1 On the solid-state theoretical description of photonic crystals

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1.1 Introduction

Since the invention of the laser, progress in Photonics has been intimately related to the development of optical materials which allow one to control the flow of electromagnetic radiation or to modify light–matter interaction. Photonic Crystals (PhCs) represent a novel class of optical materials which elevates this principle to a new level of sophistication. These artificial structures are characterized by two–dimensional (2D) or three–dimensional (3D) periodic arrangements of dielectric material which lead to the formation of an energy band structure for electromagnetic waves propagating in them. Recent advances in micro–structuring technology provide an enormous flexibility in the choice of material composition, lattice periodicity and symmetry of these arrangements allowing one to fabricate PhCs with embedded defect structures. As a consequence, the dispersion relation and associated mode structure of PhCs may be tailored to almost any need. This results in a potential for controlling the optical properties of PhCs that may eventually rival the flexibility in tailoring the properties of their electronic counterparts, the semiconducting materials.

One of the most striking features of PhCs is associated with the fact that suitably engineered PhCs may exhibit frequency ranges over which ordinary linear propagation is forbidden, irrespective of direction. These photonic band gaps (PBGs) [1-3] lend themselves to numerous applications in linear, nonlinear and quantum optics. For instance, in the linear regime novel optical guiding characteristics through the engineering of defects such as microcavities, waveguides and their combination into functional elements, such as wavelength add-drop filters [4, 5] may be realized. Similarly, the incorporation of nonlinear materials into PBG structures is the basis for novel solitary wave propagation for frequencies inside the PBG. In the case of lattice-periodic Kerr-nonlinearities, the threshold intensities and symmetries of these solitary waves depend on the direction of propagation [6-8], whereas in the case of nonlinear waveguiding structures embedded in a 2D PBG material, the propagation characteristics strongly depend on the nature of the waveguides [9]. Finally, the existence of complete PBGs allows one to inhibit spontaneous emission for atomic transition frequencies, deep in the PBG [1] and leads to strongly non-Markovian effects, such as fractional localization of the atomic population for atomic transition frequencies in close proximity to a complete PBG [10, 11].

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Photonic Crystals: Advances in Design, Fabrication, and Characterization Edited by Kurt Busch, Stefan Lölkes, Ralf B. Wehrspohn, Helmut Föll Copyright © 2004 Wiley-VCH Verlag GmbH & Co. KGaA ISBN: 3-527-40432-5

The discovery of superrefractive phenomena such as the superprism effect [12, 13] and the resulting potential applications in telecommunication technology [14, 15] have recently attracted a lot of attention to the highly anisotropic nature of iso–frequency surfaces in the photonic band structure. Similarly, the tailoring of photonic dispersion relations and associated mode structures, group velocities, group velocity dispersions (GVDs) and effective nonlinearities through judiciously designed PhCs, allows one to explore regimes of nonlinear wave propagation in PhCs that hitherto have been virtually inaccessible. For instance, the existence of flat bands that are characteristic for 2D and 3D PhCs and the associated low group velocities may greatly enhance frequency conversion effects [16] and may lead to improved designs for distributed-feedback (DFB) laser systems [16–18]. Photonic crystals with embedded defects, such as microcavities and waveguiding structures, hold tremendous potential for the creation of photonic integrated circuits.

As in virtually any nano-photonic system, a careful theoretical analysis is of paramount importance when interpreting experimental data, and when predicting and realizing novel physical phenomena in PhCs. To date, photonic band structure calculations are used to determine and predict the dispersion relations of perfect, infinitely extended PhCs, and PhCs with simple defects such as isolated cavities and waveguides. More complex situations such as transmission and reflection from finite slabs of PhC-material or through waveguide bends are usually analyzed through direct simulations of Maxwell's equations, based on Finite-Difference Time-Domain (FDTD) or Finite Element (FE) methods. While these are perfectly legitimate approaches, which rest on some 30 years of experience, these techniques do require substantial computational resources and, as a consequence, modeling has been restricted to selected small scale PhC circuits. Moreover, certain computationally intensive aspects related to small scale PhC circuits, such as studies of the effect of fabricational tolerances and the optimization of device designs, still present serious challenges when working with FDTD or FE methods.

In this manuscript, we want to illustrate how the natural affinity of electromagnetic wave propagation in PhCs to the case of electron (wave) transport in semiconducting materials, allows us to devise a comprehensive and highly efficient theoretical framework for the qualitative, as well as quantitative determination of the optical properties of PhCs: Photonic band structure computations allow us to obtain photonic band structures and associated Bloch functions. Related physical quantities such as densities of states (DOS) and group velocities can be calculated with little additional work. Nonlinear PhCs can be studied through an appropriate multi–scale analysis that utilizes Bloch functions as carrier waves and leads to a natural generalization of the well–known slowly varying envelope approximation. Combining band structure calculations with elements from diffractive optics, enables us to determine the reflection and transmission properties of finite PhC–slabs. Finally, we show how defect structures in PhCs can be efficiently treated with the help of photonic Wannier functions. Moreover, this Wannier function approach allows us to formulate a PhC circuit theory, where a defect structure is replaced by the optical analogue of an impedance matrix.

1.2 Photonic band structure computation

The goal of photonic band structure computation is the solution of the wave equation for the perfect PhC, i.e., for an infinitely extended, strictly periodic array of dielectric material. The

1.2 Photonic band structure computation

resulting dispersion relation and associated mode structure may then be further processed to derive related physical quantities such as DOS and group velocities. For simplicity of presentation, we consider in the remainder of the manuscript only 2D PhCs in the TM–polarized case. However, we want to emphasize that analogous considerations apply to the case of TE– polarized radiation in 2D PhCs, as well as to electromagnetic wave propagation in 3D PhCs and will give references where appropriate.

For TM-polarized radiation in 2D PhCs, the wave equation reduces to a single scalar equation for the z-component $E(\vec{r})$ of the electric field:

$$\frac{1}{\varepsilon_{\mathsf{p}}(\vec{r})} \left(\partial_x^2 + \partial_y^2\right) E(\vec{r}) + \frac{\omega^2}{c^2} E(\vec{r}) = 0.$$
(1.1)

Here, c denotes the vacuum speed of light and $\vec{r} = (x, y)$ denotes a 2D position vector. The dielectric constant $\varepsilon_p(\vec{r}) \equiv \varepsilon_p(\vec{r} + \vec{R})$ contains all the structural information of the PhC and is periodic with respect to the set $\mathcal{R} = \{n_1 \vec{a}_1 + n_2 \vec{a}_2; (n_1, n_2) \in \mathbb{Z}^2\}$ of lattice vectors \vec{R} , generated by the primitive translations \vec{a}_i , i = 1, 2 which serve as a basis for the underlying PhC lattice. Equation (1.1) represents a differential equation with periodic coefficients and, therefore, its solutions obey the Bloch–Floquet theorem: The discrete translational symmetry of the lattice allows us to label the solutions with a wave vector \vec{k} that is restricted to the first Brillouin zone (BZ) of the reciprocal lattice. This back-folding of the dispersion relation $\omega(\vec{k})$ to the first BZ introduces a discrete band index n. The eigenmodes (Bloch functions) corresponding to eigenfrequency $\omega_n(\vec{k})$ exhibit the Bloch–Floquet form of modulated plane waves

$$E_{n\vec{k}}(\vec{r}) = e^{ik\vec{r}} u_{n\vec{k}}(\vec{r}).$$
(1.2)

