathbf{E}_h \cdot \hat{\mathbf{n}})) \times \hat{\mathbf{n}}) \cdot \mathbf{v}_h dS \\ &\quad + i\omega \sum_{F \in \mathcal{F}_h^b} \int_F ((\hat{\mathbf{n}} \times \mathbf{E}_h) \times \hat{\mathbf{n}}) \cdot \mathbf{v}_h dS - i\omega \sum_{F \in \mathcal{F}_h^b} \int_F (g_{y,h}v_{h,y} + g_{z,h}v_{h,z}) dS. \end{aligned} \quad (5.65)$$

The first term on the right hand side of Eq. (5.65) we denote “remainder term”. To obtain a stable discretization of this term, we need to connect the

normal component of $\mathbf{E}_h$ across adjacent faces at the computational boundary. In 3D as we consider here, the interface between two boundary faces is an edge. Whereas it is common to have integrals over faces in DG methods in 3D, it is less common to have integrals over edges as well. We therefore need to introduce some new DG notation. Some of the notation is illustrated in Fig. 5.3. Let $\partial\mathcal{F}_h^b$

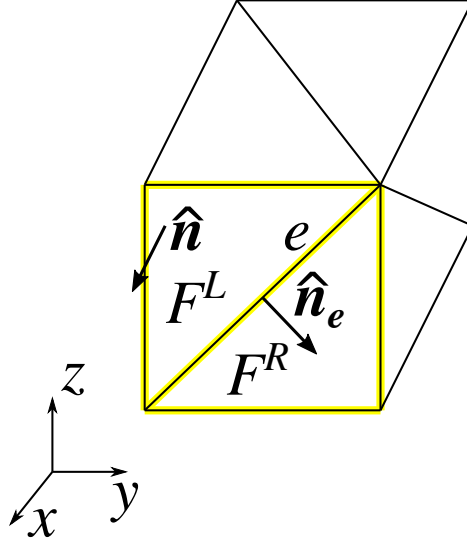


Figure 5.3: Block of five tetrahedra, where two tetrahedra have faces F^L and F^R that lie on the computational boundary. The edges in $\partial F^{L,R}$ are indicated in yellow. The unit normal vector $\hat{\mathbf{n}}$ out of Ω is shown. The edge e with adjacent faces F^L and F^R is indicated. The unit normal vector $\hat{\mathbf{n}}_e$ pointing out of F^L is also indicated.

be the set of edges on the computational boundary. Consider an edge $e \in \partial\mathcal{F}_h^b$ between face F^L and face F^R , and let $\hat{\mathbf{n}}_e^L$ and $\hat{\mathbf{n}}_e^R$ represent their respective outward pointing normal vectors inside the domain boundary. We define the y -jump, the z -jump, and the average of the scalar quantity v across edge e , and the normal jump of the vector quantity $\mathbf{v}$, respectively, as

$$[v]_{e,y} = \hat{\mathbf{n}}_{e,y}^L v^L + \hat{\mathbf{n}}_{e,y}^R v^R, \quad (5.66)$$

$$[v]_{e,z} = \hat{\mathbf{n}}_{e,z}^L v^L + \hat{\mathbf{n}}_{e,z}^R v^R, \quad (5.67)$$

$$\langle\!\langle v \rangle\!\rangle_e = (v^L + v^R)/2, \quad (5.68)$$

$$[\mathbf{v}]_{N,e} = \hat{\mathbf{n}}^L \cdot \mathbf{v}^L + \hat{\mathbf{n}}^R \cdot \mathbf{v}^R. \quad (5.69)$$

Here v^L and v^R are the values of the trace of v at ∂F^L and ∂F^R , respectively, and $\mathbf{v}^L$ and $\mathbf{v}^R$ are the values of the trace of $\mathbf{v}$ at ∂F^L , ∂F^R . Let $\partial_{h,x}$ and $\partial_{h,y}$ be the elementwise derivative operators.

We first evaluate the “remainder term” in Eq. (5.65). We start by evaluating

the expression involving the cross product of the unit normal and gradient

$$(\hat{\mathbf{n}} \times \nabla_h(\mathbf{E}_h \cdot \hat{\mathbf{n}})) \times \hat{\mathbf{n}} = \hat{\mathbf{y}}(n\partial_{h,y}E_{h,x}) + \hat{\mathbf{z}}(n\partial_{h,z}E_{h,x}),$$

with $n = \pm 1$ for the right and left boundary respectively. We then find the following expression for the “remainder term” in Eq. (5.65), and we apply integration by parts twice

$$\begin{aligned} & \sum_{F \in \mathcal{F}_h^b} \int_F ((\hat{\mathbf{n}} \times \nabla_h(\mathbf{E}_h \cdot \hat{\mathbf{n}})) \times \hat{\mathbf{n}}) \cdot \mathbf{v}_h dS \\ &= \sum_{F \in \mathcal{F}_h^b} \int_F \left((n\partial_{h,y}E_{h,x})v_{h,y} + (n\partial_{h,z}E_{h,x})v_{h,z} \right) dS \\ &+ \sum_{F \in \mathcal{F}_h^b} \int_{\partial F} \left(\hat{n}_{e,y}n(E_{h,x}^* - E_{h,x})v_{h,y} + \hat{n}_{e,z}n(E_{h,x}^* - E_{h,x})v_{h,z} \right) dl. \end{aligned} \quad (5.70)$$

We then apply the identities for $i = y, z$

$$\begin{aligned} \sum_{F \in \mathcal{F}_h^b} \int_{\partial F} \hat{n}_{e,i}(E_{h,x}^* - E_{h,x})v_{h,i} dl &= \sum_{e \in \partial \mathcal{F}_h^b} \int_e \left(\llbracket E_{h,x}^* - E_{h,x} \rrbracket_{e,i} \{ \{ v_{h,i} \} \}_e \right. \\ &\quad \left. + \{ \{ E_{h,x}^* - E_{h,x} \} \}_e \llbracket v_{h,i} \rrbracket_{e,i} \right) dl. \end{aligned} \quad (5.71)$$

These relations can be directly proven by inserting the jump relations (5.66)-(5.69) into Eq. (5.71). If we use the central numerical flux

$$E_{h,x}^* = \{ \{ E_{h,x} \} \}_e,$$

then we obtain the following expression for the “remainder term” in Eq. (5.65)

$$\begin{aligned} & \sum_{F \in \mathcal{F}_h^b} \int_F ((\hat{\mathbf{n}} \times \nabla_h(\mathbf{E}_h \cdot \hat{\mathbf{n}})) \times \hat{\mathbf{n}}) \cdot \mathbf{v}_h dS \\ &= \sum_{F \in \mathcal{F}_h^b} \int_F \left((n\partial_{h,y}E_{h,x})v_{h,y} + (n\partial_{h,z}E_{h,x})v_{h,z} \right) dS \\ &- \sum_{e \in \partial \mathcal{F}_h^b} \int_e \left(\llbracket nE_{h,x} \rrbracket_{e,y} \{ \{ v_{h,y} \} \}_e + \llbracket nE_{h,x} \rrbracket_{e,z} \{ \{ v_{h,z} \} \}_e \right) dl \end{aligned} \quad (5.72)$$

In our numerical tests we found that connecting the normal component of $\mathbf{E}_h$ across adjacent faces on the computational boundary is not sufficient for stability. To obtain a stable discretization of the Hagstrom-Warburton equation (5.57) we need to add a stabilization term *directly to the discretization* of the boundary

term Eq. (5.58), namely

$$\sum_{e \in \partial \mathcal{F}_h^b} \int_e (a/h^2) \llbracket \mathbf{E}_h \rrbracket_{N,e} \llbracket \mathbf{v}_h \rrbracket_{N,e} dl. \quad (5.73)$$

Numerical experiments show that $a = 1$ gives stable results in our numerical tests.

In summary, we have found the following discretization of the boundary term (5.58) in the mixed DG discretization that implements the Hagstrom-Warburton boundary condition at a planar computational boundary $x = \text{constant}$

$$\begin{aligned} & \sum_{F \in \mathcal{F}_h^b} \int_F (\hat{\mathbf{n}} \times \nabla_h \times \mathbf{E}_h) \cdot \mathbf{v}_h dS \\ &= \sum_{F \in \mathcal{F}_h^b} \int_F \left((n \partial_{h,y} E_{h,x}) v_{h,y} + (n \partial_{h,z} E_{h,x}) v_{h,z} \right) dS \\ & - \sum_{e \in \partial \mathcal{F}_h^b} \int_e \left(\llbracket n E_{h,x} \rrbracket_{e,y} \{v_{h,y}\}_e + \llbracket n E_{h,x} \rrbracket_{e,z} \{v_{h,z}\}_e \right) dl \\ & + i\omega \sum_{F \in \mathcal{F}_h^b} \int_F ((\hat{\mathbf{n}} \times \mathbf{E}_h) \times \hat{\mathbf{n}}) \cdot \mathbf{v}_h dS \\ & - i\omega \sum_{F \in \mathcal{F}_h^b} \int_F (g_{y,h} v_{h,y} + g_{z,h} v_{h,z}) dS \\ & + \sum_{e \in \partial \mathcal{F}_h^b} \int_e (a/h^2) \llbracket \mathbf{E}_h \rrbracket_{N,e} \llbracket \mathbf{v}_h \rrbracket_{N,e} dl. \end{aligned} \quad (5.74)$$

5.5.2 Discretization of auxiliary equations

In this section we discretize the Hagstrom-Warburton auxiliary equation (5.38) with Bassi-Rebay type numerical fluxes [42]. We multiply Eq. (5.38) with scalar-valued test functions $\psi_h^i \in Q_{h,d-1}^l$, and integrate over all the boundary faces in $\mathcal{F}_h^b$

$$\begin{aligned} & \sum_{F \in \mathcal{F}_h^b} \int_F (-l_{1,0} \omega^2 E_{h,i} \psi_h^i - l_{1,1} \omega^2 g_{i,h} \psi_h^i) dA \\ &= \sum_{F \in \mathcal{F}_h^b} \int_F c^2 (m_{1,0} (\partial_y \lambda_h^{i,y}) \psi_h^i + m_{1,0} (\partial_z \lambda_h^{i,z}) \psi_h^i \\ & + m_{1,1} (\partial_y \sigma_h^{i,y}) \psi_h^i + m_{1,1} (\partial_z \sigma_h^{i,z}) \psi_h^i) dA \quad i = y, z. \end{aligned} \quad (5.75)$$

In order to obtain a Bassi-Rebay type discretization, we integrate the integral in the first term on the right of Eq. (5.75) by parts, express the sum over boundaries into a sum over face edges, analogous to Eq. (5.71), and use a central numerical

flux,

$$\lambda_h^{i,y*} = \{\!\!\{\lambda_h^{i,y}\}\!\!\}_e \quad i = y, z,$$

resulting for the first term on the right of Eq. (5.75) in

$$\begin{aligned} \sum_{F \in \mathcal{F}_h^b} \int_F (\partial_y \lambda_h^{i,y}) \psi_h^i dA &= - \sum_{F \in \mathcal{F}_h^b} \int_F \lambda_h^{i,y} \partial_y \psi_h^i dA \\ &\quad + \int_{\partial \mathcal{F}_h^b} \{\!\!\{\lambda_h^{i,y}\}\!\!\}_e \llbracket \psi_h^i \rrbracket_{e,y} dl \quad i = y, z. \end{aligned}$$

We also apply the same procedure to the other terms in the auxiliary equations for the Hagstrom-Warburton boundary condition. After combining all terms this results in the following DG discretization of the auxiliary equations

$$\begin{aligned} &\sum_{F \in \mathcal{F}_h^b} \int_F (-l_{1,0} \omega^2 E_{h,i} \psi_h^i - l_{1,1} \omega^2 g_{i,h} \psi_h^i) dA \\ &+ \sum_{F \in \mathcal{F}_h^b} \int_F \left(c^2 m_{1,0} \lambda_h^{i,y} \partial_y \psi_h^i + c^2 m_{1,0} \lambda_h^{i,z} \partial_z \psi_h^i \right. \\ &\quad \left. + c^2 m_{1,1} \sigma_h^{i,y} \partial_y \psi_h^i + c^2 m_{1,1} \sigma_h^{i,z} \partial_z \psi_h^i \right) dA \\ &- \sum_{e \in \partial \mathcal{F}_h^b} \int_e \left(c^2 m_{1,0} \{\!\!\{\lambda_h^{i,y}\}\!\!\}_e \llbracket \psi_h^i \rrbracket_{e,y} + c^2 m_{1,0} \{\!\!\{\lambda_h^{i,z}\}\!\!\}_e \llbracket \psi_h^i \rrbracket_{e,z} \right. \\ &\quad \left. + c^2 m_{1,1} \{\!\!\{\sigma_h^{i,y}\}\!\!\}_e \llbracket \psi_h^i \rrbracket_{e,y} + c^2 m_{1,1} \{\!\!\{\sigma_h^{i,z}\}\!\!\}_e \llbracket \psi_h^i \rrbracket_{e,z} \right) dl = 0 \quad i = y, z. \end{aligned}$$

For the discretization of the auxiliary variables $\sigma_h^{i,y}, \sigma_h^{i,z}, \lambda_h^{i,y}, \lambda_h^{i,z}$, given by Eqns. (5.41)-(5.44), we follow the same procedure used for the auxiliary equations in the Hagstrom-Warburton boundary condition, but we perform a second integration by parts. This results in the following equations for $i = y, z$

$$\begin{aligned} \sum_{F \in \mathcal{F}_h^b} \int_F \sigma_h^{i,y} \xi_h^{i,y} dA &= \sum_{F \in \mathcal{F}_h^b} \int_F (\partial_y g_{i,h}) \xi_h^{i,y} dA - \sum_{e \in \partial \mathcal{F}_h^b} \int_e \llbracket g_{i,h} \rrbracket_{e,y} \{\!\!\{\xi_h^{i,y}\}\!\!\}_e dl, \\ \sum_{F \in \mathcal{F}_h^b} \int_F \sigma_h^{i,z} \xi_h^{i,z} dA &= \sum_{F \in \mathcal{F}_h^b} \int_F (\partial_z g_{i,h}) \xi_h^{i,z} dA - \sum_{e \in \partial \mathcal{F}_h^b} \int_e \llbracket g_{i,h} \rrbracket_{e,z} \{\!\!\{\xi_h^{i,z}\}\!\!\}_e dl, \\ \sum_{F \in \mathcal{F}_h^b} \int_F \lambda_h^{i,y} \zeta_h^{i,y} dA &= \sum_{F \in \mathcal{F}_h^b} \int_F \partial_y E_{h,i} \zeta_h^{i,y} dA - \sum_{e \in \partial \mathcal{F}_h^b} \int_e \llbracket E_{h,i} \rrbracket_{e,y} \{\!\!\{\zeta_h^{i,y}\}\!\!\}_e dl, \\ \sum_{F \in \mathcal{F}_h^b} \int_F \lambda_h^{i,z} \zeta_h^{i,z} dA &= \sum_{F \in \mathcal{F}_h^b} \int_F \partial_z E_{h,i} \zeta_h^{i,z} dA - \sum_{e \in \partial \mathcal{F}_h^b} \int_e \llbracket E_{h,i} \rrbracket_{e,z} \{\!\!\{\zeta_h^{i,z}\}\!\!\}_e dl. \end{aligned}$$

Finally, we add the following additional stabilization terms to the left hand

side of the mixed DG formulation (5.55)

$$\begin{aligned} \sum_{e \in \partial \mathcal{F}_h^b} \int_e (a/h^2) & \left([g_{i,h}]_{e,y} [\psi_h^i]_{e,y} + [g_{i,h}]_{e,z} [\psi_h^i]_{e,z} + [\sigma_h^{i,y}]_{e,y} [\xi_h^{i,y}]_{e,y} \right. \\ & + [\sigma_h^{i,y}]_{e,z} [\xi_h^{i,y}]_{e,z} + [\sigma_h^{i,z}]_{e,y} [\xi_h^{i,z}]_{e,y} + [\sigma_h^{i,z}]_{e,z} [\xi_h^{i,z}]_{e,z} + [\lambda_h^{i,y}]_{e,y} [\lambda_h^{i,y}]_{e,y} \\ & \left. + [\lambda_h^{i,y}]_{e,z} [\lambda_h^{i,y}]_{e,z} + [\lambda_h^{i,z}]_{e,y} [\lambda_h^{i,z}]_{e,y} + [\lambda_h^{i,z}]_{e,z} [\lambda_h^{i,z}]_{e,z} \right) dl, \quad i = y, z. \end{aligned}$$

Numerical results show that the addition of these stabilization terms results in a stable and accurate numerical discretization, see Section 5.6.

5.6 Results

We have tested the Hagstrom-Warburton nonreflecting boundary condition by calculating an exact plane-wave solution of the Maxwell equations. The goal is to obtain a spurious reflection error that is smaller than the discretization error. We begin by presenting 2D results. We test the boundary condition for $P = 0$ and $P = 1$ and employ second-order Nédélec basis functions on triangular elements.

The incident wave has spatial periodicities $(\lambda_x, \lambda_y) = (2\pi/\cos(\theta), 2\pi/\sin(\theta))$ in the x and y directions, where θ is the incidence angle. The spatial frequencies are given by $(k_x, k_y) = (2\pi/\lambda_x, 2\pi/\lambda_y)$.

In Fig. 5.2 (page 122) we show the rectangular computational domain in the (x, y) plane. We choose the dimensions of the domain to be equal to the spatial periodicities: $(L_x, L_y) = (\lambda_x, \lambda_y)$. At the left ($x = x_{left}$) and right ($x = x_{right}$) boundary the Hagstrom-Warburton boundary condition of order P is imposed. The Hagstrom-Warburton boundary condition at the left boundary also generates the incident wave. At the top ($y = y_{top}$) and bottom ($y = y_{bottom}$) boundaries the periodic boundary condition is imposed.

