Density of states for finite photonic crystals

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There is a twofold way to study wave propagation: one can deal with infinite structures and solve a spectral problem through Bloch waves or deal with a finite size device and solve a diffraction problem. In this work, we concentrate on scattering theory and we define a notion of scattering measure or reciprocal density of states, which plays the role of the classical local density of states for finite structures.

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I. INTRODUCTION

Photonic band-gap materials are periodically modulated structures that offer the possibility of controlling the propagation of light in all directions of space through forbidden band effects.[1–3] Defects may be introduced so as to create cavities with a very high quality factor, but also to design waveguides.[4–9] Among the various approaches to the theoretical study of these objects we can distinguish Bloch-wave theory,[3] grating theory,[10] the finite differences in time domain (FDTD) method and scattering theory.[11] By using Bloch waves, it is possible to obtain the dispersion curves of the device, supposed to extend at infinity, and also some related interesting quantities, such as the density of states. However, this method does not allow one to compute the result of a scattering experiment, and the coupling of an exterior incident field to a resonant mode cannot be taken into account. The use of grating theory, describing the photonic crystal as a stack of diffraction gratings, permits one to solve a scattering problem, but also to compute the band structure of the crystal. However, both these approaches cannot handle directly the problem of the defects or the boundary effects: some geometric periodization has to be introduced. Though widely used, such a technique can lead to spurious phenomena and remove some interesting properties. The two last techniques, that of the FDTD method and that of the scattering matrix, can handle finite structures, i.e., made out of a finite number of scatterers arbitrarily placed in space, and so it can handle easily the case of defects and also the coupling with an exterior field. From nuclear physics and quantum chemistry, where scattering theory takes its roots, it is known that it is possible to reconstruct the fundamental properties of the harmonic scattering matrix from the knowledge of the evolution of the field in time domain—for instance, by using complex scaling.[12] We shall therefore concentrate on the scattering theory, which furnishes directly mathematical tools.

Such notions as that of the density of states or local density of states, which are crucial in the description of the coupling between field and matter—for instance, for considering the spontaneous emission of an atom embedded in a photonic crystal—cannot be straightforwardly defined for finite structures. Some previous attempts have been made to generalize this notion to finite-size structures.[13–16] In the present work, we define a reciprocal density of states derived from the resonances of the scattering matrix. This quantity takes into account the shape of the modes but also the coupling of the modes with plane waves.

II. SCATTERING THEORY

In order to examplify the concepts, we use a bidimensional finite-size photonic crystal and a crystal made of a stack of diffraction gratings as well. For the numerical computations, we use a multiple-scattering rigorous theory of diffraction[17–19] that has been successfully compared with experiment[19] and a grating code using the differential method for gratings. Throughout the study, we use a time-harmonic field with a time dependence of $\exp(-i\omega t)$.

The main theoretical tool in dealing with a finite structure is the scattering matrix. It is the operator that gives the diffracted field from the incident one. It is obtained in the following way. Considering a two-dimensional(2D) structure, i.e., made of infinite parallel rods, and *s*-polarized waves, the electric field satisfies $\Delta E+k_0^2\varepsilon E=0$ (k_0 is the wave number in vacuum). Denoting by E^i the incident field and $E^d=E-E^i$ the diffracted one, we have $(\Delta+k_0^2)E^d=k_0^2(1-\varepsilon)E$, hence, denoting $R(k_0)=(\Delta+k_0^2)^{-1}$ and $R(k_0,\varepsilon)=(1/\varepsilon\Delta+k_0^2)^{-1}$ we have $E^d=R(k_0,\varepsilon)k_0^2(1-1/\varepsilon)E^i$ and so $R(k_0,\varepsilon)=[I-R(k_0)k_0^2(1-\varepsilon)]^{-1}R(k_0)$. From a practical point of view, an explicit expression is obtained by using a Fourier-Bessel expansion of the field.[11] The position of the rods being denoted by $\{\mathbf{r}^j=(r^j,\theta^j)\}$, we write the diffracted field outside the rods in the form

$$E^d(\mathbf{r})=\sum_j\sum_{n=-\infty}^{n=+\infty} b_n^j H_n^{(1)}(k_0|\mathbf{r}-\mathbf{r}^j|)e^{in\theta_j}.$$

