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Photonic band structure in the nearly plane wave approximation

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Abstract. For photons propagating in a periodic dielectric lattice, the dispersion curve forms photonic bands separated by forbidden gaps. When the dielectric lattice deviates only slightly from being homogenous, the photonic band structure resembles the linear dispersion relation for photons folded into the first Brillouin zone, *i.e.*, the so-called empty lattice bands. Using group theoretical technique, we calculate the splitting of the accidental degeneracies in the empty lattice bands at symmetry points for a simple cubic dielectric lattice.

PACS. 71.15.-m Methods of electronic structure calculations – 78.20.-e Optical properties of bulk materials and thin films

1 Introduction

Recently there has been some interest [1–28] in the problem of propagation of electromagnetic waves through a fabricated dielectric structure, either periodic or disordered. For a periodic structure, the photon dispersion curve takes the form of allowed frequency bands separated by forbidden gaps, analogous to the electronic bands in crystals [1,2]. On the other hand, in a disordered structure, there are possibilities for photon localization [2–9].

Apart from confirmation [10–18] of the existence of photonic gaps in a periodic structure, there exist calculations of certain specific photonic band structure. In several of these theoretical works, a plane-wave expansion of the photonic Bloch wave is made, and the resulting eigenvalue equation is solved numerically.

In the present work, we also calculate the photonic band structure using the plane- wave expansion. At the same time, we make the assumption that the dielectric lattice is only slightly different from being a homogenous medium. Under this assumption the photonic bands resemble closely the empty lattice bands, *i.e.*, the linear dispersion relation $\omega = ck$ folded into the first Brillouin zone. The only significant change is that certain accidental degeneracies at symmetry points and along symmetry directions will now be lifted due to photon scattering from the periodic lattice. The advantage of adopting this nearly plane wave approximation is that we can calculate these splittings analytically. As usual, analytic results will provide more useful guidelines as to, for example, how can one adjust various parameters involved in order to manufacture a true photonic gap in the band structure.

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It is quite obvious that the present method is analogous to the nearly free electron approximation in determining the electronic band structure of simple metals. The essential difference between the two cases is that while the electron is represented by a scalar wave function satisfying the Schrodinger equation, the photon is a vector field governed by Maxwell's equations. So despite the close analogy, one still needs to illustrate the nearly-plane-wave method as applied to photons. This is the purpose of the present paper. Since at this stage we are not trying to interpret any specific set of data, we shall just assume a simple model consisting of a simple cubic dielectric lattice with each unit cell made of two kinds of dielectric material. This model will be quantitatively defined and then solved in Section 3 after we have presented the general method in Section 2. We conclude the paper by making some brief remarks in Section 4.

2 Plane wave method

For EM wave in dielectric medium, the $\mathbf{E}$ and $\mathbf{H}$ fields satisfy Maxwell's equations

$$\boldsymbol{\nabla} \times \mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{B}}{\partial t}, \ \boldsymbol{\nabla} \times \mathbf{H} = \frac{1}{c}\frac{\partial \mathbf{D}}{\partial t} \cdot \tag{2.1}$$

Assuming linear and isotropic dielectrics and neglecting magnetic effects, we have the following two constitutive equations

$$\mathbf{D} = \epsilon(\mathbf{r})\mathbf{E}, \ \mathbf{B} = \mathbf{H}, \tag{2.2}$$

where ϵ is a position-dependent dielectric constant. It follows that the **H**-field satisfies the equation

$$\boldsymbol{\nabla} \times \left(\frac{1}{\epsilon(\mathbf{r})} \boldsymbol{\nabla} \times \mathbf{H} \right) = -\frac{1}{c^2} \frac{\partial^2 \mathbf{H}}{\partial t^2} \cdot \tag{2.3}$$

In a periodic medium, the **H** field behaves like a Bloch wave, *i.e.*, a plane wave with its amplitude modulated as represented by

$$\mathbf{H} = \mathbf{u}(\mathbf{r})\, \mathrm{e}^{i(\mathbf{k}\cdot\mathbf{r} - \omega t)} \tag{2.4}$$

where the vector amplitude **u** has the periodicity of the lattice.

