Generalized Wannier function method for photonic crystals

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(Received 18 October 1999)

The concept of generalized Wannier functions, adopted from the electronic theory of solids, is used to build a localized representation of electromagnetic waves in dielectric materials. For two-dimensional photonic crystals, we demonstrate the existence of such a localized state basis, and we establish an efficient computational method, allowing a tight-binding-like parameter free modelization of any dielectric structure deviating from periodicity. Numerical simulations of a T-shaped photonic crystal waveguide prove its ability to deal with large-scale systems and complex structures.

Over the past few years much effort has been devoted to the study of the propagation of electromagnetic (EM) waves in periodic dielectric structures. The possibility of creating, under favorable circumstances, frequency ranges for which EM wave propagation is forbidden has attracted much theoretical and experimental attention.[1–4] The study of localized or extended defects in these photonic band-gap (PBG) materials is now becoming a field of growing activity owing to the potential applications of these perturbed structures in the realization of high-quality waveguides or microcavities.[5] The next step will be the development of integrated photonic devices which will require modelization techniques to deal with very large systems. From a theoretical point of view the plane-wave method (PWM) has been largely used to calculate the band structures and defect modes in photonic crystals. Much less attention has been given to the possibility of an expansion of the EM wave field on localized functions in a similar way to the tight-binding (TB) description of the electron states in solids. Since the approach uses small sets of basis functions, the computational effort is smaller than that required by methods based on plane waves. It then allows one to consider complex systems with large unit cells where plane-wave methods come to their limits of applicability. However, the essence of this approach, and its efficiency to modelize complex systems, relies on the existence of localized basis states. Unlike the electron case where atomic orbitals localized on individual atoms constitute a natural basis, in the case of light propagating in a dielectric material only scattering extended states can be associated with the individual scattering centers. Thus the extension of the TB method to PBG materials appears not to be trivial. We will contend ourselves here to its implementation in the two-dimensional (2D) case, where one can get rid of the complications arising from the vectorial nature of the wave field while keeping the basic features of the problem. In this paper we demonstrate that a set of localized basis states associated with a periodic 2D photonic crystal exists and can be constructed. We then establish an efficient computational procedure allowing large-scale simulations on complex PBG structures.

Our work is rooted to the concept of generalized Wannier functions[6] whose construction is performed in photonic crystals. This construction only requires a prior knowledge of the Bloch fields and frequencies of a periodic structure taken as a reference system. The calculation strategy goes as follows: in a first stage a TB empirical parametrization of the band structure of this reference system is performed. Together with the Bloch functions already determined, it then allows the construction of the Wannier functions of the periodic lattice.[7–9] Any perturbation of the reference system can be characterized by calculating explicitly and without any additional assumption all the relevant matrix elements in this basis. The determination of the corresponding perturbed eigenmodes can then finally be obtained by employing a Green's-function-based technique or a TB formalism coupled with a supercell method which is more competitive for large-scale simulations.

Once the basis states are determined, this method can deal with any dielectric structure within a ''first-principles'' scheme. This approach differs fundamentally from the mixed TB-plane-wave empirical framework recently proposed by Lidorikis *et al.*[10] for the treatment of 2D PBG structures with a high dielectric contrast. The homogeneous and localized nature of the basis states used here avoids all the complications arising from the coupling between localized and extended states. Furthermore, the nonempirical modelization of perturbations adopted here allows us to deal with a far wider class of defects such as changes in the dielectric constant in some units, where an empirical scheme appears difficult to apply.

This photonic version of the TB method will now be presented by studying a model system.[11] It consists of a periodic array of infinitely long dielectric rods whose vertical axes are arrayed on a square lattice of lattice constant d. The rods have a dielectric constant of 11.56, a radius of $0.2d$, and are embedded in vacuum. As in Refs. 10 and 11, we will limit ourselves here to a study of the propagation of waves with electric field parallel to the rod axis (TM waves). This working model is sufficiently standard to ensure that no conceptual nor numerical difficulties should be expected when dealing with others different 2D problems.

Considering first the fully periodic structure, which is taken as the reference system, the scalar wave equation obeyed by the electric field can be written as

$$(-\nabla^2)E_n(\mathbf{k},\mathbf{r}) = \varepsilon_p(\mathbf{r})\frac{\omega_n^2(\mathbf{k})}{c^2}E_n(\mathbf{k},\mathbf{r}), \qquad (1)$$

where $\varepsilon_p(\mathbf{r})$ stands for the dielectric function of the periodic medium. A band index n and a 2D vector $\mathbf{k}$ lying in the first Brillouin zone have been used to label the band modes $E_n(\mathbf{k},\mathbf{r})$ and their associated frequency $\omega_n(\mathbf{k})$.