Resonances are due to the existence of poles of the scattering matrix in the complex plane of wavelengths. The following generalized Laurent expansion for the scattering matrix, as an operator in $\mathcal{L}(l^2)$ on $(b_n^j)_{j,n}$, holds:

$$S(k)=\sum_p \frac{S_p}{k-k_p}+S_0(k), \tag{1}$$

where $S_p=(1/2i\pi)\oint S(z)dz$ is a projector (i.e., $S_p^2=\mu S_p$) on the kernel of $(1/\varepsilon)\Delta+k_p^2$ (see Ref. 20 for a numerical approach to this notion) and $S_0(k)$ is a regular (holomorphic)

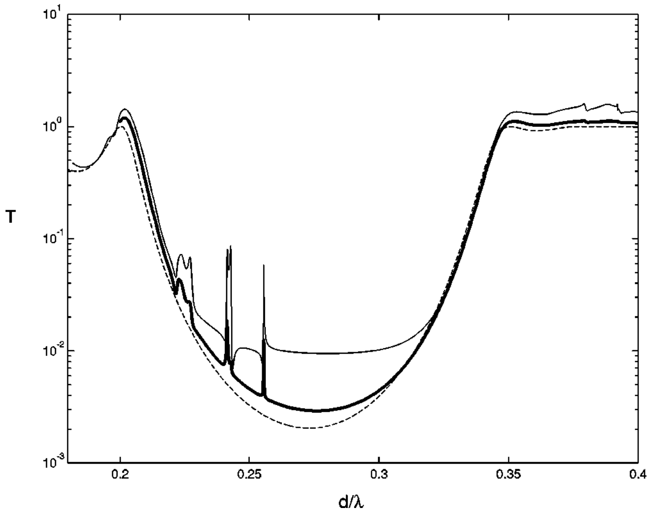

FIG. 1. Transmission in normal incidence. Light solid line: finite structure with an incident plane wave. Bold solid line: finite structure with an incident Gaussian beam. Dashed line: stack of gratings for an incident plane wave.

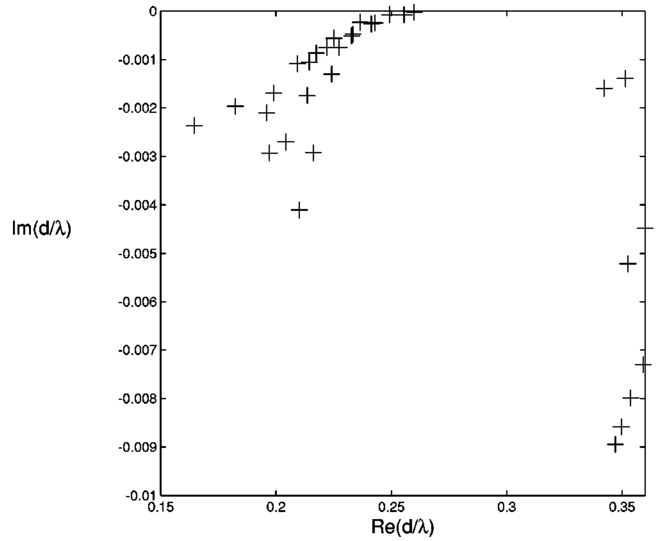

FIG. 2. Location of some poles of the scattering matrix in the complex plane of wavelengths.

operator. The (possibily degenerated) modes $\{|\phi_p\rangle\}_p$ associated with the poles belong to the kernel of $S^{-1}(k_p)$, and the associated characteristic space is the image of S_p: it is the eigenspace generated by $|\phi_p\rangle$. It is important to remark that S_p is not necessarily an orthonormal projector so that we can only write $S_p = |\phi_p\rangle\langle\phi_p^*|$ where $|\phi_p^*\rangle = S_p^*|\phi_p\rangle$ and the operator S_p^* is the adjoint of operator S_p for the ℓ^2 inner product.