In the Hagstrom-Warburton boundary condition of order P , we can choose P incidence angles θ_i to be exactly absorbed in addition to the normal incidence angle. For all of these angles, however, we set $\theta_i = 0$ (normal incidence). The theoretical reflection coefficient of the Hagstrom-Warburton boundary condition is then [28]:

$$R = \left(\frac{1 - \cos(\theta)}{1 + \cos(\theta)} \right), \quad \text{for } P = 0, \quad (5.76)$$

and

$$R = \left(\frac{1 - \cos(\theta)}{1 + \cos(\theta)} \right) \left(\frac{\cos(0.22\pi) - \cos(\theta)}{\cos(0.22\pi) + \cos(\theta)} \right)^2, \quad \text{for } P = 1.$$

Since both the left and right boundaries induce a spurious reflection, there will be a series of multiply spuriously reflected waves. The exact solution is (see Appendix 5.B)

$$\mathbf{E}_{exact} = \begin{bmatrix} \sin(\theta) \\ -\cos(\theta) \end{bmatrix} \frac{1}{1 - R^2} e^{-i(k_x x + k_y y)} + \begin{bmatrix} \sin(\theta) \\ \cos(\theta) \end{bmatrix} \frac{R}{1 - R^2} e^{-i(-k_x x + k_y y)}. \quad (5.77)$$

We verify that the discretization error of the DG method is not affected by the nonreflecting boundary condition. In calculations with nonreflecting boundary conditions the real and imaginary part of the field are coupled. To interpret the discretization error, however, it is easier to consider only the real part. The discretization error for the real part of the field is defined as

$$|\mathbf{E}_{diff}(\mathbf{x})| = \frac{|\operatorname{Re}(\mathbf{E}_h(\mathbf{x})) - \operatorname{Re}(\mathbf{E}_{exact}(\mathbf{x}))|}{|\mathbf{E}_{exact}(\mathbf{x})|},$$

with $\mathbf{x}$ a point in the mesh, $\mathbf{E}_{exact}$ the exact solution from Eq. (5.77) that includes the spuriously reflected waves, $\mathbf{E}_h$ the DG approximation, and where we divide by the modulus of the complex field to avoid division by zero at some positions in the mesh. In Fig. 5.4 we show the discretization error for the real part of the field in the (x, y) plane for the $P = 1$ Hagstrom-Warburton boundary condition. The error appears to have a high spatial frequency component, which

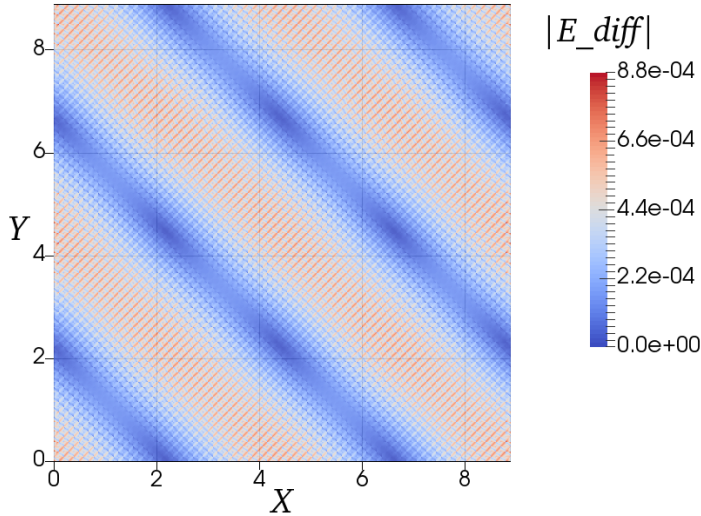


Figure 5.4: Discretization error in the (x, y) plane for the real part of the field for the $P = 1$ Hagstrom-Warburton nonreflecting boundary condition with $\theta_0 = 0$ and $\theta_1 = 0.22\pi = 39.6^\circ$. Note, the exact solution here also contains the contribution from the reflected wave due to the $P = 1$ Hagstrom-Warburton boundary condition. There are 92×92 elements in the x and y directions, divided into triangles, and second-order Nédélec basis functions are employed.

is typical for finite element discretizations. We also do not see any perturbation at the boundaries. It therefore appears that the discretization error of the DG method is not affected by the nonreflecting boundary condition. To compare the discretization error of the DG discretization with and without nonreflecting boundaries, we quantify the rate of convergence, that is, we calculate the convergence order. We assume that the grid spacing h is sufficiently refined for the

error in the L^2 -norm to asymptotically approach zero as

$$\|\mathbf{E}_{exact} - \mathbf{E}_h\|_{L^2(\Omega)} / \|\mathbf{E}_{exact}\|_{L^2(\Omega)} \cong Ch^p, \quad (5.78)$$

for a grid spacing h , and C a constant.

In Fig. 5.5 we show the error in the L^2 -norm for the field for the $P = 1$ Hagstrom-Warburton boundary condition. We see that the error reduces with

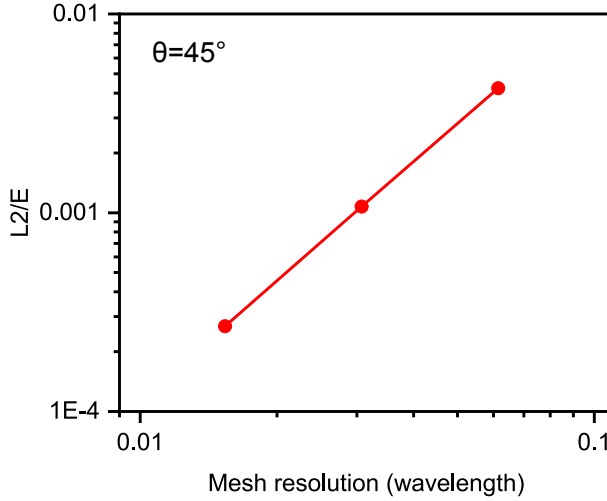


Figure 5.5: Error in the L^2 norm for the electric field (5.78) for a computational domain with the $P = 1$ Hagstrom-Warburton nonreflecting boundary condition with $\theta_0 = 0$ and $\theta_1 = 0.22\pi = 39.6^\circ$. A grid with triangular elements and second-order Nédélec basis functions is employed.

$O(h^2)$ as the mesh size h reduces, see also Table 5.1. The values for the L^2 -norm are also given in Table 5.1. Therefore, we conclude that the discretization error of the DG method is not affected by the nonreflecting boundary condition.

Table 5.1: Error in the L^2 -norm for the electric field and the Lagrange parameter versus the mesh resolution for the $P = 0$ ($\theta_0 = 0$) and $P = 1$ ($\theta_0 = 0$, $\theta_1 = 0.22\pi = 39.6^\circ$) Hagstrom-Warburton nonreflecting boundary conditions. Here $\mathbf{E}_{exact}$ is the exact electric field, $p_{exact} = 0$ the exact value of the Lagrange multiplier and $\mathbf{E}_h, p_h$, respectively, their DG approximations. Note, the exact solution here also contains the contribution from the reflected wave due to the Hagstrom-Warburton boundary condition. The mesh resolution n_y is given as the number of elements for one spatial period of the wave in the y -direction.

n_y	$\ \mathbf{E}_{exact} - \mathbf{E}_h\ _{L^2(\Omega)} / \ \mathbf{E}_{exact}\ _{L^2(\Omega)}$	order for $\mathbf{E}_h$	$\ p_{exact} - p_h\ _{L^2(\Omega)}$
$P = 0$ Hagstrom-Warburton boundary condition			
23	0.00463929	1.9782	$7.4457 \cdot 10^{-4}$
46	0.001177195		$8.9667 \cdot 10^{-5}$
92	$2.9462 \cdot 10^{-4}$		$1.1029 \cdot 10^{-5}$
$P = 1$ Hagstrom-Warburton boundary condition			
23	0.00423427	1.9769	$7.2284 \cdot 10^{-4}$
46	0.00107542		$8.7005 \cdot 10^{-5}$
92	$2.6863 \cdot 10^{-4}$		$1.0637 \cdot 10^{-5}$

We next study the performance of the Hagstrom-Warburton nonreflecting boundary condition with $P = 0$. In this boundary condition, there are no auxiliary variables and it is equivalent to the well-known Sommerfeld boundary condition. In Fig. 5.6 we show the x -component of the field. We consider an incidence angle of the incident wave of $\theta = 45^\circ$, for which the spurious reflection coefficient is $R_{\text{spurious}} = 0.17$. The incident wave is visibly modulated by a spuriously reflected wave, which is not desired in electromagnetic scattering calculations.

In Fig. 5.7 we show the x -component of the field for the $P = 1$ Hagstrom-Warburton boundary condition. We again consider an incidence angle of $\theta = 45^\circ$, for which the spurious reflection coefficient is now $R_{\text{spurious}} < 10^{-2}$. The incident wave is not visibly distorted at the boundaries, as desired, and in contrast to Fig. 5.6.

To investigate quantitatively whether the spurious reflection error is smaller than the discretization error for the $P = 1$ boundary condition, we calculate the relative error of the x -component of the field with respect to the incident wave $|E_{diff,rel,x}| = \frac{|E_x - E_{x,inc}|}{|E_{x,inc}|}$. The relative error is averaged over the line $x = L_x/2$, where the x -components of the incident wave and the spuriously reflected waves in Eq. (5.77) positively interfere. In Fig. 5.8 we show the relative error versus the order P of the Hagstrom-Warburton boundary condition. We see that the error decreases as the order of the boundary condition is increased from $P = 0$ to $P = 1$, so the $P = 0$ boundary condition has not converged yet to the level of discretization error. Since we do not have a data point for $P = 2$, we cannot at this time conclude whether the $P = 1$ boundary condition has converged.

For a boundary condition that has converged to the level of discretization error, we expect the relative error to be highly sensitive to the grid spacing, since

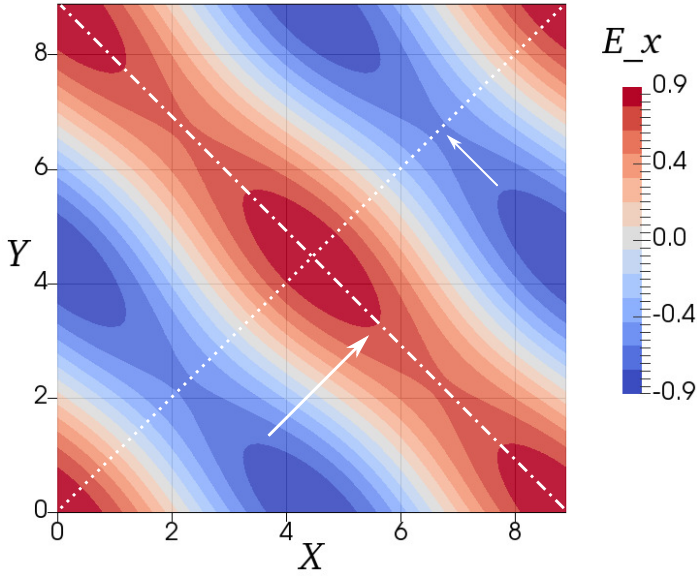


Figure 5.6: x -component of the field in the (x, y) plane for the $P = 0$ Hagstrom-Warburton boundary condition with $\theta_0 = 0$. The modulus of the incident wave is normalized to unity. The incident wave moves in the $(+x, +y)$ -diagonal direction, as indicated by the large arrow. Two phasefronts of the incident wave are indicated with dash-dotted lines. The spuriously reflected wave moves in the $(-x, +y)$ -diagonal direction, as indicated by the small arrow. A phasefront of the spuriously reflected wave is indicated with a dotted line. There are 92×92 elements in the x and y direction, divided into triangles. The spurious reflection coefficient is $R_{\text{spurious}} = 0.17$.

the relative error in that case consists primarily of the discretization error. We therefore investigate the grid spacing dependence of the relative error. The grid spacing for the triangular elements is defined as the length of the edges in the y -direction (L_y/n_y), where n_y is the number of edges in the y -direction, normalized by the wavelength λ of the incident wave

$$h = \frac{(L_y/n_y)}{\lambda}.$$

Fig. 5.9 shows the relative error versus the grid spacing. The relative error for the $P = 0$ boundary condition is insensitive to the grid spacing, which agrees with our observation that there are spuriously reflected waves. For the $P = 1$ boundary condition, the maximum relative error decreases as the grid spacing decreases from coarse ($h = 0.061$) to fine ($h = 0.015$). Therefore, we conclude that the $P = 1$ boundary condition has converged to at least the level of the discretization error of the DG discretization in the interior, as desired, and the spurious reflection error is smaller than the discretization error. We expect that for even finer meshes the relative error eventually levels out to a fixed level

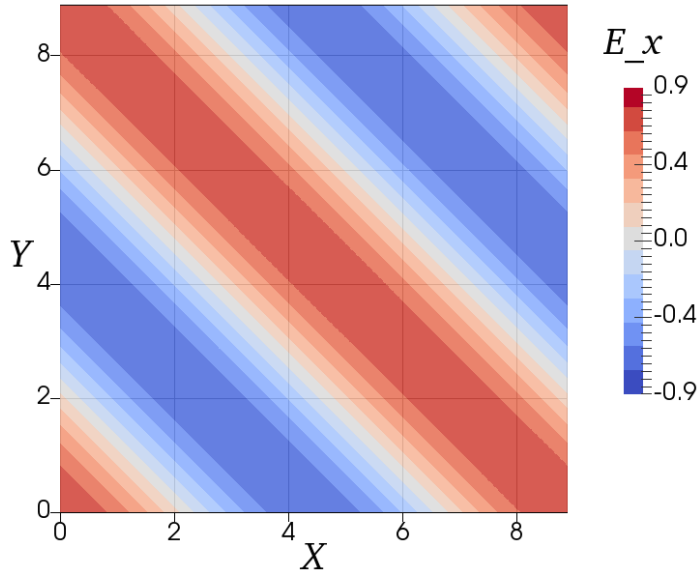


Figure 5.7: x -component of the field E_x in the (x, y) plane for the $P = 1$ Hagstrom-Warburton boundary condition with $\theta_0 = 0$ and $\theta_1 = 0.22\pi = 39.6^\circ$. The modulus of the incident wave is normalized to unity. The incident wave moves in the $(+x, +y)$ -diagonal direction. There are 92×92 pairs of triangular elements in the x and y direction.

independent of h , since even for $h \rightarrow 0$ there is still a small spurious reflection error for the Hagstrom-Warburton boundary condition for finite values of P .

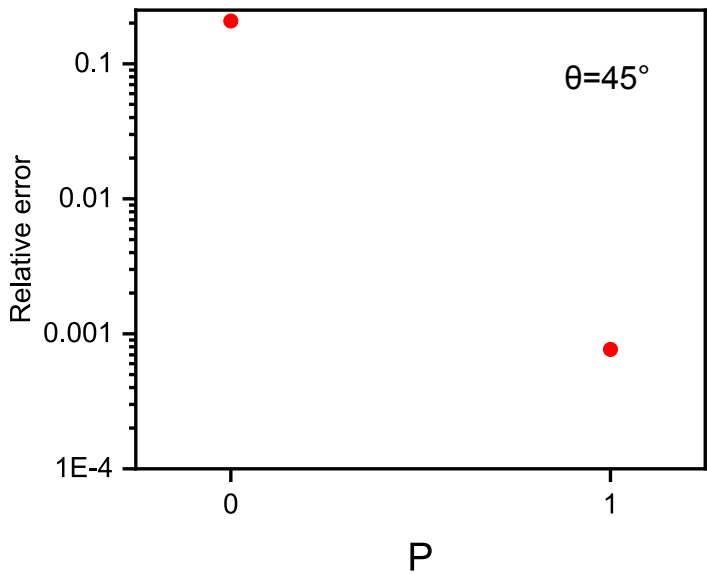


Figure 5.8: Relative error in the x -component of the field E_x versus order P of the Hagstrom-Warburton boundary condition. The $P = 0$ boundary condition has $\theta_0 = 0$ and the $P = 1$ boundary condition has $\theta_0 = 0$ and $\theta_0 = 0.22\pi$. The incidence angle of the incident wave is $\theta = 45^\circ$. There are 92×92 pairs of triangular elements in the x and y directions.

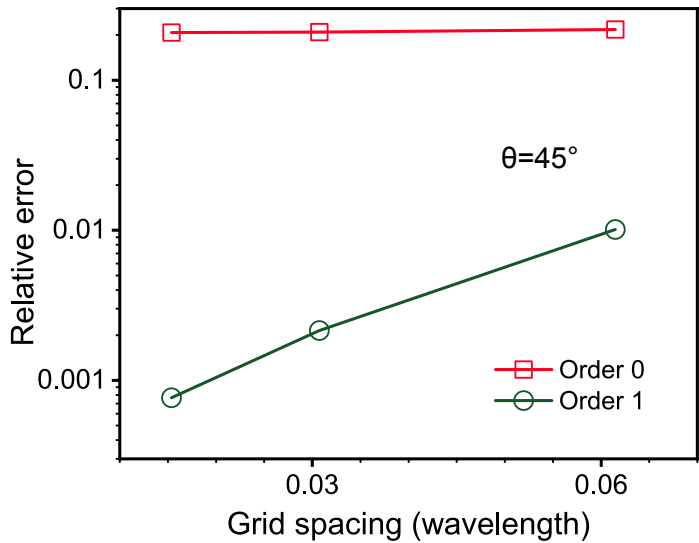


Figure 5.9: Relative error in the x -component of the field versus the grid spacing. The incidence angle of the incident wave is $\theta = 45^\circ$.