Here, $u_{n\vec{k}}(\vec{r} + \vec{R}) = u_{n\vec{k}}(\vec{r})$ is periodic with the lattice. A straightforward way of solving Eq. (1.1) and (1.2) is to expand all the periodic functions into a Fourier series over the reciprocal lattice \mathcal{G}

$$\frac{1}{\varepsilon_{p}(\vec{r})} = \sum_{\vec{G}} \eta_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} , \qquad E_{\vec{k}}(\vec{r}) = \sum_{\vec{G}} a_{\vec{G}}^{\vec{k}} e^{i\left(\vec{k}+\vec{G}\right)\cdot\vec{r}} .$$
(1.3)

The Fourier coefficients $\eta_{\vec{G}}$ are given by

$$\eta_{\vec{G}} = \frac{1}{V_{\text{wsc}}} \int_{\text{wsc}} d^2 \vec{r} \frac{1}{\varepsilon_{\text{p}}(\vec{r})} e^{-i\vec{G}\cdot\vec{r}} , \qquad (1.4)$$

where we have designated the volume of the Wigner-Seitz cell (WSC) by V_{wsc} . Inserting this expansion into Eq. (1.1) and defining the coefficients $b_{\vec{G}}^{\vec{k}} \equiv |\vec{k} + \vec{G}| a_{\vec{G}}^{\vec{k}}$, transforms the differential equation into an infinite matrix eigenvalue problem

$$\sum_{\vec{G}'} |\vec{k} + \vec{G}| |\vec{k} + \vec{G}'| \eta_{\vec{G} - \vec{G}'} b_{\vec{G}'}^{\vec{k}} = \frac{\omega_{\vec{k}}^2}{c^2} b_{\vec{G}}^{\vec{k}} , \qquad (1.5)$$

which must be suitably truncated to become accessible to an approximate numerical solution. Further details of the plane wave method (PWM) for 2D TE and 3D isotropic systems can be found, for instance, in [19] and for anisotropic 3D systems in [20].

In Fig. 1.1(b), we show the band structure for TM-polarized radiation in a 2D PhC consisting of a square lattice (lattice constant *a*) of cylindrical air pores (radius $R_{\text{pore}} = 0.475a$) in a silicon matrix ($\varepsilon = 12$) (for details on the fabrication of this structure, we would like to refer the reader to Chapter 4 of this book). This structure exhibits two complete 2D bandgaps. The larger, fundamental bandgap (20% of the midgap frequency) extends between $\omega = 0.238 \times 2\pi c/a$ to $\omega = 0.291 \times 2\pi c/a$ and the smaller, higher order bandgap (8% of the midgap frequency) extends from $\omega = 0.425 \times 2\pi c/a$ to $\omega = 0.464 \times 2\pi c/a$. In the remainder



Figure 1.1: Density of states (a) and photonic band structure (b) for TM–polarized radiation in a square lattice (lattice constant *a*) of cylindrical air pores of radius $R_{pore} = 0.475a$ in dielectric with $\varepsilon = 12$ (silicon). This PhC exhibits a large fundamental gap extending from $\omega = 0.238 \times 2\pi c/a$ to $\omega = 0.291 \times 2\pi c/a$. A higher order band gap extends from $\omega = 0.425 \times 2\pi c/a$ to $\omega = 0.464 \times 2\pi c/a$.

of this chapter, this particular PhC will serve as the model problem for which we illustrate our solid state theoretical approach to the optical properties of PhCs.

1.2.1 Density of states

The photonic dispersion relation $\omega_n(\vec{k})$ gives rise to a photonic density of states (DOS), which plays a fundamental role for the understanding of the quantum optical properties of active material embedded in PhCs [11]. The photonic DOS $N(\omega)$ is defined by "counting" all allowed states with a given frequency ω

$$N(\omega) = \sum_{n} \int_{BZ} d^2k \ \delta(\omega - \omega_n(\vec{k})).$$
(1.6)

In Fig. 1.1(a) we depict the DOS for our model system, where the photonic band gaps are manifest as regions of vanishing DOS. Characteristic for 2D systems is the linear behavior for small frequencies as well as the logarithmic singularities, the so-called van Hove singularities, associated with vanishing group velocities for certain frequencies inside the bands. However, for applications to quantum optical experiments in photonic crystals, it is necessary to investigate not only the (overall) availability of modes with frequency ω , but also the local coupling strength of an emitter at a certain position \vec{r} in the PhC to the electromagnetic environment

provided by the PhC. Consequently, it is the overlap matrix element of the emitter's dipole moment to the eigenmodes (Bloch functions) that is determining quantum optical properties such as decay rates etc. [11]. This may be combined into the local DOS (LDOS), $N(\vec{r}, \omega)$, defined as

$$N(\vec{r},\omega) = \sum_{n} \int_{BZ} d^{2}k \ |E_{n\vec{k}}(\vec{r})|^{2} \,\delta(\omega - \omega_{n}(\vec{k})).$$
(1.7)

For an actual calculation, the integrals in Eq. (1.6) and Eq. (1.7) must be suitably discretized and one may again revert to the methods of electronic band structure calculations (see Ref. [19]).

1.2.2 Group velocity and group velocity dispersion

In order to understand pulse propagation in linear and nonlinear PhCs, it is necessary to obtain group velocities and the group velocity dispersion (GVD) from the photonic band structure. In principle, this can be done through a simple numerical differentiation of the band structure, but in particular for the GVD, this becomes computationally complicated and great care must be exercised in order to avoid numerical instabilities. Therefore, we want to demonstrate how to obtain group velocities and GVD through an adaptation of the so-called $\vec{k} \cdot \vec{p}$ -perturbation theory (kp–PT) of electronic band structure theory. This approach has been applied to systems of arbitrary dimensions [21–23] and will be particularly useful for the investigation of nonlinear effects in PhCs.

With the help of the Bloch–Floquet theorem Eq. (1.2), we may rewrite the wave equation (1.1) as an equation of motion for the lattice-periodic functions $u_{\vec{k}}(\vec{r})$

$$\left(\Delta + 2i\,\nabla \cdot \vec{k} - \vec{k}^2\right) u_{\vec{k}}(\vec{r}) + \frac{\omega_{\vec{k}}^2}{c^2}\,\varepsilon_{\rm p}(\vec{r})\,u_{\vec{k}}(\vec{r}) = 0\,,\tag{1.8}$$

where, $\Delta = \partial_x^2 + \partial_y^2$. An inspection of Eq. (1.8) for the lattice-periodic $u_{\vec{k}+\vec{q}}(\vec{r})$

$$\left(\Delta + 2i\,\nabla \cdot \vec{k} - \vec{k}^2\right)\,u_{\vec{k}+\vec{q}}(\vec{r}) + \vec{q}\cdot\left(2\hat{\Omega} - \vec{q}\right)\,u_{\vec{k}+\vec{q}}(\vec{r}) + \frac{\omega_{\vec{k}+\vec{q}}^2}{c^2}\,\varepsilon_{\rm p}(\vec{r})\,u_{\vec{k}+\vec{q}}(\vec{r}) = 0\,\,,\,\,(1.9)$$

at a nearby wave vector $\vec{k} + \vec{q}$ ($|\vec{q}| \ll \pi/a$) suggests that we treat the second term on the l.h.s. as a perturbation to Eq. (1.8). In writing Eq. (1.9), we have introduced $\hat{\Omega} = i(\nabla + i\vec{k})$. Comparing the perturbation series with a Taylor–expansion of frequency $\omega_{\vec{k}+\vec{q}}$ around \vec{k} , connects group velocities $\vec{v}_{\vec{k}} = \partial_{\vec{k}}\omega_{\vec{k}}$ and GVD tensor elements $M_{\vec{k}}^{ij} = \partial_{k_i}\partial_{k_j}\omega_{\vec{k}}$, i = 1, 2 to expressions familiar from second order perturbation theory [21–23]. Explicitly [22], we obtain for the group velocity

$$\vec{v}_{n\vec{k}} = \frac{c^2}{\omega_{n\vec{k}}} \langle n\vec{k} | (-i\nabla) | n\vec{k} \rangle , \qquad (1.10)$$



