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Reciprocity theorem and perturbation theory for photonic crystal waveguides

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Starting from Maxwell's equations we derive a reciprocity theorem for photonic crystal waveguides. A set of strongly coupled discrete equations results, which can be applied to the simulation of perturbed photonic crystal waveguides. As an example we analytically study the influence of the dispersion of a two level system on the band structure of a photonic crystal waveguide. In particular, the formation of polariton gaps is discussed.

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Photonic crystals (PCs) are regarded as a very promising and variable material base of a future photonic integration. In particular photonic crystal waveguides (PCWs), which are aligned defects in PCs, allow for an efficient transport of optical signals in highly integrated all-optical circuits. Modes of straight PCWs are determined by band structure calculations [1,2]. However, to analyze the field evolution in perturbed, bent, or mutually interacting PCWs, the complete set of Maxwell's equations has to be solved via a finite difference time domain (FDTD) scheme [3]. The latter is extremely time and memory consuming in particular because stationary states appear only in the limit of temporally infinite calculations. Furthermore FDTD simulations do not often provide for a deeper insight into the physics of the investigated structures. Therefore some simpler modeling or even analytical descriptions of the field dynamics in perturbed PCWs are desirable.

Starting from a strict orthogonality relations for PCWs we derive a set of simple evolution equations, which allow one to determine the field distribution in a PCW for a fixed frequency ω and for given initial conditions. In analogy to the derivation of the reciprocity theorem for conventional waveguides [4] we start from a set of stationary unperturbed electric $\vec{E}_1$ and magnetic $\vec{H}_1$ fields, which serves as a reference. These fields belong to an ideal Bloch mode with the Bloch vector q_1 and the shapes $\vec{E}_1=\vec{e}_{q_1}(x,y,z)\exp(iq_1z)$ and $\vec{H}_1=\vec{h}_{q_1}(x,y,z)\exp(iq_1z)$, which propagate along the PCW in the z direction. A second set of fields is subject to possible perturbations, which influence respective electrical $\vec{E}_2$ and magnetic $\vec{H}_2$ fields via an additional polarization $\vec{P}_{\text{pert}}$. The interaction is characterized by Maxwell's equations such as $\text{rot}(\vec{E}_2)=i\omega\mu_0\vec{H}_2$ and $\text{rot}(\vec{H}_2)=-i\omega\varepsilon_0\varepsilon\vec{E}_2-i\omega\vec{P}_{\text{pert}}$, where ε defines the dielectric structure of the ideal unperturbed photonic crystal waveguide. Both electromagnetic fields are linked together by the following relation: $\text{div}(\vec{E}_2\times\vec{H}_1^*+\vec{E}_1^*\times\vec{H}_2)=i\omega\vec{E}_1^*\vec{P}_{\text{pert}}$. After integrating over one unit cell [see the inset of Fig. 1(a)] and subsequent transformations, we obtain

$$\int\int_{\substack{\text{surface}\\ \text{unit cell}}}(\vec{E}_2\times\vec{H}_1^*+\vec{E}_1^*\times\vec{H}_2)d\vec{A}=i\omega\int\int\int_{\substack{\text{volume}\\ \text{unit cell}}}\vec{E}_1^*\vec{P}_{\text{pert}}dV. \quad (1)$$

In what follows we chose the boundaries of the unit cell extends perpendicularly to the original waveguide (x-y plane). For a vanishing perturbation $\vec{P}_{\text{pert}}=0$ the second field can also be assumed to be a Bloch state with a wave number q_2. Taking into account the periodicity of the Bloch states we obtain $\sin[(q_1-q_2)L/2]\int_{-\infty}^{+\infty}dx\int_{-\infty}^{+\infty}dy[\vec{e}_{q_2}\times\vec{h}_{q_1}^*+\vec{e}_{q_1}^*\times\vec{h}_{q_2}]_z=0$, where L is the extension of the unit cell and only the z component of the respective vector products enters the integration. Because the actual position of a unit cell is arbitrary the integration can be performed on each fixed z. Consequently an orthogonality relation for PCW modes at a fixed frequency can be expressed as

$$\int_{-\infty}^{+\infty}dx\int_{-\infty}^{+\infty}dy[\vec{e}_{q_2}\times\vec{h}_{q_1}^*+\vec{e}_{q_1}^*\times\vec{h}_{q_2}]_z=\delta_{q_1q_2}s(q_1), \quad (2)$$