Since **u** has the lattice periodicity, it can be Fourier expanded as

$$\mathbf{u}(\mathbf{r}) = \sum_{\mathbf{k}} \mathbf{u}(\mathbf{K}) \mathrm{e}^{i\mathbf{K}\cdot\mathbf{r}}, \tag{2.5}$$

involving reciprocal lattice vector **K**. Likewise, the inverse dielectric constant can be expressed as a Fourier series

$$\frac{1}{\epsilon}(\mathbf{r}) = \sum_{\mathbf{K}} \left(\frac{1}{\epsilon} \right)_{\mathbf{K}} \mathrm{e}^{i\mathbf{K}\cdot\mathbf{r}}. \tag{2.6}$$

It is then convenient to work out equation (2.3) in the reciprocal lattice space. To do this we must first determine the direction of the vector amplitude $\mathbf{u}(\mathbf{K})$ for each plane wave with wave vector $\mathbf{k}+\mathbf{K}$. From the Maxwell equation $\boldsymbol{\nabla} \cdot \mathbf{H} = 0$, we have

$$(\mathbf{k}+\mathbf{K}) \cdot \mathbf{u}(\mathbf{K}) = 0. \tag{2.7}$$

In other words, for each $\mathbf{k}+\mathbf{K}$, there are two independent modes, each having its polarization transverse to $\mathbf{k}+\mathbf{K}$. Let us label the two independent polarizations by mutually perpendicular unit vectors $\hat{\mathbf{e}}_1(\mathbf{k}+\mathbf{K})$ and $\hat{\mathbf{e}}_2(\mathbf{k}+\mathbf{K})$. Since **H** field is an axial vector field, we further specify that the three mutually perpendicular vectors $\hat{\mathbf{e}}_1$, $\hat{\mathbf{e}}_2$ and $\mathbf{k}+\mathbf{K}$ form a right handed rectangular coordinate system with

$$\hat{\mathbf{e}}_1 \times \hat{\mathbf{e}}_2 = \frac{\mathbf{k}+\mathbf{K}}{|\mathbf{k}+\mathbf{K}|} \cdot \tag{2.8}$$

In reciprocal lattice space, equation (2.3) becomes

$$\frac{\omega^2}{c^2} \mathbf{u}(\mathbf{K}) = -\sum_{\mathbf{K}'} \left(\frac{1}{\epsilon} \right)_{\mathbf{K}-\mathbf{K}'} (\mathbf{k}+\mathbf{K}) \times [(\mathbf{k}+\mathbf{K}') \times \mathbf{u}(\mathbf{K}')]. \tag{2.9}$$

Based on (2.8) we see that for either polarization of $\mathbf{u}\,(\mathbf{K}')$, the cross product inside the bracket above can be written as

$$(\mathbf{k}+\mathbf{K}') \times \mathbf{u}(\mathbf{K}') = |\mathbf{k}+\mathbf{K}'| u(\mathbf{K}') \quad [\text{either} - \hat{\mathbf{e}}_1(\mathbf{k}+\mathbf{K}') \text{ or } \hat{\mathbf{e}}_2(\mathbf{k}+\mathbf{K}')]. \tag{2.10}$$

Taking scalar product with $\hat{\mathbf{e}}_i(\mathbf{k}+\mathbf{K})$ on both sides of (2.9), we obtain the following equation

$$\frac{\omega^2}{c^2} u(\mathbf{K})\ I = \sum_{\mathbf{K}'} |\mathbf{k}+\mathbf{K}||\mathbf{k}+\mathbf{K}'| \left(\frac{1}{\epsilon} \right)_{\mathbf{K}-\mathbf{K}} u(\mathbf{K})\ p(\mathbf{K},\mathbf{K}') \tag{2.11}$$

where I is a 2×2 unit matrix and p matrix involves the polarization vectors as follows:

$$p(\mathbf{K},\mathbf{K}') = \begin{pmatrix} \hat{\mathbf{e}}_2(\mathbf{k}+\mathbf{K}) \cdot \hat{\mathbf{e}}_2(\mathbf{k}+\mathbf{K}') & -\hat{\mathbf{e}}_1(\mathbf{k}+\mathbf{K}) \cdot \hat{\mathbf{e}}_2(\mathbf{k}+\mathbf{K}') \\ -\hat{\mathbf{e}}_2(\mathbf{k}+\mathbf{K}) \cdot \hat{\mathbf{e}}_1(\mathbf{k}+\mathbf{K}') & \hat{\mathbf{e}}_1(\mathbf{k}+\mathbf{K}) \cdot \hat{\mathbf{e}}_1(\mathbf{k}+\mathbf{K}') \end{pmatrix}.$$

