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An averaged-field approach for obtaining the band structure of a dielectric photonic crystal

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Abstract. An averaged-field approach is suggested for obtaining the explicit form of the dispersion equation for electromagnetic waves propagating in a three- or two-dimensional dielectric photonic crystal when the dimension of the inclusions is small compared with the longest period of the rectangular lattice of the photonic crystal. The band structure is obtained in an explicit and simple way. The method is verified numerically by comparing with the conventional plane-wave expansion method for a special case.

1. Introduction

A photonic crystal is a periodic dielectric structure which is used to control and manipulate the propagation of light [1–4]. Intensive investigations on photonic crystals have been carried out recently following the discovery of photonic band-gap materials, which is a new and exciting development in physics. Most of the potential applications of photonic crystals rely on their band structures of the dispersion curves [5–8]. The band structure of a photonic crystal is usually computed by the plane-wave expansion method, in which the fields and the dielectric constant are expanded in infinite series of plane waves and the problem is reduced to an infinite-dimensional eigenvalue problem [9–13]. Since the plane-wave expansion converges slowly, a large number of terms in the truncated series are required. Furthermore, such a numerical method does not provide much physical insight into how the band structure is formed. In this paper we introduce an analytic method for obtaining the band structure of a three- or two-dimensional dielectric photonic crystal when the dimension of the inclusions is small compared with the longest period of the rectangular lattice of the photonic crystal. This method allows one to obtain an explicit and simple dispersion equation which involves a dispersion coefficient. This dispersion coefficient can be expressed in terms of the response of the individual inclusion element to the local field and the response to the field generated by the whole lattice. Explicit solutions for special cases are useful for the insight they provide and as references in establishing benchmarks for general numerical algorithms. The analytic method is verified numerically for a special case (the *H*-polarization of the two-dimensional case) by comparing with the conventional plane-wave expansion method. Compared with other

analytic approaches such as the generalized Rayleigh method [14, 15], the present approach gives the simplest formulation.

2. The averaged-field approach

Consider a photonic crystal (with a rectangular lattice) as shown in figure 1. The centres of the inclusion elements form an infinite periodic lattice with period l along the z -direction and periods l_x, l_y along the x - and y -directions, respectively (assume that $l \geq l_x, l_y$; i.e., we choose the z -axis along the direction with the longest period). We view this lattice as a set of grid points on many parallel planes $z = 0, \pm l, \pm 2l, \pm 3l, \dots$. Denote the maximum length of the inclusion along the z -direction by d . We consider the case when the phase shift of the eigenwave is small over the distance d (i.e., $kd < 1$, where k is the wavenumber in the medium). We also assume that $d \ll l$. We define region n as the region $(n-3)l/2 + d/2 < z < (n-1)l/2 - d/2$ when n is odd or the region $(n-2)l/2 - d/2 < z < (n-2)l/2 + d/2$ when n is even (see figure 1). In regions $\pm 1, \pm 3, \pm 5, \dots$, the medium is homogeneous (the background medium) with permittivity ϵ_b and permeability μ and the homogeneous Maxwell's equations hold in these regions. The inclusions have permittivity ϵ_a and the same permeability as the background medium. The time dependence of the fields is assumed to be $\exp(-i\omega t)$.

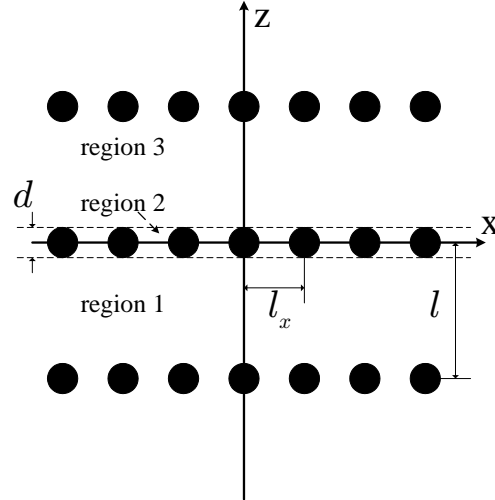


Figure 1. The configuration for a 2D periodic rectangular array of inclusions in a background material.

Our goal is to derive an explicit dispersion relation for the photonic crystals. Instead of the dispersion relation for the true electromagnetic fields, the dispersion relation for the transversely averaged fields (over the region $[x - l_x/2, x + l_x/2] \times [y - l_y/2, y + l_y/2]$) will be considered. A transversely averaged function for a function $f(x, y, z)$ is defined and denoted by

$$\langle f \rangle(x, y, z) = \frac{1}{l_x} \frac{1}{l_y} \int_{x-l_x/2}^{x+l_x/2} \int_{y-l_y/2}^{y+l_y/2} f(x', y', z) dx' dy'. \quad (1)$$

From the linearity of the averaging operator it follows that the same Maxwell's equations hold in regions 1, 2, 3, \dots , for the averaged fields [16]. We then take the following spatial

Fourier transform for these averaged fields in region 1 ($-l + d/2 < z < -d/2$) and region 3 ($d/2 < z < l - d/2$):

$$\hat{f}(\mathbf{k}, z) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} f(x, y, z) e^{ik_x x + ik_y y} dx dy \quad (2)$$

where $\mathbf{k} = (k_x, k_y)$. In the conventional theory for photonic crystals one considers the true fields and obtains the band structure numerically by e.g. a plane-wave expansion method. In the present paper we consider the averaged fields and obtain an analytic expression for the band structure. Since the eigenwaves in a photonic crystal are spatial plane harmonics (with periods $l_x/m, l_y/n$ and l/p in x -, y - and z -directions, respectively, where m, n, p are integers) [2], the operation of averaging (defined by equation (1)) does not change the spatial dependence of the eigenwaves. The averaged fields have the same expansion in terms of the averaged eigenwaves for the same wave vector and, hence, the dispersion relation for the averaged fields is the same as that for the true fields.