We use the following structure: the crystal is made out of 5×10 parallel rods, with relative permittivity $\varepsilon_r = 9$, the radius over period of the rods is $r/d = 0.3$, with square symmetry, and we use *s*-polarized incident fields. Dealing with a finite device, we define the transmission ratio as the flux of the Poynting vector through a segment situated near the lower face of the crystal over the flux of the Poynting vector of the incident field. In order to allow for comparison with the infinite case, we also consider a structure made of a stack of five gratings, with the same basic cell as that of the finite structure.

We first compute the transmission ratio for an incident plane wave for both the finite structure (light solid line in Fig. 1) and the stack of gratings (dashed line in Fig. 1).

Remark: It should be noted that this transmission ratio may be superior to 1.

Contrarily to what happens in case of diffraction gratings, in the finite-size case shallow acceptor modes[21] appear in the first gap. These resonances appear for wavelengths that are of the order of the size of the crystal, and so the question may arise as to whether these peaks are linked to the finiteness of the structure and can be removed, for instance, by illuminating the structure with a Gaussian beam whose waist is smaller than the size of the side of the photonic crystal, i.e., when the incident field does not "see" the boundary. The direct numerical computation for incident Gaussian beams (bold solid line in Fig. 1) shows that there are still peaks, though their widths and heights are diminished.

The key to the understanding of these phenomena lies in the pole structure of the photonic crystal.[18] We compute the poles of the scattering matrix of the crystal. We find poles with real parts very near to that of the peaks of Fig. 1 (see Fig. 2). A different insight may be gained by computing the Bloch dispersion diagram of the structure (Fig. 3). It can be seen that the gap depends strongly on the angle of incidence and that there is a complete gap for *s*-polarized waves, that is, a gap for all incidence, only for the interval $d/\lambda \in [0.26, 0.34]$ (it is the gray zone in Fig. 3): this is precisely the pole-free region of the scattering matrix as seen in the pole structure diagram of Fig. 2. The apparent gap in normal incidence that is seen on the transmission through the stack

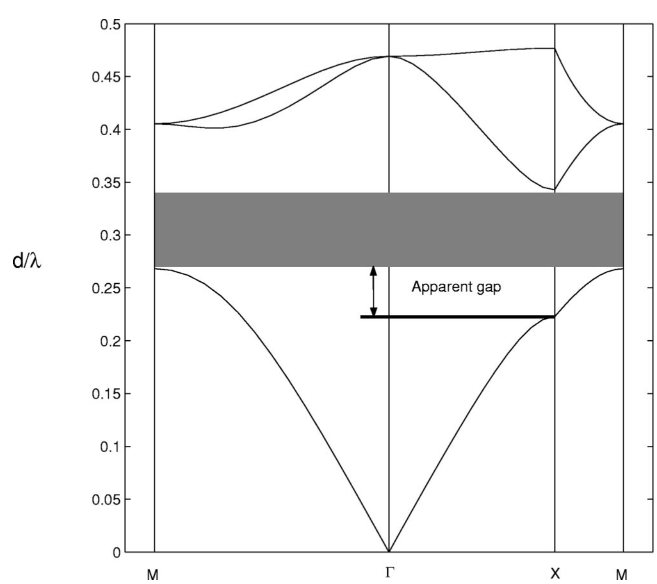

FIG. 3. Bloch diagram of the infinite crystal. The grey band indicates the true gap; the arrow indicates the apparent gap in normal incidence for the stack of gratings.

of gratings corresponds to the Γ-M region of the Bloch diagram (see arrow in Fig. 3). Consequently, the peaks on the right side of the transmission diagram correspond to poles associated with Bloch waves with a non zero horizontal component, i.e., the X-M and M-Γ regions in Fig. 3.

