Photonic Band Gaps: Noncommuting Limits and the "Acoustic Band"

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We study the photonic "acoustic band" for both square arrays of dielectric and infinite refractive index cylinders. We show that the effective refractive index defined by this band does not have a continuous limit as the cylinder refractive index approaches infinity, and we explain this physically.

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The idea that singly, doubly, and triply periodic dielectric lattices can be designed to possess photonic band gaps has attracted wide attention, both theoretically and experimentally [1,2]. The absence of electromagnetic modes inside a photonic band gap can lead to unusual physical phenomena. Thus, atoms or molecules embedded in such a structure, called a dielectric crystal, can be locked in an excited state if the energy of this state, relative to the ground state, falls within the photonic band gap. In this case, the atoms (or molecules) are also expected to exhibit an anomalous Lamb shift. At the same time, in a dielectric crystal new types of electron-photon interactions appear leading to a specific behavior of light.

The most widely used theoretical approach in calculating the photonic band structures relies on the treatment of the full vector Maxwell equations by means of plane wave expansions [3–5]. In this method, the field and the dielectric constant are expanded in infinite series of plane waves, so that the problem is reduced to an infinite-dimensional eigenvalue problem. Because plane wave expansions converge slowly, this method requires a large number of terms in the series, in order to obtain accurate numerical results. By truncating the series, the high frequency components are removed. Also, the dielectric constant is poorly estimated near spatial discontinuities [6–8]. For metallic systems at high frequencies the dielectric constant may exhibit a very large imaginary part and the plane wave expansions become impractical [9]. The numerical techniques used to avoid these difficulties still require the evaluation of large determinants by complicated and time consuming algorithms.

In a series of papers we have extended Rayleigh's technique [10] from electrostatic to full electromagnetic problems, for singly [11–13], doubly [14–16], and triply [17] periodic systems. Rayleigh's method involves a set of lattice sums which consists of sums over terms with a function evaluated at each lattice point, and the evaluation of lattice sums is the most important and subtle part of this technique. The main reason is that the definition of lattice sums involves conditionally converging series over the direct lattice, and a direct evaluation is thus impractical if high accuracy is needed. The lattice sums involved in our method are represented in terms of absolutely converging series over the reciprocal lattice, and, in contrast to the method used by Ewald [18], these series may be accelerated by succesive integrations to any order. By introducing the lattice sums, we obtain a representation of Green's function in terms of a rapidly convergent Neumann series. Also, the representation in terms of absolutely converging series allows us to have some physical insight into the analytic properties of the lattice sums. For the coefficients in the multipole expansions of fields we have obtained a generalized Rayleigh identity.

Our method is capable of studying, numerically and analytically, problems in which the dielectric constant is piecewise constant and may take finite or infinite values. Because there are no series expansions of the dielectric constant, the method may also be applied in cases when the dielectric constant takes on imaginary values. This method is also consistent with an approach which has been used for static studies of composites, and is therefore suitable for studying the homogenization problem (in which an effective uniform refractive index is attributed to a composite material) [19].

In this Letter, we consider the diffraction of a plane electromagnetic wave by a periodic array of dielectric cylinders embedded in a host medium. The geometry of the system is specific to photonic band gap studies; i.e., the cylinders have the axes parallel to the z axis and the incident plane wave has the wave vector $\mathbf{k}_0$ perpendicular to the axes of the cylinders. Consequently, the components of the fields are independent of z.

In the case when the host medium is an isotropic homogeneous dielectric in which the electromagnetic wave has the wave number k, the equations for the components of the electric $(\mathbf{E})$ and magnetic $(\mathbf{H})$ field decouple and each field component satisfies the two-dimensional Helmholtz equation. At the same time, the problem can be reduced to solving two independent problems: (i) for s polarization, when the electric field is along the z axis perpendicular to the plane of propagation, and (ii) for p polarization, when the electric field is parallel to the plane of propagation.

