Influence of weak dissipation on the photonic band structure of periodic composites

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We study dissipation in an otherwise perfect photonic crystal. A perturbational calculation (for small dissipation) leads to formulas for the imaginary part of the eigenfrequency (if the wavevector is real) and for the imaginary part of the wave vector (if the frequency is real). We also calculate the density of states (DOS) in the vicinity of a band edge ω_c of a complete photonic band gap. There is a smoothing effect, namely, the density of states becomes finite inside the gap. In this region the DOS is inversely proportional to $(\omega - \omega_c)^{1/2}$ (three-dimensional periodicity) or to $(\omega - \omega_c)$ (two-dimensional periodicity). We also present a semiquantitative argument which suggests that, inside the band gap, the importance of finite crystal size is considerably less than that of absorption.

I. INTRODUCTION

In the past few years the theory of propagation of electromagnetic (EM) waves in periodic dielectric structures has been intensively developed. Three-dimensional (3D) and two-dimensional (2D) periodic structures possessing a photonic band gap have been predicted theoretically and fabricated experimentally.¹ Different methods borrowed from the theory of electronic band structure were used to calculate the photonic band structure with high accuracy. These methods include the plane-wave expansion,² the Korringa-Kohn-Rostoker method,³ and the $\mathbf{k} \cdot \mathbf{p}$ method.⁴ They are relevant for calculation of the EM spectra of ideal photonic crystals, i.e., ideally periodic, infinite, and nondissipative structures. However the experiment deals with finite-size slabs fabricated from low-loss dielectrics. The measurable quantity is the transmission coefficient which drops drastically in the frequency region corresponding to the gap.

Different methods allowing one to calculate directly the transmission coefficient of a slab with scatterers have been proposed.⁵⁻⁷ One of them—the finite element method introduced by Pendry and McKinnon⁵—has the advantage that it is also applicable for the absorbing photonic crystals. The influence of absorption on the transmission coefficient of 2D periodic array of cylinders was studied by Sigalas *et al.*⁸ It was shown that finite absorption as well as finite size of a sample give rise to pseudogaps rather than strictly forbidden band gaps.

In this paper we analyze the influence of weak dissipation on the damping of photonic eigenmodes and on the density of photonic states (DOS). The DOS determines the transport properties of a periodic structure as well as the rate of the spontaneous emission of an excited atom embedded in it.

The paper is planned as follows. In Sec. II we calculate the temporal damping of the eigenmodes (i.e., the imaginary part of eigenfrequency) in the linear approximation. In Sec. III we obtain the functional connection between the temporal and spatial decrements of the same mode. In Sec. IV we calculate the DOS in an absorbing photonic crystal. It is shown that dissipation smooths the singularities of the DOS at the band edge and gives rise to the finite DOS inside the gap. We also calculate the asymptotic behavior of the DOS inside the gap for 2D and 3D periodic photonic crystals. Finally in Sec. V we estimate the influence of the finite crystal size for a 1D superlattice.

II. EIGENVALUE PROBLEM IN PERIODIC MEDIA WITH WEAK DISSIPATION

We consider propagation of EM waves in dissipative periodic media. The medium can be discribed by the position-dependent complex dielectric constant

$$\epsilon(\mathbf{r}) = \epsilon'(\mathbf{r}) + i\epsilon''(\mathbf{r}), \quad \epsilon'' > 0$$
 (1a)

or by the reciprocal dielectric constant

$$\eta({f r}) \;=\; {1\over \epsilon({f r})} \;=\; \eta'({f r}) \;-\; i\eta''({f r}) \;,\;\; \eta''>0 \;.$$
 (1b)

The periodic functions $\epsilon'(\mathbf{r})$, $\epsilon''(\mathbf{r})$, $\eta'(\mathbf{r})$, and $\eta''(\mathbf{r})$ can be expanded in Fourier series,

$$\epsilon'(\mathbf{r}) = \sum_{\mathbf{G}} \epsilon'(\mathbf{G}) \exp(i\mathbf{G} \cdot \mathbf{r}) ,$$

$$\epsilon''(\mathbf{r}) = \sum_{\mathbf{G}} \epsilon''(\mathbf{G}) \exp(i\mathbf{G} \cdot \mathbf{r}) ; \qquad (2a)$$

$$\eta'(\mathbf{r}) = \sum_{\mathbf{G}} \eta'(\mathbf{G}) \exp(i\mathbf{G} \cdot \mathbf{r}) ,$$

$$\eta''(\mathbf{r}) = \sum_{\mathbf{G}} \eta''(\mathbf{G}) \exp(i\mathbf{G} \cdot \mathbf{r}) , \qquad (2b)$$

where ${\bf G}$ are the reciprocal-lattice vectors. The Fourier coefficients

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$$\begin{aligned} \epsilon'(\mathbf{G}) &= \frac{1}{Vc} \int_{Vc} \epsilon'(\mathbf{r}) \exp(-\mathbf{G} \cdot \mathbf{r}) d\mathbf{r}, \\ \epsilon''(\mathbf{G}) &= \frac{1}{Vc} \int_{Vc} \epsilon''(\mathbf{r}) \exp(-i\mathbf{G} \cdot \mathbf{r}) d\mathbf{r}; \end{aligned} (3a)$$

$$\eta'(\mathbf{G}) = \frac{1}{Vc} \int_{Vc} \frac{\epsilon'(\mathbf{r})}{|\epsilon(\mathbf{r})|^2} \exp(-i\mathbf{G}\cdot\mathbf{r}) ,$$

$$\eta''(\mathbf{G}) = \frac{1}{Vc} \int_{Vc} \frac{\epsilon''(\mathbf{r})}{|\epsilon(\mathbf{r})|^2} \exp(-i\mathbf{G}\cdot\mathbf{r})$$
(3b)

obey the following property (for brevity we give the formulas only for ϵ):

$$\epsilon'(-\mathbf{G}) = \epsilon'^*(\mathbf{G}) , \quad \epsilon''(-\mathbf{G}) = \epsilon''^*(\mathbf{G}) .$$
 (4)

The integration in Eqs. (3a) and (3b) runs over the volume of the unit cell V_c .

In periodic structures the space distribution of any components of the EM field $[\mathbf{E}(\mathbf{r}), \mathbf{D}(\mathbf{r}), \text{ or } \mathbf{H}(\mathbf{r})]$ follows the Bloch theorem. For instance, for the magnetic field **H** the expansion over Bloch states takes the form

$$\mathbf{H}(\mathbf{r}) = \exp(i\mathbf{k}\cdot\mathbf{r})\sum_{\mathbf{G}}\mathbf{h}(\mathbf{G})\exp(i\mathbf{G}\cdot\mathbf{r}) , \qquad (5)$$

where **k** is the quasiwave (Bloch) vector and the dependence of **h** on **k** is suppressed. For fixed **k** a discrete sequence of eigenfrequencies $\omega_n(\mathbf{k})$ (n = 1, 2, ...) gives rise to bands (labeled by the integer n) when **k** changes continuously inside the Brillouin zone.