From Maxwell's equations, one obtains the following equations for the Fourier-transformed averaged fields in the homogeneous region 1 ($-l + d/2 \leq z \leq -d/2$) and region 3 ($d/2 \leq z \leq l - d/2$):

$$\nabla \times \langle \hat{\mathbf{E}} \rangle = -i\omega\mu \langle \hat{\mathbf{H}} \rangle \quad (3)$$

$$\nabla \times \langle \hat{\mathbf{H}} \rangle = i\omega\epsilon_b \langle \hat{\mathbf{E}} \rangle \quad (4)$$

which can be rewritten in the following form:

$$\mathbf{k} \times \partial_z \langle \hat{\mathbf{E}}_t \rangle(\mathbf{k}, z) = i\omega\mu z_0 \mathbf{k} \cdot \langle \hat{\mathbf{H}}_t \rangle(\mathbf{k}, z) \quad (5)$$

$$\mathbf{k} \times \partial_z \langle \hat{\mathbf{H}}_t \rangle(\mathbf{k}, z) = -i\omega\epsilon_b z_0 \mathbf{k} \cdot \langle \hat{\mathbf{E}}_t \rangle(\mathbf{k}, z) \quad (6)$$

$$\partial_z \langle \hat{\mathbf{E}}_z \rangle(\mathbf{k}, z) = i\mathbf{k} \cdot \langle \hat{\mathbf{E}}_t \rangle \quad (7)$$

where the subscript t refers to the tangential component of the fields, and z_0 is the unit vector along the z -direction. The solutions to these equations can be expressed in the following form (in both regions 1 and 3):

$$C(\mathbf{k}, z) = \vec{C}(\mathbf{k}) \exp(i\sqrt{k_0^2 - k^2}z) + \overleftarrow{C}(\mathbf{k}) \exp(-i\sqrt{k_0^2 - k^2}z) \quad (8)$$

where $C(\mathbf{k}, z)$ denotes $\langle \hat{\mathbf{H}} \rangle$ or $\langle \hat{\mathbf{E}} \rangle$ and $k_0 = \omega\sqrt{\epsilon_b\mu}$ is the wavenumber in the background medium. The coefficients $\vec{C}(\mathbf{k})$, $\overleftarrow{C}(\mathbf{k})$ in equation (8) are the amplitudes of the two waves propagating in the positive or negative z -direction.

On the other hand, from the Bloch theorem one knows that $\langle \hat{\mathbf{E}} \rangle$ and $\langle \hat{\mathbf{H}} \rangle$ can be written in the following form [2]:

$$C(\mathbf{k}, z) = \vec{F}(\mathbf{k}, z) \exp(ik_z z) + \overleftarrow{F}(\mathbf{k}, z) \exp(-ik_z z) \quad (9)$$

where k_z is the z -axis propagation constant of the periodic photonic crystal (as a medium) which belongs to the first Brillouin zone ($0 < k_z < \pi/l$), and the functions $\vec{F}(\mathbf{k}, z)$ and $\overleftarrow{F}(\mathbf{k}, z)$ are periodic in z with period l . This periodicity allows one to express the amplitudes of the two waves in region 3 ($\vec{C}^{(3)}$ and $\overleftarrow{C}^{(3)}$) in terms of the amplitudes of these waves in region 1 ($\vec{C}^{(1)}$ and $\overleftarrow{C}^{(1)}$) as follows:

$$\vec{C}^{(3)}(\mathbf{k}) = \vec{C}^{(1)}(\mathbf{k}) e^{i(\sqrt{k_0^2 - k^2} - k_z)l} \quad \overleftarrow{C}^{(3)}(\mathbf{k}) = \overleftarrow{C}^{(1)}(\mathbf{k}) e^{i(\sqrt{k_0^2 - k^2} + k_z)l}. \quad (10)$$

In the conventional theory of photonic crystals there is only one eigenwave $\vec{F}(\mathbf{k}, z) \exp(ik_z z)$ in the representation (9) (see e.g. [2]). However, our approach is quite different. We derive the jumps in the averaged fields over each inclusion layer (with thickness d). These jumps

indicate an ‘averaged’ reflection of the electromagnetic wave from these inclusion layers, and thus we cannot drop the back-propagation term in equation (8) or equation (9) (one can find an analogy in the well-known coupled-wave theory [17]). Otherwise, we will obtain a trivial result

$$k_z = \sqrt{k_0^2 - k^2}.$$

Since each inclusion layer is quite thin ($kd < 1$), we may neglect the phase shift of the electromagnetic field over the spatial interval $-d/2 < z < d/2$. We consider the inclusion layer centred at the plane $z = 0$ as a very thin layer of electrical dipole polarization (induced by the propagating waves). For this inclusion layer we introduce an equivalent averaged surface polarization $\langle \mathbf{P} \rangle(x, y)$ referred to its central plane $z = 0$. We may also describe the tangential polarization of this layer in terms of the following effective surface polarization current (cf. equations (5.2) and (6.87) of [18]):

$$\langle \mathbf{J} \rangle(x, y) = -i\omega \langle \mathbf{P}_t \rangle(x, y). \quad (11)$$

The above relation follows from the continuity equation. The same relation holds for the bulk polarization \mathbf{p}_{bulk} and the bulk polarization current \mathbf{j}_{bulk} [16]. One then has

$$\langle \mathbf{P} \rangle \equiv \langle \mathbf{P}_t \rangle + z_0 \langle P_z \rangle = d \langle \mathbf{p}_{bulk} \rangle|_{[-d/2 < z < d/2]}. \quad (12)$$

Over this dipolar layer the averaged transverse fields have the following jumps:

$$\Delta \langle \mathbf{H}_t \rangle \equiv z_0 \times (\langle \mathbf{H} \rangle|_{z=d/2} - \langle \mathbf{H} \rangle|_{z=-d/2}) = -\langle \mathbf{J} \rangle = i\omega \langle \mathbf{P}_t \rangle \quad (13)$$

$$\langle \mathbf{E}_t \rangle|_{z=d/2} - \langle \mathbf{E}_t \rangle|_{z=-d/2} = -i \frac{\mathbf{k}}{\epsilon_b} \langle P_z \rangle. \quad (14)$$

Equation (14) follows from the well-known expression for the potential drop in a dipole layer with thickness d . Relations (13) and (14) for the averaged fields are true for arbitrary x, y , and, therefore, also hold for the Fourier-transformed averaged fields.