5.6.1 Exact reflection coefficient

In this section we describe how we compute the reflection coefficient from the relative error. In Appendix 5.B we derive the full exact 2D wave field

$$\mathbf{E}_{exact} = \begin{bmatrix} \sin(\theta) \\ -\cos(\theta) \end{bmatrix} (1 + R^2 + R^4 + \dots) e^{-i(k_x x + k_y y)} + \begin{bmatrix} \sin(\theta) \\ \cos(\theta) \end{bmatrix} R(1 + R^2 + R^4 + \dots) e^{-i(-k_x x + k_y y)},$$

with R the spurious reflection coefficient of the Hagstrom-Warburton condition. Subtracting the incident wave field and taking the x -component we can compute the relative error

$$|E_{diff,rel,x}| = \frac{|E_{exact,x} - E_{inc,x}|}{|E_{inc,x}|} = |(R^2 + R^4 + R^6 + \dots) e^{-i(k_x x)} + (R + R^3 + R^5 + \dots) e^{-i(-k_x x)}|.$$

Using $k_x x = \frac{2\pi}{\lambda_x} x = \frac{2\pi}{L_x} x = \frac{2\pi}{L_x} \frac{L_x}{2} = \pi$ and after summation of all R terms given by the geometric series we find

$$|E_{diff,rel,x}| = R \left(\frac{1}{1 - R} \right).$$

We can solve for the reflection coefficient in terms of the maximum relative error:

$$R = \frac{|E_{diff,rel,x}|}{|E_{diff,rel,x}| + 1}.$$

In a calculation we do not compute $\mathbf{E}_{exact}$, but the DG solution $\mathbf{E}_h \simeq \mathbf{E}_{exact}$ that will have a discretization error. The relative error $|E_{diff,rel,x}| = \frac{|E_x - E_{inc,x}|}{|E_{inc,x}|}$ found in the calculations is therefore potentially position-dependent. To use all the data available in the calculations, we average therefore $|E_{diff,rel,x}| = \frac{|E_x - E_{inc,x}|}{|E_{inc,x}|}$ in y at $k_x x = \pi$.

We next confirm that the calculated reflection coefficients agree with the ones estimated in Eq. (5.76). In Fig. 5.10 we show the spurious reflection coefficient versus the angle of incidence. We observe that the reflection coefficients extracted from the calculations agree with the estimated ones. This confirms the known and important property of the Hagstrom-Warburton boundary condition that it has a robust error estimate [17].

To investigate the influence of the discretization on the numerically obtained reflection coefficient, we perform a calculation with angle of incidence $\theta = 0.22\pi = 39.6^\circ$, where the reflection coefficient is zero at the continuous level. We calculated numerically the reflection coefficient $R = 0.0013$, in contrast to $R = 0.0021$ for incidence angle $\theta = 0.25\pi = 45^\circ$. This agrees with our previous conclusion that the error is dominated by the discretization error.

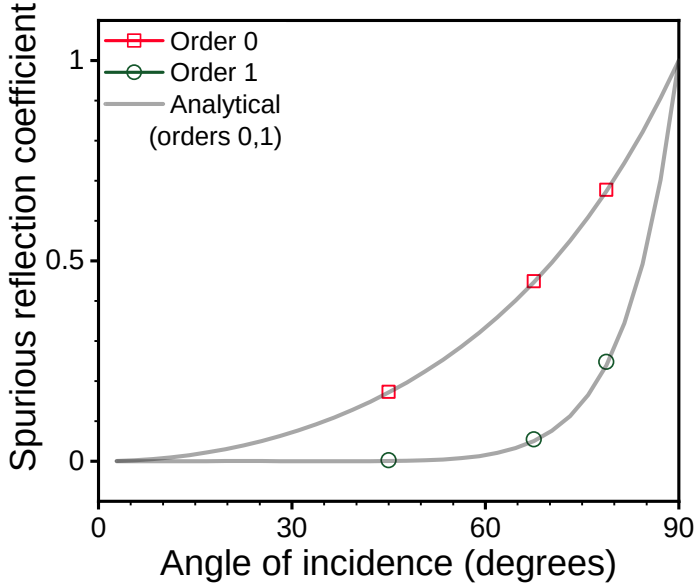


Figure 5.10: Spurious reflection coefficient versus angle of incidence for the $P = 0$ and $P = 1$ Hagstrom-Warburton nonreflecting boundary conditions. The $P = 0$ boundary condition has $\theta_0 = 0$ and the $P = 1$ boundary condition has $\theta_0 = 0$ and $\theta_0 = 0.22\pi$. The spurious reflection coefficient is normalized to the modulus of the incident wave. The extracted spurious reflection coefficients are shown as well as the ones estimated in Eq. (5.76). There are 46×46 , 84×35 , and 165×33 pairs of triangular elements in the x and y directions for the data points at, respectively, $\theta = 45^\circ$, $\theta = 67.5^\circ$ and $\theta = 78.75^\circ$. Second-order Nédélec basis functions are employed.

5.6.2 3D results

Finally, we present results in 3D where we employ tetrahedral elements. In Fig. 5.11 we show the x -component of the field for the $P = 1$ Hagstrom-Warburton boundary condition. We do not see any distortions in the wave profile, that appears to be well absorbed at the boundary. The values of the L^2 -norm are given in Table 5.2 We see that the L^2 error reduces with $O(h^p)$ with $p = 1.9521$ for the $P = 1$ Hagstrom-Warburton boundary condition as the mesh size h reduces. The small deviation of the convergence rate from the theoretical rate $p = 2$ in the absence of a boundary condition is expected given the relatively coarse mesh. The calculated reflection coefficient $R = 0.1867$ for the $P = 0$ boundary condition is reasonably close to the estimated $R = 0.17157$ and the small mismatch can be explained by the small mesh size. For the $P = 1$ boundary condition, the calculated $R = 0.02128$ is $67\times$ larger than the estimated $R = 3.1593 \cdot 10^{-4}$, which can be explained by the relatively coarse mesh. We therefore conclude that the 3D DG discretizations of the $P = 0$ and $P = 1$ Hagstrom-Warburton boundary conditions are stable and accurate.

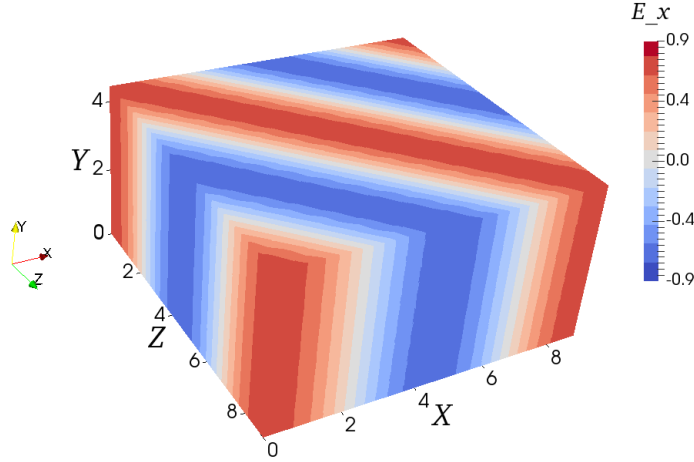


Figure 5.11: x -component of the field in the (x, y, z) plane for the $P = 1$ Hagstrom-Warburton boundary condition with $\theta_0 = 0$ and $\theta_1 = 0.22\pi = 39.6^\circ$. The incident angle of the incident wave is $\theta = 45^\circ$. The modulus of the incident wave is normalized to unity. The incident wave moves in the $(+x, -z)$ -diagonal direction. There are $16 \times 8 \times 16$ blocks of five tetrahedral elements in the x -, y - and z -direction, respectively.

Table 5.2: Error in the L^2 -norm for the electric field and the Lagrange parameter versus the mesh resolution for the $P = 0$ ($\theta_0 = 0$) and $P = 1$ ($\theta_0 = 0$, $\theta_1 = 0.22\pi = 39.6^\circ$) Hagstrom-Warburton nonreflecting boundary conditions, as well as the calculated reflection coefficients. Here $\mathbf{E}_{exact}$ is the exact electric field, $p_{exact} = 0$ the exact value of the Lagrange multiplier and $\mathbf{E}_h, p_h$, respectively, their DG approximations. Note, the exact solution here also contains the contribution from the reflected wave due to the Hagstrom-Warburton boundary condition. The mesh resolution n_x is given as the number of elements for one spatial period of the wave in the x -direction. The incident angle of the incident wave is $\theta = 45^\circ$. The estimated reflection coefficients for the $P = 0$ (Eq. (5.76)) and $P = 1$ (Eq. (5.77)) are $R = 0.17157$ and $R = 3.1593 \cdot 10^{-4}$

n_x	L^2 -error in $\mathbf{E}$ (5.78)	order for $\mathbf{E}_h$	$\ p_{exact} - p_h\ _{L^2(\Omega)}$	R
$P = 0$ Hagstrom-Warburton boundary condition				
8	0.0419729	1.91261	0.066036	0.2289
16	0.0111489		0.00931155	0.1867
$P = 1$ Hagstrom-Warburton boundary condition				
8	0.0391402	1.9521	0.0630077	0.07690
16	0.0101155		0.0088893	0.02128

5.7 Summary

We have developed and implemented nonreflecting boundary conditions for a mixed DG discretization of the time-harmonic Maxwell equations. The boundary conditions are obtained by applying the well-known Hagstrom-Warburton boundary conditions separately to the tangential components of the electric field in the time-harmonic Maxwell equations. The auxiliary equations for the Hagstrom-Warburton boundary conditions are discretized with a DG method using Bassi-Rebay type numerical fluxes and combined with a mixed discontinuous Galerkin discretization for the time-harmonic Maxwell equations. This is the first time that the Hagstrom-Warburton boundary condition is combined with an element-wise curl-conforming discretization of the Maxwell equations. The discretized Hagstrom-Warburton boundary condition successfully describes unboundedness with only small spurious reflections that are accurately predicted by an estimate at the continuous level. These new nonreflecting boundary conditions will allow accurate computations of the behavior of light in finite structures.

5.A Derivation of the mixed DG discretization

In this Appendix we give a brief summary of the derivation of the mixed discontinuous Galerkin discretization for the time-harmonic Maxwell equations given by Eq. (5.54). First, we introduce an auxiliary variable $\mathbf{M}$, such that the time-harmonic Maxwell equations (5.35)-(5.36) can be written as a coupled first order system

$$\mathbf{M} - \nabla \times \mathbf{E} = 0 \text{ in } \Omega, \quad (5.79)$$

$$\nabla \times \mathbf{M} - \omega^2 \epsilon \mathbf{E} - \epsilon \nabla p = \mathbf{j} \text{ in } \Omega, \quad (5.80)$$

$$\nabla \cdot (\epsilon \mathbf{E}) = 0 \text{ in } \Omega. \quad (5.81)$$

Multiplying Eqns. (5.79)–(5.80), respectively, by arbitrary test functions $\mathbf{w}, \mathbf{v} \in \mathbf{V}_h^l$, replacing $\mathbf{E}$ with $\mathbf{E}_h \in \mathbf{V}_h^l$ and p with $p_h \in Q_{h,d}^l$, and integrating by parts (twice for Eq. (5.80)) over the domain Ω , we obtain

$$(\mathbf{M}_h, \mathbf{w})_\Omega = \sum_{K \in \mathcal{T}_h} \int_K (\nabla \times \mathbf{E}_h) \cdot \mathbf{w} d\mathbf{x} + \sum_{K \in \mathcal{T}_h} \int_{\partial K} (\hat{\mathbf{n}} \times (\mathbf{E}_h^* - \mathbf{E}_h)) \cdot \mathbf{w} dS, \quad (5.82)$$

$$(\mathbf{j}, \mathbf{v})_\Omega = \sum_{K \in \mathcal{T}_h} \int_K \left((\nabla \times \mathbf{M}_h) \cdot \mathbf{v} - \omega^2 \epsilon \mathbf{E}_h \cdot \mathbf{v} - \epsilon \nabla p_h \cdot \mathbf{v} \right) d\mathbf{x}, \quad (5.83)$$

where $\mathbf{E}_h^* : \mathcal{F}_h \rightarrow \mathbb{C}^3$ denotes the numerical flux for $\mathbf{E}_h$. The numerical flux $\mathbf{E}^*$ is introduced since $\mathbf{E}_h \in \mathbf{V}_h$ has a multivalued trace at the element faces. We now introduce a mathematical identity, which will be employed several times in

this Chapter. First, for any $\mathbf{u}_h, \mathbf{v} \in \mathbf{V}_h$, we have

$$\begin{aligned} \sum_{K \in \mathcal{T}_h} \int_{\partial K} (\hat{\mathbf{n}} \times \mathbf{u}_h) \cdot \mathbf{v} dS &\equiv \sum_{F \in \mathcal{F}_h^i} \int_F \left(\llbracket \mathbf{u}_h \rrbracket_T \cdot \llbracket \mathbf{v} \rrbracket - \llbracket \mathbf{v} \rrbracket_T \cdot \llbracket \mathbf{u}_h \rrbracket \right) dS \\ &+ \sum_{F \in \mathcal{F}_h^b} \int_F \llbracket \mathbf{u}_h \rrbracket_T \cdot \llbracket \mathbf{v} \rrbracket dS. \end{aligned} \quad (5.84)$$

This relation can be easily verified by introducing the expression for the average and the tangential jump into the right hand side of Eq. (5.84). Using Eq. (5.84) in Eq. (5.82), we obtain the following relation for the auxiliary equation

$$\begin{aligned} (\mathbf{M}_h, \mathbf{w})_\Omega &= \sum_{K \in \mathcal{T}_h} \int_K (\nabla \times \mathbf{E}_h) \cdot \mathbf{w} d\mathbf{x} + \sum_{F \in \mathcal{F}_h^i} \int_F \left(\llbracket \mathbf{E}_h^* - \mathbf{E}_h \rrbracket_T \cdot \llbracket \mathbf{w} \rrbracket \right. \\ &\quad \left. - \llbracket \mathbf{w} \rrbracket_T \cdot \llbracket \mathbf{E}_h^* - \mathbf{E}_h \rrbracket \right) dS + \sum_{F \in \mathcal{F}_h^b} \int_F \llbracket \mathbf{E}_h^* - \mathbf{E}_h \rrbracket_T \cdot \llbracket \mathbf{w} \rrbracket dS. \end{aligned} \quad (5.85)$$

Introducing the lifting operators, defined in Eqns. (5.51) and (5.52), into Eq. (5.85), yields

$$(\mathbf{M}_h, \mathbf{w})_\Omega = (\nabla_h \times \mathbf{E}_h, \mathbf{w})_\Omega + (\mathcal{R}(\llbracket \mathbf{E}_h^* - \mathbf{E}_h \rrbracket_T), \mathbf{w})_\Omega - (\mathcal{L}(\llbracket \mathbf{E}_h^* - \mathbf{E}_h \rrbracket), \mathbf{w})_\Omega,$$

where ∇_h indicates the element-wise nabla operator. Since $\mathbf{w} \in \mathbf{V}_h$ is an arbitrary test function, we deduce the expression

$$\mathbf{M}_h = \nabla_h \times \mathbf{E}_h + \mathcal{R}(\llbracket \mathbf{E}_h^* - \mathbf{E}_h \rrbracket_T) - \mathcal{L}(\llbracket \mathbf{E}_h^* - \mathbf{E}_h \rrbracket) \quad (5.86)$$

almost everywhere in Ω . Next, we consider Eq. (5.83), rewritten as

$$(\mathbf{j}, \mathbf{v})_\Omega = \sum_{K \in \mathcal{T}_h} \int_K \left(\nabla \cdot (\mathbf{M}_h \times \mathbf{v}) + \mathbf{M}_h \cdot (\nabla_h \times \mathbf{v}) - \omega^2 \epsilon \mathbf{E}_h \cdot \mathbf{v} - \epsilon \nabla p_h \cdot \mathbf{v} \right) d\mathbf{x}.$$

Using the divergence theorem and Eq. (5.84) we can express the contribution from the element boundaries as a sum over all faces in $\mathcal{T}_h$

$$\begin{aligned} (\mathbf{j}, \mathbf{v})_\Omega &= (\mathbf{M}_h, \nabla_h \times \mathbf{v})_\Omega - (\omega^2 \epsilon \mathbf{E}_h, \mathbf{v})_\Omega - (\nabla_h p_h, \epsilon \mathbf{v})_\Omega \\ &+ \sum_{F \in \mathcal{F}_h^i} \int_F \left(\llbracket \mathbf{M}_h^* \rrbracket_T \cdot \llbracket \mathbf{v} \rrbracket - \llbracket \mathbf{v} \rrbracket_T \cdot \llbracket \mathbf{M}_h^* \rrbracket \right) dS \\ &+ \sum_{F \in \mathcal{F}_h^b} \int_F \llbracket \mathbf{M}_h^* \rrbracket_T \cdot \llbracket \mathbf{v} \rrbracket dS. \end{aligned} \quad (5.87)$$

Next, we substitute the expression for $\mathbf{M}_h$, given by Eq. (5.86), into Eq. (5.87) and after replacing the lifting operators with their respective definitions given by