These band modes have to first be calculated by an *ab initio* method. With the PWM, 441 plane waves were amply sufficient to ensure a good convergence for the low-frequency bands of interest and their associated Bloch fields. These latter are then orthonormalized on the 2D crystal surface as

$$\int_S E_n^*(\mathbf{k},\mathbf{r})\varepsilon_p(\mathbf{r})E_{n'}(\mathbf{k}',\mathbf{r})d^2\mathbf{r}=\delta_{nn'}\delta_{\mathbf{k}\cdot\mathbf{k}'}. \tag{2}$$

In the present work we are interested in modes whose frequencies lie in the vicinity of the first gap, between the first two bands. A convenient localized basis for their expansion is then obtained by constructing the Wannier functions associated with a group of bands situated in this frequency range. These Wannier functions can be classified according to the irreducible representations of the square group (C_{4v}).[12] We have found that eight functions per lattice site are sufficient to obtain a good description: two functions with symmetry A_1(s type), four functions with symmetry E (two p_x types and two p_y types), one function with symmetry B_1($d_{x^2-y^2}$ type), and one function with symmetry B_2(d_{xy} type). Since they are unitary transforms of the Bloch functions, the Wannier functions obey the orthonormality condition

$$\int_S a_m^*(\mathbf{r}-\mathbf{R})\varepsilon_p(\mathbf{r})a_{m'}(\mathbf{r}-\mathbf{R}')d^2\mathbf{r}=\delta_{mm'}\delta_{\mathbf{R}\cdot\mathbf{R}'}, \tag{3}$$

where an index $m=1,8$ has been used to label the functions centered at lattice site $\mathbf{R}$. A TB-like parametrization of the bands can then be performed. Writing Eq. (1) in this basis, it is found that the operator $\Theta=-\nabla^2$ has to satisfy the following eigenvalue equation:

$$\sum_{m'}\Theta_{mm'}(\mathbf{k})U_{m'n}(\mathbf{k})=\frac{\omega_n^2(\mathbf{k})}{c^2}U_{mn}(\mathbf{k}), \tag{4}$$

where $U_{mn}(\mathbf{k})$ are the eigenvectors. Here

$$\Theta_{mm'}(\mathbf{k})=\sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}}\int a_m^*(\mathbf{r})(-\nabla^2)a_{m'}(\mathbf{r}-\mathbf{R})d^2\mathbf{r}. \tag{5}$$

The matrix representation of this operator is obtained by using the standard Slater-Koster method. The symmetry properties of the basis functions allow the $\mathbf{k}$-dependent terms $\Theta_{mm'}(\mathbf{k})$ to be expressed in terms of a reduced number of integrals. These are then considered as free parameters in the procedure where the solutions Ω of the determinantal 8×8 equation,

$$\det|\Theta_{mm'}(\mathbf{k})-\Omega\,\delta_{mm'}|=0, \tag{6}$$

are fitted to the results $\omega_n^2(\mathbf{k})/c^2$ of the plane-wave calculation. Taking into account only first-neighbor interactions, the fit involves the determination of 26 independent parameters. The resulting band-structure scheme calculated along high-symmetry directions in the BZ is shown in Fig. 1, together

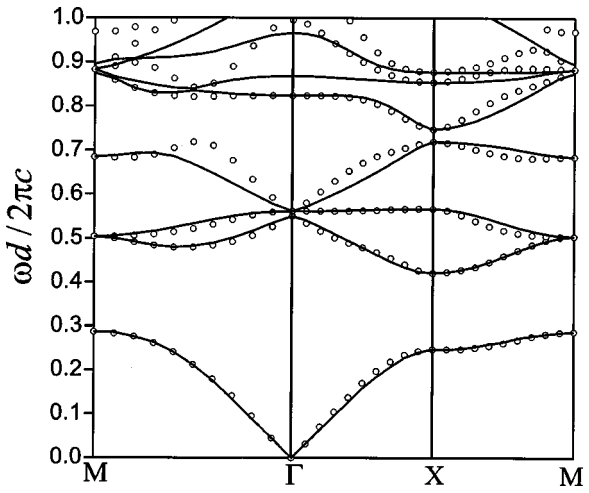

FIG. 1. TM photonic band structure of a 2D square lattice (period d) of dielectric rods ($\varepsilon=11.6$) with radius $0.2d$. Solid lines correspond to numerical results from the PWM, while circles correspond to a TB fit. Only the lower-frequency region which is relevant for the present study is shown.