Since inside the inclusions $\mathbf{p}_{bulk} = (\epsilon_a - \epsilon_b)\mathbf{E}$, there exists a 3×3 matrix $\overline{\overline{\beta}}(\mathbf{k})$ which relates the Fourier-transformed averaged surface polarization at the plane $z = 0$ and the Fourier-transformed averaged electric field at the same plane in the following form:

$$\langle \hat{\mathbf{P}} \rangle(\mathbf{k}) = \overline{\overline{\beta}}(\mathbf{k}) \cdot \langle \hat{\mathbf{E}} \rangle(\mathbf{k})|_{z=0}. \quad (15)$$

Since the inclusion layer is thin, we may write

$$\langle \hat{\mathbf{E}} \rangle|_{z=0} = \frac{1}{2} (\langle \hat{\mathbf{E}} \rangle|_{z=-d/2} + \langle \hat{\mathbf{E}} \rangle|_{z=d/2}). \quad (16)$$

From equation (7) one has

$$\partial_z \langle \hat{\mathbf{E}}_z \rangle|_{z=\pm d/2} = i\mathbf{k} \cdot \langle \hat{\mathbf{E}}_t \rangle|_{z=\pm d/2}. \quad (17)$$

Expressing the z -derivative of $\langle \hat{\mathbf{E}}_z \rangle$ in terms of the fields with equation (9) and using the periodicity condition (10) for both $\langle \hat{\mathbf{E}}_z \rangle$ and $\langle \hat{\mathbf{E}}_t \rangle$, it follows from equation (17) that

$$\begin{aligned} \langle \hat{\mathbf{E}}_z \rangle|_{z=d/2} + \langle \hat{\mathbf{E}}_z \rangle|_{z=-d/2} &= \frac{\mathbf{k}}{K_z(b-a)} \left[(b \langle \hat{\mathbf{E}}_t \rangle|_{z=-d/2} - \langle \hat{\mathbf{E}}_t \rangle|_{z=d/2})(a+1) \right. \\ &\quad \left. + (a \langle \hat{\mathbf{E}}_t \rangle|_{z=-d/2} - \langle \hat{\mathbf{E}}_t \rangle|_{z=d/2})(b+1) \right] \end{aligned}$$

where

$$K_z \equiv \sqrt{k_0^2 - k^2}$$

and

$$a = e^{i[K_z(l-d)+k_zl]} \quad b = e^{-i[K_z(l-d)-k_zl]}. \quad (18)$$

Using the above relation and equation (16) one can eliminate $\langle \hat{E}_z \rangle(\mathbf{k})|_{z=0}$ in equation (15) and obtain the following equation:

$$\begin{aligned} \langle \hat{P} \rangle(\mathbf{k}) &= \frac{\bar{\bar{\beta}}}{2} \cdot (\langle \hat{E}_t \rangle|_{z=-d/2} + \langle \hat{E}_t \rangle|_{z=+d/2}) \\ &+ \frac{\bar{\bar{\beta}}}{2} \cdot \frac{z_0}{K_z(b-a)} \mathbf{k} \cdot \left[(b\langle \hat{E}_t \rangle|_{z=-d/2} - \langle \hat{E}_t \rangle|_{z=d/2})(a+1) \right] \\ &+ \frac{\bar{\bar{\beta}}}{2} \cdot \frac{z_0}{K_z(b-a)} \mathbf{k} \cdot \left[(a\langle \hat{E}_t \rangle|_{z=-d/2} - \langle \hat{E}_t \rangle|_{z=d/2})(b+1) \right]. \end{aligned} \quad (19)$$

Substituting the representation (8) for both $\langle \hat{E}_t \rangle$ and $\langle \hat{H} \rangle$ into equations (5) and (6) and using the periodicity condition (10), one obtains the following relation between tangential fields at $z = \pm d/2$:

$$\begin{aligned} \Delta \langle \hat{H}_t \rangle &\equiv z_0 \times (\langle \hat{H} \rangle|_{z=d/2} - \langle \hat{H} \rangle|_{z=-d/2}) \\ &= \frac{K_z}{\omega\mu(a-b)} \left[(a\langle \hat{E}_t \rangle|_{z=-d/2} - \langle \hat{E}_t \rangle|_{z=d/2})(b-1) \right. \\ &\quad \left. + (b\langle \hat{E}_t \rangle|_{z=-d/2} - \langle \hat{E}_t \rangle|_{z=d/2})(a-1) \right] \end{aligned} \quad (20)$$

where a and b are given by equation (18).

We now have four vector homogeneous equations (13), (14), (19) and (20) for four unknown vectors $\langle \hat{E}_t \rangle|_{z=-d/2}$, $\langle \hat{E}_t \rangle|_{z=d/2}$, $\langle \hat{P} \rangle$ and $\Delta \langle \hat{H}_t \rangle$. In order for this homogeneous system of equations to have a non-trivial solution, the determinant of the coefficient matrix must vanish, and this gives an *explicit* dispersion equation if the susceptibility tensor $\bar{\bar{\beta}}$ is known.

In a special case when the inclusions are symmetric, the cross-components of $\bar{\bar{\beta}}$ are identically zero. Thus, equation (19) can be split into the following two equations:

$$\langle \hat{P}_t \rangle = \frac{\bar{\bar{\beta}}_t \cdot (\langle \hat{E}_t \rangle|_{z=-d/2} + \langle \hat{E}_t \rangle|_{z=+d/2})}{2} \quad (21)$$

$$\begin{aligned} \langle \hat{P}_z \rangle &= \frac{\beta_{zz}}{2K_z(b-a)} \left[(b\langle \hat{E}_t \rangle|_{z=-d/2} - \langle \hat{E}_t \rangle|_{z=d/2})(a+1) \right] \\ &+ \frac{\beta_{zz}}{2K_z(b-a)} \left[(b\langle \hat{E}_t \rangle|_{z=-d/2} - \langle \hat{E}_t \rangle|_{z=d/2})(a+1) \right] \end{aligned} \quad (22)$$

where $\bar{\bar{\beta}}_t$ is the transverse part of $\bar{\bar{\beta}}$, i.e.,

$$\bar{\bar{\beta}}_t \equiv \beta_{xx} \mathbf{x}_0 \mathbf{x}_0 + \beta_{yy} \mathbf{y}_0 \mathbf{y}_0 + \beta_{xy} \mathbf{x}_0 \mathbf{y}_0 + \beta_{yx} \mathbf{y}_0 \mathbf{x}_0.$$