Eq. (5.51) and Eq.(5.52), we obtain

$$\begin{aligned}
 (\mathbf{j}, \mathbf{v})_\Omega &= (\nabla_h \times \mathbf{E}_h, \nabla_h \times \mathbf{v})_\Omega - (\omega^2 \epsilon \mathbf{E}_h, \mathbf{v})_\Omega - (\nabla_h p_h, \epsilon \mathbf{v})_\Omega \\
 &+ \sum_{F \in \mathcal{F}_h^i} \int_F \left([\mathbf{M}_h^*]_T \cdot \{\mathbf{v}\} - [\mathbf{v}]_T \cdot \{\mathbf{M}_h^*\} \right. \\
 &+ [\mathbf{E}_h^* - \mathbf{E}_h]_T \cdot \{\nabla \times \mathbf{v}\} \\
 &- \{\mathbf{E}_h^* - \mathbf{E}_h\} \cdot [\nabla \times \mathbf{v}]_T \Big) dS \\
 &+ \sum_{F \in \mathcal{F}_h^b} \int_F \left([\mathbf{M}_h^*]_T \cdot \{\mathbf{v}\} + [\mathbf{E}_h^* - \mathbf{E}_h]_T \cdot \{\nabla \times \mathbf{v}\} \right) dS,
 \end{aligned} \tag{5.88}$$

with $\mathbf{M}_h^* : \mathcal{F}_h \rightarrow \mathbb{C}^3$ the numerical flux for $\mathbf{M}_h$. The Lagrange multiplier contribution can be further evaluated using integration by parts and a DG identity similar to Eq. (5.84) yielding

$$\begin{aligned}
 (\nabla_h p_h, \epsilon \mathbf{v})_\Omega &= \sum_{F \in \mathcal{F}_h^i} \int_F \left([p_h^*] \cdot \{\epsilon \mathbf{v}\} + [\epsilon \mathbf{v}]_N [p_h^*] \right) dS \\
 &+ \sum_{F \in \mathcal{F}_h^b} \int_F [p_h^*] \cdot \{\epsilon \mathbf{v}\} dS - (p_h, \nabla_h \cdot (\epsilon \mathbf{v}))_\Omega,
 \end{aligned} \tag{5.89}$$

with $p_h^* : \mathcal{F}_h \rightarrow \mathbb{C}$ the numerical flux for p_h . Now, substituting relation (5.89) for $(\nabla_h p_h, \epsilon \mathbf{v})_\Omega$ into Eq. (5.88) and a second integration by parts of the Lagrange multiplier contribution containing p gives the relation

$$\begin{aligned}
 (\mathbf{j}, \mathbf{v})_\Omega &= (\nabla_h \times \mathbf{E}_h, \nabla_h \times \mathbf{v})_\Omega \\
 &- \omega^2 (\epsilon \mathbf{E}_h, \mathbf{v})_\Omega \\
 &- (\nabla_h p_h, \epsilon \mathbf{v})_\Omega \\
 &+ \sum_{F \in \mathcal{F}_h} \int_F [\mathbf{E}_h^* - \mathbf{E}_h]_T \cdot \{\nabla_h \times \mathbf{v}\} dS \\
 &- \sum_{F \in \mathcal{F}_h^i} \int_F \{\mathbf{E}_h^* - \mathbf{E}_h\} \cdot [\nabla_h \times \mathbf{v}]_T dS \\
 &+ \sum_{F \in \mathcal{F}_h} \int_F [\mathbf{M}_h^*]_T \cdot \{\mathbf{v}\} dS - \sum_{F \in \mathcal{F}_h^i} \int_F [\mathbf{v}]_T \cdot \{\mathbf{M}_h^*\} dS \\
 &- \sum_{F \in \mathcal{F}_h} \int_F [p_h^* - p_h] \cdot \{\epsilon \mathbf{v}\} dS - \sum_{F \in \mathcal{F}_h^i} \int_F \{p_h^* - p_h\} [\epsilon \mathbf{v}]_N dS,
 \end{aligned} \tag{5.90}$$

which will be the starting point for the derivation of the mixed DG discretization with Brezzi-type numerical fluxes. The discontinuous Galerkin formulation for the divergence constraint can be obtained analogously. Multiplying Eq. (5.81) with arbitrary test functions $q \in Q_{h,d}^i$, integrating over each element $K \in \mathcal{T}_h$ and

using a DG identity similar to Eq. (5.84) gives

$$0 = -(\epsilon \mathbf{E}_h, \nabla_h q)_\Omega + \sum_{F \in \mathcal{F}_h} \int_F \llbracket q \rrbracket \cdot \{(\epsilon \mathbf{E}_h)^*\} dS + \sum_{F \in \mathcal{F}_h^i} \int_F \{q\} \llbracket (\epsilon \mathbf{E}_h)^* \rrbracket_N dS, \quad (5.91)$$

with $(\epsilon \mathbf{E}_h)^* : \mathcal{F}_h \rightarrow \mathbb{C}^3$ the numerical flux for $(\epsilon \mathbf{E}_h)$.

The Brezzi-type numerical fluxes in the present Chapter are similar to the Brezzi-type numerical fluxes for the non-mixed method in Sármany *et al.* [50] and given by

$$\begin{aligned} \mathbf{E}_h^* &= \{\mathbf{E}_h\} && \text{at } \mathcal{F}_h^i, \\ \mathbf{M}_h^* &= \{\mathbf{M}_h\} - \alpha_F \mathcal{R}_F(\llbracket \mathbf{E}_h \rrbracket_T) && \text{at } \mathcal{F}_h^i, \\ \hat{\mathbf{n}} \times \mathbf{E}_h^* &= \hat{\mathbf{n}} \times \mathbf{E}_h && \text{at } \mathcal{F}_h^b, \\ \mathbf{M}_h^* &= \mathbf{M}_h && \text{at } \mathcal{F}_h^b, \end{aligned}$$

where α_F is a positive stabilization parameter that could potentially depend on the face F . Considering the Brezzi numerical flux in Arnold *et al.* [42] it seems reasonable to define the numerical fluxes p_h^* and $(\epsilon \mathbf{E}_h)^*$ as

$$\begin{aligned} p_h^* &= \{p_h\} - \beta_F \mathcal{S}_F(\llbracket \epsilon \mathbf{E}_h \rrbracket_N) && \text{at } \mathcal{F}_h^i, \\ p_h^* &= 0 && \text{at } \mathcal{F}_h^b, \\ (\epsilon \mathbf{E}_h)^* &= \{\epsilon \mathbf{E}_h\} - \gamma_F \mathcal{R}_F(\llbracket p_h \rrbracket) && \text{at } \mathcal{F}_h. \end{aligned}$$

Inserting these numerical fluxes into the expression derived from the divergence constraint (5.91) gives

$$\begin{aligned} 0 &= -(\epsilon \mathbf{E}_h, \nabla_h q)_\Omega + \sum_{F \in \mathcal{F}_h} \int_F \llbracket q \rrbracket \{(\epsilon \mathbf{E}_h)^*\} dS \\ &\quad - \sum_{F \in \mathcal{F}_h} \int_F \gamma_F \llbracket q \rrbracket \cdot \{\mathcal{R}_F(\llbracket p_h \rrbracket)\} dS. \end{aligned} \quad (5.92)$$

Next, using the expression for the lifting operator (5.53) we will rewrite expression (5.92) to show the symmetry of the last term

$$0 = -(\epsilon \mathbf{E}_h, \nabla_h q)_\Omega + \sum_{F \in \mathcal{F}_h} \int_F \llbracket q \rrbracket \{(\epsilon \mathbf{E}_h)^*\} dS - \sum_{F \in \mathcal{F}_h} \int_\Omega \gamma_F \mathcal{R}_F(\llbracket q \rrbracket) \cdot \mathcal{R}_F(\llbracket p_h \rrbracket) d\mathbf{x}. \quad (5.93)$$

Note, the actual support of the local lifting operators is confined to elements adjacent to the face hence only contributions from elements connected to face F contribute to the last integral in Eq. (5.93). Moreover, we note that this last term is now symmetric with respect to p_h and q .

Next, we consider the curl-curl expression (5.90). Inserting fluxes in the right-

hand side of Eq. (5.90) and using Eq. (5.86) yields

$$\begin{aligned} - \sum_{F \in \mathcal{F}_h} \int_F [\mathbf{v}]_T \cdot \{\{\mathbf{M}_h^*\}\} dS &= - \sum_{F \in \mathcal{F}_h} \int_F [\mathbf{v}]_T \cdot \{\{\nabla_h \times \mathbf{E}_h\}\} dS \\ - \sum_{F \in \mathcal{F}_h} \int_F [\mathbf{v}]_T \cdot \mathcal{R}([\mathbf{E}_h^* - \mathbf{E}_h]_T) dS &+ \sum_{F \in \mathcal{F}_h^i} \int_F \alpha_F [\mathbf{v}]_T \{\{\mathcal{R}_F([\mathbf{E}_h]_T)\}\} dS. \end{aligned} \quad (5.94)$$

For the second term on the right hand side of Eq. (5.94) we find that by using the lifting operator (5.52)

$$- \sum_{F \in \mathcal{F}_h} \int_F \{\{\mathcal{R}([\mathbf{E}_h^* - \mathbf{E}_h]_T)\}\} \cdot [\mathbf{v}]_T dS = -(\mathcal{R}([\mathbf{E}_h^* - \mathbf{E}_h]_T), \mathcal{R}([\mathbf{v}]_T))_\Omega, \quad (5.95)$$

and using the definition of the local lifting operator (5.53) we can apply a similar lifting to the third term on the right-hand side of Eq. (5.94). While the term (5.95) could be implemented directly, it has a relatively large sparsity pattern as it includes integrals with contribution from basis functions of neighbours of neighbours. Therefore it is standard in the field of DG methods (see Brezzi *et al.* [48]) to approximate this term by

$$(\mathcal{R}([\mathbf{E}_h^* - \mathbf{E}_h]_T), \mathcal{R}([\mathbf{v}]_T))_\Omega \approx \sum_{F \in \mathcal{F}_h} \sum_{T \in \mathcal{T}_h} n_T (\mathcal{R}_F([\mathbf{E}_h^* - \mathbf{E}_h]_T), \mathcal{R}_F([\mathbf{v}]_T))_T, \quad (5.96)$$

where n_T is the number of faces to element T , and $(\cdot, \cdot)_T$ is the L^2 -inner product over the element T . This double sum (5.96) might seem inefficient, but the inner sum over the elements can be restricted to the elements adjacent to the face F since the contribution of other elements is zero. Therefore, the sum only involves couplings between basis functions in adjacent elements. Combining all terms gives the mixed DG discretization (5.54).

5.B Derivation of exact solution

We define the total wave field in 2D as

$$\mathbf{E} = \begin{bmatrix} \sin(\theta) \\ -\cos(\theta) \end{bmatrix} e^{-i \cos(\theta)x - i \sin(\theta)y} + R \begin{bmatrix} \sin(\theta) \\ \cos(\theta) \end{bmatrix} e^{-i(-\cos(\theta)x + i \sin(\theta)y)}. \quad (5.97)$$

We will apply the zeroth-order Hagstrom-Warburton boundary condition at the right boundary $x = x_{right}$, given by

$$(\partial_x + i\omega)(\hat{n} \times \mathbf{E}) \times \hat{n} = 0. \quad (5.98)$$

If we insert Eq. (5.97) into Eq. (5.98) then we obtain

$$E_y = -\cos(\theta)e^{-i\cos(\theta)x-i\sin(\theta)y} + R\cos(\theta)e^{i\cos(\theta)x-i\sin(\theta)y}, \quad (5.99)$$

$$\partial_x E_y = i\cos^2(\theta)e^{-i\cos(\theta)x-i\sin(\theta)y} + iR\cos^2(\theta)e^{i\cos(\theta)x-i\sin(\theta)y}. \quad (5.100)$$

We consider the normalized frequency $\omega = 1$. Substituting expression (5.99) into boundary condition (5.98) and eliminating the common phase factor we obtain

$$i\cos^2(\theta)e^{-i\cos(\theta)x} + iR\cos^2(\theta)e^{i\cos(\theta)x} - i\cos(\theta)e^{-i\cos(\theta)x} + iR\cos(\theta)e^{i\cos(\theta)x} = 0.$$

Eliminating the common factor of i yields

$$R = \frac{-(\cos^2(\theta) - \cos(\theta))e^{-i\cos(\theta)x}}{(\cos^2(\theta) + \cos(\theta))e^{i\cos(\theta)x}},$$

and rearranging terms we obtain the reflection coefficient

$$R = \left(\frac{1 - \cos(\theta)}{1 + \cos(\theta)} \right) e^{-2i\cos(\theta)x}.$$

Next, we consider the boundary condition at the left side of the domain $x = x_{left}$

$$(-\partial_x + i\omega)((\hat{\mathbf{n}} \times \mathbf{E}) \times \hat{\mathbf{n}}) = 0. \quad (5.101)$$

Using the same procedure as for $x = x_{right}$, we obtain the reflection coefficient

$$R = \left(\frac{1 - \cos(\theta)}{1 + \cos(\theta)} \right) e^{2i\cos(\theta)x}.$$

We consider now a domain with sides $L_x = 2\pi/\cos(\theta)$ and $L_y = 2\pi/\cos(\theta)$ and calculate the solution for the incident wave

$$\mathbf{E}_{inc} = \begin{bmatrix} \sin(\theta) \\ -\cos(\theta) \end{bmatrix} e^{-i\cos(\theta)x-i\sin(\theta)y}.$$

We employ the zeroth-order Hagstrom-Warburton boundary condition

$$(\partial_n + i)((\hat{\mathbf{n}} \times \mathbf{E}) \times \hat{\mathbf{n}}) = (\partial_n + i)((\hat{\mathbf{n}} \times \mathbf{E}_{inc}) \times \hat{\mathbf{n}}).$$

The Hagstrom-Warburton boundary conditions at the left and right sides of the domain both have the reflection coefficients

$$R = \frac{(1 - \cos(\theta))}{1 + \cos(\theta)}.$$

The waves will be multiply spuriously reflected and we obtain a solution that is

a power series

$$\begin{aligned}
 \mathbf{E} &= (1 + R^2 + R^4 + \dots) \begin{bmatrix} \sin(\theta) \\ -\cos(\theta) \end{bmatrix} e^{-i \cos(\theta)x - i \sin(\theta)y} \\
 &+ (R + R^3 + R^5 + \dots) \begin{bmatrix} \sin(\theta) \\ \cos(\theta) \end{bmatrix} e^{-i(-\cos(\theta)x + \sin(\theta)y)} \\
 &= \begin{bmatrix} \sin(\theta) \\ -\cos(\theta) \end{bmatrix} \frac{1}{1 - R^2} e^{-\cos(\theta)x - i \sin(\theta)y} \\
 &+ \begin{bmatrix} \sin(\theta) \\ \cos(\theta) \end{bmatrix} \frac{R}{1 - R^2} e^{\cos(\theta)x - i \sin(\theta)y}.
 \end{aligned} \tag{5.102}$$

The reflection coefficient for the first-order Hagstrom-Warburton boundary condition is [28]

$$R = \left(\frac{1 - \cos(\theta)}{1 + \cos(\theta)} \right)^3. \tag{5.103}$$

In our numerical tests with the first-order Hagstrom-Warburton boundary condition, we observe convergence to Eq. (5.102) with R substituted from Eq. (5.103).