The dispersion relation $\omega = \omega_n(\mathbf{k})$ for the EM waves in a periodic medium is obtained as a solution of the eigenvalue problem. This problem can be formulated for the Fourier components of either the electric, the magnetic, or the displacement field. It was shown⁹ that those three eigenvalue problems lead to the same dispersion relation $\omega = \omega_n(\mathbf{k})$. Here we prefer to consider the eigenvalue problem for the Fourier component $\mathbf{h}(\mathbf{G})$ of the magnetic field. The eigenvalue equation is

$$\sum_{\mathbf{G}'} [\eta'(\mathbf{G} - \mathbf{G}') - i\eta''(\mathbf{G} - \mathbf{G}')] [(\mathbf{k} + \mathbf{G}) \cdot (\mathbf{k} + \mathbf{G}')\delta_{ij}]$$

$$-(\mathbf{k} + \mathbf{G}')_i(\mathbf{k} + \mathbf{G})_j]\mathbf{h}_j(\mathbf{G}') = \frac{\omega^2}{c^2}\mathbf{h}_i(\mathbf{G}) ,$$

$$i, j = x, y, z. \qquad (6)$$

In Eq. (6) and further we use the Einstein summation convention for the vector component indices.

In a lossless medium $(\epsilon'' = \eta'' = 0)$ the eigenvalue problem (6) is Hermitian and the eigenvalues ω_n^2/c^2 are real. But in a dissipative medium the matrix which operates on the eigenvectors $\mathbf{h}_j(\mathbf{G}')$ in Eq. (6) is not Hermitian, therefore the eigenvalues ω_n^2/c^2 are complex, which leads to the decay of eigenmodes.

If the imaginary part of the eigenfrequency

$$\omega_n(\mathbf{k}) = \omega'_n(\mathbf{k}) - i\omega''_n(\mathbf{k}) , \ \omega''_n > 0 \tag{7}$$

is comparable to its real part, the dissipation is rather strong and EM waves do not propagate. Usually in this case EM waves decay within a short distance (a few lattice periods). But for the case of weak dissipation, i.e.,

$$\omega_n'' \ll \omega_n' \tag{8}$$

the typical decay length is much greater than the lattice period. Of course, inequality (8) can be valid only if $\epsilon'' \ll \epsilon'$. The latter allows one to use the standard perturbation theory to calculate the deformation of the EM spectrum, using the Hermitian eigenvalue problem (6) with $\epsilon'' = 0$ as a zero-order approximation. It is clear from general considerations that for frequencies outside the gap, $\epsilon'' \neq$ 0 should lead to absorption in the photonic crystal. It was shown⁸ that at high frequencies the transmissivity of an absorbing photonic crystal decreases drastically in comparison with the perfect crystal. This means that the conditions for the perturbation theory to be valid are more stringent at high frequencies.

For the frequencies inside the gap there is an opposite effect of weak dissipation on the optical properties of photonic crystals. Here dissipation gives rise to a finite density of states (DOS) inside the gap and, hence, finite transmissivity of light. The corresponding DOS, which is the subject of the present paper, is small, so instead of a true gap there is a pseudogap in the spectrum of an absorbing photonic crystal.

We start from the calculation of the imaginary part of frequency ω''_n . The unperturbed Hamiltonian $\mathcal{H}^{(0)}$ is given by the matrix

$$\mathcal{H}_{ij}^{(0)}(\mathbf{G},\mathbf{G}') = \eta'(\mathbf{G}-\mathbf{G}')[(\mathbf{k}+\mathbf{G})\cdot(\mathbf{k}+\mathbf{G}')\delta_{ij} - (\mathbf{k}_i+\mathbf{G}'_i)(\mathbf{k}_j+\mathbf{G}_j)], \qquad (9)$$

and the perturbation $\mathcal{H}^{(1)}$ by the anti-Hermitian matrix

$$\mathcal{H}_{ij}^{(1)}(\mathbf{G},\mathbf{G}') = -i\eta''(\mathbf{G}-\mathbf{G}')[(\mathbf{k}+\mathbf{G})\cdot(\mathbf{k}+\mathbf{G}')\delta_{ij} - (\mathbf{k}_i+\mathbf{G}'_i)(\mathbf{k}_j+\mathbf{G}_j)].$$
(10)

We assume that the bands near a given Bloch vector \mathbf{k} are not degenerate. Therefore the linear correction $\Delta \lambda_n$ to the eigenvalue $\lambda_n = \omega_n^2/c^2$ is simply the diagonal matrix element of $\mathcal{H}^{(1)}$, namely

$$\Delta\lambda_n = \langle n \mid \mathcal{H}^{(1)} \mid n \rangle$$

$$\equiv \sum_{\mathbf{G},\mathbf{G}'} \mathcal{H}^{(1)}_{ij}(\mathbf{G},\mathbf{G}') \mathbf{h}^{*(n)}_i(\mathbf{G}) \mathbf{h}^{(n)}_j(\mathbf{G}') .$$
(11)

Here $\mathbf{h}_{i}^{(n)}(\mathbf{G})$ is the *i* component of the eigenvector $|n\rangle$ of the Hamiltonian $\mathcal{H}^{(0)}$, corresponding to the eigenvalue λ_{n} . The set of eigenvectors $|n\rangle$ forms an orthonormal basis in Hilbert space:

$$\langle n \mid n' \rangle = \sum_{\mathbf{G}} \mathbf{h}^{*(n)}(\mathbf{G}) \cdot \mathbf{h}^{(n')}(\mathbf{G}) = \delta_{nn'} .$$
 (12)

Equation (11) can be substantially simplified in the important case of a binary photonic crystal made from two different materials: material a ("atoms") and material b ("background"). Then the Fourier components (3a) and

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(3b) can be expressed through the structural factor

$$F(\mathbf{G}) = \frac{1}{V_c} \int_{V_a} e^{-i\mathbf{G}\cdot\mathbf{r}} d\mathbf{r}$$
(13)

as follows:

$$\eta'(\mathbf{G}) = (\eta'_a - \eta'_b)F(\mathbf{G}) ,$$

$$\eta''(\mathbf{G}) = (\eta''_a - \eta''_b)F(\mathbf{G}) , \ \mathbf{G} \neq 0 ,$$
(14)

$$\eta'(0) = f\eta'_a + (1-f)\eta'_b , \ \eta''(0) = f\eta''_a + (1-f)\eta''_b .$$
(15)

Here $\eta'_a \approx 1/\epsilon'_a$, $\eta'_b \approx 1/\epsilon'_b$, $\eta''_a \approx \epsilon''_a/\epsilon'^2_a$, $\eta''_b \approx \epsilon''_b/\epsilon'^2_b$ and f is the filling fraction of the component a. In Eq. (13) integration runs over the volume occupied by the component a in a unit cell.