with that obtained by the PWM. The agreement between the two calculations is quite good for the lowest-frequency bands. Because of our limitation to first-neighbor interactions, the quality of the fit slightly decreases with increasing frequency. However, it will be shown that this worsening does not seriously affect the determination of the defect modes in which we are interested. The basis functions involved in this TB parametrization procedure can then be effectively constructed by performing two successive unitary transformations on the Bloch waves already calculated by the PWM. Generalized Bloch functions are first defined for each $\mathbf{k}$ in the BZ zone by taking linear combinations of the Bloch functions as

$$\Phi_m(\mathbf{k},\mathbf{r})=\sum_n U_{mn}^*(\mathbf{k})E_n(\mathbf{k},\mathbf{r}), \tag{7}$$

where the unitary 8×8 matrix $U_{mn}(\mathbf{k})$ is formed by the orthonormalized eigenvectors obtained in solving Eq. (6). Then the Wannier functions are obtained by Fourier transforming these generalized Bloch functions $\Phi_m(\mathbf{k},\mathbf{r})$,

$$a_m(\mathbf{r}-\mathbf{R})=\frac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}}\Phi_m(\mathbf{k},\mathbf{r}), \tag{8}$$

where N is the number of unit cells in the 2D periodic lattice. Symmetry considerations allow the summation to be restricted to the irreducible wedge of the BZ. 67 $\mathbf{k}$ vectors in this reduced zone have been considered. An idea of the localization of the resulting Wannier functions can be inferred from Fig. 2, where we plot two functions with respective symmetries A_1 and E. These plots are made in the (10) direction, which is the direction of their slowest decrease. A strong localization of these Wannier functions about their origin, followed by small decaying oscillations around successive lattice sites, can be observed. This rapid decay of the amplitudes beyond the first-neighbor site is coherent with the limitation to first-neighbor interactions in the parametrization

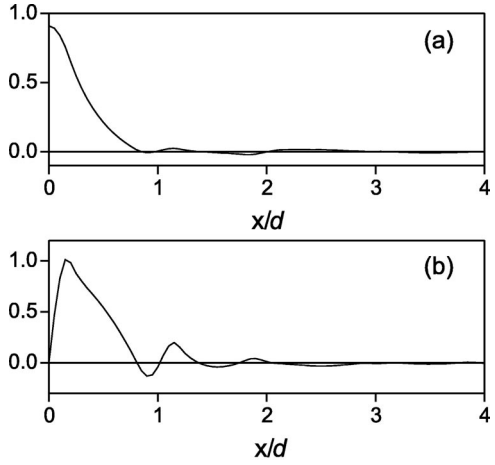

FIG. 2. Wannier functions of the square lattice with A_1 (a) and E (b) symmetries plotted along the (10) direction. The integer values of x/d correspond to successive neighbors in this direction.

procedure, and gives a clear indication of the validity of this TB-like approach for the description of the periodic structure.

We next consider structures containing defects. These perturbed structures are characterized by the local deviation $\Delta\varepsilon(\mathbf{r})$ of the dielectric constant from its original periodic value $\varepsilon_p(\mathbf{r})$ in the reference system. The wave equation in this case takes the following form:

$$\left\{-\nabla^2-\frac{\omega^2}{c^2}[\varepsilon_p(\mathbf{r})+\Delta\varepsilon(\mathbf{r})]\right\}E(\mathbf{r})=0. \tag{9}$$

Within the TB formalism the perturbation can be completely characterized by constructing the matrix representation of $\Delta\varepsilon(\mathbf{r})$ in the Wannier function basis. This is greatly facilitated by the short-range properties of these functions: the only non-negligible matrix elements are those which involve functions centered in the close vicinity of the perturbed domain. These are easily obtained by 2D numerical integration.

Equation (9) can then be solved by using the TB method, coupled with either the Green's function method (TBGF method) or with the supercell approximation (TBSC approximation). In the former case, the Green's matrix associated with the $(-\nabla^2)$ operator in the periodic structure can be constructed from the solutions of Eq. (6), while in the second case only the TB representation of the Θ operator previously determined is needed. Both methods are used here to study the two types of point defects obtained by reducing and expanding the initial radius of a single rod, respectively. These two calculations will allow an appreciation of the validity of the TB determination of the defect modes in the two characteristic situations where these are extracted from the bands lying above or below the gap. The specific values attributed to the radius are respectively zero, corresponding to the creation of a vacancy, and $0.3d$. For both cases it was found that a 3×3 supercell suffices, in the TBSC approximation, to obtain results agreeing with those obtained with the TBGF method. In the first case a single nondegenerate A_1-type monopole defect mode appears in the gap at a reduced frequency $\omega d/2\pi c=0.390$, while in the second case a doubly degenerate mode with E symmetry is found at 0.384. Both