Figure 1.2: Group velocities for bands 1, 3, and 5 of our model system (see Fig. 1.1). The group velocities of these bands exhibit extreme variations which may have numerous application in superrefractive phenomena and classical nonlinear optics. This illustrates the huge parameter space of effective parameters accessible with PhCs.

and for the GVD tensor

$$\vec{q} \cdot \mathcal{M}_{n\vec{k}} \cdot \vec{q} = |\vec{q}|^2 \frac{c^2}{2\omega_{n\vec{k}}} \langle n\vec{k}|n\vec{k}\rangle - \frac{1}{2\omega_{n\vec{k}}} \left(\vec{q} \cdot \vec{v}_{n\vec{k}}\right)^2 + \frac{2c^4}{\omega_{n\vec{k}}} \sum_{m \neq n} \frac{\langle n\vec{k}|(-i\vec{q} \cdot \nabla)|m\vec{k}\rangle \langle m\vec{k}|(-i\vec{q} \cdot \nabla)|n\vec{k}\rangle}{\omega_{n\vec{k}}^2 - \omega_{m\vec{k}}^2} .$$
(1.11)

Here, we have used the notation $\int_{\text{wsc}} d^2 r E_{n\vec{k}}^*(\vec{r}) \hat{O} E_{m\vec{k}}(\vec{r}) = \langle n\vec{k} | \hat{O} | m\vec{k} \rangle$ for matrix elements of the operator \hat{O} between Bloch functions $E_{n\vec{k}}(\vec{r})$ and $E_{m\vec{k}}(\vec{r})$.

Despite their complicated appearance, these expressions can be evaluated rather easily using standard PWM and obtain very accurate, efficient and numerically stable results. In Fig. 1.2, we display the variation of the group velocities associated with bands 1, 3, and 5 of our model system. Clearly visible, are the extreme variations ranging from 0.5c for band 1 in the long wavelength (effective medium) limit, all the way to the almost vanishing group velocity of band 5 along the entire Γ -X direction. This illustrates the huge parameter space of effective group velocities that can *simultaneously* be realized in PhCs.

1.3 Nonlinear photonic crystals

For large intensities of the light propagating through the photonic crystal, we should also account for the nonlinear polarization $P_{\text{NL}}(\vec{r}, t)$, representing the nonlinear response of the materials that comprise the PhC. In this case, Maxwell's equations for the TM-polarized light propagating in PhCs take the form

$$\left(\partial_x^2 + \partial_y^2\right) E(\vec{r}, t) - \frac{\varepsilon_{\rm p}(\vec{r})}{c^2} \partial_t^2 E(\vec{r}, t) = \frac{4\pi}{c^2} \partial_t^2 P_{\rm NL}(\vec{r}, t) .$$

$$(1.12)$$

In writing this equation we have neglected the linear dispersion of the constituent materials, which is usually negligible compared to the dispersion associated with the photonic band structure.

1.3 Nonlinear photonic crystals

The existence of PBGs, the tailoring of photonic dispersion relations and mode structures through judiciously designed PhCs, represent a novel paradigm for nonlinear wave interactions. To date, only a few works have been carried out for Kerr–nonlinearities [6–8] or for $\chi^{(2)}$ –nonlinearities [16,24] in PhCs. Moreover, the approximations involved in some of these works seriously limit the applicability of these theories to real PhCs. For instance, the study of Kerr–nonlinearities in 2D PhCs [6] has been limited to weak modulations in the linear index of refraction. Similarly, the recent investigation of second harmonic generation in 2D PhCs [16,24] failed to reproduce the well–known results for the limiting case of homogeneous materials.

In this section, we outline a systematic approach to quantitative calculations of the optical properties of nonlinear PhCs that is based on a multi–scale approach [25]. Since optical nonlinearities are generally quite weak, Eq. (1.12) should be solved in a perturbative way, taking into account that the effect of the nonlinearity accumulates only on time and spatial scales that are much slower and longer, respectively, than the natural scales of the underlying linear problem. For electromagnetic wave propagation in PhCs, these natural scales of the linear problem are determined through the inverse optical period and the associated wavelength of the light. Therefore, key simplifications to Eq. (1.12) arise from separating the fast from slow scales in space and time in the electromagnetic field [21]

$$E(\vec{r},t) = \mu e_1(\vec{r}_0,\vec{r}_1,\cdots;t_0,t_1,\cdots) + \mu^2 e_2(\vec{r}_0,\vec{r}_1,\cdots;t_0,t_1,\cdots) + \cdots, \quad (1.13)$$

by formally replacing the space and time variables, \vec{r} and t, with a set of independent variables $\vec{r}_n \equiv \mu^n \vec{r}$ and $t_n \equiv \mu^n t$. Here, we denote the fastest spatial scale corresponding to the wavelength of the electromagnetic waves propagating in the linear PhC by \vec{r}_0 . Likewise, we denote the associated fastest temporal scale by t_0 . Depending on the type of nonlinearity, the hierarchy is suitably truncated and a closed set of equations is obtained by collecting terms of equal order in μ . To express the results in terms of the original physical variables, one has to set $\mu = 1$ at the end of the calculation [21].

As an illustration, we consider the case of the Kerr-nonlinear material, for which the refractive index depends on the light intensity leading to the nonlinear polarization $P_{\text{NL}}(\vec{r},t) = \chi^{(3)}(\vec{r})E^3(\vec{r},t)$. Here, we have neglected the nonlinear material dispersion. In this case, substituting Eq. (1.13) into Eq. (1.12) and assuming that third-harmonic generation effects are not phase-matched and, hence, can be neglected, we obtain in the third order in μ that

$$e_1(\vec{r_0}, \vec{r_1}, \cdots; t_0, t_1, \cdots) = a_{n\vec{k}}(\vec{z_1}; \vec{r_2}, \cdots; t_1, \cdots) E_{n\vec{k}}(\vec{r_0}) e^{i\omega_{n\vec{k}}t_0} + c.c. , \quad (1.14)$$

where $\vec{z_1} \equiv \vec{r_1} - \vec{v_{n\vec{k}}}t_1$ with the group velocity $\vec{v_{n\vec{k}}}$ given by Eq. (1.10), the Bloch function $E_{n\vec{k}}(\vec{r_0})$ represents a carrier wave and the envelope function $a_{n\vec{k}}(\vec{r_1}, \dots; t_1, \dots)$ has to be determined from the 2D nonlinear Schrödinger equation

$$\begin{bmatrix} i \left(\vec{v}_{n\vec{k}} \cdot \nabla_{\vec{r}_{2}} + \partial_{t_{2}} \right) + \nabla_{\vec{z}_{1}} \cdot \mathcal{M}_{n\vec{k}} \cdot \nabla_{\vec{z}_{1}} \end{bmatrix} a_{n\vec{k}} (\vec{z}_{1}; \vec{r}_{2} \cdots ; t_{2}, \cdots) + \alpha_{n\vec{k}} |a_{n\vec{k}} (\vec{z}_{1}; \vec{r}_{2} \cdots ; t_{2}, \cdots)|^{2} a_{n\vec{k}} (\vec{z}_{1}; \vec{r}_{2} \cdots ; t_{2}, \cdots) = 0,$$
(1.15)

where the GVD tensor $\mathcal{M}_{n\vec{k}}$ is given in Eq. (1.11) and the effective nonlinearity

$$\alpha_{n\vec{k}} = 6\pi \,\omega_{n\vec{k}} \int_{\text{wsc}} d^2 r \,\chi^{(3)}(\vec{r}) \,|E_{n\vec{k}}(\vec{r})|^4 \tag{1.16}$$

reflects how the carrier wave $E_{n\vec{k}}(\vec{r})$ samples the spatial distribution $\chi^{(3)}(\vec{r})$ of nonlinear material within the PhC.