The scattering matrix only depends on the wave number and not on the horizontal Bloch component contrarily to what happens for the scattering matrix of a stack of gratings which is written as $(k,\theta)\rightarrow S(k,\theta)$. Consequently, the scattering matrix accounts for all possible generalized modes and, whatever the angle of incidence, there is some coupling between the incident field and the scattering modes, even if they do not have the same horizontal component as that of the incident field. This remark is crucial for a proper definition of the density of states in finite photonic crystals. More precisely, let us write, at least formally, the scattered field as

$$|u^d\rangle=\sum_p \frac{1}{k_0-k_p}\int d\alpha A(\alpha)\langle \phi_p^*|u^i(\alpha)\rangle|\phi_p\rangle+S_0(k_0)|u^i\rangle \tag{2}$$

for an incident monochromatic field $|u^i\rangle=\int d\alpha A(\alpha)|\psi_\alpha\rangle$, where $|\psi_\alpha\rangle$ is the ket associated with $e^{i\mathbf{k}_0(\alpha)\mathbf{r}}$. This shows that the actual excitation of a resonance pole is linked to both the amplitude of the field and the *spectral amplitude on mode p* defined as $\langle\phi_p^*|\psi_\alpha\rangle$. On the sphere at infinity, the scattering mode can be written as $|\phi_p\rangle=\int d\alpha\langle\psi_\alpha|\phi_p\rangle|\psi_\alpha\rangle$. The total field then is written as

$$u=\int d\alpha'\left[A(\alpha')+\int d\alpha A(\alpha)\rho(\alpha,\alpha')\right]|\psi_{\alpha'}\rangle,$$

where we define the *off-shell scattering amplitude* for the finite structure as[22]

$$\rho(\alpha,\alpha';k_0)=\sum_p \frac{\langle\phi_p^*|\psi_\alpha\rangle\overline{\langle\phi_p|\psi_{\alpha'}\rangle}}{k_0-k_p}+S_0(k_0), \tag{3}$$

the spectral scattering measure, which is an operator-valued measure,

$$M(dk)=\sum_p |\phi_p\rangle\langle\phi_p^*|\otimes\delta_{k_p}+S_0\otimes dk, \tag{4}$$

and the *scattering measure* or *reciprocal density of states* (RDOS)

$$m(\alpha,\alpha';dk)=\langle\psi_{\alpha'}|M(dk)|\psi_\alpha\rangle \tag{5}$$

$$=\sum_p \langle\phi_p^*|\psi_\alpha\rangle\overline{\langle\phi_p|\psi_{\alpha'}\rangle}\delta(k-k_p)+\langle\psi_{\alpha'}|S_0|\psi_\alpha\rangle dk, \tag{6}$$

and we can write

$$\rho(\alpha,\alpha';k_0)=\int\frac{m(\alpha,\alpha';dk)}{k_0-k},$$

$$S(k_0)=\int\frac{M(dk)}{k_0-k}. \tag{7}$$

Both measures can be split into a regular and a singular part, as in the Lebesgue theorem for the decomposition of measures: $M(dk)=M_{sg}(dk)+M_{ac}(dk)$, $m(\alpha,\alpha';dk)=m_{sg}(\alpha,\alpha';dk)+m_{ac}(\alpha,\alpha';dk)$ where

$$M_{sg}(dk)=\sum_p |\phi_p\rangle\langle\phi_p^*|\otimes\delta_{k_p},M_{ac}(dk)=S_0\otimes dk,$$

$$m_{sg}(\alpha,\alpha';dk)=\sum_p \langle\phi_p^*|\psi_\alpha\rangle\overline{\langle\phi_p|\psi_{\alpha'}\rangle}\delta(k-k_p),$$

$$m_{ac}(\alpha,\alpha';dk)=\langle\psi_{\alpha'}|S_0|\psi_\alpha\rangle dk, \tag{8}$$

this leads to a similar decomposition for r and S.

Remarks: (1) All these quantities are independent of the incident field [defined by $A(\alpha)$] and are intrinsic properties of the photonic crystal, and (2) As $m(dk)$ is not a measure on the real line, then ρ is not the Stieljes transform of $m(dk)$, and consequently $m(dk)\neq(1/\pi)\mathrm{Im}(\rho(k_0+i0))$.[23]

Let us now denote by $\{|\phi_n\rangle\}_n$ the canonical basis of $l^2(\mathbb{Z},\mathbb{C})$, i.e., $\langle\theta|\phi_n\rangle=e^{in\theta}$. The basis can be expanded as an integral of plane waves:

$$|\phi_n\rangle=\int_{\mathbb{T}^1} i^n e^{-in\alpha}|\psi_\alpha\rangle d\alpha.$$