where δ is the Kronecker symbol and s denotes the energy flux in the respective mode. Going back to the general case $\vec{P}_{\text{pert}}\neq 0$ we express the perturbed fields $\vec{E}_2$ and $\vec{H}_2$ as superpositions of Bloch modes $\vec{E}_2=\Sigma_q a_q(z)\vec{e}_q(\vec{r})+b_q(z)\vec{e}_q^*(\vec{r})$ and $\vec{H}_2=\Sigma_q a_q(z)\vec{h}_q(\vec{r})-b_q(z)\vec{h}_q^*(\vec{r})$. In the case of unperturbed waveguides the amplitudes of forward and backward propagating fields $a_q(z)$ and $b_q(z)$ simplify to $\exp(\pm iqz)$. But in the presence of a perturbation the dynamics of these amplitudes changes. In order to obtain a respective evolution

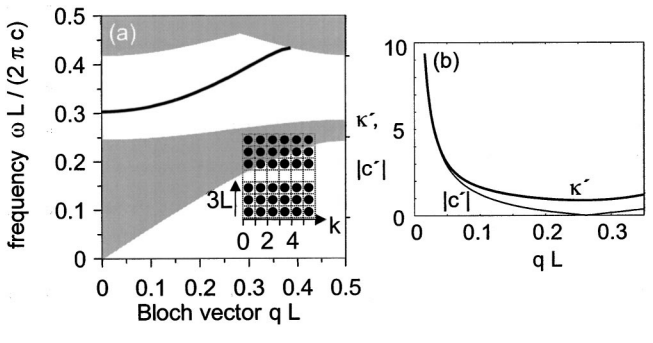

FIG. 1. Unperturbed W1 photonic crystal waveguide (PCW) and its sensitivity on perturbations, (a) band structure of a PCW; inset: scheme of a PCW; k: index of unit cells; L: period of the PC (b) self-coupling and cross-coupling coefficients as a function of the Bloch vector; parameters: rods: $\varepsilon=12$, radius/$L=0.2$.

equation we insert the mode expansion into the integral equation (1) and make use of the discrete translational symmetry of the Bloch modes. In so doing we obtain a set of discrete equations

$$\begin{aligned} a_q[(k+1)L]\exp[-iq(k+1)L]-a_q[kL]\exp[-iqkL] &= \frac{i\omega}{s(q)}\int_{-\infty}^{\infty}dx\int_{-\infty}^{\infty}dy\int_{kL}^{(k+1)L}dz\vec{e}_q^{\,*}\vec{P}_{\text{pert}}\exp(-iqz), \\ b_q[(k+1)L]\exp[iq(k+1)L]-b_q[kL]\exp[iqkL] &= -\frac{i\omega}{s(q)}\int_{-\infty}^{\infty}dx\int_{-\infty}^{\infty}dy\int_{kL}^{(k+1)L}dz\vec{e}_q\vec{P}_{\text{pert}}\exp(iqz), \end{aligned} \tag{3}$$

where we have assumed the kth unit cell to extend between $kL \leqslant z=(k+1)L$. Equations (7) can be used to describe a variety of problems with linear and/or nonlinear perturbations. The most significant frequency dependence is incorporated into the Bloch vector $q(\omega)$. For an infinitesimally small period of the PC ($L\to 0$) Eqs. (3) pass over to the well known coupled mode equations for conventional waveguides of integrated optics [4]. Besides the discrete nature of Eqs. (3) there is a further essential difference between the coupled mode equations of PCWs and conventional waveguides. For conventional waveguides the coupling between forward and backward propagating fields can usually be neglected, because of the big mismatch between respective propagation constants. In contrast, arbitrary perturbations induce a strong coupling between forward and backward modes in PCWs, especially close to the Γ point.