Equation (2.11) may be looked upon as a matrix equation in $(\mathbf{K},\mathbf{K}')$. The ω *vs.* k dispersion relations can be obtained by diagonalizing this matrix. This method was used by Ho *et al.* [22] in their calculation of the photonic band structure.

3 A simple cubic dielectric lattice

Consider a simple cubic dielectric lattice of lattice constant a. The lattice is made of two kinds of dielectric material of dielectric constant ϵ_1 and ϵ_2. They are distributed in the way specified as follows: in each unit cell, space with coordinates $-\frac{a}{4} < x < \frac{a}{4}, -\frac{a}{4} < y < \frac{a}{4}, -\frac{a}{4} < z < \frac{a}{4}$ is filled with dielectric ϵ_1, and the rest of the cell has dielectric constant ϵ_2. It is trivial to calculate the Fourier coefficient of the inverse dielectric constant in this model. It is given by

$$\left(\frac{1}{\epsilon} \right)_{n_1 n_2 n_3} = \left(\frac{1}{\epsilon_1} - \frac{1}{\epsilon_2} \right) \frac{1}{n_1 n_2 n_3 \pi^3} \sin\frac{n_1\pi}{2} \sin\frac{n_2\pi}{2} \sin\frac{n_3\pi}{2} + \frac{1}{\epsilon_2} \frac{1}{n_1 n_2 n_3 \pi^3} \sin\ n_1\pi\ \sin\ n_2\pi\ \sin\ n_3\pi \tag{3.1}$$

for reciprocal lattice vector

$$\mathbf{K} = \frac{2\pi}{a}(n_1\hat{\mathbf{x}} + n_2\hat{\mathbf{y}} + n_3\hat{\mathbf{z}}).$$

It is clear that the second term in (3.1) only contributes to the average $\left(\frac{1}{\epsilon}\right)_{000}$, and that $\left(\frac{1}{\epsilon}\right)_{n_1 n_2 n_3} = 0$ if any of the three integers is a non-zero even integer. It is also useful to give the explicit form of a few Fourier coefficients below:

$$\left(\frac{1}{\epsilon} \right)_{000} = \frac{1}{8}\frac{1}{\epsilon_1} + \frac{7}{8}\frac{1}{\epsilon_2}$$
$$\left(\frac{1}{\epsilon} \right)_{100} = \frac{1}{4\pi} \left(\frac{1}{\epsilon_1} - \frac{1}{\epsilon_2} \right)$$
$$\left(\frac{1}{\epsilon} \right)_{110} = \frac{1}{2\pi^2} \left(\frac{1}{\epsilon_1} - \frac{1}{\epsilon_2} \right)$$
$$\left(\frac{1}{\epsilon} \right)_{111} = \frac{1}{\pi^3} \left(\frac{1}{\epsilon_1} - \frac{1}{\epsilon_2} \right).$$