It follows from Eqs. (9), (10), (14), and (15) that there is a simple linear relation between the matrix elements of the operators $\mathcal{H}^{(0)}$ and $\mathcal{H}^{(1)}$:

$$\mathcal{H}^{(1)}(\mathbf{G},\mathbf{G}') = -i\frac{\eta_a'' - \eta_b'}{\eta_a' - \eta_b'} \mathcal{H}^{(0)}(\mathbf{G},\mathbf{G}') \text{ if } \mathbf{G} \neq \mathbf{G}' , (16)$$

 and

$$\mathcal{H}^{(1)}(\mathbf{G},\mathbf{G}) = -i \frac{f \eta_a'' + (1-f) \eta_b''}{f \eta_a' + (1-f) \eta_b'} \mathcal{H}^{(0)}(\mathbf{G},\mathbf{G}) \ .$$

Inserting Eq. (16) in Eq. (11) one can transform the sum over G' to the following form:

$$\sum_{\mathbf{G}'} \mathcal{H}_{ij}^{(1)}(\mathbf{G}', \mathbf{G}') \mathbf{h}_{j}^{(n)}(\mathbf{G}')$$

$$= -i \frac{\eta_{a}'' - \eta_{b}''}{\eta_{a}' - \eta_{b}'} \sum_{\mathbf{G}' \neq \mathbf{G}} \mathcal{H}_{ij}^{(0)}(\mathbf{G}, \mathbf{G}') \mathbf{h}_{j}^{(n)}(\mathbf{G}')$$

$$-i \frac{f \eta_{a}'' + (1 - f) \eta_{b}''}{f \eta_{a}' + (1 - f) \eta_{b}''} \mathcal{H}_{ij}^{(0)}(\mathbf{G}, \mathbf{G}) \mathbf{h}_{j}^{(n)}(\mathbf{G}) . \quad (17)$$

Now this sum can be calculated keeping in mind that $\mathcal{H}^{(0)} \mid n \rangle = \lambda_n \mid n \rangle$. Using the transversality of the magnetic field, i.e.,

$$(\mathbf{k} + \mathbf{G}) \cdot \mathbf{h}^{(n)}(\mathbf{G}) = 0 , \qquad (18)$$

one obtains that

$$\sum_{\mathbf{G}'} \mathcal{H}_{ij}^{(1)} (\mathbf{G}, \mathbf{G}') \mathbf{h}_{j}^{(n)}(\mathbf{G}')$$

$$= -i \frac{\mathbf{h}_{i}^{(n)}(\mathbf{G})}{\eta_{a}' - \eta_{b}'} [\lambda_{n}(\eta_{a}'' - \eta_{b}'')$$

$$+ |\mathbf{k} + \mathbf{G}|^{2} (\eta_{b}'' \eta_{a}' - \eta_{a}'' \eta_{b}')] .$$
(19)

To get the correction $\Delta \lambda_n$ we insert Eq. (19) in Eq. (11) and use the orthogonality condition (12). Finally we get

$$\begin{aligned} \Delta\lambda_n &= \langle n \mid \mathcal{H}^{(1)} \mid n \rangle \\ &= -\frac{i}{\eta'_a - \eta'_b} \bigg[\lambda_n (\eta''_a - \eta''_b) \\ &+ (\eta''_b \eta'_a - \eta''_a \eta'_b) \sum_{\mathbf{G}} \mid \mathbf{k} + \mathbf{G} \mid^2 \mid \mathbf{h}^{(n)}(\mathbf{G}) \mid^2 \bigg] . \end{aligned}$$

$$(20)$$

This linear correction to the eigenvalue $\lambda_n = \omega_n^2/c^2$ gives rise to the damping of the *n*th eigenmode. Because

$$\lambda_n \equiv \lambda_n^{(0)} + \Delta \lambda = \frac{(\omega_n' - i\omega_n'')^2}{c^2} \simeq \frac{\omega_n'^2}{c^2} - 2i\frac{\omega_n''}{c^2},$$

we get

$$\frac{\omega_n''(\mathbf{k})}{\omega_n'(\mathbf{k})} = -\frac{\Delta\lambda_n}{2i} \frac{c^2}{\omega_n'^2(\mathbf{k})}$$
$$= \frac{1}{2(\eta_a' - \eta_b')} \left[\eta_a'' - \eta_b'' - (\eta_a''\eta_b' - \eta_b''\eta_a') \frac{c^2}{\omega_n'^2(\mathbf{k})} \times \sum_{\mathbf{G}} |\mathbf{k} + \mathbf{G}|^2 |\mathbf{h}^{(n)}(\mathbf{G})|^2 \right].$$
(21)

According to the approximation we have used, $\omega''_n(\mathbf{k})$ is a linear function of η''_a and η''_b . It is worthwhile to transform the sum on the right-hand sides of Eq. (21). With this in mind we multiply both sides of Eq. (6) (in which we put $\eta'' = 0$) by $\mathbf{h}_i^{*(n)}(\mathbf{G})$ and sum over \mathbf{G} (and *i*). Then using Eqs. (12), (14), and (18) one obtains

$$\sum_{\mathbf{G}} |\mathbf{k} + \mathbf{G}|^{2} |\mathbf{h}^{(n)}(\mathbf{G})|^{2} = \frac{\omega_{n}^{\prime 2}(\mathbf{k})}{\eta^{\prime}(0)c^{2}} - \frac{\eta_{a}^{\prime} - \eta_{b}^{\prime}}{\eta^{\prime}(0)} \sum_{\mathbf{G}} \sum_{\mathbf{G}^{\prime} \neq \mathbf{G}} F(\mathbf{G} - \mathbf{G}^{\prime}) \times \left[(\mathbf{k} + \mathbf{G}) \cdot (\mathbf{k} + \mathbf{G}^{\prime}) \mathbf{h}^{\star(n)}(\mathbf{G}) \cdot \mathbf{h}^{(n)}(\mathbf{G}^{\prime}) - (\mathbf{k} + \mathbf{G}^{\prime}) \cdot \mathbf{h}^{\star(n)}(\mathbf{G})(\mathbf{k} + \mathbf{G}) \cdot \mathbf{h}^{(n)}(\mathbf{G}^{\prime}) \right].$$
(22)

We subsitute Eq. (22) in Eq. (21) with the result

$$\frac{\omega_n''(\mathbf{k})}{\omega_n'(\mathbf{k})} = \frac{\overline{\eta}_1''}{2\overline{\eta}'} + \frac{\eta_n''\eta_b' - \eta_b''\eta_a'}{2\overline{\eta}'} \frac{c^2}{\omega_n'^2(\mathbf{k})} \sum_{\mathbf{G}} \sum_{\mathbf{G}'\neq\mathbf{G}} F(\mathbf{G} - \mathbf{G}') \\
\times \left[(\mathbf{k} + \mathbf{G}) \cdot (\mathbf{k} + \mathbf{G}') \mathbf{h}^{*(n)}(\mathbf{G}) \cdot \mathbf{h}^{(n)}(\mathbf{G}') - (\mathbf{k} + \mathbf{G}') \cdot \mathbf{h}^{*(n)}(\mathbf{G})(\mathbf{k} + \mathbf{G}) \cdot \mathbf{h}^{(n)}(\mathbf{G}') \right].$$
(23)

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Here $\overline{\eta}' = \eta'(0)$ and $\overline{\eta}'' = \eta''(0)$ are average characteristics of the dielectric composite, defined by Eq. (15). Equation (23) is a general result for the temporal damping correspondig to the band $\omega_n(\mathbf{k})$. Next let us consider two special cases.

The first term on the right-hand side of Eq. (23) gives the dominant contribution to the damping if

$$\mid \eta_a^{\prime\prime} \eta_b^{\prime} - \eta_b^{\prime\prime} \eta_a^{\prime} \mid \ll \overline{\eta} \ \overline{\eta}^{\prime\prime} \ . \tag{24}$$

This inequality means that the "contrast" is very small and the periodic medium can be considered as approximately homogeneous. In this limit Eq. (23) gives the result

$$\frac{\omega_n''(\mathbf{k})}{\omega_n'(\mathbf{k})} = \frac{\overline{\eta}''}{2\overline{\eta}'} , \qquad (25)$$

which coincides with the well-known formula

$$\frac{\omega''}{\omega'} = \frac{\epsilon''}{2\epsilon'} \approx \frac{\eta''}{2\eta'} \tag{26}$$

for the damping of EM waves in a homogeneous medium with weak dissipation.