The discussion of the solutions to Eq. (1.15) is outside the scope of the present work and we refer the reader to references on the inverse scattering theory and other methods [26]. However, we want to emphasize that, as a result of the foregoing analysis, we have obtained a generalization of the slowly varying envelope approximation. Within this approximation, the problem of pulse propagation in nonlinear PhCs is mapped onto the problem of an envelope function propagating in an effective homogeneous medium with group velocity $\vec{v}_{n\vec{k}}$, GVD tensor $\mathcal{M}_{n\vec{k}}$, and effective nonlinearity $\alpha_{n\vec{k}}$ that are determined by the carrier wave, which, in turn, is given by a Bloch function of the linear PhC. Therefore, the effective PhC parameters can be obtained from band structure theory via Eqs. (1.10), (1.11), and (1.16) and quantitative investigations become possible. Furthermore, we note that the above considerations are not limited to 2D TM-polarized radiation and have recently been extended to 3D systems by Bhat and Sipe [7]. Moreover, the above framework of multi–scale analysis in conjunction with $\vec{k} \cdot \vec{p}$ – perturbation theory can be applied to other nonlinear PhC systems such as PhCs consisting of nonresonant $\chi^{(2)}$ [27] material and resonant distributed feedback lasing systems [18]. In the present case of Kerr-nonlinearities, other effects such as nonresonant soliton interactions can be considered and lead to interesting applications [28].

1.4 Finite structures

We now consider the problem of how a plane wave couples into a PhC of finite spatial extent. Our basic approach is to apply the Maxwell continuity conditions to the electric and magnetic fields inside and outside the crystal. However, unlike in the preceding subsections, we treat the fields inside the PhC as a linear superposition of plane waves, rather than explicitly using the Bloch functions of the crystal. We then use a scattering–matrix (S–matrix) to determine the amplitudes and phases of the fields everywhere in the system. While the S–matrix is slightly more complicated than the more familiar transfer matrix (T–matrix), it has the advantage that it deals more effectively with the highly evanescent modes that appear naturally in these types of problems.

The S-matrix approach for a fully 3D system is described in detail by Whittaker and Culshaw [29]. However, their formulation does not allow for an effective investigation of lossy PhCs. Therefore, in this section we indicate how to re-formulate the method of Whittaker and Culshaw to account for losses. We first consider the model system shown in Figure 1.3, where light in the x-z plane impinges from the left upon a metallo-dielectric grating structure. The system is finite in the z-direction, but infinite and periodic in the x-direction, with period a and fundamental lattice vector of magnitude $G = 2\pi/a$. This problem can be described in terms of a transverse-electric (TE) or a transverse-magnetic (TM) problem, where following the PhC convention, for the TE (TM) problem the electric (magnetic) field lies in the x-z plane. In the following we consider the TE problem. We divide the finite structure into a number of slices along the z-direction. Within each slice, we assume that the structure is well approximated by a grating that does not vary in the z-direction. For the model system of Fig. 1.3, this slicing process is fairly straightforward. We assume that the incident light has frequency ω , and wave vector $\vec{k} = (k_x, k_z)$. Since each slice is periodic in the x-direction,

1.4 Finite structures



Figure 1.3: Model finite structure, in which a gold grating sits atop a buffer layer (green) and a substrate (blue). Light is incident from the left at an arbitrary angle to the normal, so that the k-vector is separated into a k_x and k_z component. Inset is the reflectivity of the structure as a function of the number of modes used in the solution for the improved choice of Töplitz matrices given in the text (black line) and for the usual choice (red dashed line, see [29]).

propagation through the system will generate a number of diffracted orders, characterized by a propagation constant q_n . Following the notation of Whittaker and Culshaw [29], we use Fourier series to express the x-dependence of the quantities of interest, so that, for example

$$H_y^p(x,z) = \sum_{\alpha} \widetilde{H}_y^p(\alpha,z) e^{i(k_x + \alpha G)x},$$

$$\widetilde{H}_y^p(\alpha,z) = \frac{1}{a} \int_0^a dx \, H_y^p(x,z) \, e^{-i\alpha Gx},$$
(1.17)

where α is an integer, and where for the remainder of this section the *p*-superscript indicates the p^{th} slice. We also define the Töplitz matrices $\hat{\varepsilon}^p_{\alpha\alpha'}$ and $\hat{\eta}^p_{\alpha\alpha'}$, which we discuss in more detail below, and the diagonal matrix $(\hat{k}_x)_{\alpha\alpha'} = \delta_{\alpha\alpha'} (k_x + \alpha G)$. With these definitions, we write our electric and magnetic fields in the p^{th} slice as

$$\widetilde{H}_{y}^{p}(\alpha,z) = \sum_{n} \left(a_{n}^{p} e^{iq_{n}^{p}(z-z_{p})} + b_{n}^{p} e^{iq_{n}^{p}(z_{p+1}-z)} \right) \widetilde{\phi}_{n}^{p},$$

$$(1.18)$$

$$\widetilde{E}_x^p(\alpha, z) = \sum_n \frac{1}{q_n^p} \left(a_n^p e^{iq_n^p(z-z_p)} - b_n^p e^{iq_n^p(z_{p+1}-z)} \right) \left(\mathsf{A}^p \widetilde{\phi}_n^p \right), \tag{1.19}$$

where z_p is the value of z at the *left* edge of the p^{th} layer, a_n^p and b_n^p are the amplitudes of forward and backward propagating light in the n^{th} mode, and where $A^p = \omega^2 - \hat{k}_x \hat{\eta}^p \hat{k}_x$. The value of \tilde{E}_z^p can be determined from Maxwell's equations. The quantity $\tilde{\phi}_n^p(\alpha)$ is the Fourier series of the mode in the p^{th} slice associated with the propagation constant q_n^p . Using (1.18) and (1.19) in Maxwell's equations, we find an eigenvalue equation for q and $\tilde{\phi}$:

$$\widehat{\varepsilon}\left(\omega^2 - \widehat{k}_x \widehat{\eta} \widehat{k}_x\right) \widetilde{\phi} = q^2 \widetilde{\phi},\tag{1.20}$$

where we have dropped the p-superscripts. This equation is a reduced version of Eq. (3.7) in Whittaker and Culshaw [29].