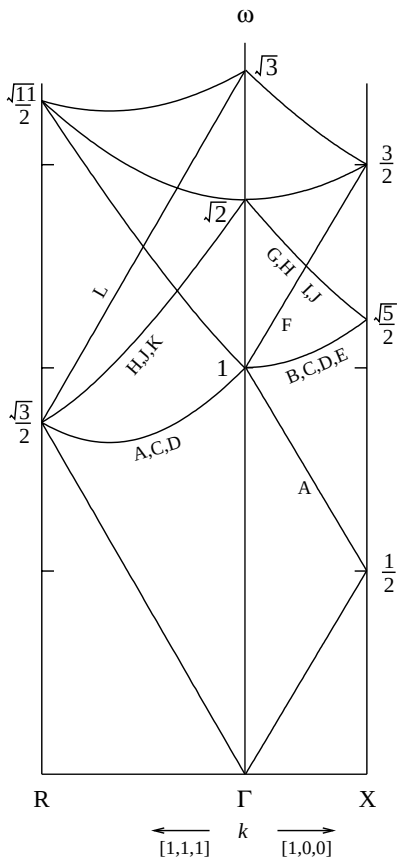

Fig. 1. Empty lattice photonic band along $(1,0,0)$ and $(1,1,1)$ directions. The frequency is in units of $c\sqrt{\left(\frac{1}{\epsilon}\right)_{000}}\frac{2\pi}{a}$. The reciprocal lattice vectors involved in the folding are labeled as follows: A: $(\overline{1},0,0)$, B: $(0,1,0)$, C: $(0,\overline{1},0)$, D: $(0,0,\overline{1})$, E: $(0,0,1)$, F: $(1,0,0)$, G: $(\overline{1},1,0)$, H:$(\overline{1},\overline{1},0)$, I: $(\overline{1},0,1)$, J: $(\overline{1},0,\overline{1})$, K: $(0,\overline{1},\overline{1})$, L: $(\overline{1},\overline{1},\overline{1})$.

Now we use the plane wave method developed in the last section to obtain the photonic band structure for the case where

$$|\frac{1}{\epsilon_1}-\frac{1}{\epsilon_2}|<\left(\frac{1}{\epsilon}\right)_{000}. \tag{3.2}$$

For this case, it is expected that the amplitude of a plane EM wave propagating through the dielectric lattice is only weakly modulated and the dispersion curve resembles the linear relationship for EM wave traveling through a homogenous medium except that now gaps may open up at symmetry points in the Brillouin zone.

To appreciate the effect of the periodic lattice, we first look at the empty lattice drawing of the linear dispersion relation $\omega=c\sqrt{\left(\frac{1}{\epsilon}\right)_{000}}k$ folded into the first Brillouin zone along two selected directions, $[1,0,0]$ and $[1,1,1]$ in Figure 1. As can be seen, some highly degenerate modes occur at symmetry points and along symmetry directions. At the center of the zone, *i.e.* Γ point, the $\omega=1$ mode is 12-fold degenerate. At X *i.e.* $\left(\frac{\pi}{a},0,0\right)$ point on the zone surface, the $\omega=\frac{1}{2}$ mode is 4-fold degenerate while the $\omega=\sqrt{5}/2$ mode is 16-fold degenerate. At the corner of the zone, *i.e.* R point with coordinates $\left(\frac{\pi}{a},\frac{\pi}{a},\frac{\pi}{a}\right)$, the $\omega=\sqrt{3}/2$ mode is 16-fold degenerate. These accidental degeneracies in the empty lattice band structure should be lifted once the scattering effect of the dielectric lattice is taken into account.

To obtain the splitting of the degeneracy at symmetry points or along symmetry directions, one may use group theoretical technique to diagonalize the matrix in (2.11). When a degenerate mode at a symmetry point splits, each of its split mode must transform according to one of the small representations of the group of $\mathbf{k}$ vector for that symmetry point. Working with the character table, one can find out the symmetry type for all the split modes, and then construct symmetrized linear combination of vector waves, $\sum_{\mathbf{K},\lambda}A_{\mathbf{k}+\mathbf{K},\lambda}\hat{\mathbf{e}}_\lambda e^{i(\mathbf{k}+\mathbf{K})\cdot\mathbf{r}}$, accordingly, where $\hat{\mathbf{e}}_1$ and $\hat{\mathbf{e}}_2$ are the two polarization vectors perpendicular to $\mathbf{k}+\mathbf{K}$. Using the symmetrized plane waves as a basis, the matrix in (2.11) is greatly simplified. We further simplify the calculation by dealing only with the block matrix connecting plane waves belonging to the same degenerate state and thus neglecting all other band interactions.

In presenting the results we begin with a discussion of the splitting of the mode $\omega=1$ at $\Gamma\left(\omega \text{ in units of } c\sqrt{\left(\frac{1}{\epsilon}\right)_{000}}\frac{2\pi}{a}\right)$. Due to scattering by the dielectric lattice this state splits into several modes. We give each of the split states by specifying its symmetry type (in commonly used notation for the irreducible representation), its degeneracy (indicated by the bracketed number), the explicit form of its **H**-field and its frequency. In this list the wave vector will be expressed in units of $\frac{2\pi}{\mathbf{a}}$, the frequency in units of $c\sqrt{\left(\frac{1}{\epsilon}\right)_{000}}\frac{2\pi}{a}$. The three unit vectors along the cubic axes will be denoted by $\hat{\mathbf{x}},\hat{\mathbf{y}},\hat{\mathbf{z}}$.