Now let us consider a 2D photonic crystal with cylindrical "atoms" arranged periodically in air $(\eta_b'' = 0, \eta_b' = 1)$. In a 2D periodic system modes with E and H polarizations are decoupled.¹⁰ In the E mode the electric field is parallel to the rods, and in the H mode it is the magnetic field that is parallel to the rods. Thus for the Hmode the second term in the square bracket of Eq. (23) vanishes as

$$(\mathbf{k} + \mathbf{G}) \cdot \mathbf{h}^{(n)}(\mathbf{G}') = 0 \tag{27}$$

even for $\mathbf{G}' \neq \mathbf{G}$. However, for the *E* mode this term does not vanish and contributes to the damping.

Here we have used perturbation theory for the nondegenerate states. The spectra of photonic crystals contain many points of degeneracy where the dispersion curves $\omega_n(\mathbf{k})$ corresponding to different band numbers n are crossing. This degeneracy is the consequence of the high symmetry of the crystal lattice. In quantum mechanics perturbations usually have lower symmetry than the zero-order Hamiltonian, leading to repulsion of levels. In our case the situation is different, namely the perturbation $\mathcal{H}^{(1)}$ has the same symmetry as the nonperturbed Hamiltonian $\mathcal{H}^{(0)}$. This is so because dissipation does not break the spatial symmetry of the lattice and therefore does not lead to additional splitting of the dispersion curves. Thus the ordinary perturbation theory is valid even at the points of degeneracy.

III. TWO DIFFERENT APPROACHES IN THE PROBLEM OF WEAK DISSIPATION: TEMPORAL AND SPATIAL DAMPING OF WAVES

The dispersion relation for the EM wave propagating in any medium may be written in a general form as

$$f(\omega, \mathbf{k}) = 0, \tag{28}$$

where the function f depends on the dielectric properties of the medium. In a nondissipative medium a propagating wave is characterized by a real frequency ω , which is a solution of Eq. (28):

$$\omega = \omega(\mathbf{k}) \ . \tag{29}$$

In a periodic medium Eq. (29) corresponds to the band structure with allowed frequency zones separated by gaps. For every given direction of propagation $\nu = \mathbf{k}/k$ Eq. (29) can be solved with respect to the length k of the wave vector. If ω is inside an allowed band with band index n this solution is real and gives a point $\mathbf{k} = (\nu, k_n)$ lying inside the Brillouin zone:

$$k_n = k_n(\omega, \nu) . \tag{30}$$

A set of points (ν, k_n) form an isofrequency surface

$$\mathbf{k} = \mathbf{k}_n(\omega) \;, \tag{31}$$

when ν sweeps the surface of the unit sphere. Inside the band gap, the solution (30) is complex and an EM wave cannot propagate in the (infinite) crystal. In the presence of dissipation the situation becomes more complicated. Absorption (due to a nonzero imaginary part of the dielectric constant) cause the solutions of Eq. (28) to be complex. For instance, these solutions can be represented in the form of Eq. (29) (temporal decay, $\omega = \omega' - i\omega''$ and real \mathbf{k}), or in the form of Eq. (31) (spatial decay, $\mathbf{k} = \mathbf{k}' + i\mathbf{k}''$ and real ω). Note that in the presence of absorption $k'' \neq 0$ even if ω' corresponds to an allowed frequency. Then the question arises: what kind of decay (temporal, spatial, or mixed), that is, what kind of experimental situation do we consider? This question has been discussed in detail in connection with excitation of surface waves.^{11,12} In that case the answer is rather nontrivial because of the presence of a special prism leading to the excitation of such waves. The Bloch waves in photonic crystals are excited directly by the incident EM wave with a fixed frequency ω . Therefore the decay has to be considered as spatial: the amplitude decreases exponentially with the distance from the surface of incidence of the sample. However, Eq. (23) describes temporal decay, given by ω'' .

In order to calculate the spatial decay, as described by \mathbf{k}'' , we use the fact that the function f in Eq. (28) is a functional of $\epsilon(\mathbf{r})$:

$$f(\omega, \mathbf{k}) = f(\omega, \mathbf{k}, [\epsilon(\mathbf{r})]) . \qquad (32)$$

If the dissipation is weak $(\epsilon'' \ll \epsilon')$, the functional (32) can be expanded and in the linear approximation one obtains

$$egin{aligned} f &pprox f(\omega,\mathbf{k},[\epsilon'(\mathbf{r})]) + irac{\delta f}{\delta\epsilon}\delta\epsilon''(\mathbf{r}) \ &= f'(\omega,\mathbf{k}) + if''(\omega,\mathbf{k}) = 0 \;. \end{aligned}$$

Linearizing Eq. (33) in the small quantities ω'' or k'' one obtains the temporal decay decrement (experiment with real \mathbf{k})

$$\omega'' = \frac{f''(\omega, \mathbf{k})}{\partial f' / \partial \omega} . \tag{34}$$

On the other hand for purely spatial decay $\omega'' = 0$ and Eq. (33b) gives

$$\mathbf{k}'' \cdot \frac{\partial f'}{\partial \mathbf{k}} = -f''(\omega, \mathbf{k}) . \qquad (35)$$

Eliminating f'' from Eqs. (34) and (35) and using the identity

$$\frac{\partial \omega}{\partial \mathbf{k}} = -\frac{\partial f'/\partial \mathbf{k}}{\partial f'/\partial \omega}$$
(36)

we obtain the relation between the temporal and spatial decay decrements in the following form:

$$\omega'' = \mathbf{k}'' \cdot \mathbf{v} . \tag{37}$$

Here $\mathbf{v} = \partial \omega / \partial \mathbf{k}$ is the group velocity of the wave. Formula (37) is not valid at the edge of the Brillouin zone where the group velocity vanishes.

In the ideal crystal ($\epsilon'' = 0$) complex solutions of Eq. (30) can be interpreted to describe surface excitations of a finite photonic crystal with ω inside the gap.^{13,7} The amplitudes of these excitations decrease exponentially from the surface of photonic crystal. This decay is due to strong Bragg reflection inside the periodic medium. Now Bragg reflection is a reversable process which does not lead to the heating of the sample. Unlike this, damping of EM waves in an absorbing medium is a dissipative process which is accompanied by an increase of the entropy.