One can then easily eliminate $\langle \hat{P} \rangle$ and $\Delta \langle \hat{H}_t \rangle$ from the system of equations (13), (14), (19) and (20). Substituting equations (20), (21) and (22) into equations (13) and (14), one obtains the following two relations between the tangential electric fields at $z = \pm d/2$:

$$\bar{\bar{S}}_{11} \cdot \langle \hat{E}_t \rangle|_{z=-d/2} + \bar{\bar{S}}_{12} \cdot \langle \hat{E}_t \rangle|_{z=d/2} = 0 \quad (23)$$

$$\bar{\bar{S}}_{21} \cdot \langle \hat{E}_t \rangle|_{z=-d/2} + \bar{\bar{S}}_{22} \cdot \langle \hat{E}_t \rangle|_{z=d/2} = 0 \quad (24)$$

where

$$\begin{aligned}\bar{\bar{S}}_{11} &= \frac{K_z(e^{ik_z l} - \cos[K_z(l-d)])}{\omega\mu \sin[K_z(l-d)]} \bar{\bar{I}}_t + \frac{\omega\bar{\bar{\beta}}_t}{2} \\ \bar{\bar{S}}_{12} &= \frac{K_z(e^{-ik_z l} - \cos[K_z(l-d)])}{\omega\mu \sin[K_z(l-d)]} \bar{\bar{I}}_t + \frac{\omega\bar{\bar{\beta}}_t}{2} \\ \bar{\bar{S}}_{21} &= \frac{\mathbf{k}\mathbf{k}\beta_{zz}(e^{ik_z l} + \cos[K_z(l-d)])}{\epsilon_b K_z \sin[K_z(l-d)]} - \bar{\bar{I}}_t \\ \bar{\bar{S}}_{22} &= -\frac{\mathbf{k}\mathbf{k}\beta_{zz}(e^{-ik_z l} + \cos[K_z(l-d)])}{\epsilon_b K_z \sin[K_z(l-d)]} + \bar{\bar{I}}_t\end{aligned}$$

and where $\bar{\bar{I}}_t$ is the unit planar dyadic (i.e., $\bar{\bar{I}}_t = \mathbf{x}_0\mathbf{x}_0 + \mathbf{y}_0\mathbf{y}_0$) and we have used the following properties:

$$\begin{aligned}2ab \pm (a+b) &= 2e^{ik_z l} (e^{ik_z l} \pm \cos[K_z(l-d)]) \\ 2 \pm (a+b) &= 2e^{ik_z l} (e^{-ik_z l} \pm \cos[K_z(l-d)]) \\ b-a &= 2ie^{ik_z l} \sin[K_z(l-d)].\end{aligned}$$

The determinant of the coefficient matrix for the system of equations (23) and (24) must vanish, which gives an explicit dispersion equation for the case of symmetric inclusions if the susceptibility tensor $\bar{\bar{\beta}}$ is known.

Thus the remaining problem is to determine the susceptibility matrix $\bar{\bar{\beta}}$, which depends on the shape of the inclusions. This is considered in the next section.

3. Determination of the susceptibility matrix $\bar{\bar{\beta}}(\mathbf{k})$

In this section we describe an approach for the determination of the dyadic $\bar{\bar{\beta}}(\mathbf{k})$, which relates the Fourier-transformed averaged electric field and the Fourier-transformed averaged polarization density on the plane $z=0$ (cf. the definition (15)).

Assume that the inclusion layer in region 2 is excited by a plane wave \mathbf{E}^{ext} which has the following x, y -dependence on the plane $z=0$:

$$\mathbf{E}^{ext}(x, y) = \mathbf{E}^{ext}(0, 0)e^{i(k_x x + k_y y)}. \quad (25)$$

Here the external field \mathbf{E}^{ext} is produced by all sources but the reference inclusion layer. It includes the field produced by all the other inclusion layers. The averaged surface polarization $\langle \mathbf{P} \rangle(x, y)$ can be expressed in terms of the total averaged field $\langle \mathbf{E} \rangle(x, y)$ on the plane $z=0$. In particular, one has the following relation at the origin:

$$\langle \mathbf{P} \rangle(0) = \bar{\bar{\beta}}'(k_x) \cdot \langle \mathbf{E} \rangle(0, 0). \quad (26)$$

It can be shown easily that $\bar{\bar{\beta}}'(k_x)$ in the above relation is identical to $\bar{\bar{\beta}}(k_x)$ in equation (15).

The periodicity of the grid then leads to the following expression for the dipole moment \mathbf{p} (per unit length) of the (n, m) -numbered cylinder (centred at the point $x = nl_x, y = ml_y, z = 0$) on the plane $z=0$:

$$\mathbf{p}(x = nl_x, y = ml_y) = \mathbf{p}(0, 0)e^{-i(k_x l_x n + k_y l_y m)} \quad (27)$$

where the 0-numbered cylinder is centred at the origin (i.e., $x = y = z = 0$). Note that the fields considered later are either at the origin or on the plane $z=0$, unless specified otherwise.

Consider the doubly periodic grid excited by the wave (25). Assume that the polarizability $\bar{\bar{\alpha}}$ is known for the inclusions, and we have

$$\mathbf{p}(0, 0) = \bar{\bar{\alpha}} \cdot \mathbf{E}^{loc}(0, 0) \quad (28)$$

where the local field $\mathbf{E}^{loc}(0, 0)$ is the field applied to the reference inclusion (centred at the origin) from all the *other* sources. The local field \mathbf{E}^{loc} can be written in the following two parts:

$$\mathbf{E}^{loc}(0, 0) = \mathbf{E}^{int}(0, 0) + \mathbf{E}^{ext}(0, 0) \quad (29)$$

where \mathbf{E}^{int} is called the interaction field, i.e. the field produced at the origin by all the inclusions except the reference inclusion centred at the origin. We assume that the external field at the origin is produced by sources far from the reference cylinder, and thus practically equals the averaged external field at the same point, i.e.,

$$\mathbf{E}^{ext}(0, 0) = \langle \mathbf{E}^{ext} \rangle(0, 0). \quad (30)$$

To ensure the validity of the approximation (30) we have already chosen the z -axis to be along the direction with the longest period (so that the inclusions at other inclusion layers have a larger distance from the reference cylinder than the neighbouring inclusions at the plane $z = 0$). The external field \mathbf{E}^{ext} may be written in the following form:

$$\mathbf{E}^{ext} = \langle \mathbf{E} \rangle - \langle \mathbf{E}^{grid} \rangle \quad (31)$$

where $\langle \mathbf{E} \rangle$ is the total averaged field and $\langle \mathbf{E}^{grid} \rangle$ is the contribution of all inclusions at the reference plane $z = 0$ to the averaged field.