To demonstrate some applications of Eq. (3) we investigate the influence of the material dispersion on the band structure of a PCW. Conventional band structure calculations [1,2] usually neglect the frequency dependence of the dielectric function. Nowadays there are efficient numerical methods to include the dispersion of the media, such as the transfer matrix method [5] or a plane wave formalism [6]. Nevertheless for a deeper physical insight into the influence of dispersion on the band structure of a PCW, analytical investigations are helpful. Provided that the dispersion of ε can be regarded as a perturbation the discrete coupled mode [Eqs. (3)] can be applied. Here we assume homogeneously distributed two level dopants, as e.g., quantum dots with

$$\Delta\varepsilon(\omega)=\frac{f(\omega_0-\omega)}{(\omega_0-\omega)^2+\gamma^2},$$

where the induced perturbation polarization reads $\vec{P}_{\text{pert}}=\varepsilon_0\Delta\varepsilon[a_q(z)\vec{e}_q(\vec{r})+b_q(z)\vec{e}_q(\vec{r})^*]$. Equation (3) suggests concentrating on a set of discrete amplitudes, which are given at the boundaries of the elementary cell as $A_k=a_q(kL)$ and $B_k=b_q(kL)$. Assuming that deviations from a Bloch wave are small we approximate the field within the kth unit cell by respective values at the boundaries as

$$a_q(z)\approx\{A_k\exp(-iqkL)+A_{k+1}\times\exp[-iq(k+1)L]\}/2\exp(iqz)$$

and

$$b_q(z)\approx\{B_k\exp(iqkL)+B_{k+1}\exp[iq(k+1)L]\}/2\times\exp(-iqz).$$

In this way we map the evolution on a discrete set of fields. Now Eqs. (3) simplify to

$$\begin{aligned} A_{k+1}\exp(-iqL)-A_k &= i\kappa[A_k+A_{k+1}\exp(-iqL)]+c[B_k+B_{k+1}\exp(iqL)], \\ B_{k+1}\exp(iqL)-B_k &= -i\kappa[B_k+B_{k+1}\exp(iqL)]+c^*[A_k+A_{k+1}\exp(-iqL)], \end{aligned} \tag{4}$$

where the parameters in Eqs. (4) are proportional to the dielectric function of the perturbation $\kappa=\Delta\varepsilon\kappa'$, $c=\Delta\varepsilon c'$.

$$\kappa'=\frac{\omega\varepsilon_0}{2s(q)}\int_{-\infty}^{\infty}dx\int_{-\infty}^{\infty}dy\int_0^L dz|\vec{e}|^2$$

is the coefficient of the self-coupling and

$$c'=\frac{i\omega\varepsilon_0}{2s(q)}\int_{-\infty}^{\infty}dx\int_{-\infty}^{\infty}dy\int_0^L dz\vec{e}^{*2}\exp(-2iqz)$$

represents the cross-coupling between forward and backward propagating waves. Both coefficients are exclusively determined by the band structure of the unperturbed PCW and do not depend on the perturbation. They describe the sensitivity of the PCW on spatially homogeneous perturbations [see Fig. 1(b)]. Equation (4) can be rewritten in a matrix representation as

$$\begin{pmatrix}A_{k+1}\\B_{k+1}\end{pmatrix}=\hat{M}\begin{pmatrix}A_k\\B_k\end{pmatrix}, \tag{5}$$

$$\hat{M}=\frac{1}{1+\kappa^2-|c|^2}\times\begin{pmatrix}[(1+i\kappa)^2+|c|^2]\exp(iqL) & 2c\exp(iqL)\\ 2c^*\exp(-iqL) & [(1-i\kappa)^2+|c|^2]\exp(-iqL)\end{pmatrix}.$$

Although spatially homogeneous, the perturbation couples forward and backward propagating modes. Consequently new eigenmodes appear which can be expressed in terms of the unperturbed ones. To do so we have to determine eigenvalues and eigenvectors of the matrix $\hat{M}$. Finally we express each field in the perturbed PCW as a linear combination of these new modes as

$$\begin{pmatrix}A_k\\B_k\end{pmatrix}=\alpha_+\lambda_+^k\begin{pmatrix}1\\e_+\end{pmatrix}+\alpha_-\lambda_-^k\begin{pmatrix}1\\e_-\end{pmatrix}, \tag{6}$$

with $\lambda_\pm=\pm\sqrt{[\mathrm{Re}(\eta)]^2-1}+\mathrm{Re}(\eta)$,

$$e_\pm=\frac{1+\kappa^2-|c|^2}{2c}[\pm\sqrt{[\mathrm{Re}(\eta)]^2-1}-i\,\mathrm{Im}(\eta)]\exp(-iqL),$$