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- [37] We start with the boundary condition (5.6)

$$(i\omega\sqrt{1 - (ck_y/\omega)^2 - (ck_z/\omega)^2} + c\partial_x)\hat{u}|_{x=0} = 0. \quad (5.104)$$

Using the second approximation of Engquist and Majda [23] in Eq. (5.8) $\sqrt{1 - x^2} \simeq 1 - \frac{1}{2}x^2 + O(|x|^4)$ we find the following approximation to the boundary condition

$$(i\omega - \frac{i\omega}{2}(ck_y/\omega)^2 - \frac{i\omega}{2}(ck_z/\omega)^2 + c\partial_x)\hat{u}|_{x=0} = 0. \quad (5.105)$$

We multiply with the factor $i\omega$ to obtain

$$(-\omega^2 + \frac{1}{2}c^2k_y^2 + \frac{1}{2}c^2k_z^2 + i\omega c\partial_x)\hat{u} = 0. \quad (5.106)$$

Fourier transforming this boundary condition back to real-space tangential variables yields the second Engquist-Majda boundary condition (5.11)

$$\mathcal{B}_1 u|_{x=0} = (-\omega^2 + i\omega c\partial_x - \frac{1}{2}\nabla_t^2)u|_{x=0} = 0. \quad (5.107)$$

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- [38] This Lemma is shown by induction [26]. We start with the operator appearing in the second Engquist-Majda boundary condition (5.11)

$$\mathcal{B}_1 u = (-\omega^2 + i\omega c\partial_x - \frac{1}{2}\nabla_t^2)u. \quad (5.108)$$

Employing the wave equation (5.5) to eliminate the tangential derivatives we obtain

$$\mathcal{B}_1 u = (-\omega^2 + i\omega c\partial_x + \frac{1}{2}\omega^2 + \frac{1}{2}c^2\partial_x^2)u \quad (5.109)$$

$$= \frac{1}{2}(i\omega + c\partial_x)^2 u. \quad (5.110)$$

Assume by the induction hypothesis that

$$\mathcal{B}_p u|_{x=0} = \frac{1}{2^p} (i\omega + c\partial_x)^{p+1} u. \quad (5.111)$$

We then find by the Engquist-Majda recursion (5.13) that

$$\mathcal{B}_{p+1} u = i\omega \mathcal{B}_p(u) - \frac{1}{4} \nabla_t^2 \mathcal{B}_{p-1}(u) \quad (5.112)$$

$$= i\omega \frac{1}{2^p} (i\omega + c\partial_x)^{p+1} u - \frac{1}{4} \nabla_t^2 \frac{1}{2^{p-1}} (i\omega + c\partial_x)^p u \quad (5.113)$$

$$= i\omega \frac{1}{2^p} (i\omega + c\partial_x)^{p+1} u - \frac{1}{4} \frac{1}{2^{p-1}} (i\omega + c\partial_x)^p \nabla_t^2 u \quad (5.114)$$

$$= i\omega \frac{1}{2^p} (i\omega + c\partial_x)^{p+1} u + \frac{1}{4} \frac{1}{2^{p-1}} (\omega^2 + c^2 \partial_x^2) (i\omega + c\partial_x)^p u \quad (5.115)$$

$$= i\omega \frac{1}{2^p} (i\omega + c\partial_x)^{p+1} u - \frac{1}{4} \frac{1}{2^{p-1}} (i\omega - c\partial_x)(i\omega + c\partial_x) \times \\ (i\omega + c\partial_x)^p u \quad (5.116)$$

$$= \frac{1}{2^p} (i\omega + c\partial_x)^{p+1} (i\omega - \frac{1}{4} \cdot 2(i\omega - c\partial_x)) \quad (5.117)$$

$$= \frac{1}{2^p} (i\omega + c\partial_x)^{p+1} (\frac{1}{2} i\omega + \frac{1}{2} c\partial_x) \quad (5.118)$$

$$= \frac{1}{2^{p+1}} (i\omega + c\partial_x)^{p+2}, \quad (5.119)$$

where in Eq. (5.115) we employed the wave equation (5.5). 116

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$$(a_p i\omega + c\partial_x)(a_p i\omega + c\partial_x)\phi_p = (-a_p^2 \omega^2 + 2a_p i\omega c\partial_x + c^2 \partial_x^2)\phi_p \quad (5.120)$$

$$= (-a_p^2 \omega^2 + 2a_p i\omega c\partial_x - \omega^2 - c^2 \nabla_t^2)\phi_p \quad (5.121)$$

$$= (-(a_p^2 + 1)\omega^2 + 2a_p i\omega c\partial_x - c^2 \nabla_t^2)\phi_p. \quad (5.122)$$

For the right hand side of Eq. (5.21) the derivation is similar, and for the operator $(a_p \omega - c\partial_x)$ and the left and right hand sides Eq. (5.21) too. 119

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CHAPTER 6

Well posedness of nonreflecting boundary conditions for Maxwell's equations

In Chapter 5 we adapted the Hagstrom-Warburton nonreflecting boundary conditions to a mixed DG discretization of the Maxwell equations. While the Hagstrom-Warburton nonreflecting boundary conditions have been applied before to a nodal DG discretization of the Maxwell equations [1–3], in that case the boundary conditions are applied to characteristic combinations of the electric and magnetic fields. The mixed DG discretization considered in Chapter 5 is formulated in terms of only the electric field. It is therefore essential to formulate the Hagstrom-Warburton nonreflecting boundary conditions also only in terms of the electric field.

In Chapter 5 we followed the approach of Mur [4] who adapted the Engquist-Majda nonreflecting boundary conditions to the Maxwell equations [5, 6], and numerically investigated the accuracy of the resulting boundary condition. This approach is based on the fact that each field component separately satisfies the Helmholtz equation. It is stated by Monk [7] that from the Stratton-Chu formula [8] we can see that each field component also satisfies the radiation condition appropriate for the Helmholtz equation. Hence, it is possible to use nonreflecting boundary conditions appropriate for the Helmholtz equation on each component of the scattered field. In fact, we apply the Hagstrom-Warburton boundary condition only to the tangential components of the electric field, as is done for the perfect electric conductor condition [9], but not for the Silver-Müller boundary condition [7]. The application of the boundary condition to only the tangential components of the field is reasonable, since for a plane-wave incident at the boundary under an oblique angle these are the only independent components. In the present Chapter we show for the *first time* that the application of the zeroth-order Engquist-Majda nonreflecting boundary condition to the tangential components of the electric field, which results in the Mur boundary condition [4], leads to a well posed problem at the continuous level.

The zeroth-order Engquist-Majda nonreflecting boundary condition corresponds to the zeroth-order Hagstrom-Warburton boundary condition, and it is likely that the result of well posedness could be extended to the high-order Hagstrom-Warburton nonreflecting boundary conditions. Indeed, the high-order Hagstrom-Warburton nonreflecting boundary conditions are modifications of the high-order Higdon nonreflecting boundary conditions, where the operator in the zeroth-order Engquist-Majda nonreflecting boundary condition is simply applied

several times at the boundary, but we do not analyze the higher order Hagstrom-Warburton boundary conditions in this Chapter.

Well posedness at the continuous level is important for developing a stable discretization, since it implies that there are no spurious modes at the continuous level that could potentially be excited by numerical inaccuracies. Well posedness at the continuous level does not, however, show that a particular discretization converges to the correct solution, which requires further analysis. For symmetric hyperbolic problems, well posedness can often be shown with an energy estimate that is derived from integration by parts [10–12], but for nonsymmetric problems, including problems described by the Maxwell equations, other techniques are needed. Alternatively, the theory developed by Kreiss [13, 14] for strictly hyperbolic problems, which is based on the construction of a “symmetrizer”, shows well posedness for problems with inhomogeneous coefficients and curved, but smooth, boundaries, and can also be applied to nonsymmetric problems. The theory by Kreiss is based on previous work by Hersh [15] and was interpreted in terms of characteristic variables by Higdon [16]. The Maxwell’s equations are not strictly hyperbolic as they have two tangential characteristics at the boundary (in addition to two incoming characteristics and two outgoing characteristics) [3], but the theory was later extended by Majda and Osher to cover the Maxwell’s equations as well [17].

However, a crucial ingredient in the theory of well posedness [13, 14, 17] is an estimate of the Fourier-Laplace components of the solution at the boundary in terms of the boundary data, called the uniform Kreiss condition, in the case of the scalar wave equation formulated as

$$|\hat{u}(0, \omega, s)|^2 \leq C |\hat{g}(\omega, s)|^2,$$

with $\hat{u}(0, \omega, s)$ the Fourier-Laplace components of the solution at the boundary $x = 0$, ω the dual Fourier variable to the tangential spatial variables, s the dual Laplace variable to time, $|\cdot|$ the modulus, C a constant independent of s and ω , and $\hat{g}(\omega, s)$ the Fourier-Laplace components of the boundary data. For Sommerfeld-type nonreflecting boundary conditions (like the zeroth-order Engquist-Majda condition we consider) one needs to employ an estimate with a different scaling in the Fourier-Laplace dual variables [18, 19]

$$|\hat{u}(0, \omega, s)|^2 \leq \frac{C}{|s|^2 + \omega^2} |\hat{g}|^2.$$

The scaling factor reflects the fact that the Sommerfeld-type nonreflecting boundary conditions have a generalized eigenvalue [16, 20] for $s = 0$: the solutions $u = \text{constant}$ satisfy the boundary condition in isolation of forcing. Hence, in a discretized solution as $s \rightarrow 0$ (*i.e.* that is nearly constant), the application of the boundary operator to the incident wavefield and the spuriously reflected wavefield results in both cases in small values, and the spurious reflection coefficient may be large due to round-off error. While it is plausible that the theory of Majda *et al.* [17] pertains also to boundary conditions with the modified estimate, a proof of this has not appeared in the literature. Hence, we not only show the

appropriate uniform Kreiss condition, but also explicitly derive an estimate of the solution in terms of the boundary data for a problem with constant coefficients and a planar boundary, which establishes well posedness at least for this problem and makes plausible well posedness for general problems.

Analyses of well posedness of boundary conditions for Maxwell's equations have been given for the Joly-Mercier boundary condition [21] in Assous *et al.* [22], for the Collino-Joly boundary conditions [23], and for boundary conditions by Hall and Kabakian [24].

We will consider the following problem. Let Ω be the computational domain in 3D and $\partial\Omega$ the computational boundary. The boundary $\partial\Omega$ is planar and located at $x = 0$, and we denote the unit outward normal vector by $\hat{\mathbf{n}}$. The domain is located on the side of the boundary with $x < 0$. The domain is shown in Fig. 6.1.

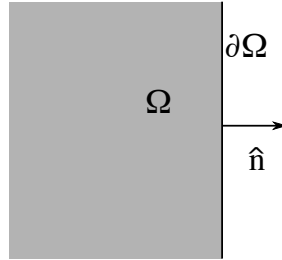


Figure 6.1: Illustration of the domain employed in the analysis of well posedness. The domain Ω is shown in grey. The computational boundary $\partial\Omega$ as well as the unit normal vector $\hat{\mathbf{n}}$ are also shown.

We consider the Maxwell equations for the electric field in the time-domain with an incident field that is generated by the boundary, and we impose the zeroth-order Engquist-Majda condition (5.10) as adapted to the vector Maxwell equations by Mur [4]

$$\nabla \times \nabla \times \mathbf{E}(\mathbf{r}, t) + \partial_t^2 \mathbf{E}(\mathbf{r}, t) = 0, \quad \mathbf{r} \in \Omega, \quad t > 0, \quad (6.1)$$

$$(\partial_t + \partial_n) \mathbf{E}_T(\mathbf{r}, t) = (\partial_t + \partial_n) \mathbf{E}_T^{inc}(\mathbf{r}, t), \quad \mathbf{r} \in \partial\Omega, \quad t > 0, \quad (6.2)$$

$$\mathbf{E}(\mathbf{r}, 0) = 0, \quad \mathbf{r} \in \Omega, \quad (6.3)$$

with $\mathbf{E}(\mathbf{r}, t)$ the electric field, $\partial_n \equiv \hat{\mathbf{n}} \cdot \nabla$ the normal derivative, $\mathbf{E}_T \equiv (\hat{\mathbf{n}} \times \mathbf{E}) \times \hat{\mathbf{n}}$ the tangential part of the field, and $\mathbf{E}^{inc}$ the incident field. In Eq. (6.1) we assumed that the magnetic permeability $\mu = 1$ and the dielectric permittivity $\epsilon = 1$, but a “symmetrizer” construction may allow an extension of the results to inhomogeneous coefficients, which requires further work. We denote the L^2 -norm over all space and time by

$$\|\cdot\|_{L^2(\Omega \times [0, \infty))} = \sqrt{\int_0^\infty \int_\Omega |\cdot|^2 d\mathbf{r} dt}.$$

We denote the tangential part of the position vector by

$$\mathbf{y} \equiv \begin{bmatrix} y \\ z \end{bmatrix}, \quad (6.4)$$

and the L^2 -norm over the boundary and all time by

$$\|\cdot\|_{L^2(\partial\Omega \times [0, \infty))} = \sqrt{\int_0^\infty \int_{\partial\Omega} |\cdot|^2 d\mathbf{y} dt}.$$

The components of the field are $E_x = \hat{\mathbf{x}} \cdot \mathbf{E}$, $E_y = \hat{\mathbf{y}} \cdot \mathbf{E}$ and $E_z = \hat{\mathbf{z}} \cdot \mathbf{E}$. We introduce the following notation for the boundary data

$$\mathbf{g} \equiv \begin{bmatrix} g_y \\ g_z \end{bmatrix} \equiv (\partial_t + \partial_n) \mathbf{E}_T^{inc}. \quad (6.5)$$

In the analysis we will use a Fourier transform in the tangential directions, with dual variable (wave vector)

$$\omega \equiv \begin{bmatrix} \omega_y \\ \omega_z \end{bmatrix}. \quad (6.6)$$

We will take a Laplace transform in time, with dual variable

$$s = \eta + i\xi, \quad (6.7)$$

where we assume $\eta > 0$. Let $\hat{g}_y$ and $\hat{g}_z$ be the Fourier transforms in the tangential part of the position vector with dual variables ω , and Laplace transform in time with dual variable s , of the boundary data. In this Chapter we will show that problem (6.1)-(6.3) is well posed.

Theorem 1. *Assume that the inverse Fourier-Laplace transform of $\frac{1}{\sqrt{|s|^2 + |\omega|^2}} \hat{g}_y$ and $\frac{1}{\sqrt{|s|^2 + |\omega|^2}} \hat{g}_z$ exists. We also assume that the inverse Fourier-Laplace transform of $\frac{\omega_y \hat{g}_y(\omega, s)}{|\sqrt{s^2 + \omega^2}| \sqrt{|s|^2 + \omega^2}}$ and $\frac{\omega_z \hat{g}_z(\omega, s)}{|\sqrt{s^2 + \omega^2}| \sqrt{|s|^2 + \omega^2}}$ exists. Under these conditions, problem (6.1)-(6.3) has a unique solution.*

For $\eta > 0$, the tangential components satisfy the following estimate with respect to the incident field

$$\|(\partial_x E_y) e^{-\eta t}\|_{L^2(\Omega \times [0, \infty))}^2 \leq \frac{C}{\eta} \|((\partial_t + \partial_n) E_y^{inc}) e^{-\eta t}\|_{L^2(\partial\Omega \times [0, \infty))}^2, \quad (6.8)$$

$$\|(\partial_x E_z) e^{-\eta t}\|_{L^2(\Omega \times [0, \infty))}^2 \leq \frac{C}{\eta} \|((\partial_t + \partial_n) E_z^{inc}) e^{-\eta t}\|_{L^2(\partial\Omega \times [0, \infty))}^2, \quad (6.9)$$

with C a constant independent of s and ω .

In the remainder of this Chapter, we will give a proof of Theorem 1, by solving Eqns. (6.1)-(6.3) with Fourier and Laplace transforms. We first make a number of remarks:

1. By setting $\mathbf{E}^{inc} = 0$ in Eq. (6.2) an eigenvalue problem is obtained that has a mode where the light is propagating tangentially to the boundary, *i.e.*, $(E_x, E_y, E_z) = (e^{i\omega \cdot \mathbf{y} + i\xi t}, 0, 0)$, with $\omega = (\omega_y, \omega_z)$ the wave vector tangential to the boundary, and ξ the frequency. We note that the Silver-Müller boundary condition [7], which is formulated in terms of normal components as well, is not consistent with this tangential wave.
2. A factor $e^{-\eta t}$ is included in estimates (6.8) and (6.9) to obtain finite norms for problems where the incident field does not tend to zero as $t \rightarrow \infty$, for instance a plane wave incident field that is smoothly turned on starting from $t = 0$.
3. It is possible to obtain estimates as well with respect to interior forcing in the Maxwell equations and initial data by employing Fourier and Laplace transforms, but this is outside the scope of the present Chapter.

To prove Theorem 1, we first show that the electromagnetic wave equation is equivalent to the first-order Maxwell equations. Suppose that we have a solution $\mathbf{E}$ of Eqns. (6.1)-(6.3). We will show that it is also a solution of problem (6.1)-(6.3) with the electromagnetic wave equation replaced by the first-order Maxwell equations, and with an appropriately defined magnetic field. We introduce the magnetic field by integrating the curl of the electric field over time

$$\mathbf{B} = - \int_0^t \nabla \times \mathbf{E} \, d\tau. \quad (6.10)$$

Taking the time derivative of Eq. (6.10) yields Faraday's law [9]

$$\partial_t \mathbf{B} = -\nabla \times \mathbf{E}. \quad (6.11)$$

Replacing the curl of the field in the wave equation (6.1) with (6.11) yields

$$-\nabla \times \partial_t \mathbf{B} + \partial_t^2 \mathbf{E} = 0. \quad (6.12)$$

Integrating Eq. (6.12) with respect to time, and using that the electric and magnetic fields are zero at the initial time, yields

$$-\nabla \times \mathbf{B} + \partial_t \mathbf{E} = 0. \quad (6.13)$$

Collecting Eqns. (6.2), (6.3), (6.11), (6.13) and (6.5) we obtain the system

$$\partial_t \begin{bmatrix} \mathbf{E}(\mathbf{r}, t) \\ \mathbf{B}(\mathbf{r}, t) \end{bmatrix} - \begin{bmatrix} 0 & \nabla \times \\ -\nabla \times & 0 \end{bmatrix} \begin{bmatrix} \mathbf{E}(\mathbf{r}, t) \\ \mathbf{B}(\mathbf{r}, t) \end{bmatrix} = 0, \quad \mathbf{r} \in \Omega, \quad t > 0, \quad (6.14)$$

$$(\partial_t + \partial_n) \mathbf{E}_T(\mathbf{r}, t) = \mathbf{g}(\mathbf{r}, t), \quad \mathbf{r} \in \partial\Omega \quad t > 0, \quad (6.15)$$

$$\begin{bmatrix} \mathbf{E}(\mathbf{r}, 0) \\ \mathbf{B}(\mathbf{r}, 0) \end{bmatrix} = 0, \quad \mathbf{r} \in \Omega. \quad (6.16)$$

Conversely, the derivation of the wave equation (6.1) from the first-order Maxwell equations (6.14) is well-known and given in many textbooks [9]. It is therefore sufficient to prove Theorem 1 for the problem (6.14)-(6.16).