$\Gamma'_{15}(3)$

$$\begin{bmatrix}\hat{\mathbf{x}}\sin y-\hat{\mathbf{y}}\sin x\\ \hat{\mathbf{y}}\sin z-\hat{\mathbf{z}}\sin y\\ \hat{\mathbf{z}}\sin x-\hat{\mathbf{x}}\sin z\end{bmatrix}$$

$$\omega=(1+2B+D)^{1/2}$$

$$B=\frac{\left(\frac{1}{\epsilon}\right)_{110}}{\left(\frac{1}{\epsilon}\right)_{000}},\quad D=\frac{\left(\frac{1}{\epsilon}\right)_{200}}{\left(\frac{1}{\epsilon}\right)_{000}}$$

$\Gamma_{15}(3)$

$$\begin{bmatrix}\hat{\mathbf{x}}(\cos y+\cos z)\\ \hat{\mathbf{y}}(\cos z+\cos x)\\ \hat{\mathbf{z}}(\cos x+\cos y)\end{bmatrix}$$

$$\omega=(1-D)^{1/2}$$

$\Gamma'_{25}(3)$

$$\begin{bmatrix}\hat{\mathbf{x}}\sin y+\hat{\mathbf{y}}\sin x\\ \hat{\mathbf{y}}\sin z+\hat{\mathbf{z}}\sin y\\ \hat{\mathbf{z}}\sin x+\hat{\mathbf{x}}\sin z\end{bmatrix}$$

$$\omega = (1 - 2B + D)^{1/2}$$

$\Gamma_{25}(3)$

$$\begin{bmatrix} \hat{\mathbf{x}}(\cos y - \cos z) \\ \hat{\mathbf{y}}(\cos z - \cos x) \\ \hat{\mathbf{z}}(\cos x - \cos y) \end{bmatrix}$$

$$\omega = (1 - D)^{1/2}.$$

As can be seen from above, the $\omega = 1$ state splits into three states, $\omega = \sqrt{1 - 2B + D}$ (3 modes), $\omega = \sqrt{1 - D}$ (6 modes), and $\omega = \sqrt{1 + 2B + D}$ (3 modes). In our present model, $D = 0$.

For X point, we discuss the splitting of $\omega = 1/2$ and $\omega = \sqrt{5}/2$ states. First, the state at $\omega = 1/2$ splits into two states.

$X_5(2)$

$$\begin{bmatrix} \hat{\mathbf{y}} \sin \frac{1}{2}x \\ \hat{\mathbf{z}} \sin \frac{1}{2}x \end{bmatrix}$$

$$\omega = \frac{1}{2}(1 + A)^{1/2}$$

$$A = \frac{\left(\frac{1}{\epsilon}\right)_{100}}{\left(\frac{1}{\epsilon}\right)_{000}}$$

$X_5'(2)$

$$\begin{bmatrix} \hat{\mathbf{y}} \cos \frac{x}{2} \\ \hat{\mathbf{z}} \cos \frac{x}{2} \end{bmatrix}$$

$$\omega = \frac{1}{2}(1 - A)^{1/2}\,.$$

As for the $\omega = \sqrt{5}/2$ state, it splits into the following states:

$X_1(1)$

$$-\hat{\mathbf{x}}\, 2 \sin \frac{x}{2}(\cos y + \cos z) + \hat{\mathbf{y}} \cos \frac{x}{2} \sin y + \hat{\mathbf{z}} \cos \frac{x}{2} \sin z$$

$$\omega = \frac{\sqrt{5}}{2}(1 - A - D + E)^{1/2}$$

$X_1'(1)$

$$\hat{\mathbf{z}} \sin \frac{x}{2} \sin y - \hat{\mathbf{y}} \sin \frac{x}{2} \sin z$$

$$\omega = \frac{\sqrt{5}}{2}(1 - \frac{3}{5}A + \frac{8}{5}B - \frac{8}{5}C + \frac{3}{5}D - E)^{1/2}$$

$$C = \frac{\left(\frac{1}{\epsilon}\right)_{111}}{\left(\frac{1}{\epsilon}\right)_{000}}, \quad E = \frac{\left(\frac{1}{\epsilon}\right)_{210}}{\left(\frac{1}{\epsilon}\right)_{000}}$$