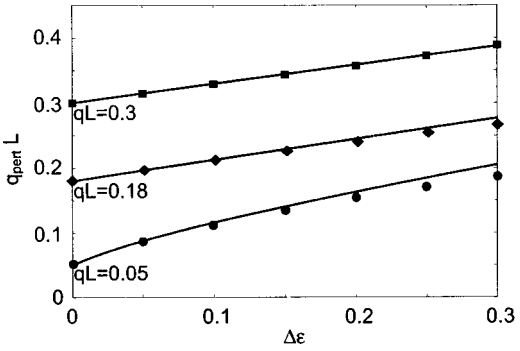

FIG. 2. Bloch vector q_{pert} of the mode of the PCW displayed in Fig. 1 as a function of the perturbation $\Delta\varepsilon$ for a set of fixed frequencies (solid line: analytical theory; points: numerical simulation).

and

$$\eta = \frac{(1+i\kappa)^2+|c|^2}{1+\kappa^2-|c|^2}\exp(iqL).$$

$\alpha_{\pm}$ are the amplitudes of the forward and backward propagating modes. Two cases have to be distinguished: For $\mathrm{Re}(\eta)\leqslant 1$ the eigenvalues of the new modes are complex, $\lambda_{\pm}=\mathrm{Re}(\eta)\pm i\sqrt{1-[\mathrm{Re}(\eta)]^2}$, with an absolute value of 1. Therefore they can be expressed as $\lambda_{\pm}=\exp(iq_{\mathrm{pert}}L)$, where the Bloch vector of the perturbed waveguide q_{pert} reads $q_{\mathrm{pert}}=\arctan[\sqrt{1-\mathrm{Re}(\eta)^2}/\mathrm{Re}(\eta)]/L$. Hence, the field evolution is characterized by a simple phase evolution of respective modes. In contrast for $|\mathrm{Re}(\eta)|>1$ eigenvalues become purely real. Thus the former propagating modes pass over to an evanescent behavior. Figure 2 shows a comparison of our analytical theory with band structure calculations for the PCW displayed in Fig. 1(a). Obviously the results obtained with exact numerical calculations and with our quasianalytical perturbation theory coincide very well.

In order to study the effect of self- and cross-coupling on the band structure of perturbed PCWs we look at some limiting cases. Let us first assume a vanishing cross-coupling $c'=0$. In this case the eigenvalues have the simple form

$$\lambda_{\pm}=\frac{1\pm\iota k}{1\mp i\kappa}\exp(\pm iqL),$$

with an absolute value of 1. Therefore self-coupling exclusively leads to a change of the Bloch vector and therefore causes a *shift* or a *deformation* of the original band. In contrast for dominant cross-coupling ($\kappa'=0$) the eigenvalues reads

$$\lambda_{\pm}=\frac{1+|c|^2}{1-|c|^2}\cos(qL)\pm\sqrt{\left[\frac{1+|c|^2}{1-|c|^2}\cos(qL)\right]^2-1}$$

At $qL=\pi/2$ the Bloch vector remains at the same value, i.e., the new eigenvalue is $\lambda_{\pm}=\pm i$. But, evanescent waves symmetric to $qL=\pi/2$ will occur at Bloch vectors, for which

$$\left|\frac{1+|c|^2}{1-|c|^2}\cos(q_{\pm}^{\mathrm{even}}L)\right|\geqslant 1$$

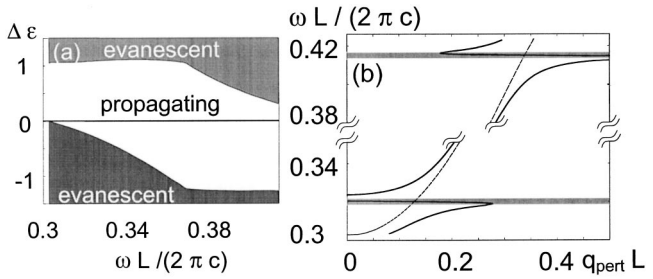

FIG. 3. Photonic crystal waveguide in the presence of a two level polarization perturbation, (a) sensitivity of the band for the emergence of evanescent waves due to an homogeneous perturbation of the dielectric function ε, shaded region: evanescent waves, none-shaded region: propagating waves, (b) Comparison of the band structure in the presence of a two level polarization perturbation (thick lines) with an unperturbed band structure (thin, dashed line); lower curves: two level resonance close to the Γ point ($\omega_0=0.32$); upper curves: two level resonance close to the boundary of the band ($\omega_0=0.415$); parameters: same as in Fig. 1, $\gamma=7.7\,e$-3, $f=7.7\,e$-3.