The eigenvalue problem (1.20) is solved by retaining a definite number N of plane waves in the Fourier series, so that the matrices involved in (1.20) are size $N \times N$. As $N \to \infty$, the Töplitz matrices $\hat{\varepsilon}^p$ and $\hat{\eta}^p$ can be generated directly from the Fourier series of $\varepsilon^p(x)$ and $\eta^p = 1/\varepsilon^p(x)$. However, for smaller values of N one must be slightly careful because these Töplitz matrices facilitate the transition from the real-space representation of Maxwell's equations to the Fourier space representation. When executing this transition, one encounters quantities such as $\varepsilon(x) E_x(x)$, for which the Fourier transform is most logically

$$\varepsilon(x) E_x(x) \to \sum_{\alpha'} \widetilde{\varepsilon}(\alpha - \alpha') \widetilde{E}_x(\alpha'),$$
(1.21)

where $\tilde{\varepsilon}(\alpha - \alpha')$ is determined by the Fourier integral of the real-space dielectric constant $\varepsilon(x)$. This leads to the definition of the Töplitz matrix $\hat{\varepsilon}_{\alpha\alpha'} = \tilde{\varepsilon}(\alpha - \alpha')$. However, such a formulation ignores the fact that in many of our slices, the real-space functions $\varepsilon(x)$ and $E_x(x)$ are discontinuous. In such a situation, Li [30] has shown that the expansion (1.21) is inappropriate. Following Li's approach, the appropriate Töplitz matrices of our TE problem are given by first defining the intermediate matrices

$$\overline{\varepsilon}_{\alpha\alpha'} = \widetilde{\varepsilon} \left(\alpha - \alpha' \right), \qquad \overline{\eta}_{\alpha\alpha'} = \widetilde{\eta} \left(\alpha - \alpha' \right), \tag{1.22}$$

and then defining the final matrices

$$\widehat{\varepsilon} = (\overline{\eta})^{-1}, \qquad \widehat{\eta} = (\overline{\varepsilon})^{-1}.$$
 (1.23)

This choice of Töplitz matrices is also appropriate for the full 3D problem.

Once the eigenvalue problem (1.20) is solved, the fields within a given slice are characterized by the values of a_n^p and b_n^p . The only remaining difficulty is the application of the Maxwell continuity conditions (that H_y and E_x must be continuous) at each interface. Typically, this is done by constructing a T-matrix that ultimately relates the set (a_n^0, b_n^0) to the set (a_n^P, b_n^P) , where p = P indexes the last layer of interest. However, it is numerically more stable to build an S-matrix that relates waves entering the structure (a_n^0, b_n^P) to those leaving the structure (a_n^P, b_n^0) . An appropriate methodology for building this S-matrix is given in Whittaker and Culshaw [29].

In the inset of Figure 1.3, we plot the total reflection from the metallo-dielectric grating structure. For simplicity we assume that the structure has a semi-infinite substrate with index of refraction n = 1.46. We also include a 20 nm-thick buffer layer with n = 1.95, and a 20 nm-thick grating composed of gold, for which the frequency-dependent value of n is taken from ref. [31]. The elements of the grating are 32 nm wide, and have a period in the x-direction of 400 nm. We simulate normally-incident TE-polarized light with vacuum wavelength 650 nm. The solid curve uses the Töplitz matrices suggested in (1.23), while the red dashed curve uses those suggested by Whittaker and Culshaw [29]. The results with the new Töplitz matrices are significantly improved convergence behavior. We have also verified that the new Töplitz matrices are significantly better for the analysis of scattering loss in finite 3D PhCs, such as the Woodpile PhCs currently being fabricated via two-photon photopolymerization (see Chapter 9 in this book).

1.4 Finite structures



Figure 1.4: Left: Sketch of a typical setup for characterizing 2D PhC–slabs in Litrow–geometry. Right: Calculation of the reflection spectra (intensity) in Litrow–geometry for our model system when the 2D PhC is oriented along the Γ –M direction (see left panel). In this setup, only light reflected into the direct backscattering direction is collected. Clearly visible, are the different diffraction orders that are "decorated" with bulk PhC–effects. The parameters of the PhC–slab are given in the text.

We now use the S-matrix technique to consider transmission and reflection in the PhC model system, assuming that it has been cleaved along the Γ -M direction, such that it is finite in the z-direction but infinite and periodic in the x-direction (see Fig. 1.4, left panel). We further assume that the cleaving at z = 0 and z = L cut through the center of the air pores. The cleaved structure includes 20 unit cells along the z-direction. To accurately model the circular pores, we divide the PhC into a large number of very thin layers, each of which is homogeneous along the z-direction. We find that the resulting staircase approximates the shape of the pores sufficiently well if we use about 100 layers per pore. In Fig. 1.4 right panel, we display the calculated reflection spectra (intensity) for this 2D-PhC slab in Litrowgeometry. Clearly visible, are the different diffraction orders that are "decorated" with bulk PhC-effects: The periodicity along the x-axis makes this PhC-slab an effective grating with a complicated frequency-dependent coupling to the incoming plane wave. For certain frequencies of the incoming radiation, there is no mode to which it could couple. As a result, the wave is completely reflected from the slab, albeit not entirely into the backscattering direction (incomplete blazing). For other frequencies, the light partially couples to propagating Bloch modes inside the PhC-slab, leading to a reduction in reflection. The strength of this coupling depends on the overlap of the incoming plane wave with a Bloch function at that frequency and the parallel crystal momentum, and therefore, depends both on the exact surface termination as well as on the symmetry of the Bloch function. To illustrate the latter point, we have calculated the frequency dependence of the total transmission through the PhC-slab for normal incidence. In Fig. 1.5, we compare these results with the corresponding band structure along the Γ -M direction. The wildly ranging coupling strengths are clearly visible, leading to corresponding variations in the total transmission. Also visible are the sharp Fabry-Perot resonances associated with multiple reflections at the front and end surfaces. However, while the total transmission for frequencies just above $\omega a/2\pi c = 0.5$ is almost zero due to a very weak but non-vanishing coupling constant, there exists an extended frequency band just below $\omega a/2\pi c = 0.8$ where the total transmission vanishes exactly although the photonic band structure suggests the presence of a band. This apparent discrepancy is resolved when considering the symmetry of the corresponding Bloch functions: The Bloch functions for the band in question exhibit an odd parity across the slab surface. Because the incoming plane wave by



Figure 1.5: Comparison between transmission calculations (normal incidence) through a 2D PhC–slab oriented along the Γ –M direction with the corresponding photonic band structure for our model system. Uncoupled bands are marked by dashed lines. Bloch functions for a coupled and an uncoupled band are shown in the left panel, revealing the odd parity of the uncoupled bands. The direction of the incoming radiation is indicated by yellow arrows and the surface termination of the PhC is represented through the vertical dashed lines.

construction has an even parity across the slab surface, we have that in this case the coupling between plane wave and Bloch function vanishes exactly due to an incompatible symmetry. This is a manifestation of a profound difference between PhCs and electronic crystals: Although both types of crystals provide Bloch functions (modes), the PhC modes are generally "empty", i.e., contain no photons. In order to transmit energy through a PhC, one has to couple an external radiation source to PhC modes. As a consequence, care must be taken when interpreting transmission and reflection data from PhC–slabs. However, the existence of these so–called uncoupled bands can always be inferred through a symmetry analysis [16,32] of the photonic Bloch functions. In Fig. 1.5, we have indicated the uncoupled bands for the Γ –M direction of our model system with dashed lines.