IV. PHOTONIC DENSITY OF STATES

Aplications of photonic crystals are associated with the inhibition of spontaneous emission. For emission within the band gap the decay rate of an excited atom or the recombination rate of electron-hole pairs can be reduced. This, in turn, is expected to be applicable to the improvement of semiconductor lasers.^{14,15} The rate of spontaneous emission is proportional to the density of photonic states in the environment medium.¹⁶ In the Born approximation the DOS is also proportional to the squared modulus of the matrix element of the operator $\mathbf{E} \cdot \boldsymbol{\mu}$, where \mathbf{E} is the amplitude of zero-point fluctuations of the eigenmode and μ is the atomic dipole moment.¹⁶ In the lossless photonic crystal the density of states (DOS) vanishes in-side the gap. But, as it has been shown,¹⁷ absorption can modify the rate of spontaneous emission for frequencies close to the resonances of a homogeneous dielectric giving rise to the finite rate of spontaneous emission in the forbidden frequency region. Then in the band-gap structures we can expect that absorption will modify the rate of emission for the frequencies close to the gap. In this region the DOS $[\rho = \rho(\omega)]$ changes abruptly, leading to a singularity of $d\rho/d\omega$. Even a weak dissipation is

expected to spread this singularity, giving rise to a finite rate of spontaneous emission inside the gap. In the Born approximation this smoothing effect increases with absorption and the rate of spontaneous emission increases proportionally to the DOS. This is true in the limit of weak dissipation.¹⁷ If dissipation becomes great enough $(\epsilon'' \sim \epsilon')$ one needs to take into account the decreasing of **E** with ϵ'' (damping of eigenmodes). However in the Born approximation one should neglect this effect, otherwise the accuracy is exceeded.

In order to calculate the effect of weak dissipation on the DOS we start from the general definition, widely applicable to quasiparticles with complex dispersion law,

$$\rho(\omega) = \frac{1}{N} \sum_{\mathbf{k}} \delta[\omega(\mathbf{k}) - \omega] = \frac{V_c}{(2\pi)^3} \int_{\omega(\mathbf{k}) = \omega} \frac{dS_{\mathbf{k}}}{|\nabla_{\mathbf{k}}\omega(\mathbf{k})|} .$$
(38)

Here $dS_{\mathbf{k}}$ is an element of the isofrequency surface $\omega(\mathbf{k}) = \omega$ in \mathbf{k} space and N is the number of unit cells in the crystal.¹⁸ For rather high frequencies the isofrequency surface may be represented by several closed or open sheets.

Equation (38) is applicable only for a lossless medium. In an absorbing medium photonic states decay with the rate given by Eq. (23). A finite dissipation shifts the pole of the photonic Green function from the real axis¹⁹ and the δ function in Eq. (38) must be replaced by a Lorentzian line shape with the width corresponding to the damping rate $\omega''(\mathbf{k})$, namely

$$\delta[\omega(\mathbf{k}) - \omega] \longrightarrow \frac{1}{\pi} \frac{\omega''(\mathbf{k})}{[\omega'(\mathbf{k}) - \omega]^2 + \omega''^2(\mathbf{k})} .$$
(39)

We substitute Eq. (39) in Eq. (38) and replace the summation over **k** by integration in **k** space. In turn the integration over **k** is converted to integration over the isofrequency surface $\omega'(\mathbf{k}) = z$ and integration over z.²⁰ The Jacobian of this transformation is $|\nabla_{\mathbf{k}}\omega'(\mathbf{k})|^{-1}$. Finally, instead of the right-hand expression (38) for the DOS, we get the following one:

$$\rho(\omega) = \frac{V_c}{\pi (2\pi)^3} \int_0^\infty dz \oint_{\omega'(\mathbf{k})=z} \frac{dS_{\mathbf{k}}}{|\nabla_{\mathbf{k}}\omega'(\mathbf{k})|} \times \frac{\omega''(\mathbf{k})}{(\omega-z)^2 + \omega''^2(\mathbf{k})} .$$
(40)

A. Three-dimensional periodicity

Assuming that the dissipation is weak, the dispersion relation $\omega'(\mathbf{k})$ in Eq. (40) can be approximated by the dispersion relation $\omega(\mathbf{k})$ for the lossless medium. Henceforth we shall suppress the prime on $\omega'(\mathbf{k})$. For frequencies well inside the allowed bands the influence of damping is rather small, so Eqs. (38) and (40) give the same

result. On the other hand, when ω is near to the edge of the gap $(\omega \to \omega_c)$ the DOS of an ideal 3D crystal vanishes according to the square-root law. For example, near the lower edge of a gap one obtains from Eq. (38) that

$$\rho(\omega) \sim \sqrt{\omega_c - \omega} , \ \omega < \omega_c ,
\rho(\omega) = 0 , \ \omega > \omega_c .$$
(41)

In the presence of dissipation the integrals in Eq. (40) do not vanish in the region $\omega > \omega_c$, giving rise to the propagation of EM waves in the forbidden zone and to a finite decay rate of spontaneous emission. We use Eq. (40) to calculate the DOS in the vicinity of the band edge $(\omega = \omega_c)$, assuming that only a single band contributes. When ω approaches ω_c , the volume inside the isofrequency surface goes to zero as there is no isofrequency surface for $\omega > \omega_c$. In other words the isofrequency surface converges to some point **K** in **k** space when $\omega \to \omega_c$. We expand the dispersion relation $\omega(\mathbf{k}) = \omega$ near this point:

$$\omega = \omega_c - \frac{1}{2} \beta_{ij} \Delta \mathbf{k}_i \Delta \mathbf{k}_j , \ \Delta \mathbf{k} = \mathbf{k} - \mathbf{K} .$$
 (42)

The linear term is absent in the expansion (42) because the group velocity $\nabla_{\mathbf{k}}\omega$ vanishes at the band edge.²¹ If ω_c is the lower edge of a band gap, then β_{ij} is a positive defined matrix.

Equation (42) can be rewritten in the form

$$(\Delta \mathbf{k})^2 = \frac{2(\omega_c - \omega)}{\beta_{ij} \mathbf{z}_i \mathbf{z}_j}, \ \mathbf{z} = \frac{\Delta \mathbf{k}}{\Delta k},$$
 (43)

which is the equation of an ellipsoid, centered at the point $\mathbf{k} = \mathbf{K}$. Then the surface element $dS_{\mathbf{k}}$ can be represented through the solid angle $d\Omega$ as follows:

$$dS_{\mathbf{k}} = \frac{|\nabla_{\mathbf{k}}\omega|}{|\mathbf{\boldsymbol{x}}\cdot\nabla_{\mathbf{k}}\omega|} (\Delta\mathbf{k})^2 d\Omega$$
$$= \sqrt{2(\omega_c - z)} \frac{|\nabla_{\mathbf{k}}\omega| d\Omega}{(\beta_{ij}\mathbf{\boldsymbol{x}}_{i}\mathbf{\boldsymbol{x}}_{j})^{3/2}} .$$
(44)

Now we substitute Eq. (44) in Eq. (40) and take into account that the surface integral

$$\int_{z=\omega(\mathbf{k})} \frac{dS_{\mathbf{k}}}{\mid \nabla_{\mathbf{k}} \omega \mid}$$

vanishes for $z > \omega_c$. Then the infinite upper limit in the integral over z in Eq. (40) can be replaced by ω_c . It is worthwhile to introduce the dimensionless dispersion and damping parameters

$$\Delta ~=~ (\omega/\omega_c) - 1 \; ,$$

 $\delta ~=~ \omega''({f k})/\omega_c \; .$

Note that Δ is positive (negative) above (below) the lower edge of the gap. In principle δ is given by Eq. (23) and depends on **k** in a very complicated manner, requiring a complete solution of the band-structure problem. In order to make our calculations manageable and our results transparent, we shall assume that δ is a constant parameter. After simple calculations we get the following formula for the DOS:

$$\rho(\omega) = QF(\Delta, \delta) . \tag{45}$$

Here

$$Q = \frac{V_c \sqrt{2\omega_c}}{\pi (2\pi)^3} \int \frac{d\Omega}{(\beta_{ij} \mathbf{a}_i \mathbf{a}_j)^{3/2}}$$
(46)

is a constant determined by the topology of isofrequency surface, and

$$F(\Delta, \delta) = \delta \int_0^1 \frac{\sqrt{x} dx}{(x+\Delta)^2 + \delta^2}$$
(47)

is the dimensionless DOS. Equations (45)–(47) are valid only for small values of Δ and δ as we consider a weak dissipation ($\delta \ll 1$) and frequencies near to the band edge ($|\Delta| \ll 1$). However, it is just this region of parameters that is interesting in an experiment.