We use a Fourier transform of the electric field and magnetic field in the tangential directions $\mathbf{y}$ with dual variables ω and a Laplace transform in time with dual variable s for $\eta > 0$ (see Eqns. (6.4), (6.6) and (6.7)). The Fourier-Laplace transforms of the field components are defined as

$$\begin{pmatrix} \hat{E}_x(x, \omega, s) \\ \hat{E}_y(x, \omega, s) \\ \hat{E}_z(x, \omega, s) \\ \hat{B}_x(x, \omega, s) \\ \hat{B}_y(x, \omega, s) \\ \hat{B}_z(x, \omega, s) \end{pmatrix} = \int_0^\infty \int_{\mathbb{R}^2} e^{-st - i\omega \cdot \mathbf{y}} \begin{pmatrix} E_x(\mathbf{r}, t) \\ E_y(\mathbf{r}, t) \\ E_z(\mathbf{r}, t) \\ B_x(\mathbf{r}, t) \\ B_y(\mathbf{r}, t) \\ B_z(\mathbf{r}, t) \end{pmatrix} d\mathbf{y} dt.$$

In this Chapter it will be shown that the Fourier-Laplace transforms indeed converge for $\eta > 0$. Taking a Fourier-Laplace transform of the Maxwell equations (6.14) yields

$$s\hat{E}_x = i\omega_y \hat{B}_z - i\omega_z \hat{B}_y, \quad (6.17)$$

$$\partial_x \hat{B}_z = i\omega_z \hat{B}_x - s\hat{E}_y,$$

$$\partial_x \hat{B}_y = s\hat{E}_z + i\omega_y \hat{B}_x,$$

$$s\hat{B}_x = -i\omega_y \hat{E}_z + i\omega_z \hat{E}_y, \quad (6.18)$$

$$\partial_x \hat{E}_z = s\hat{B}_y + i\omega_z \hat{E}_x,$$

$$\partial_x \hat{E}_y = -s\hat{B}_z + i\omega_y \hat{E}_x.$$

We see that the normal components of the field (6.17) and (6.18) can be expressed in terms of the tangential components. We collect the tangential Fourier-Laplace transforms in a vector

$$\hat{\mathbf{v}}(x, \omega, s) \equiv \begin{pmatrix} \hat{E}_y(x, \omega, s) \\ \hat{E}_z(x, \omega, s) \\ \hat{B}_y(x, \omega, s) \\ \hat{B}_z(x, \omega, s) \end{pmatrix}. \quad (6.19)$$

In the following we will work with the normalized dual variables

$$s' = \frac{s}{\sqrt{|\omega|^2 + |s|^2}}, \quad \xi' = \frac{\xi}{\sqrt{|\omega|^2 + |s|^2}}, \quad (6.20)$$

$$\omega' = \frac{\omega}{\sqrt{|\omega|^2 + |s|^2}}, \quad \eta' = \frac{\eta}{\sqrt{|\omega|^2 + |s|^2}}, \quad (6.21)$$

that are well-defined since $\eta > 0$. Taking the Fourier-Laplace transform of problem (6.14)-(6.16) and then making the substitutions (6.17) and (6.18) everywhere

for the normal variables yields the following problem

$$\partial_x \hat{\mathbf{v}} = \sqrt{|s|^2 + \omega^2} M(\omega', s') \hat{\mathbf{v}}, \quad x < 0, \quad (6.22)$$

$$s' \begin{pmatrix} \hat{E}_y \\ \hat{E}_z \end{pmatrix} + \frac{1}{\sqrt{|s|^2 + \omega^2}} \partial_x \begin{pmatrix} \hat{E}_y \\ \hat{E}_z \end{pmatrix} = \hat{\mathbf{g}}', \quad x = 0, \quad (6.23)$$

$$\hat{\mathbf{v}} \in (L^2((-\infty, 0]))^4, \quad (6.24)$$

$$\eta' > 0, \quad (6.25)$$

with

$$\hat{\mathbf{g}}' = \hat{\mathbf{g}} / \sqrt{|s|^2 + |\omega|^2},$$

the Fourier-Laplace transform of the boundary data, and with the system matrix

$$M(\omega', s') = \begin{pmatrix} 0 & 0 & \frac{\omega'_y \omega'_z}{s'} & -(s' + \frac{\omega'^2_y}{s'}) \\ 0 & 0 & (s' + \frac{\omega'^2_z}{s'}) & -\frac{\omega'_y \omega'_z}{s'} \\ -\frac{\omega'_y \omega'_z}{s'} & (s' + \frac{\omega'^2_y}{s'}) & 0 & 0 \\ -(s' + \frac{\omega'^2_z}{s'}) & \frac{\omega'_y \omega'_z}{s'} & 0 & 0 \end{pmatrix}. \quad (6.26)$$

We note that Eq. (6.24) corresponds to the requirement that the Fourier-Laplace transform converges, that remains to be verified. To interpret the preceding steps, the Maxwell's equations have two outgoing characteristics, two incoming characteristics, and two tangential characteristics [16]. As we will see, the equations (6.22)-(6.23) are a problem for only the outgoing and incoming characteristics for $\eta' > 0$. A similar approach is used in Majda *et al.* [17] and Assous *et al.* [22].

We will solve the problem (6.22)-(6.23) by determining the eigenvalues and eigenvectors of the matrix M . The system matrix (6.26) has eigenvalues κ' and $-\kappa'$, both with multiplicity two, given by

$$\kappa' = (s'^2 + \omega'^2_y + \omega'^2_z)^{1/2},$$

where we define the argument of the square root in the following way. We also define the following variable

$$\kappa = \kappa' \sqrt{|\omega|^2 + |s|^2}. \quad (6.27)$$

Let $\omega'^2 \equiv \omega'^2_y + \omega'^2_z$ so that

$$\kappa'^2 = s'^2 + \omega'^2. \quad (6.28)$$

We define the argument so that

$$-\pi < \arg(s'^2 + \omega'^2) \leq \pi, \quad \arg \sqrt{s'^2 + \omega'^2} = \frac{1}{2} \arg(s'^2 + \omega'^2). \quad (6.29)$$

The system matrix (6.26) has the following eigenvectors (see Ref. [22]), that we

collect in a matrix

$$Q = \begin{bmatrix} s'\kappa' & 0 & -\omega'_y\omega'_z & s'^2 + \omega_y'^2 \\ 0 & s'\kappa' & -(s'^2 + \omega_z'^2) & \omega'_y\omega'_z \\ -\omega'_y\omega'_z & s'^2 + \omega_y'^2 & s'\kappa' & 0 \\ -(s'^2 + \omega_z'^2) & \omega'_y\omega'_z & 0 & s'\kappa' \end{bmatrix}. \quad (6.30)$$

It is straightforward to verify by hand that they are indeed eigenvectors of the matrix (6.26). The inverse matrix of eigenvectors is

$$Q^{-1} = \frac{1}{2s'^2\kappa'^2} \begin{bmatrix} \kappa's' & 0 & \omega'_y\omega'_z & -(s'^2 + \omega_y'^2) \\ 0 & \kappa's' & s'^2 + \omega_z'^2 & -\omega'_y\omega'_z \\ \omega'_y\omega'_z & -(s'^2 + \omega_y'^2) & \kappa's' & 0 \\ s'^2 + \omega_z'^2 & -\omega'_y\omega'_z & 0 & \kappa's' \end{bmatrix} \quad (6.31)$$

Lemma 2. For $\text{Re}(s') > 0$ we have $\text{Re}(\kappa') > 0$.

Proof. We first show that κ'^2 either has a nonzero imaginary component or it is a positive real number. We substitute $s' = \eta' + i\xi'$ in the definition (6.28) and find

$$\kappa'^2 = s'^2 + \omega_y'^2 + \omega_z'^2 = \eta'^2 - \xi'^2 + \omega_y'^2 + \omega_z'^2 + 2i\eta'\xi'. \quad (6.32)$$

We make a case distinction between $\xi' = 0$ and $\xi' \neq 0$.

- If $\xi' = 0$ then we find

$$\kappa'^2 = \eta'^2 + \omega_y'^2 + \omega_z'^2.$$

The assumption $\eta' > 0$ implies that κ'^2 must be a positive real number if $\xi' = 0$.

- If $\xi' \neq 0$ then, given that by the assumption $\eta' > 0$, we have that κ'^2 has nonzero imaginary part.

Now, write κ'^2 in polar notation

$$\kappa'^2 = \rho e^{i\phi},$$

with the modulus ρ , and where the argument takes values in the interval $-\pi < \phi \leq \pi$ by definition (6.29). Since κ'^2 either has a nonzero imaginary component, or it is a positive real number, we must have $\rho > 0$. Since κ'^2 cannot be a negative real number, we have $\phi \neq \pi$ so $-\pi < \phi < \pi$. We have that for the principal square root

$$\kappa' = \sqrt{\rho} e^{i\theta} \quad (6.33)$$

with $\theta = \phi/2$. It can be seen that $\pi/2 < \theta < \pi/2$. Since we also have that $\rho > 0$, this means that $\text{Re}(\kappa') > 0$. $\square$

To interpret this result, we have now shown that the equations (6.22)-(6.23) are a problem for only the outgoing and incoming characteristics with $\eta' > 0$, see also Ref. [16].

By Lemma 2 the expression $s'^2 \kappa'^2$ appearing in the prefactor of the inverse matrix of eigenvectors (6.31) has nonzero modulus. Therefore, the inverse matrix of eigenvectors is well-defined. It can be verified by hand that it is indeed the inverse matrix of eigenvectors. The components of the Fourier-Laplace transformed fields in the eigenvector basis are

$$\tilde{\mathbf{v}} = Q^{-1} \hat{\mathbf{v}},$$

with components

$$\tilde{\mathbf{v}} \equiv \begin{bmatrix} \tilde{v}_1 \\ \tilde{v}_2 \\ \tilde{v}_3 \\ \tilde{v}_4 \end{bmatrix}.$$

Premultiplying the Fourier-Laplace transformed equations (6.22) with Q^{-1} we obtain the system in the eigenvector basis

$$\partial_x \tilde{\mathbf{v}} = \sqrt{|s|^2 + \omega^2} \begin{bmatrix} \kappa' & 0 & 0 & 0 \\ 0 & \kappa' & 0 & 0 \\ 0 & 0 & -\kappa' & 0 \\ 0 & 0 & 0 & -\kappa' \end{bmatrix} \tilde{\mathbf{v}}, \quad x < 0. \quad (6.34)$$

Solving Eq. (6.34) we find that the components in the eigenvector basis have the form

$$\tilde{v}_1 = \tilde{v}_1(0, \omega', s') e^{\kappa x}, \quad (6.35)$$

$$\tilde{v}_2 = \tilde{v}_2(0, \omega', s') e^{\kappa x}, \quad (6.36)$$

$$\tilde{v}_3 = \tilde{v}_3(0, \omega', s') e^{-\kappa x}, \quad (6.37)$$

$$\tilde{v}_4 = \tilde{v}_4(0, \omega', s') e^{-\kappa x}. \quad (6.38)$$

By Lemma 2 and the solutions (6.35)-(6.38) we see that

$$\tilde{v}_1 \in L^2((-\infty, 0]),$$

$$\tilde{v}_2 \in L^2((-\infty, 0]),$$

$$\tilde{v}_3 \in L^2((-\infty, 0]) \quad \text{if and only if} \quad \tilde{v}_3(0, \omega', s') = 0,$$

$$\tilde{v}_4 \in L^2((-\infty, 0]) \quad \text{if and only if} \quad \tilde{v}_4(0, \omega', s') = 0.$$

Since the eigenvector matrix (6.30) is invertible, and since we have the requirement (6.24) that the Fourier-Laplace transformed fields all have finite energy, we see from Lemma 2 that

$$\tilde{v}_3 = 0 \quad \text{and} \quad \tilde{v}_4 = 0.$$

We then find the following relations between the Fourier-Laplace transformed

electric field and its components in the eigenvector basis

$$\hat{E}_y = \{\hat{\mathbf{v}}\}_1 = \{Q\tilde{\mathbf{v}}\}_1 = s'\kappa'\tilde{v}_1 - \omega'_y\omega'_z\tilde{v}_3 + (s'^2 + \omega_y'^2)\tilde{v}_4 = s'\kappa'\tilde{v}_1, \quad (6.39)$$

$$\hat{E}_z = \{\hat{\mathbf{v}}\}_2 = \{Q\tilde{\mathbf{v}}\}_2 = s'\kappa'\tilde{v}_2 - (s'^2 + \omega_z'^2)\tilde{v}_3 + \omega'_y\omega'_z\tilde{v}_4 = s'\kappa'\tilde{v}_2. \quad (6.40)$$

For the Fourier-Laplace transforms of the tangential components of the magnetic field we have

$$\hat{B}_y = \{\hat{\mathbf{v}}\}_3 = \{Q\tilde{\mathbf{v}}\}_3 = -\omega'_y\omega'_z\tilde{v}_1 + (s'^2 + \omega_y'^2)\tilde{v}_2 \quad (6.41)$$

$$= -\omega'_y\omega'_z\frac{\hat{E}_y}{s'\kappa'} + (s'^2 + \omega_y'^2)\frac{\hat{E}_z}{s'\kappa'}, \quad (6.42)$$

$$\hat{B}_z = \{\hat{\mathbf{v}}\}_4 = \{Q\tilde{\mathbf{v}}\}_4 = -(s'^2 + \omega_z'^2)\tilde{v}_1 + \omega'_y\omega'_z\tilde{v}_2 \quad (6.43)$$

$$= -(s'^2 + \omega_z'^2)\frac{\hat{E}_y}{s'\kappa'} + \omega'_y\omega'_z\frac{\hat{E}_z}{s'\kappa'}. \quad (6.44)$$

We substitute expressions for the coordinates in terms of the electric field (6.39), (6.40), the fields (6.35) and (6.36) in the Fourier-Laplace transformed boundary condition (6.23) and find

$$(s' + \kappa')\hat{E}_y(0, \omega, s) = \hat{g}'_y, \quad (6.45)$$

$$(s' + \kappa')\hat{E}_z(0, \omega, s) = \hat{g}'_z. \quad (6.46)$$

To estimate the components in terms of the boundary data, we need the following Lemma.

Lemma 3. *Let $\eta' > 0$. There is a $\delta > 0$ independent of s' and ω' such that for κ' defined by Eq. (6.21) and Eq. (6.27) we have that*

$$|s' + \kappa'| > \delta. \quad (6.47)$$

Remark 1. *Estimate (6.47) corresponds to the well-known uniform Kreiss condition for hyperbolic problems, that is adapted here to nonreflecting boundary conditions [13, 16–19].*

Proof. This proof is a modification of the proof of Proposition 2.2 in Ref. [22]. We will prove Lemma 3 by contradiction. Consider the set

$$D \equiv \{(s', \omega') : \operatorname{Re}(s') > 0, |s'|^2 + |\omega'|^2 = 1\},$$

that is bounded. Note that $s' = \eta' + i\xi'$ by Eqns. (6.7), (6.20) and (6.21). The function κ'^2 , repeated here,

$$\kappa'^2 = s'^2 + |\omega'|^2 = \eta'^2 - \xi'^2 + 2\eta'\xi'i + |\omega'|^2,$$

is uniformly continuous with respect to η' , ξ' and ω' in D , since the gradient of a polynomial function on a bounded set is finite. In particular, the real and imaginary parts $p \equiv \operatorname{Re}(\kappa'^2)$ and $q \equiv \operatorname{Im}(\kappa'^2)$ are uniformly continuous. An

explicit expression for the principal square root κ' [25] is given by

$$\kappa' = \sqrt{\frac{\sqrt{p^2 + q^2} + p}{2}} \pm i \sqrt{\frac{\sqrt{p^2 + q^2} - p}{2}},$$

where the sign of the imaginary part of the root is taken to be the same as the sign of the imaginary part of κ'^2 , or positive when zero. Since the square root of a uniformly continuous real function is uniformly continuous [26], we see that κ' is also uniformly continuous in η' , ξ' and ω' . The functions $f_1 \equiv s'$ and $f_2 \equiv \omega'$ are trivially uniformly continuous. Therefore, we can introduce the continuous extensions $\bar{s}'$, $\bar{\omega}'$, and $\bar{\kappa}'$ on

$$\bar{D} \equiv \{(s', \omega') : \text{Re}(s') \geq 0, |s'|^2 + |\omega'|^2 = 1\}.$$

Note that the continuous extensions are continuous in $\bar{D}$. Now, suppose that the estimate (6.47) is not valid. Then there exist s'_0, ω'_0 in $\bar{D}$ such that for $s' \rightarrow s'_0$, $\omega' \rightarrow \omega'_0$ we have

$$|\bar{s}' + \bar{\kappa}'| \rightarrow 0. \quad (6.48)$$

Let $\bar{\kappa}'_0$ be the value of $\bar{\kappa}'$ at (s'_0, ω'_0) and let $\bar{s}'_0 = \bar{\eta}'_0 + i\bar{\xi}'_0$ be the value of $\bar{s}'$. Since $\bar{s}'$ and $\bar{\kappa}'$ are uniformly continuous functions in $\bar{D}$ with $\eta' > 0$ and $\text{Re}(\kappa') > 0$ in D , we have $\bar{\eta}'_0 \geq 0$ and $\text{Re}(\bar{\kappa}'_0) \geq 0$. Since $\text{Re}(\bar{s}'_0 + \bar{\kappa}'_0) = 0$ by the limit (6.48) we hence need

$$\bar{\eta}'_0 = 0 \quad \text{and} \quad \text{Re}(\bar{\kappa}'_0) = 0. \quad (6.49)$$

Now, $\bar{\kappa}'$ is the principal square root of κ'^2 on D , and the sign of the imaginary part is therefore the same if it is nonzero

$$\text{sign } \text{Im}(\kappa') = \text{sign } \text{Im}(\kappa'^2) \quad \text{if} \quad \text{Im}(\kappa'^2) \neq 0.$$

This fact about the principal square root is easily derived from the definition of the principal square root in polar notation, see Eq. (6.33). Since $\eta' > 0$ and by the definition of κ'^2 , repeated here,

$$\kappa'^2 = |\omega'|^2 + \eta'^2 - \xi'^2 + 2i\eta'\xi',$$

we have that the sign of the imaginary part of $\bar{\kappa}'$ is the same as the sign of ξ'

$$\text{sign } \text{Im}(\kappa') = \text{sign } \text{Im}(\kappa'^2) = \text{sign } \xi' \quad \text{if} \quad \xi' \neq 0.$$