1.5 Defect structures in photonic crystals

In electronic micro-circuits, electrical currents are guided by thin metal wires where electrons are bound within the cross section of the wire by the so-called work function (confining

potential) of the metal. As a result, electrical currents follow along the path prescribed by the wire without escaping to the background. The situation is very different for optical waves. Although optical fibers guide light over long distances, microscopic fiber–circuits for light do not exist, because empty space is already an ideal conductor of light waves. The light in an optical fiber can easily escape into the background electromagnetic modes of empty space if the fiber is bent or distorted on a microscopic scale. PBGs in the band structure of PhCs remove this problem by removing all the background electromagnetic modes over the relevant band of frequencies. As a consequence, light paths can be created inside a PBG material in the form of engineered waveguide channels. In terms of the resources required for the fabrication of these structures and the tremendous flexibility in the choice of parameters, the ability to design blueprints of PhC–based micro–optical devices and to investigate the effects of fabricational tolerances on the performance of the ideal structure, becomes both an economical and a practical must. Perhaps, even more important may be the investigation of novel operating principles of such devices.

As alluded to above, the overwhelming majority of theoretical investigations of waveguiding to date has been carried out using FDTD and/or FE techniques. However, applying general purpose methodologies such as FDTD or FE methods to defect structures in PhCs, largely disregards information about the underlying PhC structure which is readily available from photonic band structure computation. As a result, only relatively small systems can be investigated and the physical insight remains limited.

1.5.1 Maximally localized photonic Wannier functions

A more natural description of localized defect modes in PhCs consists of an expansion of the electromagnetic field into a set of localized basis functions which have encoded into them all the information of the underlying PhC. Therefore, the most natural basis functions for the description of defect structures in PhCs are the so–called photonic Wannier functions $W_{n\vec{R}}(\vec{r})$, which are formally defined through a lattice Fourier transform

$$W_{n\vec{R}}(\vec{r}) = \frac{V_{\text{wsc}}}{(2\pi)^2} \int_{\text{BZ}} d^2\vec{k} \, e^{-i\vec{k}\vec{R}} \, E_{n\vec{k}}(\vec{r}) \tag{1.24}$$

of the extended Bloch functions, $E_{n\vec{k}}(\vec{r})$. The above definition associates the photonic Wannier function $W_{n\vec{R}}(\vec{r})$ with the frequency range covered by band n, and centers it around the corresponding lattice site \vec{R} . In addition, the completeness and orthogonality of the Bloch functions translate directly into corresponding properties of the photonic Wannier functions. Computing the Wannier functions directly from the output of photonic band structure programs via Eq. (1.24) leads to functions with poor localization properties and erratic behavior (see, for instance, Fig. 2 in ref. [33]). These problems originate from an indeterminacy of the global phases of the Bloch functions. It is straightforward to show that for a group of several bands (we define their number as N_w) there exists, for every wave vector \vec{k} , a free unitary transformation between the bands which leaves the orthogonality relation of Wannier functions unchanged. A solution to this unfortunate situation is provided by recent advances in electronic band structure theory. Marzari and Vanderbilt [34, 35] have outlined an efficient scheme for the computation of maximally localized Wannier functions by numerically determining a unitary transformation between the bands that minimizes an appropriate spread



Figure 1.6: Photonic Wannier functions, $W_{n\vec{0}}(\vec{r})$, for the six bands that are most relevant for the description of the localized defect mode shown in Fig.1.7(a). These optimally localized Wannier functions have been obtained by minimizing the corresponding spread functional, Eq. (1.25). Note, that in contrast to the other bands, the Wannier center of the eleventh band is located at the air pore. The parameters of the underlying PhC are the same as those in Fig. 1.1.

functional \mathcal{F}

$$\mathcal{F} = \sum_{n=1}^{N_{\rm W}} \left[\langle n\vec{0} | \, r^2 \, | n\vec{0} \rangle - (\langle n\vec{0} | \, \vec{r} \, | n\vec{0} \rangle)^2 \right] = \text{Min} \,. \tag{1.25}$$

Here we have introduced a shorthand notation for matrix elements according to

$$\langle n\vec{R}| f(\vec{r}) | n'\vec{R}' \rangle = \int_{\mathbf{R}^2} d^2 r \, W^*_{n\vec{R}}(\vec{r}) \, f(\vec{r}) \, \varepsilon_{\mathbf{p}}(\vec{r}) \, W_{n'\vec{R}'}(\vec{r}) \,, \tag{1.26}$$

for any function $f(\vec{r})$. For instance, the orthonormality of the Wannier functions in this notation reads as

$$\langle n\vec{R}| \, |n'\vec{R}'\rangle = \int_{\mathbf{R}^2} d^2 r \, W^*_{n\vec{R}}(\vec{r}) \, \varepsilon_{\mathbf{p}}(\vec{r}) \, W_{n'\vec{R}'}(\vec{r}) = \delta_{nn'} \delta_{\vec{R}\vec{R}'} \, . \tag{1.27}$$

The field distributions of the optimized Wannier functions belonging to the six most relevant bands of our model system are depicted in Fig. 1.6 (see also the discussion in Section 1.5.3). Their localization properties as well as the symmetries of the underlying PhC structure are clearly visible. It should be noted that the Wannier centers of all calculated bands (except of the eleventh band) are located halfway between the air pores, i.e. inside the dielectric (see Refs. [34, 35] for more details on the Wannier centers). It should be pointed out that instead of working with the electric field [33,36,37], Eq. (1.1), one may equally well construct photonic Wannier functions for the magnetic field, as recently demonstrated by Whittaker and Croucher [38].

1.5.2 Wannier description of defect structures

The description of defect structures embedded in PhCs starts with the corresponding wave equation in the frequency domain

$$\nabla^2 E(\vec{r}) + \left(\frac{\omega}{c}\right)^2 \left\{ \varepsilon_{\rm p}(\vec{r}) + \delta \varepsilon(\vec{r}) \right\} E(\vec{r}) = 0 .$$
(1.28)

Here, we have decomposed the dielectric function into the periodic part $\varepsilon_p(\vec{r})$, and the contribution $\delta \varepsilon(\vec{r})$, that describes the defect structures. Within the Wannier function approach, we expand the electromagnetic field according to

$$E(\vec{r}) = \sum_{n,\vec{R}} E_{n\vec{R}} W_{n\vec{R}}(\vec{r}) , \qquad (1.29)$$

with unknown amplitudes $E_{n\vec{R}}$. Inserting this expansion into the wave equation (1.28) and employing the orthonormality relations, Eq. (1.27), leads to the basic equation for lattice models of defect structures embedded in PhCs

$$\sum_{n',\vec{R}'} \left\{ \delta_{nn'} \delta_{\vec{R}\vec{R}'} + D_{\vec{R}\vec{R}'}^{nn'} \right\} E_{n'\vec{R}'} = \left(\frac{c}{\omega}\right)^2 \sum_{n',\vec{R}'} A_{\vec{R}\vec{R}'}^{nn'} E_{n'\vec{R}'} .$$
(1.30)

The matrix $A_{\vec{R}\vec{R}'}^{nn'}$ depends only on the Wannier functions of the underlying PhC and is defined by

$$A_{\vec{R}\vec{R}'}^{nn'} = -\int_{\mathbf{R}^2} d^2 \vec{r} \ W_{n\vec{R}}^*(\vec{r}) \,\nabla^2 \,W_{n'\vec{R}'}(\vec{r}) \ . \tag{1.31}$$

The localization of the Wannier functions in space leads to a very rapid decay of the magnitude of matrix elements with increasing separation $|\vec{R} - \vec{R}'|$ between the lattice sites, effectively making the matrix $A_{\vec{R}\vec{R}'}^{nn'}$ sparse. Furthermore, it may be shown that the matrix $A_{\vec{R}\vec{R}'}^{nn'}$ is Hermitian and positive definite. Similarly, once the Wannier functions of the underlying PhC are determined, the matrix $D_{\vec{R}\vec{R}'}^{nn'}$ depends solely on the overlap of these functions, mediated by the defect structure:

$$D_{\vec{R}\vec{R}'}^{nn'} = \int_{\mathbf{R}^2} d^2 \vec{r} \ W_{n\vec{R}}^*(\vec{r}) \,\delta\varepsilon(\vec{r}) \,W_{n'\vec{R}'}(\vec{r}) \;.$$
(1.32)