is yielded. Thus cross-coupling leads to the emergence of evanescent waves and therefore causes band *shrinkage*. Now let us have a closer look at the symmetry points of the PC lattice. At the Γ point both coefficients diverges for $q\rightarrow 0$ [see Fig. 1(b)]. A similar behavior is observed at the X point. The reason is the normalization of the field by means of the energy flux $s(q)$ which goes to zero at symmetry point. An expansion of the self- and cross coupling in a small neighborhood δq of the symmetry point yields: $\kappa=\alpha/\delta q+\cdots$ and $c=i\alpha/\delta q+\cdots$, where

$$\alpha=\frac{\Delta\varepsilon}{\gamma_2}\frac{\omega(q=0,\pi/L)\varepsilon_0}{4U(q=0,\pi/L)}\int_{-\infty}^{\infty}dx\int_{-\infty}^{\infty}dy\int_0^L dz|\vec{e}(q=0,\pi/L)|^2.$$

$U(q)$ is the spatially averaged electromagnetic energy density and γ_2 is the curvature of the band at the corresponding symmetry point $\omega(q=0,\pi/L+\delta q)=\omega(q=0,\pi/L)+\gamma_2(\delta q)^2+\cdots$. For a first order approximation of the eigenvalues in δq and $\Delta\varepsilon$ close to the symmetry points one gets $\lambda_{\pm}(q=0)=1-2\alpha L\pm\sqrt{[1-2\alpha L]^2-1}$ and $\lambda_{\pm}(q=\pi/L)=-1+2\alpha L\pm\sqrt{[1-2\alpha L]^2-1}$. Therefore, evanescent waves occur for any negative α factor, i.e., if the change of the dielectric function $\Delta\varepsilon$ and the curvature γ_2 of the band have opposite signs. As a consequence any negative (positive) $\Delta\varepsilon$ perturbation will shift the mode to higher (lower) frequencies provided the curvature of the band is positive (negative). In other words, a band with a positive (negative) curvature at a symmetry point is sensitive for the emergence of evanescent waves close to this symmetry point if an negative (positive) $\Delta\varepsilon$ perturbation occurs. Figure 3(a) illustrates this fact for the PCW of Fig. 1(a). The shaded regions represent evanescent waves whereas the white region stands for propagating ones. One clearly sees that close to the Γ point the band is sensitive for the emergence of evanescent waves if an negative $\Delta\varepsilon$ perturbation occurs, because the curvature of the band is positive at $q=0$. In the center of the band it

becomes rather insensitive for any kind of perturbation, whereas the sensitivity for positive $\Delta\varepsilon$ perturbation increases for larger Bloch vectors. The reason for this is that the band now has a negative curvature and becomes close to the *X* point.

Consequently polaritons can have a considerably different influence [7,8] on the band structure. Although propagation can be suppressed due to strong absorption in the center of the resonance [shaded area in Fig. 3(b)] additional gaps can open up. If the two-level resonance is close to the Γ point a polariton gap occurs even for a very small oscillation strength. It emerges above the two level resonance because the band is very sensitive for any negative $\Delta\varepsilon$ [see Fig. 3(b)]. For a two level resonance in the center of the PCW band a rather huge oscillation strength is required to create a gap, and in most cases only a slight deformation of the band is observed. Again a two level resonance close to the upper band edge (*X* point) of the PCW mode creates a polariton gap, but for positive $\Delta\varepsilon$, i.e., below the resonance frequency [see Fig. 3(b)], opposite to polaritons in homogeneous media [9]. In addition, new propagating Bloch modes may appear for Bloch vectors at the edge of the Brillouin zone (close to the *X* point) where the unperturbed PCW has no bound eigenmodes.

In conclusion, we have derived a reciprocity theorem and an orthogonality relation for photonic crystal waveguide modes. A set of strongly coupled, discrete equations is constructed, which can be applied to the simulation of various types of perturbed PCWs. As an example, we studied the influences of polaritons on a PCW band structure analytically. The eigenmodes of the PCWs were computed using the freely available software package of MIT [1].

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