$X_2(1)$

$$-\hat{\mathbf{x}}\, 2 \sin \frac{x}{2}(\cos y - \cos z) + \hat{\mathbf{y}} \cos \frac{x}{2} \sin y - \hat{\mathbf{z}} \cos \frac{x}{2} \sin z$$

$$\omega = \frac{\sqrt{5}}{2}(1 - A - D + E)^{1/2}$$

$X_2'(1)$

$$\hat{\mathbf{z}} \sin \frac{x}{2} \sin y + \hat{\mathbf{y}} \sin \frac{x}{2} \sin z$$

$$\omega = \frac{\sqrt{5}}{2}(1 - \frac{3}{5}A - \frac{8}{5}B + \frac{8}{5}C + \frac{3}{5}D - E)^{1/2}$$

$X_3'(1)$

$$-\hat{\mathbf{x}}\, 2 \cos \frac{x}{2}(\cos y + \cos z) - \hat{\mathbf{y}} \sin \frac{x}{2} \sin y - \hat{\mathbf{z}} \sin \frac{x}{2} \sin z$$

$$\omega = \frac{\sqrt{5}}{2}(1 + A - D - E)^{1/2}$$

$X_3(1)$

$$\hat{\mathbf{y}} \cos \frac{x}{2} \sin z + \hat{\mathbf{z}} \cos \frac{x}{2} \sin y$$

$$\omega = \frac{\sqrt{5}}{2}(1 + \frac{3}{5}A - \frac{8}{5}B - \frac{8}{5}C + \frac{3}{5}D + E)^{1/2}$$

$X_4'(1)$

$$\hat{\mathbf{x}}\, 2 \cos \frac{x}{2}(\cos y + \cos z) + \hat{\mathbf{y}} \sin \frac{x}{2} \sin y + \hat{\mathbf{z}} \sin \frac{x}{2} \sin z$$

$$\omega = \frac{\sqrt{5}}{2}(1 + A - D - E)^{1/2}$$

$X_4(1)$

$$\hat{\mathbf{z}} \cos \frac{x}{2} \sin y - \hat{\mathbf{y}} \cos \frac{x}{2} \sin z$$

$$\omega = \frac{\sqrt{5}}{2}(1 + \frac{3}{5}A + \frac{8}{5}B + \frac{8}{5}C + \frac{3}{5}E + D)^{1/2}$$

$X_5(2)$

$$\begin{bmatrix} -\hat{\mathbf{x}}\, 2 \cos \frac{x}{2} \sin y + \hat{\mathbf{y}} \sin \frac{x}{2} \cos y \\ \hat{\mathbf{x}}\, 2 \cos \frac{x}{2} \sin z - \hat{\mathbf{z}} \sin \frac{x}{2} \cos z \end{bmatrix}$$

$$\omega = \frac{\sqrt{5}}{2}(1 + A + D + E)^{1/2}$$

$X_5'(2)$

$$\begin{bmatrix} \hat{\mathbf{z}} \cos\frac{x}{2}\cos y \\ -\hat{\mathbf{y}} \cos\frac{x}{2}\cos z \end{bmatrix}$$

$$\omega = \frac{\sqrt{5}}{2}(1 + \frac{3}{5}A - \frac{3}{5}D - E)^{1/2}$$

$X_5'(2)$

$$\begin{bmatrix} \hat{\mathbf{x}}\ 2\sin\frac{x}{2}\sin y + \hat{\mathbf{y}} \cos\frac{x}{2}\cos y \\ \hat{\mathbf{x}}\ 2\sin\frac{x}{2}\sin z + \hat{\mathbf{z}} \cos\frac{x}{2}\cos z \end{bmatrix}$$