The DOS Eq. (47) has different asymptotic forms inside and outside the gap.

(a) Inside the gap ($\delta \ll \Delta$, or $\omega'' \ll \omega - \omega_c \ll \omega_c$). In this region the damping δ can be neglected in the denominator of Eq. (47) and one obtains that

$$F(\Delta, \delta) \simeq \delta \int_0^1 \frac{\sqrt{x} dx}{(x+\Delta)^2} = \frac{\pi \delta}{2\sqrt{\Delta}}$$
 (48)

Thus there is a finite DOS inside the gap, and it is proportional to the damping ω''/ω_c and inversely proportional to $\sqrt{\omega - \omega_c}$.

(b) Outside the gap $(\delta \ll -\Delta \text{ or } \omega'' \ll \omega_c - \omega \ll \omega_c)$. In this case the presence of the pole at $x = |\Delta| + i\delta$ gives the following limiting contribution to the integral:

$$F(\Delta, \delta) = \pi \int_0^1 \sqrt{x} \delta(x - |\Delta|) dx = \pi \sqrt{|\Delta|} .$$
 (49)

Substituting Eq. (49) in Eq. (45) we get the zero-order DOS,

$$\rho(\omega) = \pi Q \sqrt{(\omega - \omega_c)/\omega_c} , \qquad (50)$$

with the well-known square-root singularity. In principle the parameter Q can be determined, for a given bandedge, experimentally or theoretically from Eq. (46).

(c) Boundary between the allowed and forbidden zones $(\Delta = 0)$,

$$F(0,\delta) = \delta \int_0^1 \frac{\sqrt{x} dx}{x^2 + \delta^2} \simeq \pi \sqrt{\delta/2} , \ \omega = \omega_c .$$
 (51)

Photonic band gaps are determined by transmission rate measurments.¹⁴ But due to different reasons (finite size of a sample, absorption, etc.) the transmission rate does not drop to zero inside the gap and it is difficult to determine the position of the band edge. Equation (51) gives the position of the gap in the theoretically infinite photonic crystal fabricated from low-loss materials. The influence of the finite size of a sample on the transmission



FIG. 1. Frequency dependence of the normalized density of states for 3D periodicity for different absorption parameters $\delta = \text{Im } \omega/\omega_c$: (1) $\delta = 0$, (2) $\delta = 0.0015$, (3) $\delta = 0.003$, (4) $\delta = 0.005$, (5) $\delta = 0.01$. This has been calculated from Eq. (47).

rate has been studied in Refs. 6-8 and in the following section.

The above analysis of $F(\Delta, \delta)$ shows that, for frequencies sufficiently bellow ω_c , the DOS decreases according to the same law as for a nondissipative medium [Eq. (50)]. However, very near to the edge of the gap ($|\Delta| \lesssim \delta$) the dissipation detains this decreasing and in this region the DOS is proportional to $\sqrt{\omega''}$ [Eq. (51)]. Inside the gap the DOS decreases slowly [Eq. (48)] with frequency. Thus even a weak dissipation leads to a rounding or "smoothing" of the edge of the forbidden zone. Because of this it should be rather difficult to resolve narrow gaps experimentally.

Figure 1 shows the dependence of the dimensionless DOS Eq. (47) on the dimensionless frequency Δ , for different dampings δ . Positive (negative) Δ corresponds to the frequencies inside (outside) the gap. Examining Fig. 1, it is evident that for frequencies well below ω_c , the DOS decreases essentially in the same manner as for a nondissipative medium, represented by curve 1. So a weak dissipation does not affect the DOS for frequencies far below ω_c . In the vicinity of the gap edge $(|\Delta| \lesssim \delta)$ the square-root singularity disappears and inside the gap the DOS decreases slowly ~ $(\omega - \omega_c)^{-1/2}$ as in Eq. (48). Such behavior implies that, even if there exists a complete gap in the band structure of a *nominally* lossless crystal, the ever-present dissipation will give rise to propagation of an EM wave with frequencies inside the gap. All this is consistent with the approximate results (48)-(51). In the case when ω_c is the upper edge of the gap, the graphs on Fig. 1 must be inverted with respect to the line $\Delta = 0$.

B. Two-dimensional periodicity

Now let us consider the influence of weak dissipation on the DOS of a 2D periodic array. In the 2D case the isofrequency lines Eq. (42) are ellipses and the surface element $dS_{\mathbf{k}}$ must be replaced by the linear element

$$dl_{\mathbf{k}} = \frac{|\nabla_{\mathbf{k}}\omega|}{|\mathbf{x}\cdot\nabla_{\mathbf{k}}\omega|}\Delta kd\varphi = \frac{|\nabla_{\mathbf{k}}\omega|}{\beta_{ij}\mathbf{x}_{ij}\mathbf{x}_{ij}\mathbf{x}_{j}}\,d\varphi\;.$$
 (52)

Substituting Eq. (52) in Eq. (40) we get the formula (45) for the DOS of a 2D photonic crystal with

$$Q = \frac{S_c}{\pi (2\pi)^2} \int_0^{2\pi} \frac{d\varphi}{\beta_{ij} \mathbf{\mathfrak{E}}_i \mathbf{\mathfrak{E}}_j} , \qquad (53)$$

 and

$$F(\Delta, \delta) = \delta \int_0^1 \frac{dx}{(x+\Delta)^2 + \delta^2} \approx \frac{\pi}{2} - \operatorname{arctg} \frac{\Delta}{\delta} .$$
 (54)

Here S_c is the area of the unit sell. The dimensionless DOS Eq. (54) has the following asymptotics.