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We consider the unit cell of the array, containing one cylinder of radius a and refractive index N, centered at the origin of coordinates. For this unit cell, in the host medium, in polar coordinates (r, θ), the general solution of the two-dimensional Helmholtz equation has the form $(r \geq a)$

$$V_e^{(\gamma)}(\mathbf{r}) = \sum_{\ell=-\infty}^{\infty} [A_\ell^{(\gamma)} J_\ell(kr) + B_\ell^{(\gamma)} Y_\ell(kr)] e^{i\ell\theta}, \quad (1)$$

where $\mathbf{r}$ is the radius vector in the x-y plane, γ labels the polarization (s or p), $V_e^{(s)} = E_{e,z}$, and $V_e^{(p)} = H_{e,z}$. Also, J and Y are Bessel functions of the first and second kind, respectively. Inside the cylinder the solution is $(r \leq a)$

$$V_i^{(\gamma)}(\mathbf{r}) = \sum_{\ell=-\infty}^{\infty} C_\ell^{(\gamma)} J_\ell(Nkr) e^{i\ell\theta}, \quad (2)$$

where $V_i^{(s)} = E_{i,z}$ and $V_i^{(p)} = H_{i,z}$. The solution (1),(2) has to fulfill the boundary conditions at the surface of the cylinder, and the quasiperiodicity condition [15,16]:

$$V_{i,e}^{(\gamma)}(\mathbf{r} + \mathbf{R}_p) = e^{i\mathbf{k}_0 \cdot \mathbf{R}_p} V_{i,e}^{(\gamma)}(\mathbf{r}). \quad (3)$$

Here, $\mathbf{R}_p$ is a vector from the origin of coordinates to the center of the pth cylinder (the pth node of the array). The boundary conditions (the continuity of tangential components of $\mathbf{E}$ and $\mathbf{H}$ at the surface of each cylinder) provide us with a relation of the form $A_\ell^{(\gamma)} = -M_\ell^{(\gamma)} B_\ell^{(\gamma)}$. In the case when the host medium consists of free space (dielectric constant ε_0 and magnetic permeability μ_0), and the cylinders have the relative dielectric constant ε and the magnetic permeability μ_0, the coefficients $M_\ell^{(\gamma)}$ take the form

$$M_\ell^{(s)} = \frac{N J_\ell'(Nka) Y_\ell(ka) - J_\ell(Nka) Y_\ell'(ka)}{N J_\ell'(Nka) J_\ell(ka) - J_\ell(Nka) J_\ell'(ka)}, \quad (4)$$

$$M_\ell^{(p)} = \frac{J_\ell'(Nka) Y_\ell(ka) - N J_\ell(Nka) Y_\ell'(ka)}{J_\ell'(Nka) J_\ell(ka) - N J_\ell(Nka) J_\ell'(ka)}, \quad (5)$$

where $N = \sqrt{\varepsilon}$ represents the refractive index of the cylinders and the prime indicates the derivative of the corresponding function.

Following the extended Rayleigh method, we obtain the multipole coefficients $B_\ell^{(\gamma)}$ from the generalized Rayleigh identity [14–16]:

$$M_\ell^{(\gamma)} B_\ell^{(\gamma)} + \sum_{m=-\infty}^{\infty} (-1)^{\ell+m} S_{m-\ell}^Y(k, \mathbf{k}_0) B_m^{(\gamma)} = 0, \quad (6)$$

for $-\infty \leq \ell \leq \infty$, and with $S_{m-\ell}^Y(k, \mathbf{k}_0)$ the lattice sums for the corresponding array. For infinite refractive index cylinders, in the limit $\varepsilon \rightarrow \infty$, in the homogeneous system (5) the coefficients $M_\ell^{(\gamma)}$ are replaced by

$$M_\ell^{(s)} = \frac{Y_\ell(ka)}{J_\ell(ka)}, \quad (7)$$

$$M_\ell^{(p)} = \frac{Y_\ell'(ka)}{J_\ell'(ka)}. \quad (8)$$

The zeros of the determinant in (6), for $\mathbf{k}_0$ in the irreducible domain of the first Brillouin zone, define the dispersion curves for photons propagating through the periodic structure. In the coordinate system k vs $\mathbf{k}_0$ the lowest values of k form an "acoustic band," if for $\mathbf{k}_0 \rightarrow \mathbf{0}$ then $k \rightarrow 0$ [20]. We obtain what is termed the quasistatic limit for small k_0 if $k \sim \alpha k_0$. This is attained for p polarization at long wavelengths and normal incidence [21]. In this limit the effective refractive index of the structure is given by $N^* = 1/\alpha$. This effective refractive index is obtained by investigating the phase change of V_e across the unit cell [22]. For p polarization and in the dipole approximation [i.e., truncating the homogeneous system (6) to $-1 \leq \ell, m \leq 1$], from (6) and (5) we obtain the Maxwell-Garnett formula