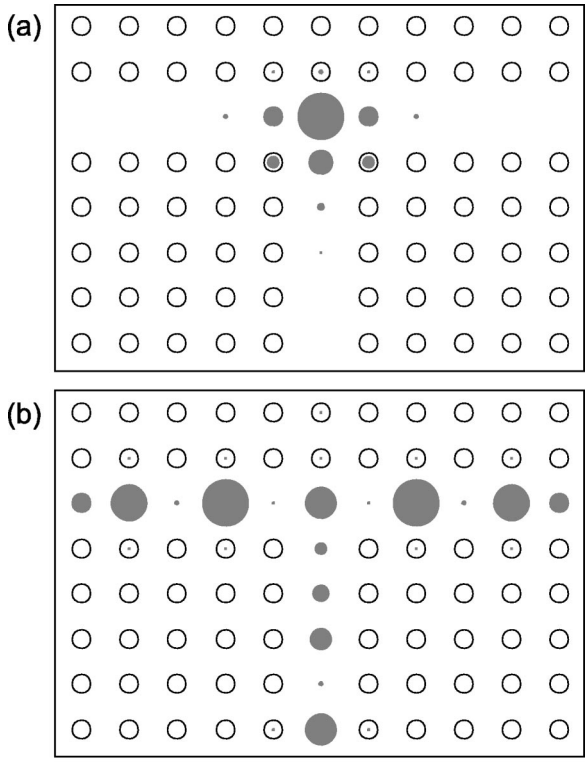

FIG. 3. Two characteristic modes of a T-shaped waveguide. The dielectric rods are represented by open circles. The intensity of the electric field is plotted with gray circles whose diameter is proportional to the intensity (in arbitrary units). The reduced frequencies of the mode are 0.308 and 0.377 for the (a) and (b) cases, respectively.

values compare favorably with the PWM results, 0.380 and 0.374, respectively.[11] It is to be noted that here only nearest neighbors have been taken into account in the TB calculations, both in periodic and perturbed structures. Inclusion of more distant interactions should improve the accuracy of the TBSC approximation which, however, appears at this stage to be quite competitive for further investigations of perturbed structures.

The potential usefulness of this approach for modeling extended PBG structures involving microcavities and waveguides will finally be assessed here by considering the specific case of a T-shaped PBG waveguide. This structure is created by removing rods in the periodic original 2D lattice (see Fig. 3). The TBSC method allows Eq. (9) to be solved for this specific configuration, obtaining the field $E_i(\mathbf{r})$ associated with the eigenfrequency ω_i as

$$E_i(\mathbf{r})=\sum_{m\mathbf{R}} C_m^i(\mathbf{R})a_m(\mathbf{r}-\mathbf{R}). \tag{10}$$

Because of the localization of the Wannier functions around their respective centers, a clear indication about the intensity variations of the wave field in the structure can then be obtained by calculating and plotting

$$I_i(\mathbf{R})=\sum_m |C_m^i(\mathbf{R})|^2 \tag{11}$$

for each site **R** in the supercell. Figure 3 plots $I_i(\mathbf{R})$ for two characteristic modes. The first one at the reduced frequency $\omega_i d/2\pi c = 0.308$ constitutes a bound state whose electric field is strongly localized at the junction of the three waveguides. The second one at 0.377 is confined inside the whole waveguide. It corresponds to a guided mode. The existence of such a mode shows the ability of PBG waveguide to guide light through cross junctions.

Such types of plot made for specific patterns of line defects in periodic structures may give useful information about their associated guiding properties for EM waves.[5] Due to the reduced number of basis functions involved (here eight basis functions per lattice site) the TBSC method appears to be appealing because of its ability to handle extended structures with reasonable matrix sizes. For comparison a PWM calculation made on the 11×8 supercell considered here would involve at least 10^4 plane waves, since more than 100 plane waves per site (as is generally accepted) are needed to obtain well-converged results. It is to be noted that, although this approach retains the simplicity and efficiency of the empirical TB method, no adjustable parameter is involved in the calculation. Instead all the necessary matrix elements characterizing any perturbation of a reference structure are explicitly calculated. Furthermore the short-range properties of the basis functions drastically reduce the effective number of those which have to be calculated. The difficulties related to the evaluation[13] and the transferability of the parameters in empirical versions of the TB method[10] are then circumvented. The efficiency of such a localized representation of EM waves should become decisive in numerical simulations on disordered or quasicrystalline structures to investigate their localization properties for light. Also, an extension of this approach to the treatment of 3D structures, with vector Wannier functions[14] replacing the scalar ones obtained here, appears feasible and promising.

As a conclusion we have shown that it is possible to calculate explicitly a localized state basis using Wannier functions in 2D photonic crystals and that a TB formalism based on these functions constitutes a very efficient tool in the description of eigenmodes associated with structures deviating from periodicity. This method offers a promising way to study large integrated photonic devices associating microcavities and waveguides.

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