The trace of the S matrix is given by

$$\mathrm{tr}(S)=\sum_p \langle\phi_p|S(k_0)\phi_p\rangle.$$

Denoting $\langle\rho\rangle=(1/2\pi)\int_{\mathbb{T}^1}\rho(\alpha,\alpha;k_0)d\alpha$, it is not difficult to see that

$$\mathrm{tr}(S)=\langle\rho\rangle=\int_{\mathbb{R}}\frac{\langle m(dk)\rangle}{k_0-k}+\int\langle m(dk)\rangle.$$

This quantity represents somehow a decomposition of the modes on plane waves, and it is linked to the cluster of scatterers only; i.e., it does not depend on the incident field [recall that $A(\alpha)$ accounts for the spectral density of the incident field].

The consequence of Eqs. (8) is that the existence of a peak on the transmission diagram, or more generally the possibility of exciting a mode, depends on three parameters: the spectral amplitude $\langle\phi_p^*|\psi_\alpha\rangle$, the distance of the wave number to the nearest pole $|k_0-k_p|$, and the amplitude of the incident field $A(\alpha)$.

Let us consider two examples—for instance, the poles $d/\lambda_1=0.2598-2.025\times10^{-5}i$ and $d/\lambda_2=0.2556-6.53\times10^{-5}i$. In Figs. 4(a) and 4(b), we have plotted the spectral amplitudes which have very strong lobes in some precise directions, corresponding to the plane waves associated with the modes. However, for the first pole, the spectral amplitude is antisymmetric with respect to the horizontal axis, and therefore it cannot be coupled by a field illuminating the structure on its largest side: the spectral amplitude is null in the vertical direction. On the contrary, the other pole can be excited in normal incidence so that there is still a peak in the corresponding transmission diagram. Therefore, the existence or not of the peaks is linked to the symmetries of the