(a) Inside the gap $(\delta \ll \Delta)$,

$$F(\Delta, \delta) \simeq \frac{\delta}{\Delta} , \ \omega > \omega_c .$$
 (55)

(b) Outside the gap $(\delta \ll |\Delta|)$,

$$F(\Delta, \delta) \simeq \pi - \frac{\delta}{\Delta}, \omega < \omega_c$$
 (56)

(c) Boundary between allowed and forbidden zones $(\Delta = 0)$,

$$F(0,\delta) = \frac{\pi}{2} \ . \tag{57}$$

Figure 2 shows the two-dimensional DOS for different dampings, calculated from Eq. (54). In the ideal case $\delta = 0$ (curve 1) the function $F(\Delta, 0)$ has a discontinuous jump. As in the case of 3D periodicity the dissipation smoothes the singular behavior (curves 2–5) in a manner that is consistent with Eq. (54). Note that inside the gap the DOS drops faster in the 2D case [Eq. (55)] than in the 3D one [Eq. (48)]. It means that the 2D band structure is more stable with respect to a perturbation in the form

3.5 3.0 F 2.5 2.0 1.5 1.0 0.5 0.0 -0.02 -0.01 0.00 0.01 0.02 0.03 0.04 0.05 Δ

FIG. 2. Frequency dependence of the normalized density of states for 2D periodicity for different absorption parameters $\delta = \text{Im } \omega/\omega_c$: (1) $\delta = 0$, (2) $\delta = 0.0015$, (3) $\delta = 0.005$, (4) $\delta = 0.05$. This figure is based on Eq. (54).

of weak dissipation than the 3D one. Moreover it looks like this conclusion is true not only for an anti-Hermitian perturbation (dissipation), but also for arbitrary perturbations. This conclusion can be confirmed by the following example. The principal macroscopic defect of any crystal is its finite size. Therefore the transmission rate (and the DOS) does not drop exactly to zero inside the gap. This effect has been studied in Refs. 6–8. According to the results of these papers the transmission rate drops much faster in a two-dimensional periodic array⁸ than in a three-dimensional one.^{6,7}

Note that in an infinite crystal dissipation always gives rise to finite DOS inside the gap. On the other hand, in a finite sample it can further increase the DOS in the gap. This occurs when the transmission rate is already big enough due to the finite size. Then dissipation leads to the usual damping of the EM modes. This situation is realized for the *E*-polarized modes propagating in a periodic array of cylinders.⁸ But for the *H*-polarized modes the transmission rate for the same sample turns out to be much smaller (than that for the *E*-polarized modes) if the dissipation is absent. In this case a weak dissipation causes additional increase of the transmission rate (and also the DOS) inside the nominal band gap.

V. INFLUENCE OF THE FINITE CRYSTALS SIZE

Throughout this work we have assumed that the dielectric composite considered deviates from perfect "crystallinity" only due to dissipation of energy. It is pertinent to discuss a different kind of "imperfection," namely the finite size of the crystal, and to compare the ensuing modifications of the band structure.

Strictly speaking, band structures and band gaps exist only for a perfect (transparent and boundless) crystal. Either absorption or a finite number of unit cells will give rise to finite DOS within the nominal gaps and a smoothing of the van Hove singularities. There are available DOS computations for two-dimensional¹⁰ and three-dimensional^{2(b),22} photonic crystals and also similar computations for "phononic crystals" (elastic composites).²³ However, these calculations were all performed for infinite and nondissipative periodic structures. We are not aware of calculations of the DOS for either a finite or for an absorptive array. Nevertheless, we can estimate the importance of finiteness of the crystal and compare it to the results reported in the preceding sections.

We do this for a modulated superlattice, assuming weak, sinusoidal modulation. In this case the band structure is given by the solutions of the Mathieu equation. The eigenvalues are^{24}

$$\omega_{\pm}(k) = \omega_c \pm \sqrt{\omega_G^2 + c_0^2 \left(k - \frac{\pi}{a}\right)^2} , \qquad (58)$$

where c_0 is the speed of light in the host (unmodulated) medium, a is the period of the modulation, $2\omega_G$ is the band gap (proportional to the modulation amplitude), and $\omega_c = \pi c_0/a$ is the midgap frequency. Even for twoor three-dimensional crystals, if one considers propagation in a high-symmetry direction, in the vicinity of a Brillouin zone boundary only two plane waves make important contributions to the diffraction process. It is well known that, for such a simplified model, the approximate band structure is also given by the two bands, Eq. (58).²⁵ Below we calculate the density of states $\rho_L(\omega)$, based on Eq. (58), for a crystal of finite length L.

For a periodic structure of length l = Na the permitted values of the Bloch vector are $k_n = (2\pi/L)n$, where $n = 0, \pm 1, \pm 2, ..., \pm N/2$ (Born–Von Karman boundary conditions).²⁶ Also taking into account the absorption, the density of states can be written down according to Eqs. (38) and (39):

$$\rho_L(\omega) = \frac{\omega''}{2\pi N} \left\{ \sum_{|n| < N/2} \left[\frac{2}{[\omega_+(k_n) - \omega]^2 + (\omega'')^2} + \frac{2}{[\omega_-(k_n) - \omega]^2 + (\omega'')^2} \right] + \frac{1}{(\omega_c - \omega_G - \omega)^2 + (\omega'')^2} + \frac{1}{(\omega_c - \omega_G - \omega)^2 + (\omega'')^2} \right\},$$
(59)

where $\omega_{\pm}(k_n)$ is given by Eq. (58). The two terms in the summation give the contributions of the upper and lower branches in Eq. (58), excluding the Brillouin zone edge. The last two terms take care of this point, $k_n = \pi/a$ (n = N/2). These terms are chosen to have one-half of the weight of the terms in the summation which leads to the correct result for the DOS in the limit $L \to \infty$ and $\omega'' \to 0$ (see below). We shift the summation number n in Eq. (59) by defining $m = n \mp N/2$ and also define $\Omega = \omega - \omega_c$, where Ω is the frequency measured from the midgap. After simple algebra Eq. (59) becomes

$$\rho_L(\Omega) = \frac{\omega''}{2\pi N} \left\{ \sum_{m=1}^{N/2} \frac{2}{\left[\sqrt{\omega_G^2 + (2\pi c_0 m/L)^2} - \Omega \right]^2 + (\omega'')^2} + \frac{1}{(\Omega - \omega_G)^2 + (\omega'')^2} + (\Omega \to -\Omega) \right\}.$$
 (60)

First we consider the infinite crystal (thermodynamic limit) $L \to \infty$. Then $2\pi m/L \to k$ and the summation over m is replaced by $(L/2\pi) \int_0^\infty dk$. This gives

$$\rho_{\infty}(\Omega) = \frac{\omega''a}{2\pi^2} \int_0^\infty \frac{dk}{(\sqrt{\omega_G^2 + k^2 c_0^2} - \Omega)^2 + (\omega'')^2} + (\Omega \to -\Omega).$$
(61)

Parenthetically we remark that, in the dissipationless limit $\omega'' \to 0$, this formula reduces to

$$\rho_{\infty}(\Omega) = \frac{\Omega a}{2\pi c_0 \sqrt{\Omega^2 - \omega_G^2}} \Theta(\Omega^2 - \omega_G^2) , \qquad (62)$$

where $\Theta(x)$ is the step function. This just reproduces the well-known singularity for 1D periodicity, thus justifying our choice, of the contributions (weights) of the last two terms in Eq. (59), corresponding to n = N/2. The DOS is infinite at both the lower and the upper edges of the gap, $\Omega = \pm \omega_G$. Dissipation removes this singularity: from Eq. (61) we find that

$$\rho\left(\pm\omega_G\right) \simeq \frac{a}{4\pi c_0} \sqrt{\frac{\omega_G}{\omega''}},\tag{63}$$

assuming that $\omega'' \ll \omega_G$. Thus the DOS at the band edges is inversely proportional to $\sqrt{\omega''}$. Inside the gap the DOS decays according to the power law if ω is far enough from the band edges. This decay is given by the following asymptotics obtained from Eq. (61) under the condition $\omega_G - \Omega \gg \omega''$:

$$\rho_{\infty}(\Omega) \simeq \frac{a\omega''\omega_G^2}{2\pi c_0(\omega_G^2 - \Omega^2)^{3/2}} . \tag{64}$$

Thus in the 1D case the DOS drops (inside the gap) faster than in 3D and 2D cases [Eqs. (48) and (55)] and we can conclude that the 1D band structure is the stablest one with respect to the weak dissipation.