Since both the external field and the distribution of the polarization are periodic functions (cf. equations (25) and (27)), one can express the interaction field in terms of the so-called interaction tensor $\bar{\bar{A}}(\mathbf{k})$ (introduced by Collin in [19] for dipolar lattices):

$$\mathbf{E}^{int}(0, 0) = \bar{\bar{A}}(\mathbf{k}) \cdot \mathbf{p}(0, 0). \quad (32)$$

An explicit expression for $\bar{\bar{A}}(\mathbf{k})$ in a special case can be found in e.g. [19] (page 784). A similar relation resulting from the periodicity of the fields can be written for the averaged grid field:

$$\langle \mathbf{E}^{grid} \rangle(0, 0) = \bar{\bar{B}}(\mathbf{k}, l_x, l_y) \cdot \mathbf{p}(0, 0). \quad (33)$$

We derive the explicit expressions for $\bar{\bar{A}}$ and $\bar{\bar{B}}$ in a special case in the appendix.

Now assume that $\bar{\bar{A}}$ and $\bar{\bar{B}}$ are already known. Substituting equations (29), (31), (32) and (33) into equation (28) and using the fact that $\langle \mathbf{P} \rangle(0, 0) = \mathbf{p}(0, 0)/l_x l_y$, one obtains

$$\langle \mathbf{P} \rangle(0, 0) = \frac{1}{l_x l_y} (\bar{\bar{I}} - \bar{\bar{\alpha}} \cdot \bar{\bar{A}} + \bar{\bar{\alpha}} \cdot \bar{\bar{B}})^{-1} \cdot \bar{\bar{\alpha}} \cdot \langle \mathbf{E} \rangle(0, 0) \quad (34)$$

which gives the following explicit expression for the susceptibility matrix $\bar{\bar{\beta}}(\mathbf{k})$:

$$\bar{\bar{\beta}} = \frac{1}{l_x l_y} (\bar{\bar{I}} - \bar{\bar{\alpha}} \cdot \bar{\bar{A}} + \bar{\bar{\alpha}} \cdot \bar{\bar{B}})^{-1} \cdot \bar{\bar{\alpha}} \quad (35)$$

where $\bar{\bar{I}}$ is the unit dyadic.

4. Numerical verification for a special case: H -polarization of the 2D case

In this section we verify our method numerically for a special case, namely, the H -polarization of the two-dimensional case. In the two-dimensional model, the inclusions are uniform along the y -direction and all the fields are independent of y . We consider the case of H -polarization, i.e., the magnetic field is perpendicular to the xz -plane (the electric field has x - and z -components).

Then the averaging operator and Fourier transformation (2) are redefined to exclude l_y and k_y in the definitions (1) and (2). For such a case, $\overline{\beta}$ is a 2×2 matrix which contains xx , xz , zx and zz elements. The zero determinant of the system of equations (13), (14), (19) and (20) leads to the following explicit dispersion equation (note that $k_0 = \omega\sqrt{\epsilon_b\mu}$):

$$Q \sin \sqrt{(\omega\sqrt{\epsilon_b\mu}l)^2 - (k_x l)^2} = \cos \sqrt{(\omega\sqrt{\epsilon_b\mu}l)^2 - (k_x l)^2} - \cos k_z l \quad (36)$$

where

$$Q = \frac{-2ik_0 l \sqrt{\mu/\epsilon_b}}{\sqrt{(k_0 l)^2 - (k_x l)^2}} \left(M_1 - \frac{[(k_0 l)^2 - (k_x l)^2]^{3/2}}{k_0^2 \omega \mu} M_2 \right) / \left(4 + \frac{\sqrt{(k_0 l)^2 - (k_x l)^2}}{\omega \epsilon_b} M_1 M_2 \right) \quad (37)$$

and where M_1 and M_2 are given by

$$M_1 = i\omega \left(\beta_{xx} - \beta_{xz} \frac{k_x}{\sqrt{k_0^2 - k_x^2}} \right) \quad (38)$$

$$M_2 = -i \frac{k_x}{\epsilon_b} \left(\beta_{zx} - \beta_{zz} \frac{k_x}{\sqrt{k_0^2 - k_x^2}} \right). \quad (39)$$

Equations (37), (38) and (39) for the symmetric case when $\beta_{zx} = \beta_{xz} = 0$ can easily be derived from the relation $S_{11}S_{22} - S_{12}S_{21} = 0$, which follows from equations (23) and (24) (the tensors \overline{S}_{ij} become scalar in the 2D case).

Note that the dimensionless dispersion coefficient Q is real when the inclusions are lossless. Also note that in general Q depends on the frequency, the dielectric parameters, the shape of the inclusions and the lattice parameters. The variables k_x and k_z in the dispersion relation (36) determine the propagation direction. For normal propagation (i.e., $k_x = 0$), equation (36) has a form similar to the well-known dispersion equation for the inductively loaded transmission line (where Q is independent of the frequency) [20]. It is also similar to the approximate dispersion relation for electron propagation in an ‘empty lattice’ when the electron energy exceeds the periodic potential barriers [21].