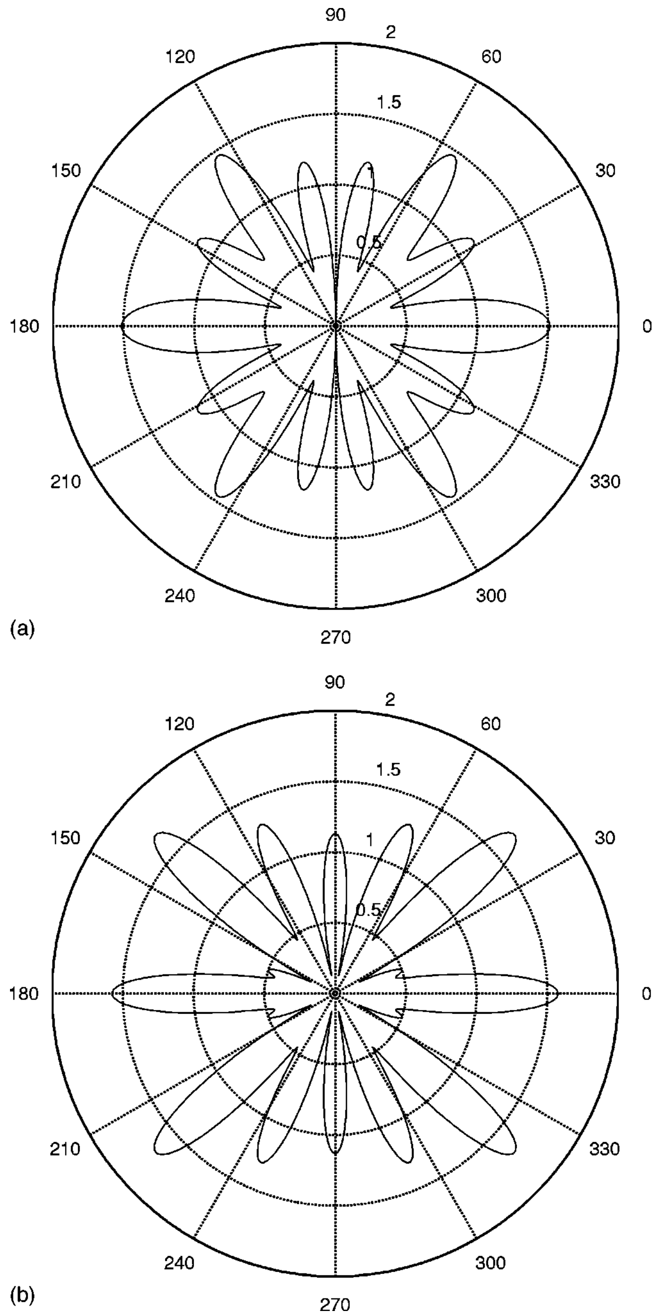

FIG. 4. Polar plot of the spectral amplitude of the modes: (a) $d/\lambda_1 = 0.2598 - 2.025\times 10^{-5} i$, (b) $d/\lambda_2 = 0.2556 - 6.53\times 10^{-5} i$.

incident field with respect to that of the modes.[24–26] We stress that for a plane wave under normal incidence, these irregularities could not be removed by using a larger structure: indeed, the peaks are due to the presence of poles of the scattering matrix which are independent of the incident field.

We see here that the global geometry of the structure is a crucial point for a clear understanding of the transmission properties or more generally the excitation of the modes of the crystal. Now the question arises to understand for what reason the peaks disappear when a Gaussian beam with sufficient small waist is used. Of course, this follows the physical intuition, but from another point of view, the poles are still there, whatever the incident field. In order to get a

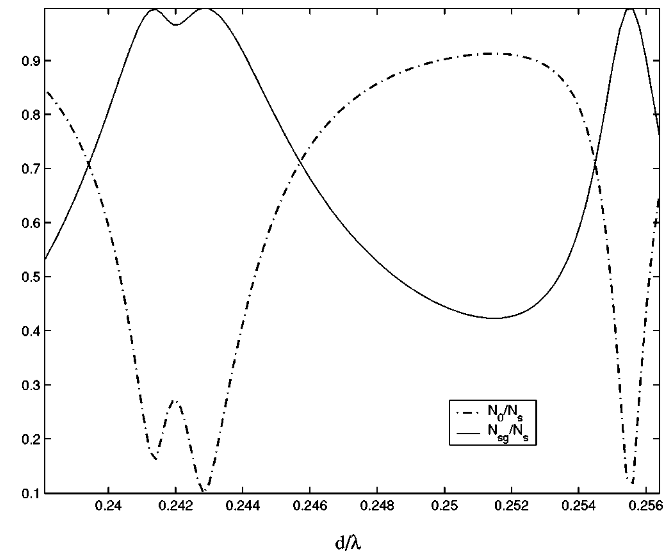

FIG. 5. Decomposition of the scattering field on resonant and evanescent modes for an incident plane wave.

deeper view into this problem, we compare the relative importance of the regular and singular parts of the scattering matrix or, in other words, of the atomic and absolutely continuous parts of the scattering matrix. We limit our investigation to the two first resonances $d/\lambda_1 = 0.2598 - 2.025 \times 10^{-5} i$ and $d/\lambda_2 = 0.2556 - 6.53\times 10^{-5} i$, we compute the residu operators associated with these poles, and we write

$$S(k_0) = \int \frac{M_{sg}(dk)}{k_0 - k} + \widetilde{S}_0(k_0),$$

where

$$M_{sg}(dk) = |\phi_1\rangle\langle\phi_1^*| \otimes \delta_{k_1} + |\phi_2\rangle\langle\phi_2^*| \otimes \delta_{k_2}.$$

Therefore we get two scattering operators, one associated with the resonances,

$$S_{sg}(k_0) = \int \frac{M_{sp}(dk)}{k_0 - k} dk, \tag{9}$$

and one which accounts for both the evanescent field and the remote resonances. Due to the positions of the other resonances, it is reasonable to assume that in a small neighborhood of λ_1 and λ_2 we have $\widetilde{S}_0 = S_0$.