As a consequence of the localization properties of both the Wannier functions and the defect dielectric function, the Hermitian matrix $D_{\vec{R}\vec{R}'}^{nn'}$ is also sparse. In the case of PhCs with inversion symmetry, $\varepsilon_p(\vec{r}) \equiv \varepsilon_p(-\vec{r})$, the Wannier functions can be chosen to be real. Accordingly, both matrices, $A_{\vec{R}\vec{R}'}^{nn'}$ and $D_{\vec{R}\vec{R}'}^{nn'}$ become real symmetric matrices. Depending on the nature of the defect structure, we are interested in (i) frequencies of

Depending on the nature of the defect structure, we are interested in (i) frequencies of localized cavity modes, (ii) dispersion relations for straight waveguides, or (iii) transmission and reflection through waveguide bends and other, more complex defect structures. In the following, we consider each of these cases separately.

1.5.3 Localized cavity modes

As a first illustration of the Wannier function approach, we consider the case of a simple cavity created by infiltrating a single pore at the defect site \vec{R}_{def} with a material of dielectric constant ε_{def} , as shown in the inset of Fig. 1.7(a). In this case, we solve Eq. (1.30) directly as a generalized eigenvalue problem for the cavity frequencies that lie within the PBG, and reconstruct the cavity modes from the corresponding eigenvectors.



Figure 1.7: (a) Frequencies of localized cavity modes created by infiltrating a single defect pore with a material of dielectric constant ε_{def} (see inset). The results of the Wannier function approach (diamonds) using $N_{\text{w}} = 10$ Wannier functions per unit cell, are in complete agreement with numerically exact results of the super-cell calculations (full line). The parameters of the underlying PhC are the same as those in Fig. 1.1. (b) Electric field distribution for the cavity mode with frequency $\omega = 0.290 \times 2\pi c/a$, created by infiltrating the pore with a polymer of $\varepsilon_{\text{def}} = 2.4$.

In Fig. 1.7(a) we compare the frequencies of these cavity modes calculated from Eq. (1.30)with corresponding calculations using PWM-based super-cell calculations [39]. Upon increasing ε_{def} , a non-degenerate cavity mode with monopole symmetry emerges from the upper edge of the bandgap. The results of the Wannier function approach using the $N_{\rm w} = 10$ most relevant Wannier functions per unit cell in Eq. (1.30), are in complete agreement with numerically exact results of the super-cell calculations. In Fig. 1.7(b), we depict the corresponding mode structure for a monopole cavity mode created by infiltration of a polymer with $\varepsilon_{def} = 2.4$ into the pore. The convergence properties of the Wannier function approach should depend on the nature and symmetry properties of the cavity modes under consideration. To discuss this issue in greater detail, it is helpful to define a measure V_n of the strength of the contributions to a cavity mode from the individual Wannier function associated with band nvia $V_n = \sum_{\vec{R}} |E_{n\vec{R}}|^2$. In Fig. 1.8, we display the dependence of the parameter V_n on the band index n for the cavity modes shown in Fig. 1.7, for two values of the defect dielectric constant, $\varepsilon_{def} = 2.4$ (solid line) and $\varepsilon_{def} = 8$ (dashed line), respectively. In both cases, the most relevant contributions to the cavity modes originate from the Wannier functions belonging to bands n = 1, 2, 3, 5, 11 and 19, and all contributions from bands n > 20 are negligible. These most relevant Wannier functions for our model system are shown in Fig. 1.6. In fact, fully converged results are obtained when we work with the 10 most relevant Wannier functions per unit cell (for a comparison with numerically exact super-cell calculations see Fig. 1.7(a)).



Figure 1.8: The strength V_n of the individual contributions from the Wannier functions of the lowest 20 bands (index *n*) to the formation of the cavity modes depicted in Fig. 1.7. The Wannier functions with $V_n \leq 10^{-3}$ may be safely left out of account. Arrows indicate the six most relevant Wannier functions depicted in Fig. 1.6. The parameters of the underlying PhC are the same as those in Fig. 1.1.

1.5.4 Dispersion relations of waveguides

The efficiency of the Wannier function approach is particularly evident when considering defect clusters consisting of several defect pores. In this case, the defect dielectric function $\delta \varepsilon(\vec{r})$, can be written as a sum over positions \vec{R}_m , of the individual defect pores so that Eq. (1.32) reduces to a sum

$$D_{\vec{R}\vec{R}'}^{nn'} = \sum_{m} D(m)_{\vec{R}-\vec{R}_m,\vec{R}'-\vec{R}_m}^{nn'} , \qquad (1.33)$$

over the matrix elements $D(m)_{\vec{R},\vec{R}'}^{nn'}$ of the individual defects (see discussion in Ref. [33] for more details). Therefore, for a given underlying PhC structure, it becomes possible to build up a database of matrix elements $D(m)_{\vec{R},\vec{R}'}^{nn'}$, for different geometries (radii, shapes) of defect pores, which allows highly efficient defect computations through simple matrix assembly procedures. This is in strong contrast to *any* other computational technique known to us.

Arguably the most important types of defect clusters in PhCs are one or several adjacent straight rows of defects. Properly designed, such defect rows form a PhC waveguide which allows the efficient guiding of light for frequencies within a PBG [40,41]. Due to the one-dimensional periodicity of such a waveguide, its guided modes $E^{(p)}(\vec{r} \mid \omega) = \sum_{n,\vec{R}} E^{(p)}_{n\vec{R}}(\omega) W_{n\vec{R}}(\vec{r})$, obey the 1D Bloch-Floquet theorem

$$E_{n\vec{R}+\vec{s}_{\rm W}}^{(p)}(\omega) = e^{i\vec{k}_p(\omega)\vec{s}_{\rm W}} E_{n\vec{R}}^{(p)}(\omega) , \qquad (1.34)$$

and thus they can be labeled by a wave vector $\vec{k}_p(\omega)$, parallel to the waveguide director $\vec{s}_w = w_1 \vec{a}_1 + w_2 \vec{a}_2$, where $\vec{a}_1 = (a, 0)$ and $\vec{a}_2 = (0, a)$ are the primitive lattice vectors of the PhC, and integers w_1 and w_2 define the direction of the waveguide (for instance, an *x*-axis directed W1-waveguide is described through $w_1 = 1$ and $w_2 = 0$). Commonly, investigations of PhC waveguides consist of calculations of the dispersion relations $\vec{k}_p(\omega)$, of all the guided



Figure 1.9: Dispersion relations of the propagating guided mode for PhC waveguides consisting of (a) one row (W1) and (b) two rows (W2) of defect pores infiltrated with a polymer with $\varepsilon_{def} = 2.4$. The calculations within the Wannier function approach (diamonds) based on Eqs. (1.30) and (1.34), in which we accounted for the interaction of 5 nearest pores along the waveguide and used 10 most relevant Wannier functions per unit cell, are in complete agreement with the results of supercell calculations (solid lines). The gray areas represent the projected band structure of the underlying model PhC (see Fig. 1.1). The red circles in the insets indicate the positions of the infiltrated pores.

modes which can be obtained by substituting Eq. (1.34) into Eq. (1.30) as we have described in detail in Ref. [33].