The matrix $\overline{\beta}$ depends on the shape of the inclusions. One can derive explicit expressions for $\overline{\beta}$ for inclusions with various special shapes. For inclusions of circular cylinders (with radius $a = d/2$ and permittivity ϵ_a), one can obtain the following explicit expression for $\overline{\beta}$ (see the appendix for a detailed derivation):

$$\beta_{xx} = \frac{2\pi a^2 \epsilon_b}{l_x (1 - \delta)} \frac{\epsilon_a - \epsilon_b}{\epsilon_a + \epsilon_b} \quad (40)$$

$$\beta_{zz} = \frac{2\pi a^2 \epsilon_b}{l_x (1 - \delta')} \frac{\epsilon_a - \epsilon_b}{\epsilon_a + \epsilon_b} \quad (41)$$

$$\beta_{xz} = \beta_{zx} = 0 \quad (42)$$

where

$$\delta = \frac{\pi(\omega\sqrt{\epsilon_b\mu}a)^2}{\omega\sqrt{\epsilon_b\mu}l_x} \frac{\epsilon_a - \epsilon_b}{\epsilon_a + \epsilon_b} \left[Y_1(\omega\sqrt{\epsilon_b\mu}l_x) \sin(k_x l_x) + k_x^2 l_x / (\omega\sqrt{\epsilon_b\mu}) \right] \quad (43)$$

$$\delta' = \frac{\pi a}{2l_x} \frac{\epsilon_a - \epsilon_b}{\epsilon_a + \epsilon_b} \quad (44)$$

and where Y_1 is the Neumann function of order 1. As shown in the appendix, the explicit expressions (40) and (41) for β_{xx} and β_{zz} are quite accurate when $k_0 < 2\pi/l_x$, and the dispersion relation for the complementary case $k_0 > 2\pi/l_x$ can be described approximately as that for the homogeneous background medium. Note that the photonic band gap usually occurs at several low bands, and thus the explicit formulae for the band structure in the low-frequency region $k_0 < 2\pi/l_x$ are particularly interesting and useful. It thus follows from equations (38), (39), (37)–(42) that the dispersion coefficient Q for the case $k_0 < 2\pi/l_x$ has the following expression for circular inclusions:

$$Q = \frac{gl_x(\omega\sqrt{\epsilon_b\mu}l)^2}{l\sqrt{(\omega\sqrt{\epsilon_b\mu}l)^2 - (k_x l)^2}} \frac{(1 - \delta') - (1 - \delta)(k_x l)^2 [(\omega\sqrt{\epsilon_b\mu}l)^2 - (k_x l)^2] / (\omega\sqrt{\epsilon_b\mu}l)^4}{(1 - \delta)(1 - \delta') + (k_x l_x)^2 g} \quad (45)$$

where

$$g = \frac{\pi a^2 (\epsilon_a - \epsilon_b)}{l_x^2 (\epsilon_a + \epsilon_b)}.$$

4.1. Numerical verification

In order to verify the analytic results obtained from our averaged-field approach, we compare the band structure obtained with our explicit formulae with the one computed by the conventional plane-wave expansion method [9]. As a simple numerical example, we choose $\epsilon_a = 100\epsilon_0$, $\epsilon_b = \epsilon_0$, $l_x/l = 0.15$ and the radius $a = 0.25l_x$ for the circular cylinders. In this case the irreducible Brillouin zone is a triangular wedge, and the rest of the Brillouin zone can be related to this triangular wedge by rotational symmetry. Therefore, we have three special points, Γ , X and M corresponding respectively to $k_{\parallel} = 0$, $k_{\parallel} = (\pi/l)\hat{z}$ and $k_{\parallel} = (\pi/l)\hat{z} + (\pi/l_x)\hat{x}$. In figures 2(a) and 2(b), the solid curves are the band structure obtained by the conventional plane-wave expansion method [9] (with 441 plane waves), and the circles are obtained from our explicit dispersion relation (36) with Q given by the approximation (45). As one can see from figure 2(a), our results give a good agreement with the results obtained by the conventional plane-wave expansion method. The dashed curves in figure 2(b) give the corresponding band structure (for a normal propagation) for the homogeneous background medium (i.e. there is no inclusion). Figure 2(b) indicates that our method has taken into account the inclusion information in a correct way. The comparison given in figures 2(a) and 2(b) verifies the present method. Our method is over 70 times faster than the plane-wave expansion method in terms of the required computational time.

5. Conclusions

An averaged-field approach has been suggested for obtaining the band structure of a photonic crystal when the dimension of the inclusions is small compared with the longest period of the rectangular lattice. The method allows one to obtain an explicit dispersion equation for a three- or two-dimensional photonic crystal. The band structure is obtained in an explicit and simple

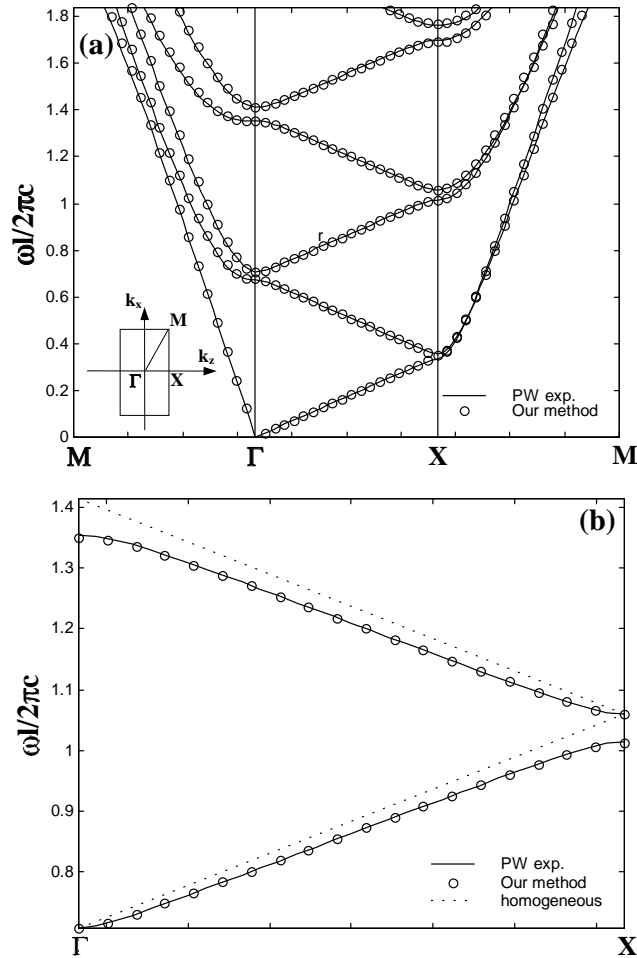


Figure 2. The band structure for a 2D photonic crystal with $\epsilon_a = 100\epsilon_0$, $\epsilon_b = \epsilon_0$, $l_x/l = 0.15$ and radius $a = 0.25l_x$ for the circular cylinders. The circles are obtained by our results, and the solid curves are obtained by the conventional plane-wave expansion method (with 289 plane waves). The dashed lines in (b) give the corresponding band structure (for a normal propagation) for the homogeneous background medium (i.e. there is no inclusion).

way. The method has been verified numerically by comparing with the conventional plane-wave expansion method for the H -polarization of the two-dimensional case. The present method can be generalized to the more complicated cases such as the case of anisotropic inclusions, etc.