We use first a plane wave in normal incidence ($\alpha = 0$) to illuminate the structure and we compute

$$N_s = \langle \psi_0 | S^* S | \psi_0 \rangle = \frac{1}{2\pi} \int_{\mathbb{T}^1} |\rho(0,\alpha')|^2 d\alpha', \tag{10}$$

which is to be compared to $N_{sg} = \langle \psi_0 | S_{sg}^* S_{sg} | \psi_0 \rangle$ and $N_0 = \langle \psi_0 | \widetilde{S}_0^* \widetilde{S}_0 | \psi_0 \rangle$. Both curves N_{sg}/N_s and N_0/N_s are given in Fig. 5. We clearly see that the scattering matrix is perfectly well represented by the singular part around the resonances, but also that the regular part plays also a non-negligible role between resonances.

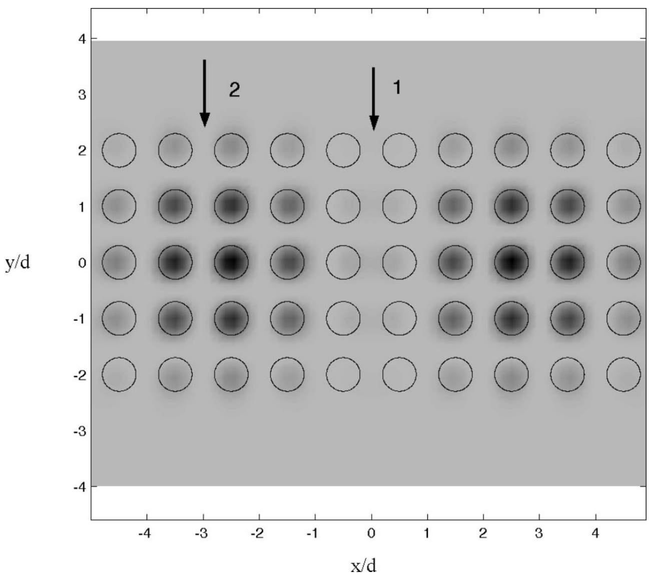

FIG. 6. Map of the mode for $d/\lambda_2 = 0.2556 - 6.53\times 10^{-5}i$. The arrows indicate the focus point of the Gaussian beam.

In a second time, we use an incident Gaussian beam focused on the center of the structure (see Fig. 6 for a map of the field at $\lambda=\lambda_2$; arrow 1 shows the focus point of the beam). The coefficients N_{sg}/N_s and N_0/N_s are given in Fig. 7. This time it is clear that it is the regular part that plays the most important role: almost all the energy is coupled to the evanescent waves instead of the resonances, which do not appear on the transmission curve, as noted above. The final experiment consists in focusing the incident beam on a part of the crystal where the intensity of the modes is maximal (see arrow 2 in Fig. 7). Under that condition, we find again that the modes can be coupled (Fig. 8).

The question of the converge of the properties of the finite structure towards that of an infinite one is then posed. The

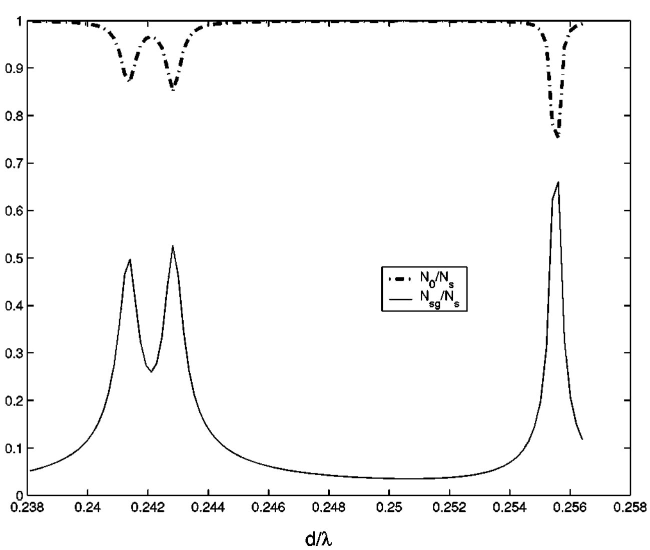

FIG. 7. Decomposition of the scattering field on resonant and evanescent modes for an incident Gaussian beam focused on the center of the crystal (see arrow 1 in Fig. 6).