If the signs of the imaginary parts of the terms in Eq. (6.48) are the same, but the limit goes to zero, then we must have

$$\text{Im}(\bar{s}'_0 + \bar{\kappa}'_0) = 0 \quad \text{if and only if} \quad \bar{\xi}'_0 = 0 \quad \text{and} \quad \text{Im}(\bar{\kappa}'_0) = 0. \quad (6.50)$$

Since both the real part (6.49) and imaginary part (6.50) of $\bar{\kappa}'$ are zero in the limit, we find

$$\bar{\kappa}'_0 = 0. \quad (6.51)$$

We will now show that this leads to a contradiction. Inside D , we have for the continuous extension $\bar{\kappa}'^2 = \kappa'^2$ and from the definition of κ'^2

$$\bar{\kappa}'^2 = |\bar{\omega}'|^2 + \bar{\eta}'^2 - \bar{\xi}'^2 + 2i\bar{\eta}'\bar{\xi}'.$$

Since the continuous extension of $\bar{\kappa}'$ is continuous it does not matter in which order we evaluate limits. We take the limit as $\bar{\eta}' \rightarrow 0$ and $\bar{\xi}' \rightarrow 0$ and find

$$\lim_{\bar{\eta}' \rightarrow 0} \lim_{\bar{\xi}' \rightarrow 0} \bar{\kappa}'^2 = |\bar{\omega}'|^2.$$

This can only go to zero (which is needed by Eq. (6.51)) if $\bar{\omega}' \rightarrow 0$. But this is impossible by the normalisation $|\bar{s}'|^2 + |\bar{\omega}'|^2 = 1$, since in the limit we already have $\bar{s}'_0 = \bar{\eta}'_0 + i\bar{\xi}'_0 = 0$. Therefore we have found a contradiction and Lemma 3 is true. $\square$

We then obtain the following Lemma

Lemma 4. *Let $\text{Im}(s') > 0$. Assume that the inverse Fourier-Laplace transform of $\frac{1}{\sqrt{|s|^2 + |\omega|^2}} \hat{g}_y$ and $\frac{1}{\sqrt{|s|^2 + |\omega|^2}} \hat{g}_z$ exists. We also assume that the inverse Fourier-Laplace transform of $\frac{\omega_y \hat{g}_y(\omega, s)}{|\sqrt{s^2 + \omega^2}| \sqrt{|s|^2 + \omega^2}}$ and $\frac{\omega_z \hat{g}_z(\omega, s)}{|\sqrt{s^2 + \omega^2}| \sqrt{|s|^2 + \omega^2}}$ exists. Then, problem (6.14)-(6.16) has a unique solution. The Fourier-Laplace transformed tangential components are*

$$\hat{E}_y(x, \omega, s) = e^{\kappa x} \hat{E}_y(0, \omega, s) = e^{\kappa x} \frac{\hat{g}_y}{s + \kappa}, \quad (6.52)$$

$$\hat{E}_z(x, \omega, s) = e^{\kappa x} \hat{E}_z(0, \omega, s) = e^{\kappa x} \frac{\hat{g}_z}{s + \kappa}, \quad (6.53)$$

which we can estimate in terms of the boundary data as

$$|\hat{E}_y(0, \omega, s)|^2 \leq \frac{1}{\delta(|s|^2 + \omega^2)} |\hat{g}_y|^2, \quad (6.54)$$

$$|\hat{E}_z(0, \omega, s)|^2 \leq \frac{1}{\delta(|s|^2 + \omega^2)} |\hat{g}_z|^2, \quad (6.55)$$

with δ the constant in Lemma 3 that is independent of s and ω .

Proof. From the substitution of the fields in the boundary condition (6.45)-(6.46) and the estimate (6.47) we find the following estimates of the Fourier-Laplace components on the boundary

$$|\hat{E}_y(0, \omega, s)|^2 \leq \frac{1}{\delta(|s|^2 + \omega^2)} |\hat{g}_y(\omega, s)|^2,$$

$$|\hat{E}_z(0, \omega, s)|^2 \leq \frac{1}{\delta(|s|^2 + \omega^2)} |\hat{g}_z(\omega, s)|^2.$$

The Fourier-Laplace transformed tangential components at the boundary (6.52)-(6.53) are obtained from Eqns. (6.35)-(6.36) and (6.39)-(6.40) and (6.45)-

(6.46). We assume that the inverse Fourier-Laplace transform of $\frac{1}{\sqrt{|s|^2+|\omega|^2}}\hat{g}_y$ and $\frac{1}{\sqrt{|s|^2+|\omega|^2}}\hat{g}_z$ exists. The estimates (6.54)-(6.55) then show that the Fourier-Laplace transforms of the tangential components of the electric field at the boundary in Eqns. (6.52)-(6.53) exist. For general x we find the estimates

$$\begin{aligned} |\hat{E}_y(x, \omega, s)| &= |e^{\operatorname{Re}(\kappa)x}||\hat{E}_y(0, \omega, s)| \leq |\hat{E}_y(0, \omega, s)|, \\ |\hat{E}_z(x, \omega, s)| &= |e^{\operatorname{Re}(\kappa)x}||\hat{E}_z(0, \omega, s)| \leq |\hat{E}_z(0, \omega, s)|. \end{aligned}$$

Therefore, we can invert the Fourier-Laplace transforms in Eqns. (6.52)-(6.53) to find the tangential components of the electric field in real space and time that are unique. The Fourier-Laplace transforms of the tangential components of the magnetic field (6.42)-(6.44) are well-defined since $\operatorname{Re}(\kappa') > 0$ for $\operatorname{Im}(s') > 0$ by Lemma 2. We then find for the Fourier-Laplace transform of the normal component of the electric field

$$\begin{aligned} \hat{E}_x &= \frac{i\omega'_y \hat{B}_z - i\omega'_z \hat{B}_y}{s'} \\ &= \frac{i\omega'_y}{s'} \left(-(s'^2 + \omega_z'^2) \frac{\hat{E}_y}{s'\kappa'} + \omega'_y \omega'_z \frac{\hat{E}_z}{s'\kappa'} \right) \\ &\quad - \frac{i\omega'_z}{s'} \left(-\omega'_y \omega'_z \frac{\hat{E}_y}{s'\kappa'} + (s'^2 + \omega_y'^2) \frac{\hat{E}_z}{s'\kappa'} \right) \\ &= -i\omega'_y \frac{\hat{E}_y}{\kappa'} - i\omega'_z \frac{\hat{E}_z}{\kappa'} \\ &= -i\omega'_y \frac{e^{\kappa x} \hat{E}_y(0, \omega, s)}{\kappa'} - i\omega'_z \frac{e^{\kappa x} \hat{E}_z(0, \omega, s)}{\kappa'} \\ &= -i\omega'_y \frac{e^{\kappa x} \hat{g}_y}{\kappa'(s + \kappa)} - i\omega'_z \frac{e^{\kappa x} \hat{g}_z}{\kappa'(s + \kappa)}. \end{aligned} \tag{6.56}$$

We can estimate this as

$$|\hat{E}_x|^2 \leq \frac{|\omega'_y|^2 |g_y(\omega, s)|^2}{\delta^2 |\kappa'|^2 (|s|^2 + \omega^2)} + \frac{|\omega'_z|^2 |g_z(\omega, s)|^2}{\delta^2 |\kappa'|^2 (|s|^2 + \omega^2)}.$$

We assume that the inverse Fourier-Laplace transform of $\frac{\omega_y \hat{g}_y(\omega, s)}{|\sqrt{s^2 + \omega^2}| \sqrt{|s|^2 + \omega^2}}$ and $\frac{\omega_z \hat{g}_z(\omega, s)}{|\sqrt{s^2 + \omega^2}| \sqrt{|s|^2 + \omega^2}}$ exists. Then we invert Eq. (6.56) to find that the normal component of the field exists and is unique. The magnetic field can be found from the integral (6.10). Therefore, problem (6.14)-(6.16) has a unique solution. $\square$

To obtain the estimates in Theorem 1 we need the following Lemma.

Lemma 5. *Let $y \in \mathbb{C}$. The solution of*

$$\partial_x y = \lambda y, \quad y(0) = g, \quad \operatorname{Re}(\lambda) > 0, \quad -\infty \leq x \leq 0, \tag{6.57}$$

with boundary data $g \in \mathbb{C}$, satisfies

$$\|y\|_{L^2((-\infty, 0])}^2 = \frac{1}{2\operatorname{Re}(\lambda)} |g|^2.$$

Proof. Define $\langle y, y \rangle = y^* y$. We have

$$\langle y, y \rangle_x = 2\operatorname{Re} \langle y_x, y \rangle \quad (6.58)$$

$$= 2(\operatorname{Re}(\lambda)) \langle y, y \rangle. \quad (6.59)$$

Equation (6.57) has the solution $y = y(0)e^{\lambda x}$, and since $\operatorname{Re}(\lambda) > 0$, we have that $y \in L^2([-\infty, 0])$. Since we have that $y \in L^2([-\infty, 0])$ we can integrate over x and find for the left hand side of Eq. (6.58)

$$\int_{-\infty}^0 \langle y, y \rangle_{x'} dx' = |y(0)|^2 - \lim_{x \rightarrow \infty} |y(x)|^2 = |y(0)|^2.$$

In the second step we used that the limit tends to zero since $y \in L^2([-\infty, 0])$. We also integrate the right hand side of Eq. (6.59) and find

$$\int_{-\infty}^0 (2(\operatorname{Re}(\lambda)) \langle y, y \rangle) dx' = 2(\operatorname{Re}(\lambda)) \|y\|_{L^2((-\infty, 0])}^2.$$

We then obtain

$$|y(0)|^2 = 2(\operatorname{Re}(\lambda)) \|y\|_{L^2((-\infty, 0])}^2.$$

After we divide by $2\operatorname{Re}(\lambda)$ we find the equality we set out to prove. $\square$

Next, we prove the Lemma

Lemma 6. *Let $\eta' > 0$. There exists some $\delta > 0$ independent of s' and ω' such that*

$$\operatorname{Re}(\kappa') \geq \delta \eta'.$$

Proof. We argue by contradiction. Suppose that such a δ does not exist. Then there exist ξ'_0, η'_0 and ω'_0 such that as $\xi' \rightarrow \xi'_0$, $\eta' \rightarrow \eta'_0 > 0$ and $\omega' \rightarrow \omega'_0$ we have $\operatorname{Re}(\kappa') \rightarrow 0$. Let κ'_0 be the limit of κ' . We use polar notation

$$\kappa'_0 = \rho e^{i\theta}.$$

If $\operatorname{Re}(\kappa'_0) = 0$ then we must either have $\theta = -\pi/2$, $\theta = \pi/2$ or $\rho = 0$. We then find

$$\kappa'^2_0 = \rho^2 e^{i\phi},$$

with $\phi = 2\theta$. We must therefore have $\phi = 2\theta = \pi$ (since we define the phase $-\pi < \phi \leq \pi$) or $\rho = 0$. Recall that

$$\kappa'^2 = |\omega'|^2 + \eta'^2 - \xi'^2 + 2\eta'\xi'i.$$

If $\rho = 0$ then $\kappa'^2 \rightarrow 0$ and hence $\xi' \rightarrow 0$, but since $\eta' \rightarrow \eta'_0 > 0$ we obtain a contradiction since κ'^2 is still positive. If $\phi = \pi$ then κ'^2 should go to some negative real number, and hence $\xi' \rightarrow 0$, but $|\omega'|^2 + \eta'^2$ then still is positive, hence $\phi = \pi$ is not possible. Hence the Lemma is true. $\square$

We find the following estimate for the Fourier-Laplace transforms of the tangential electric field components in the interior of the domain.

Lemma 7. *The unique solution to the problem, described in Lemma 4, satisfies the following interior estimate*

$$\|\hat{E}_y\|_{L^2((-\infty, 0])}^2 \leq \frac{C}{\eta} \frac{|\hat{g}_y|^2}{|s|^2 + |\omega|^2}, \quad (6.60)$$

$$\|\hat{E}_z\|_{L^2((-\infty, 0])}^2 \leq \frac{C}{\eta} \frac{|\hat{g}_z|^2}{|s|^2 + |\omega|^2}, \quad (6.61)$$

with $C > 0$ a constant that does not depend on s and ω .

Proof. By Lemma 4 and Lemma 5 we have that

$$\begin{aligned} \|\hat{E}_y\|_{L^2((-\infty, 0])}^2 &= \frac{1}{2 \operatorname{Re}(\kappa)} |\hat{E}_y(0, \omega, s)|^2 \leq \frac{1}{\operatorname{Re}(\kappa)} \frac{C}{|s|^2 + \omega^2} |\hat{g}_y|^2, \\ \|\hat{E}_z\|_{L^2((-\infty, 0])}^2 &= \frac{1}{2 \operatorname{Re}(\kappa)} |\hat{E}_z(0, \omega, s)|^2 \leq \frac{1}{\operatorname{Re}(\kappa)} \frac{C}{|s|^2 + \omega^2} |\hat{g}_z|^2. \end{aligned}$$

By Lemma 6 we have that $\operatorname{Re}(\kappa') \geq \delta \eta'$ and we obtain Eqns. (6.60)-(6.61). $\square$

We also need the following Lemma.

Lemma 8. *There is a $C > 0$ independent of s and ω such that*

$$|\kappa|^2 < C(|s|^2 + |\omega|^2).$$

Proof. We repeat Eq. (6.32)

$$\kappa'^2 = |\omega'|^2 + \eta'^2 - \xi'^2 + 2\eta'\xi'i.$$

For this to diverge, we must have either $\xi' \rightarrow \infty$, $\eta' \rightarrow \infty$ or $\omega' \rightarrow \infty$. But these are all constrained to have a maximum of one by the normalisation (6.20). We have therefore found a contradiction. $\square$

We differentiate Eqns. (6.52) and (6.53) with respect to x to find

$$\begin{aligned} \partial_x \hat{E}_y &= \kappa \hat{E}_y(0, \omega, s) e^{\kappa x} = \kappa \hat{E}_y, \\ \partial_x \hat{E}_z &= \kappa \hat{E}_z(0, \omega, s) e^{\kappa x} = \kappa \hat{E}_z. \end{aligned}$$

We then find the following estimate on the interior of the domain for the x -derivative of the Fourier-Laplace components

$$\begin{aligned}\|\partial_x \hat{E}_y\|_{L^2((-\infty, 0])}^2 &\leq |\kappa|^2 \frac{C}{\eta} \frac{|\hat{g}_y|^2}{|s|^2 + |\omega|^2} \leq \frac{C}{\eta} |\hat{g}_y|^2, \\ \|\partial_x \hat{E}_z\|_{L^2((-\infty, 0])}^2 &\leq |\kappa|^2 \frac{C}{\eta} \frac{|\hat{g}_z|^2}{|s|^2 + |\omega|^2} \leq \frac{C}{\eta} |\hat{g}_z|^2.\end{aligned}$$

In the second step we used Lemma 8. We use Parseval's relation for the Fourier transform in ξ' with $s = \eta + i\xi$ to transform this back to time, and Parseval's relation for the Fourier transform in y

$$\begin{aligned}\|\partial_x E_y e^{-\eta t}\|_{L^2(\Omega)} &\leq \frac{C}{\eta} \|g_y e^{-\eta t}\|_{L^2(\partial\Omega)}^2, \\ \|\partial_x E_z e^{-\eta t}\|_{L^2(\Omega)} &\leq \frac{C}{\eta} \|g_z e^{-\eta t}\|_{L^2(\partial\Omega)}^2.\end{aligned}$$

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CHAPTER 7

Summary and outlook

In this thesis, we have theoretically and numerically investigated novel aspects of light propagation in three-dimensional (3D) photonic band gap crystals that open up new opportunities to tune the interaction between light and matter. We have also developed highly accurate nonreflecting boundary conditions for a mixed DG discretization of the Maxwell equations on finite size computational domains.

We have explored the unconventional “Cartesian” propagation of light in a 3D cavity superlattice embedded within a 3D photonic band-gap crystal. Using the plane-wave expansion method, we calculated the dispersion relations of a 3D cavity superlattice with the cubic inverse woodpile structure that reveal five coupled-cavity bands m . These bands have quadrupolar symmetry and are the optical analogues of d-orbitals in solid-state physics. For $m = 3, 4, 5$, we observed that the dispersion bandwidth indeed looks like a quadrupolar radiation pattern. To understand the coupling between the cavities in a 3D cavity superlattice more fundamentally, we derived the coupling coefficients of light from the dispersion relations using the tight-binding method. For all converged coupled-cavity bands, we found that light hops remarkably only in a few discrete directions including the Cartesian (x, y, z) directions. Therefore we propose the name “*Cartesian light*”. The large coupling coefficients in the Cartesian directions occur simultaneously with a near vanishing dispersion bandwidth in this direction. This means that arguments for a one-dimensional (1D) coupled-resonator optical waveguide (CROW) *do not* hold for 3D cavity superlattices, in other words, our 3D cavity superlattice is not a “3D CROW”. The unusually small dispersion bandwidth in the Cartesian directions is a result of the interplay between positive and negative coupling coefficients in the Cartesian and diagonal directions.

Cartesian light propagation on a 3D superlattice of cavities differs fundamentally from other known modes of propagation in periodic nanophotonic systems, notably from the conventional 3D spatially-extended Bloch wave propagation in crystals, from light tunneling through a band gap, from coupled-resonator optical waveguiding, and also from light diffusing at the edge of a gap.