$$N^*(\varepsilon) = \left[\frac{(\varepsilon + 1) + f(\varepsilon - 1)}{(\varepsilon + 1) - f(\varepsilon - 1)}\right]^{1/2}, \quad (9)$$

where $f = \pi a^2$ is the filling fraction. Equation (9) defines another effective refractive index, usually justified by electrostatic arguments [10,23,24]. At the same time, for infinite refractive index cylinders, the same method applied to (6) and (8) leads us to the formula [22]

$$N_\infty^* = (1 + f)^{1/2}. \quad (10)$$

From (9) and (10) we may conclude that

$$N_\infty^* \neq \lim_{\varepsilon \to \infty} N^*(\varepsilon). \quad (11)$$

This difference resides in the behavior of the coefficients (5) and (8) in the quasistatic limit. Actually, we have the noncommuting limits

$$\lim_{k \to 0} \lim_{\varepsilon \to \infty} M_\ell^{(p)} \neq \lim_{\varepsilon \to \infty} \lim_{k \to 0} M_\ell^{(p)}. \quad (12)$$

To check numerically the noncommuting limits (12) we consider the dispersion curves for a square array of cylinders in air, for p polarization. The array constant is d and the ratio of the cylinders radii to the array constant is $a/d = 0.472$, corresponding to a filling fraction $f = 0.70$. First, we assume that the cylinders have a dielectric constant $\varepsilon = 50$ [see Fig. 1(a)]. In this case, the effective refractive index evaluated in the quasistatic limit is $N^* \approx 2.5184$. We compare this with the value of the effective refractive index for the same array calculated using electrostatic rather than electromagnetic theory: $N_{\rm st}^* = 2.5171$ [23]. Then, we consider that the cylinders have an infinite refractive index [see Fig. 1(b)]. Now, the effective refractive index is $N_\infty^* \approx 1.4945$, while the static effective refractive index is $N_{\rm st}^* = 2.7263$ [23]. The dipole approximation (10) gives $N_\infty^* = 1.3038$. In both cases, we have truncated the system (6) to $-12 \leq \ell, m \leq 12$. This truncation order has been chosen so that the numerical stability of the results is assured [22,23].

Also, for $d = 1$ cm the band gap exhibited by the dispersion curves for $\varepsilon = 50$ is characterized by a midgap frequency $g \approx 3.9$ GHz and a gap width $\Delta g \approx 1$ GHz ($\Delta g/g \approx 26\%$), while for infinite refractive index cylinders we have $g_\infty \approx 16.9$ GHz and $\Delta g_\infty \approx 12.5$ GHz ($\Delta g_\infty / g_\infty \approx 74\%$).

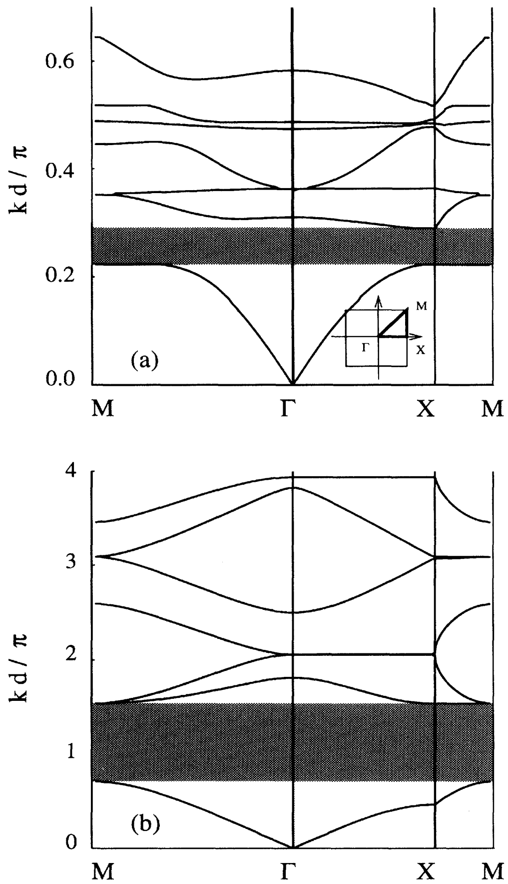

FIG. 1. Photonic band structure of a square array of cylinders in air, for p polarization. The ratio of the cylinder radii to the array constant was 0.472 (the filling fraction $f = 0.70$). The dielectric constant of the cylinders was $\varepsilon = 50$ (a) and $\varepsilon = \infty$ (b). In both cases the system (6) has been truncated to $-12 \leq \ell, m \leq 12$. The inset shows the irreducible octant of the first Brillouin zone.