Besides the resulting simple and explicit formulae, the present method has many other advantages such as that it can treat the case when the inclusions are perfectly conducting (results are presented in [25]). However, the conventional plane-wave expansion method will be complicated to apply to this case. Note that all the formulae in the present paper also hold when the permittivity of the inclusions is frequency dependent (as long as the permittivity is positive) and the band structure can be computed from our explicit dispersion relation in a straightforward way (the plane-wave expansion method, however, works only for some very special types of frequency dependence after complicated modifications [22]).

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Appendix. Derivation for $\overline{\beta}$ for the case when the inclusions are circular cylinders

The off-diagonal elements of the matrix $\overline{\beta}$ vanish if the cross-section of the centre cylinder is symmetric with respect to the plane $z = 0$ and each inclusion cylinder is treated as a line dipole with the dipole moment per unit length denoted by p .

For circular inclusions (with radius a), one has the following relation between $p(0)$ and the local field E^{loc} [23]:

$$p(0) = 2\pi a^2 \epsilon_b \frac{\epsilon_a - \epsilon_b}{\epsilon_a + \epsilon_b} E^{loc}. \quad (A1)$$

Thus, the polarization coefficient α (defined by equation (28)) is given by

$$\alpha = 2\pi a^2 \epsilon_b \frac{\epsilon_a - \epsilon_b}{\epsilon_a + \epsilon_b}. \quad (A2)$$

In the two-dimensional case, equation (34) reduces to the following relation (note that $\langle P_{x,z} \rangle(0) = p_{x,z}(0)/l_x$):

$$\langle P_{x,z} \rangle = \frac{\alpha}{l_x(1 - \alpha A_{x,z} + \alpha B_{x,z})} \langle E_{x,z} \rangle. \quad (A3)$$

Therefore, one has (cf. equation (15))

$$\beta_{xx} = \frac{\alpha}{l_x[1 - \alpha(A_x - B_x)]} \quad (A4)$$

$$\beta_{zz} = \frac{\alpha}{l_x[1 - \alpha(A_z - B_z)]}. \quad (A5)$$

To find the expressions for $A_{x,z}$ and $B_{x,z}$, we consider separately the low-frequency case $k_0 < 2\pi/l_x$ and the high-frequency case $k_0 > 2\pi/l_x$, and we start with the former.

To find the expressions for A_x and B_x , we consider an array of discrete equivalent dipoles (polarized in the x -direction) located at the centres of the cylinder inclusions. Thus, the parameter A_x can be found from the following relation [24]:

$$E_x^{int} \equiv A_x p_x(0) = \left(\sum_{n=-\infty}^{-1} + \sum_{n=1}^{\infty} \right) G(nl_x, 0) p_x(0) e^{ik_x n l_x} \quad (A6)$$

where $G(x, z)$ is Green's function describing the electric field at the origin generated by a unit line dipolar at the point (x, z) . On the plane $z = 0$ one has [24]

$$G(x, 0) = \frac{-i}{4\epsilon_b} \frac{H_1^{(1)}(k_0|x|)}{|x|}. \quad (A7)$$

We replace the summation in equation (A6) by an integration (as an approximation) using the well-known Euler formula when $k_0 < 2\pi/l_x$. One then obtains

$$E_x^{int} = \frac{p_x(0)}{l_x} \left(\int_{-\infty}^{-l_x/2} + \int_{l_x/2}^{\infty} \right) G(x, 0) e^{ik_x x} dx. \quad (A8)$$

We consider the interaction field to be the field produced by a continuous polarization distribution in the regions $x > l_x/2$ and $x < -l_x/2$, and this polarization $\langle P_x^{smooth} \rangle(x)$ is given by

$$\langle P_x^{smooth} \rangle(x) = p_x(0) e^{ik_x x} / l_x. \quad (A9)$$

Note that the exact expression for the averaged polarization $\langle P_x \rangle$ is $\langle P_x \rangle(x) = p_x(0)e^{ik_x n l_x} / l_x$, where $x \in [(n - 1/2)l_x, (n + 1/2)l_x]$ and $n = 0, \pm 1, \pm 2, \dots$. Relation (A9) comes from the smoothing of this exact expression. The function $G(x, 0)$ can be expressed in terms of the second z -derivative of $H_0^{(1)}(k_0 R)$ at $z = 0$:

$$G(x, 0) = \frac{-i}{4k_0 \epsilon_b} \frac{\partial^2}{\partial z^2} H_0^{(1)}(k_0 R) \Big|_{z=0}.$$

Since the Hankel function $H_0^{(1)}(k_0 R)$ satisfies the Helmholtz equation, it then follows from equation (A8) that

$$E_x^{int} = \frac{i p_x(0)}{4 \epsilon_b k_0 l_x} \left(k_0^2 + \frac{\partial^2}{\partial x^2} \right) \Big|_{x=0} \left(\int_{-\infty}^{-l_x/2} + \int_{l_x/2}^{\infty} \right) e^{ik_x x'} H_0^{(1)}(k_0 |x - x'|) dx'. \quad (\text{A10})$$

Using integration by parts, one can derive the following explicit expression for A_x from equation (A10):

$$A_x = \frac{\sqrt{\mu/\epsilon_b}}{2l_x} \left[\frac{k_0}{\sqrt{k_0^2 - k_x^2}} + Y_1(k_0 l_x) \sin(k_x l_x) + k_x^2 l_x / k_0 \right] \quad (\text{A11})$$

where Y_n is the Neumann function of order n .