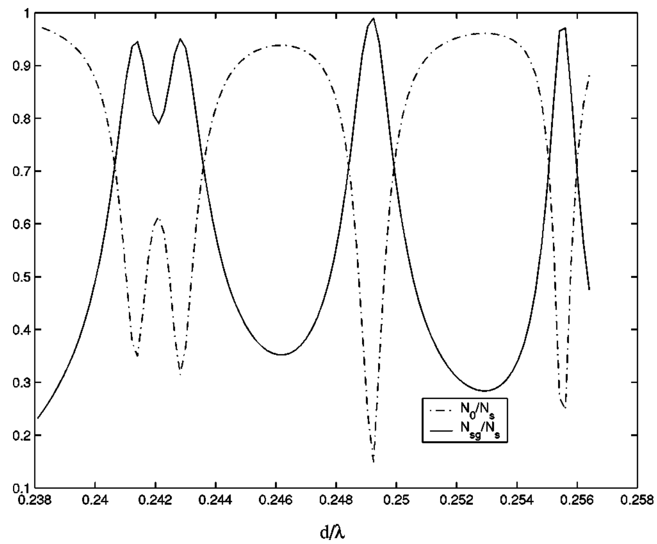

FIG. 8. Decomposition of the scattering field on resonant and evanescent modes for an incident Gaussian beam focused on the left side of the crystal (see arrow 2 in Fig. 6).

first idea that may come is to expect some sort of convergence of the poles and residues when the size of the crystal increases. In fact, there are different mathematical entities at stake here: the pole structure by itself, which is just a set of points and can be expected to converge, in a Kuratowski meaning towards a curve and, if the crystals grow in all directions, towards the Bloch spectrum on the real axis. But there are also a projection-valued measure, the spectral measure *M*, and a complex atomic measure *m*, for which convergence is not so clear. For instance, if the crystal grows in one direction only (for instance, laterally), then the pole structure should remain complex because that of the infinite grating is.

In the specific example that is given here, the finite structure behaves as an infinite one provided that we use a Gaussian beam whose waist is smaller than the spatial period of the anomalous modes or concentrated on a node of the mode. A natural question is to ask when it is possible to consider the structure as infinite. Unfortunately, this question is not well posed. For instance, if we use a plane wave as an incident field, then the above shows that the answer is ‘‘never.’’ If one wants to compute the properties of a mode associated with a cavity, then the boundary of the crystal plays such an important role that the question has no sense. Consequently, it appears to be extremely difficult to exhibit a general rule. At least can we say that some situations may be solved by common sense: for instance, if the incident field is a beam concentrated on one or two periods while the structure contains a great number of periods, then the properties of the structure should be that of the infinite one in the horizontal extend.

In some obvious cases (i.e., where a beam illuminates a structure much larger than the waist of the beam), the structure behaves as the one that is infinite in the horizontal direction. But in many physical situations, the source of light is not a well-collimated beam—let us think, for instance, of a dipole or an atom emitting inside the structure—or else the interesting quantity is the lifetime of a resonance—for instance, in the study of modes in photonic crystal fibers. In both cases, the periodization can hardly represent adequately the physical situation at issue.

III. CONCLUSION

Though pseudoperiodic boundary conditions are often considered as the cornerstone of solid-state physics, it should be noted that, unlike electrons that barely leave the crystal, photons cross the photonic crystal and hence interact strongly with the boundary. These observations, which raise the difficult problem of exhibiting a rigorous link between finite and infinite structures, plead for a specific theory. The present study is only a first step in that direction, though we have already implicitly applied similar concepts to the study of resonant cavities and nonlinear photonic crystals.[27,28] A more complete work should deal with the phenomenon of spontaneous emission, where certainly the finiteness of the structure plays an important role, and also deal with the electromagnetic field quantization, which hopefully could be performed by means of the generalized modes of the structure (important results in that direction have been obtained in Ref. 29 for one-dimensional photonic crystals). Finally, it should be noted that the above approach can be extended to deal with 3D photonic crystals.

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