A numerical check of the noncommuting limits is also presented in Tables I, II, and III. Thus, in Table I, we display the values of the effective refractive index N^* for an array of dielectric cylinders, evaluated for a truncation $-8 \leq \ell, m \leq 8$ in (6). In Table II we present the effective refractive index for the same array in an electrostatic field, the values being obtained by using the Rayleigh method [23,24]. It can be seen that the results given by the generalized Rayleigh identity (6), in the quasistatic limit, agree very well with the results given by the classical Rayleigh identity, over a large range of filling fractions and dielectric constants.

The effect of noncommuting limits (12) appears in the case of very large values of the dielectric constant of the cylinders. In such cases, displayed in the last column in Table I, the *dynamic* effective refractive index differs substantially from the *static* effective refractive index (the last column in Table II) and agrees with the *dynamic* effective refractive index for infinite refractive index cylinders (the third column in Table III).

TABLE I. The effective refractive index (N^*) of an array of dielectric cylinders as given by (6), with a truncation $-8 \leq \ell, m \leq 8$, for different values of filling fraction (f) and dielectric constant of the cylinders (ε).

	ε			
f	10	10^2	10^3	10^{10}
0.212	1.1920	1.2354	1.2403	1.1023
0.283	1.2661	1.3300	1.3373	1.1350
0.363	1.3601	1.4541	1.4651	1.1685
0.454	1.4822	1.6243	1.6416	1.2147
0.554	1.6495	1.8801	1.9101	1.2646

The fourth column in Table III displays the values of the dynamic refractive index in the dipole approximation (10). These values differ from the values in the third column as the filling fraction is increased. The explanation of this difference resides in the fact that for concentrated systems the dipole approximation is no longer valid, and we have to add higher-order terms to obtain the correct result. Thus, in the third column of Table III the dynamic effective refractive index has been obtained using a truncation $-20 \leq \ell, m \leq 20$ in (6), which assures the numerical stability of the results.

The extension of our method to other systems is straightforward. The lattice sums depend only on the geometry of the lattice and the characteristics of the incident wave, i.e., they are independent of the shape or the dielectric constant of the inclusions. We are currently working on the extension of our technique to periodic arrays of elliptical cylinders and lattices of spheres. Note that, for any shape of the inclusions, the generalized Rayleigh identity involves linear combinations of lattice sums in cylindrical (2D problems) or polar coordinates (3D problems). Also, the essential physics described here should carry over to disordered systems.

In the literature on homogenization, it is usual to state that an effective refractive index can be attributed to a composite material provided the wavelength of electromagnetic radiation is much larger than a characteristic

TABLE II. The effective refractive index (N^*_{st}) of an array of dielectric cylinders in an electrostatic field [23], for different values of filling fraction (f) and dielectric constant of the cylinders (ε).

	ε			
f	10	10^2	10^3	∞
0.212	1.1920	1.2354	1.2403	1.2408
0.283	1.2661	1.3300	1.3373	1.3381
0.363	1.3601	1.4541	1.4651	1.4663
0.454	1.4822	1.6243	1.6416	1.6435
0.554	1.6495	1.8801	1.9100	1.9135

TABLE III. The effective refractive index (N_∞^*) of an array of infinite refractive index cylinders (radius a) obtained from (6) with a truncation $-20 \le \ell, m \le 20$. The values obtained from (10) are displayed in the last column.

a	f	N_∞^*	$(1 + f)^{1/2}$
0.26	0.212	1.1013	1.1011
0.30	0.283	1.1334	1.1326
0.34	0.363	1.1736	1.1676
0.38	0.454	1.2151	1.2051
0.42	0.554	1.2782	1.2467

particle size. We have shown here that the wavelength *in all components* of the composite must satisfy this condition. If not, homogenization may not be possible, or may yield surprising results. For example, in the case of cylinders with infinite refractive index, the internal wavelength is zero, and thus is never much larger than the radius. Hence, (10) applies in the dipole approximation, rather than the expected result (9).

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