In a similar way we can derive the expression for the parameter B_x in the low-frequency case when $k_0 < 2\pi/l_x$. We use the theorem proved in [16] that the averaged field generated by discrete dipoles is equal to the field generated by the averaged dipole distribution, i.e., $\langle \mathbf{E} \rangle(\mathbf{P}) = \mathbf{E}(\langle \mathbf{P} \rangle)$. Instead of the exact representation for $\langle \mathbf{P} \rangle$, we use its smoothed approximation (A9). Using the well-known formula for the electric field produced by an infinite sheet of harmonic dipole polarization (see e.g. [23] and [24]), one obtains

$$B_x = \frac{\omega \mu}{2l_x \sqrt{k_0^2 - k_x^2}}. \quad (\text{A12})$$

Thus, substituting equations (A11) and (A12) into equation (A4), one obtains the final expression (40) for β_{xx} with δ given by equation (43).

Now we derive the expressions for A_z and B_z . We consider an array of discrete equivalent dipoles (polarized in the z -direction) located at the centres of the cylinder inclusions. We study the interaction field E_z^{int} and the averaged grid field $\langle E_z^{grid} \rangle$ at the origin in a way similar to the one used in the derivation for A_x and B_x . Using the corresponding relation (11) for the bulk polarization and the bulk current density, equations (39a), (39b) in [24] and the formula $\langle P_z^{bulk} \rangle = \langle P_z \rangle / d$, one obtains the following expression for the field increment dE_z at the origin produced by the polarization current on a small strip element dx on the plane $z = 0$ (a distance $|x|$ away from the origin):

$$dE_z = \frac{i \sqrt{\mu/\epsilon_b} \omega}{4d} (p_z(0)/l_x) e^{ik_x x} H_1^{(1)}(k_0 |x|) dx. \quad (\text{A13})$$

Integrating the above dE_z , one obtains

$$E_z^{int} \equiv A_z l_x \langle P_z \rangle(0) = \left(\int_{-\infty}^{-l_x/2} + \int_{l_x/2}^{\infty} \right) dE_z. \quad (\text{A14})$$

To find the averaged grid field $\langle E_z^{grid} \rangle$, we cannot integrate (A13) over all x on the plane $z = 0$, since this representation implies that the bulk polarization distribution has a delta-function $\delta(z)$ form and equation (A13) cannot be used to describe the field in a z -polarized strip generated by itself [24]. Thus we separate the plane $z = 0$ (with a smoothed surface polarization $\langle P_z \rangle(x)$)

into two regions, namely, the closest region $|x| < x_0$ and the far region $|x| > x_0$ (we choose the value x_0 such that $2a \leq x_0 < l_x/2$ and $k_0 x_0 \leq 1$). When evaluating the contribution from the region $|x| < x_0$ to $\langle E_z^{grid} \rangle$, denoted by $\langle E_z^{closest} \rangle$, we may neglect the phase shift of the waves and hence it behaves like a static field. Since $x_0 \geq 2a$, the two domains $x > x_0$ and $x < -x_0$ are far enough away from the origin and we can assume that the field is generated by a delta-polarization $\langle p_z^{bulk} \rangle(x, z) = \langle P_z \rangle(x) \delta(z)/d$. It then follows from equation (A13) that

$$\langle E_z^{grid} \rangle \equiv B_z l_x \langle P_z \rangle(0) = \langle E_z^{closest} \rangle + \left(\int_{-\infty}^{-x_0} + \int_{x_0}^{\infty} \right) dE_z. \quad (\text{A15})$$

The field $\langle E_z^{closest} \rangle$ is the electrostatic field on the dipole layer which is infinite along the y -axis and has a finite size $2x_0 \times d$ on the xz -plane. This field (due to the effect of bound charges) can be treated as the field inside an equivalent capacitor with the surface charge $\sigma = \langle p_z^{bulk} \rangle = \langle P_z \rangle/d$. This equivalent capacitor is formed by two infinite strips with the same transverse size. We suggest choosing $x_0 = d$. It then follows that $\langle E_z^{closest} \rangle = \langle p_z^{bulk} \rangle/2\epsilon_b = \langle P_z \rangle/2\epsilon_b d$. For the integral term in equation (A15), the contribution from the parts $x > l_x/2$ and $x < -l_x/2$ to B_z cancels out with A_z (given by equation (A14)). It thus follows from equation (A13) that

$$A_z - B_z = \frac{1}{2dl_x\epsilon_b} - \frac{i\sqrt{\mu/\epsilon_b}\omega}{2l_x^2} \int_d^{l_x/2} \cos(k_x x) H_1^{(1)}(k_0 x) dx. \quad (\text{A16})$$

An analytic estimation shows that the integral term in the above equation is very small compared to the first term. Thus one has the following approximation:

$$A_z - B_z = \frac{1}{4al_x\epsilon_b}. \quad (\text{A17})$$

Substituting the above expression into equation (A5), one obtains the expression (41) for β_{zz} with δ' given by equation (44).

Now consider the high-frequency case, i.e. $k_0 > 2\pi/l_x$. Then all the cylinders are situated more than half a wavelength away from the reference cylinder. The averaged field at the origin generated by the n -numbered cylinder ($n \neq 0$) on the plane $z = 0$ is approximately equal to the field at the origin generated by this cylinder, i.e.,

$$\langle E_{x,z}^n \rangle|_{x=0} = E_{x,z}^n|_{x=0}.$$

Since

$$\langle E_{x,z}^{grid} \rangle|_{x=0} = \sum_{n=-\infty}^{\infty} \langle E_{x,z}^n \rangle|_{x=0}$$

it follows from equations (32) and (33) that

$$B_{x,z} - A_{x,z} = \frac{1}{p_{x,z}(0)} \int_{-l_x/2}^{l_x/2} E_{x,z}^0(x) dx$$

where $E^0(x)$ is the field at the point $(x, z = 0)$ generated by the reference (i.e., 0-numbered) cylinder. This field cannot be treated as the field generated by a line dipole source, since we have to take in account the near-field structure in the closest region. The expression for the field generated by a uniformly polarized cylinder with a finite cross-section is given in [24]. Using the exact expression for $E^0(x)$ we have carried out a quite complicated study for β_{xx} and β_{zz} for the high frequency case $k_0 > 2\pi/l_x$. However, our study leads to the trivial result corresponding to the homogeneous background medium. If the frequency is so high that $k_0 l_x > 2\pi$ and $k_0 a < 1$ (the condition required for the present 'thin-layer' treatment), the polarized cylinders give an insignificant scattered field. The dispersion curves calculated with our complicated high-frequency formulae for this case give an almost linear frequency dependence of the propagation constant (as for the homogeneous background medium).

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