To date, investigations of straight PhC waveguides have concentrated on the calculation of dispersion relations for *propagating guided modes* with real wave vectors $k_p(\omega)$, only. Such calculations can also be carried out accurately by employing the supercell technique. In Fig. 1.9, we display the dispersion relations for the propagating guided modes of the W1– and W2–waveguides created by infiltrating a polymer into one row and two rows of pores, calculated within the Wannier function approach. The results of these calculations are fully converged and in complete agreement with the results of plane–wave based supercell computations. Similar to the calculations of complex cavity structures, the calculations of waveguide dispersion relations within the Wannier function approach require fairly minimal computational resources in comparison of the supercell technique.

We would like to emphasize that, in contrast to the supercell technique, the Wannier function approach enables us to also obtain the dispersion relations for *evanescent guided modes* with complex wave vectors $\vec{k}_p(\omega)$. Since such modes grow or decay along the waveguide direction, they are mainly irrelevant in perfectly periodic straight waveguides. However, they start to play an important role as soon as the perfect periodicity of the waveguide is broken either through imperfections due to fabricational tolerances, or through the deliberate creation of deviations from periodicity such as bends or coupled cavity–waveguide systems for Wavelength Division Multiplexing (WDM) applications. In such cases, these *evanescent* guided modes give rise to light localization effects and determine the non–trivial transmission and reflection properties of PhC circuits [33,42] as we will discuss below.

1.5.5 Light propagation through photonic crystal circuits

In this section, we demonstrate that the Wannier function approach provides an efficient simulation tool for the description of light through PhC circuits which allows one to overcome most of the limitations related to FDTD or FE methods. As an illustration, we consider light propagation through two-port PhC circuits such as waveguide bends or coupled cavity–waveguide systems. The common feature of these devices is that two semi-infinite straight PhC waveguides act as leads that are connected through a finite–sized region of defects. In this case, light propagation through the device at frequency ω is governed by Eq. (1.30), which should be truncated (to obtain an equal number of equations and unknowns) by prescribing certain values to the expansion coefficients $E_{n\vec{R}}$, at some sites inside the waveguiding leads. Since these values determine the amplitudes of the incoming light, it is physically more transparent to express the expansion coefficients $E_{n\vec{R}}$ within the leads through a superposition of the guided modes $\vec{\Phi}^{(p)}(\omega)$ with wave vectors $\vec{k}_p(\omega)$ of the corresponding infinite straight waveguide. In a numerical implementation, this is facilitated by replacing the expansion coefficients $E_{n\vec{R}}$ for all lattice sites \vec{R} inside each waveguiding lead W_i , i = 1, 2, according to

$$E_{n\vec{R}}^{\mathbf{w}_{i}} = \sum_{p=1}^{N} u_{\mathbf{w}_{i}}^{(p)}(\omega) E_{n\vec{R}}^{(p)}(\omega) + \sum_{p=N+1}^{2N} d_{\mathbf{w}_{i}}^{(p)}(\omega) E_{n\vec{R}}^{(p)}(\omega) , \qquad (1.35)$$

where $u_{w_i}^{(p)}$ and $d_{w_i}^{(p)}$ are amplitudes of the guided modes, and we assume that all 2N guided modes are ordered in the following way: p = 1 to N are occupied by the propagating guided modes with $\text{Re}[k_p] > 0$ and evanescent guided modes with $\text{Im}[k_p] > 0$, whereas p = N + 1 to 2N are occupied by the propagating guided modes with $\text{Re}[k_p] < 0$ and evanescent guided modes with $\text{Im}[k_p] < 0$. Assuming that the amplitudes, $u_{w_1}^{(p)}$ and $d_{w_2}^{(p)}$, of all the propagating (evanescent) guided modes which propagate (decay) in the direction of the device are known (they depend on the purpose of our calculation or on the experimental setup), we can now substitute Eq. (1.35) into Eq. (1.30) and, solving the resulting system of coupled equations, find the unknown expansion coefficients $E_{n\vec{R}}$ for the sites \vec{R} inside the domain of the device (which can be used, e.g., for visualization of the field propagation through the device), and the amplitudes $u_{w_1}^{(p)}$ and $d_{w_1}^{(p)}$, of all *outgoing propagating* and *growing evanescent* guided modes.

In Ref. [33] we have demonstrated, by comparison with the FDTD calculations [40], that the results of such transmission calculations based on the Wannier function approach are indeed very accurate and agree extremely well with FDTD calculations. Now, in Fig. 1.10, we present the results of Wannier function calculations of the transmission spectra for four different bend geometries with attached single–mode waveguide leads (see Fig. 1.9) that are embedded in our model PhC.

The efficiency of the Wannier function approach for transmission calculations becomes apparent when considering that – once the Wannier functions for the underlying PhC have been obtained – the calculation of a single data point in the reflection spectra of Fig. 1.10 reduces to the solution of a single sparse system of some 800 equations, which even on a laptop computer takes only a few seconds. Therefore, the Wannier function approach outlined above will (i) enable a reverse engineering of defect structures with prescribed functionality



Figure 1.10: Transmission spectra $|T(\omega)|^2$, for four different bend geometries embedded in our 2D model PhC. The results of the Wannier function approach are obtained with $N_{\rm R} = 5$, L = 5, and the $N_{\rm W} = 10$ most relevant Wannier functions. The parameters of the underlying PhC are the same as those in Fig. 1.1.

and (ii) allow detailed studies regarding the robustness of successful designs with respect to fabricational tolerances. Moreover, the Wannier function approach can be straightforwardly applied, with comparable efficiency, to investigations of the transmission spectra through PhC circuits made from highly dispersive and/or nonlinear materials. Of paramount importance is the fact that, in contrast to the FDTD or FE methods, the Wannier function approach permits one to accurately and efficiently calculate the complete scattering matrices of PhC devices [33]. This allows us to construct a PhC circuit theory in which *individual devices are replaced by simple equivalent scattering matrices*, which are assembled by simple scattering matrix multiplication rules to form the scattering matrix of *large-scale circuits* [43]. We want to emphasize that in some sense, these scattering matrices can be regarded as the optical analogue of the impedance matrices associated with multi-port devices in microwave technology [44].

1.6 Conclusions

In summary, we have outlined a framework based on solid state theoretical methods that allows one to qualitatively and quantitatively treat wave propagation in PhCs. Photonic band structure computation of the infinitely extended PhC provides the input necessary to efficiently obtain the properties of defect structures, embedded in PhCs via expansions into localized Wannier functions. This allows us to determine effective parameters such as DOS, group velocities, GVD tensors, and effective nonlinearities. The description of nonlinear PhCs through the generalized slowly varying envelope approximation allows us to investigate such systems using a limited number of effective parameters with transparent physical meaning. Finite structures can be treated through combining techniques from diffractive optics with photonic band structure computations. In particular, the efficiency of the Wannier function approach to defect structures in PhCs allows investigations of PhC circuits which, to date, are beyond the reach of standard simulation techniques such as FDTD or FE methods.

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Acknowledgements

This work was supported by the Center for Functional Nanostructures (CFN) of the Deutsche Forschungsgemeinschaft (DFG) within projects A 1.1, A 1.2, and A 1.3. The research of K.B., A.G.M., and L.T. is further supported by the DFG under grant Bu 1107/2-2 (Emmy-Noether program). M.F. acknowledges the support of the DFG Priority Program SP 1113 *Photonic Crystals.* The work of M.S. is funded in the framework of the DFG Research Training Group 786 *Mixed Fields and Nonlinear Interactions* at the University of Karlsruhe.

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