Superlattice Bloch modes do not give a full picture of light propagation in 3D cavity superlattices, since all the cavities are excited simultaneously. Therefore, we have analyzed the time-resolved propagation of an ultrashort input pulse that initially excites only a single cavity with frequencies within a single band m of the superlattice. We observed that light for $m = 3$ travels primarily in the Cartesian directions, for $m = 4$ it looks like a high-order Hermite-gaussian mode,

and for $m = 5$ it travels primarily in the diagonal directions. The predominant propagation directions in 3D cannot be readily inferred from either the dispersion bandwidth or from the coupling coefficients, in contrast to CROWs, which is a result of the interference between multiple hopping paths that do not exist in a CROW. The initial excitation decays much faster for the $m = 4$ band than for the other bands, which can potentially be observed in time-resolved experiments on fabricated superlattices.

We have for the first time investigated the effects of disorder on the density of states (DOS) of light in a 3D photonic band gap crystal. We employed a method that unambiguously samples all possible modes in the DOS, in contrast to previous work with externally-incident light beams that likely misses some modes. We observed that the band gap becomes narrower as the disorder strength increases from 0% to 25% of the pore radius. At a disorder strength of 25%, the band gap closes for one realization out of ten. However, at this disorder strength the structure is so thin that the real structure may collapse. The band gap is therefore remarkably robust over the entire physical range of disorder strengths. Interestingly, we observed a larger frequency shift of the lower band edge than for the upper band edge, which agrees with separate observations of states appearing in the upper half of the band gap for many parameters of defect pores used in the design of cavities.

We have developed and implemented nonreflecting boundary conditions for a mixed DG discretization of the time-harmonic Maxwell equations. The boundary conditions are obtained by applying the well-known Hagstrom-Warburton boundary conditions separately to the tangential components of the electric field. The auxiliary equations for the Hagstrom-Warburton boundary conditions are discretized with discontinuous Galerkin elements and Bassi-Rebay type fluxes and combined with the mixed DG discretization for the time-harmonic Maxwell equations. This is the first time that the Hagstrom-Warburton boundary condition is combined with an element-wise curl-conforming discretization of the Maxwell equations. The discretized Hagstrom-Warburton boundary conditions successfully describe unboundedness with only small spurious reflections that are accurately predicted by an estimate at the continuous level. These new nonreflecting boundary conditions will allow accurate computations of the behavior of light in finite structures.

Finally, we analyzed the well posedness at the continuous level of a Hagstrom-Warburton type nonreflecting boundary condition for the time-harmonic Maxwell equations. We showed that this boundary condition satisfies a uniform Kreiss condition that is appropriate to nonreflecting boundary conditions. We also derived an estimate for the electric field in the interior in terms of the boundary data.

Based on this research, I present the following outlook for further studies:

1. If the resonance frequencies of the cavities in a 3D cavity superlattice are varied according to a random distribution, an Anderson localization transition of light may occur. For strong levels of disorder, the five bands of the superlattice may couple, increasing the phase space for propagation of light and inhibiting localization. It would be very exciting to investigate

the renormalization group for the localization of multiple coupled-cavity bands.

2. We found a directionality of $D = 4$ for the $m = 4$ band of the inverse woodpile 3D cavity superlattice that has nonzero coupling coefficients only in the x - and z -directions, whereas the bands $m = 3, 5$, that have nonzero coupling coefficients in the diagonal directions as well, have higher directionalities $D = 15, 26$. It may be interesting to see whether a quantitative argument can be given that these additional coupling coefficients result in a larger contribution of interference between different hopping paths to the propagation. In addition, one could investigate whether decreasing the y -spacing of cavities gives higher coupling coefficients in the y -direction, and even higher directionalities.
3. To make a quantitative connection between the propagation directions of light in the time-domain in 3D cavity superlattices and the dispersion bandwidth, one could use the Born-von Karmann (or periodic) boundary condition at the edge of the superlattice instead of truncating it. In that case, the light would be in a superposition of superlattice modes with well-defined wave vectors, for which the group velocity $\mathbf{v}_g = \nabla_{\mathbf{k}}\omega$ can be calculated. A weighted summation over the group velocities would likely give the predominant propagation directions, and resolve the tension between the time-resolved observations and the frequency-domain ones.
4. The time-resolved calculations revealed that the initial excitation for a cavity in the superlattice decays much faster for the $m = 4$ band than for the other bands. It may be interesting to investigate whether a larger amount of disorder is necessary, as well, to localize the $m = 4$ band in a given superlattice.
5. We observed that the band gap of the inverse woodpile crystal is progressively filled with states as the disorder strength becomes larger than $\gamma = 0.20$. It would be interesting to study whether these states are localized. A measure of the propagating character of a state is the dispersion bandwidth $\Delta\omega$, from which the dimensionless conductance $\gamma = \frac{\Delta\omega}{\Delta_s\omega}$, with $\Delta_s\omega$ the average frequency separation between neighbouring states, is easily calculated. The DOS calculations in this Thesis allow to study the dispersion bandwidth of each mode. One could plot the dispersion bandwidth on a frequency axis at the mean frequencies of the bands, and then perform calculations for a larger $5 \times 5 \times 5$ crystal. If the bands are localized, we would expect to see two fixed points on the frequency axis where the variation of the dispersion bandwidth with sample size is constant.
6. It would be interesting to test the discretized Hagstrom-Warburton boundary condition by calculating the reflectivity of inverse woodpile photonic crystals, replicating calculations that have been previously carried out in the COPS group.

7. Applying the Hagstrom-Warburton boundary condition to all sides of a rectangular, or more generally, polyhedral domain, requires the discretization of special corner conditions. The Hagstrom-Warburton boundary condition has also been applied with dielectric surfaces that extend to infinity, *i.e.*, a substrate. For calculations with sources in the interior it is important to use a modified boundary condition for evanescent waves.
8. Finally, it would be worthwhile to study mathematically the well-posedness of the discretized Hagstrom-Warburton boundary conditions in combination with the mixed DG formulation for the time-harmonic Maxwell equations, guaranteeing their accuracy and robustness.

Nederlandse samenvatting

In dit proefschrift hebben we theoretisch en numeriek nieuwe aspecten onderzocht van lichtvoortplanting in driedimensionale (3D) fotonische bandkloof kristallen die nieuwe mogelijkheden creëren om de interactie tussen licht en materie af te stemmen. We hebben ook zeer nauwkeurige niet-reflecterende randcondities ontwikkeld voor een gemengde DG discretisatie van de Maxwell vergelijkingen op rekendomeinen van eindige grootte met een welbepaalde foutschatting.

We hebben voor het alleréerst de onconventionele “Cartesische” lichtvoortplanting onderzocht in een 3D rooster van trilholtten ingebed in een 3D fotonische bandkloof kristal. Het 3D rooster van trilholtten heeft toestanden waarbij het licht tussen de trilholtten springt. Met de vlakke-golf expansie methode hebben we de dispersierelaties van een 3D rooster van trilholtten met de kubische inverse woodpile structuur berekend die vijf gekoppelde-trilholte banden m laten zien. Deze banden hebben quadrupolaire symmetrie en zijn de optische analogen van d-orbitalen in de vaste stof fysica. Voor $m = 3, 4, 5$, hebben we waargenomen dat de dispersie bandbreedte er inderdaad uitziet als een quadrupolair stralingspatroon. Om de koppeling tussen de trilholtten in een 3D rooster van trilholtten fundamenteeler te begrijpen, hebben we de koppelingscoëfficiënten van licht afgeleid van de dispersierelaties met gebruik van de tight-binding methode. Het is opmerkelijk dat we voor alle gekoppelde-trilholte banden hebben gevonden dat licht slechts in een paar discrete richtingen springt, inclusief de Cartesische (x, y, z) richtingen. Daarom stellen we de naam “*Cartesisch licht*” voor. De grote koppelingscoëfficiënten in de Cartesische richtingen bestaan gelijktijdig met een bijna verwaarloosbare dispersie bandbreedte in deze richting. Dit betekent dat argumenten voor een een-dimensionale (1D) gekoppelde-resonator optische golfgeleider (CROW) niet opgaan voor 3D roosters van trilholtten. Met andere woorden, ons 3D rooster van trilholtten is geen “3D CROW”. De ongebruikelijk kleine dispersie bandbreedte in de Cartesische richtingen is een gevolg van de wisselwerking tussen positieve en negatieve koppelingscoëfficiënten in de Cartesische en diagonale richtingen.

Cartesische lichtvoortplanting op een 3D rooster van trilholtten verschilt fundamenteel van andere bekende vormen van lichtvoortplanting in periodieke nanofotonische systemen, in het bijzonder van de conventionele 3D ruimtelijk uitgebreide Bloch golf voortplanting in kristallen, van licht dat door een bandkloof springt, van gekoppelde-resonator optische golfgeleiding, en ook van licht dat diffundeert op de rand van een bandkloof.

Rooster Bloch modes geven geen volledig beeld van lichtvoortplanting in 3D roosters van trilholtten, omdat alle trilholtten tegelijk gevuld met licht zijn.

Daarom hebben we de tijdsafhankelijke voortplanting van een zeer korte input puls geanalyseerd die in eerste instantie alleen een enkele trilholte met frequenties binnen een enkele band m van het trilholte opwindt. We hebben waargenomen voor band $m = 3$ dat licht zich primair voortplant in de Cartesische richtingen, voor $m = 4$ ziet het er uit als een hogere-orde Hermite-gaussian mode, en voor $m = 5$ plant het zich vooral voort in de diagonale richtingen. De overheersende voortplantingsrichtingen in 3D kunnen niet onmiddellijk afgeleid worden uit hetzij de dispersie bandbreedte, hetzij de koppelingscoëfficiënten, in contrast tot CROWs, hetgeen een gevolg is van de interferentie tussen meervoudige sprong paden die niet bestaan in een CROW. De eerste excitatie vervalt veel sneller voor de $m = 4$ band dan voor andere banden, hetgeen potentieel waargenomen kan worden in tijdsafhankelijke experimenten op gefabriceerde roosters.

We hebben voor de eerste keer de effecten onderzocht van wanorde op de toestandsdichtheid (DOS) van licht in een 3D fotonische bandkloof kristal. We hebben een methode gebruikt die ondubbelzinnig alle mogelijke modes in de DOS bemonstert, in contrast tot eerder werk met van buiten invallende lichtbundels die waarschijnlijk sommige modes missen. We hebben waargenomen dat de bandkloof nauwer wordt als de sterkte van de wanorde toeneemt van 0% tot 25% van de porie straal. Bij een wanorde sterkte van 25% sluit de bandkloof voor één realisatie van de tien. Echter, bij deze disorder sterkte is de structuur in de berekeningen zo dun dat de echte fysieke structuur mogelijk instort. De bandkloof is daarom opmerkelijk robuust over het hele fysische gebied van wanorde sterktes. Het is interessant dat we een grotere frequentieverschuiving hebben waargenomen voor de onderste rand van de bandkloof dan voor de bovenste rand van de bandkloof, hetgeen overeenkomt met afzonderlijke waarnemingen van toestanden die tevoorschijn komen in de bovenste helft van de bandkloof voor vele parameters van defect poriën die gebruikt worden in het ontwerp van trilholtten.

We hebben niet-reflecterende randcondities ontwikkeld en geïmplementeerd voor een gemengde DG discretisatie van de tijdharmonische Maxwell vergelijkingen. De randcondities worden verkregen door de welbekende Hagstrom-Warburton randcondities afzonderlijk toe te passen op de tangentiële componenten van het elektrisch veld. De hulpvergelijkingen voor de Hagstrom-Warburton randcondities worden gediscretiseerd met discontinue Galerkin elementen en Bassi-Rebay type fluxes en gecombineerd met de gemengde DG discretisatie voor de tijdharmonische Maxwell vergelijkingen. Dit is de eerste keer dat de Hagstrom-Warburton randconditie gecombineerd wordt met een elementsgewijze curl-conforming discretisatie van de Maxwell vergelijkingen. De gediscretiseerde Hagstrom-Warburton randcondities beschrijven met succes de onbegrensde van het fysieke domein met alleen kleine kunstmatige reflecties die nauwkeurig voorspeld worden door een schatting op het continue niveau. Deze nieuwe niet-reflecterende randcondities zullen nauwkeurige berekeningen toestaan van het gedrag van licht in eindige structuren.

Tot slot, hebben we de goed gesteldheid geanalyseerd op het continuüm niveau van een Hagstrom-Warburton type niet-reflecterende randconditie voor de tijdsafhankelijke Maxwell vergelijkingen. We hebben laten zien dat deze randconditie voldoet aan een uniforme Kreiss conditie die geschikt is voor niet-reflecterende

randcondities. We hebben ook een schatting afgeleid voor het elektrisch veld in het inwendige in termen van de data op de rand.

Op basis van dit onderzoek, presenteer ik de volgende suggesties voor toekomstig onderzoek dat is geïnspireerd door mijn proefschrift:

1. Als de resonantie frequenties van de trilhouten in een 3D rooster van trilhouten worden gevarieerd volgens een kansverdeling, kan er een Anderson localisatie transitie van licht plaatsvinden. Voor sterke niveaus van wanorde kunnen de vijf banden van het rooster mogelijk gekoppeld raken, hetgeen de faseruimte voor de voortplanting van licht doet toenemen en localisatie onderdukt. Het zou fantastisch zijn om de renormalisatiegroep voor de localisatie van meervoudige gekoppelde-trilholte banden te onderzoeken.
2. We hebben een directionaliteit van $D = 4$ voor de $m = 4$ band van de inverse woodpile 3D rooster van trilhouten gevonden, die alleen in de x - en z -richtingen koppelingscoëfficiënten heeft die ongelijk aan nul zijn, terwijl de banden $m = 3$ en 5 , die ook in diagonale richtingen koppelingscoëfficiënten ongelijk aan nul hebben, hogere directionaliteiten $D = 15$ en 26 hebben. Het zou interessant kunnen zijn om te onderzoeken of er een kwantitatief argument gegeven kan worden dat deze aanvullende koppelingscoëfficiënten resulteren in een grotere bijdrage van de interferentie tussen verschillende sprong paden aan de voortplanting. In aanvulling hierop, zou men kunnen onderzoeken of het verminderen van de y -afstand tussen trilhouten grotere koppelingscoëfficiënten geeft in de y -richting, en nog hogere directionaliteiten.
3. Om een kwantitatief verband te leggen tussen de voortplantingsrichtingen van licht in het tijddomein in 3D roosters van trilhouten en de dispersie bandbreedte, kan men de Born-von Karman (of periodieke) randconditie gebruiken op de rand van het rooster in plaats van het af te kappen. In dat geval zou het licht zich bevinden in een superpositie van rooster modes met goed-gedefinieerde golf vectoren, waarvoor de groepssnelheid $\mathbf{v}_g = \nabla_{\mathbf{k}}\omega$ kan worden berekend. Een gewogen sommering over de groepssnelheden zou waarschijnlijk de overheersende voortplantingsrichtingen geven, en de verschillen verklaren tussen de tijdsafhankelijke waarnemingen en die in het frequentiedomein.
4. De tijdsafhankelijke berekeningen laten zien dat de aanvankelijke excitatie voor een trilholte in het rooster veel sneller vervalst voor de $m = 4$ band dan voor de andere banden. Het kan interessant zijn om uit te zoeken of er ook een grotere hoeveelheid wanorde nodig is om de $m = 4$ band te localiseren in een gegeven rooster.
5. We hebben waargenomen dat de bandkloof van een inverse woodpile kristal progressief gevuld raakt met toestanden wanneer de wanorde sterkte groter wordt dan $\gamma = 0.20$. Het zou interessant zijn om te bestuderen of deze toestanden gelocaliseerd zijn. Een maat voor het propagerende karakter

van een toestand is de dispersie bandbreedte $\Delta\omega$, op basis waarvan de dimensieloze geleiding $\gamma = \frac{\Delta\omega}{\Delta_s\omega}$, met $\Delta_s\omega$ de gemiddelde frequentiescheiding tussen naburige toestanden, gemakkelijk berekend kan worden. De DOS berekeningen in dit proefschrift maken het mogelijk om de dispersie bandbreedte van iedere mode te bestuderen. Men zou de dispersie bandbreedte op een frequentie-as bij de gemiddelde frequenties van de banden kunnen plotten, en vervolgens berekeningen kunnen doen op een groter $5 \times 5 \times 5$ kristal. Als de banden gelocaliseerd zijn, zouden we verwachten dat we twee vaste punten zien op de frequentie-as waar de variatie van de dispersie bandbreedte met kristal grootte constant is.

6. Het zou interessant zijn om de gediscretiseerde Hagstrom-Warburton randconditie te testen door de reflectiviteit te berekenen van inverse woodpile fotonische kristallen, waarmee we berekeningen zouden repliceren die eerder uitgevoerd zijn binnen de COPS groep.
7. Het toepassen van de Hagstrom-Warburton randconditie op alle zijden van een rechthoekig, of meer in het algemeen, een veelvlakig domein, vereist de discretisatie van speciale hoek condities. De Hagstrom-Warburton randconditie is ook toegepast met diëlektrische grensvlakken die doorlopen tot het oneindige, in andere woorden, een substraat. Voor berekeningen met bronnen in het inwendige is het belangrijk om een aangepaste randconditie voor evanescente golven te gebruiken.
8. Tot slot, zou het de moeite waard zijn om wiskundig de goed gesteldheid van de gediscretiseerde Hagstrom-Warburton randcondities te onderzoeken in combinatie met de gemengde DG formulering voor de tijdharmonische Maxwell vergelijkingen, hetgeen hun nauwkeurigheid en robuustheid garandeert.

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