In Fig. 3 we examine the importance of taking into account the fact that, in practice, the length L is finite. The solid line gives the dimensionless DOS $F(x) = \omega_G \rho_L(\Omega)$ vs the dimensionless frequency $x = \Omega/\omega_G$ for a superlattice with N = 50 periods, calculated from Eq. (60). This is compared with the DOS for the infinite superlattice, Eq. (61), dashed line. The only appreciable difference occurs outside the band gap, where the DOS oscillates strongly. This is then a notable effect of a finite number of periods N. In fact, with a choice N = 10, the amplitude and the period of oscillations strongly increase. However, the DOS *inside* the gap (not very near to the band edges) remains practically unaffected. We stress



FIG. 3. Frequency dependence of the normalized density of states for 1D periodicity for a finite N = 50 [solid line, Eq. (60)] and an infinite [dashed line, Eq. (6)] superlattice. The gap to midgap ratio $2a\omega_G/\pi c_0 = 0.25$ and the damping $\omega''/\omega_G = 0.05$.

this point by an analytic calculation of the DOS at the midgap point $\Omega = 0$ — for infinite and for finite L. In the first case, if $\omega'' \ll \omega_G$, we get from Eq. (64) that

$$\rho_{\infty}(0) \simeq \frac{a\omega''}{2\pi c_0 \omega_G}.$$
(65)

For finite L this expression is multiplied by coth $(L\omega_G/2c_0)$, provided that $N^{-1} \ll 2\omega_G/\omega_0 \ll 1$; this is satisfied for reasonable values of the parameters. If we choose the gap to midgap ratio $2\omega_G a/\pi c_0 = 0.25$ then, for N = 10, this correction factor is only about 1.04. In fact, it is easy to verify that

$$\rho_L(0) - \rho_\infty(0) \simeq \frac{a\omega''}{\pi c_0 \omega_G} \exp(-L\omega_G/c_0) .$$
 (66)

Thus our conclusion is that, well inside the band gap, the finite length of the superlattice gives only an exponentially small contribution.

The considerations in this section suggest that, *inside* the band gaps of (2D and 3D) photonic crystals, effects of absorption are considerably more important than those of the finite crystal size.

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¹ For a recent review see E. Yablonovich, J. Phys. Condens. Matter 5, 2443 (1993); *Photonic Band Gaps and Localization*, edited by C.M. Soukoulis (Plenum, New York, 1993).

² See, e.g., (a) K.M. Leung and Y.F. Liu, Phys. Rev. Lett. **65**, 2646 (1990); (b) Z. Zhang and S. Satpathy, *ibid.* **65**,

^{2650 (1990); (}c) K.M. Ho, C.T. Chan, and C.M. Soukoulis, *ibid.* **65**, 3152 (1990); (d) M. Plihal, A. Shambrook, and A.A. Maradudin, Opt. Commun. **80**, 199 (1991); (e) H.S. Sözüer, J.W. Haus, and R. Inguva, Phys. Rev. B **45**, 13962 (1992).

- ³ W. Lamb, D.M. Wood, and N.W. Ashcroft, Phys. Rev. B 21, 2248 (1980); K.M. Leung and Y.F. Liu, *ibid.* 41, 10188 (1990); K.M. Leung and Y. Qiu, *ibid.* 48, 7767 (1993).
- ⁴ N.F. Johnson and P.M. Hui, Phys. Rev. B 48, 10118 (1993); N.F. Johnson, P.M. Hui, and K.H. Luk, Solid State Commun. 90, 229 (1994).
- ⁵ J.B. Pendry and A. McKinnon, Phys. Rev. Lett. **69**, 2772 (1992).
- ⁶ N. Stefanou, V. Karathanos, and A. Modinos, J. Phys. Condens. Matter 4, 3789 (1992).
- ⁷ Kenneth W.-K. Shung and Y.C. Tsai, Phys. Rev. B 48, 11 265 (1993).
- ⁸ M. Sigalas, C.M. Soukoulis, E.N. Economou, C.T. Chan, and K.M. Ho, Phys. Rev. B **48**, 14121 (1993); M.M. Sigalas, C.M. Soukoulis, C.T. Chan, and K.M. Ho, Phys. Rev. B **49**, 11080 (1994).
- ⁹ A. Krokhin and P. Halevi (unpublished).
- ¹⁰ M. Plihal and A.A. Maradudin, Phys. Rev. B 44, 8565 (1991).
- ¹¹ K.L. Kliewer and R. Fuchs, Adv. Chem. Phys. 27, 355 (1974).
- ¹² P. Halevi and R. Fuchs, J. Phys. C 17, 3869 (1984).
- ¹³ R.D. Meade, K.D. Brommer, A.M. Rappe, and J.D. Joannopoulos, Phys. Rev. B 44, 10 961 (1991).
- ¹⁴ E. Yablonovitch, Phys. Rev. Lett. **60**, 1711 (1988); E. Yablonovitch and T.J. Gmitter, *ibid.* **63**, 1950 (1989).
- ¹⁵ Jordi Martorell and N.M. Lawandy, Phys. Rev. Lett. 65, 1877 (1990).

- ¹⁶ R. Loudon, *The Quantum Theory of Light*, 2nd ed. (Oxford University Press, Oxford, 1983); D. Marcuse, *Principles of Quantum Electronics* (Academic, New York 1980).
- ¹⁷ S. M. Barnett, B. Huttner, and R. Loudon, Phys. Rev. Lett. **68**, 3698 (1992).
- ¹⁸ We assume that only one isofrequency surface corresponds to a certain frequency ω . Otherwise every isofrequency surface gives an independent contribution to the DOS.
- ¹⁹ E.M. Lifshitz and P.L. Pitaevskii, *Statistical Physics* (Pergamon, Oxford, 1980), Chap. IX, Pt. 2.
- ²⁰ I.M. Lifshitz, M.Ya Azbel, and M.I. Kaganov, *Electron Theory of Metals* (Consultant Bureau, New York, 1972).
- ²¹ In the presence of absorption, strictly speaking, the group velocity does not vanish at a Brillouin zone boundary. This is so because $\nabla_{\mathbf{k}}\omega' \neq \nabla_{\mathbf{k}}\omega = 0$. However, in our low-dissipation limit, ω' is replaced by ω in the first approximation.
- ²² Joseph W. Hause, H. Sami Sözuer, and R. Inguva (unpublished).
- ²³ See, for example, J.O. Vasseur, B. Djafari-Rouhani, L. Dobrzynski, M.S. Kushwaha, and P. Halevi, J. Phys. Condens. Matter 6, 8759 (1994).
- ²⁴ Pochi Yeh, Optical Waves in Layered Media (Wiley, New York, 1988).
- ²⁵ See, for example, C. Kittel, Introduction to Solid State Physics (Wiley, New York, 1976), 5th. ed.
- ²⁶ In order to avoid complications we assume that the number of periods N of the modulated superlattice is even.