$$\omega = \frac{\sqrt{5}}{2}(1 - A + D - E)^{1/2}$$

$X_5(2)$

$$\begin{bmatrix} \hat{\mathbf{z}} \sin\frac{x}{2}\cos y \\ -\hat{\mathbf{y}} \sin\frac{x}{2}\cos z \end{bmatrix}$$

$$\omega = \frac{\sqrt{5}}{2}(1 - \frac{3}{5}A - \frac{3}{5}D + E)^{1/2}\,.$$

In our model, $D = E = 0$. The $\omega = \sqrt{5}/2$ state splits into eight states, *i.e.* $\omega = \frac{\sqrt{5}}{2}(1-A)^{1/2}$ (4 modes), $\omega = \frac{\sqrt{5}}{2}(1+A)^{1/2}$ (4 modes), $\omega = \frac{\sqrt{5}}{2}(1-\frac{3}{5}A)^{1/2}$ (2 modes), $\omega = \frac{\sqrt{5}}{2}(1+\frac{3}{5}A)^{1/2}$ (2 modes), $\omega = \frac{\sqrt{5}}{2}(1-\frac{3}{5}A+\frac{8}{5}B-\frac{8}{5}C)^{1/2}$ (1 mode), $\omega = \frac{\sqrt{5}}{2}(1-\frac{3}{5}A-\frac{8}{5}B+\frac{8}{5}C)^{1/2}$ (1 mode), $\omega = \frac{\sqrt{5}}{2}(1+\frac{3}{5}A-\frac{8}{5}B-\frac{8}{5}C)^{1/2}$ (1 mode), $\omega = \frac{\sqrt{5}}{2}(1+\frac{3}{5}A+\frac{8}{5}B+\frac{8}{5}C)^{1/2}$ (1 mode).

As for the bands along the cubic x-axis, *i.e.* Δ, the lowest two bands remain transverse modes, each with two possible polarizations; they transform like Δ_5 irreducible representation. The next 8-fold degenerate band splits into six bands. Neglecting interaction with other bands, we obtain the following bands:

$\Delta_1(1)$

$$\mathrm{e}^{i\lambda x}[-\hat{\mathbf{x}}(\cos y + \cos z) + i\lambda\hat{\mathbf{y}}\sin y + i\lambda\hat{\mathbf{z}}\sin z]$$

$$\omega = (1+\lambda^2)^{1/2}(1-D)^{1/2}$$

$\Delta_1'(1)$

$$\mathrm{e}^{i\lambda x}(\hat{\mathbf{z}}\sin y - \hat{\mathbf{y}}\sin z)$$

$$\omega = (1+\lambda^2)^{1/2}(1 + \frac{2}{1+\lambda^2}B + \frac{1-\lambda^2}{1+\lambda^2}D)^{1/2}$$

$\Delta_2(1)$

$$\mathrm{e}^{i\lambda x}[-\hat{\mathbf{x}}(\cos y - \cos z) + i\lambda\hat{\mathbf{y}}\sin y - i\lambda\hat{\mathbf{z}}\sin z]$$

$$\omega = (1+\lambda^2)^{1/2}(1-D)^{1/2}$$

$\Delta_2'(1)$

$$\mathrm{e}^{i\lambda x}(\hat{\mathbf{z}}\sin y + \hat{\mathbf{y}}\sin z)$$

$$\omega = (1+\lambda^2)^{1/2}(1 - \frac{2}{1+\lambda^2}B + \frac{1-\lambda^2}{1+\lambda^2}D)^{1/2}$$

$\Delta_5(2)$

$$\begin{bmatrix} \mathrm{e}^{i\lambda x}(i\ \hat{\mathbf{x}}\sin y - \lambda\ \hat{\mathbf{y}}\cos y) \\ \mathrm{e}^{i\lambda x}(i\ \hat{\mathbf{x}}\sin z - \lambda\ \hat{\mathbf{z}}\cos z) \end{bmatrix}$$

$$\omega = (1+\lambda^2)^{1/2}(1+D)^{1/2}$$

$\Delta_5(2)$

$$\begin{bmatrix} \hat{\mathbf{z}}\mathrm{e}^{i\lambda x}\cos y \\ \hat{\mathbf{y}}\mathrm{e}^{i\lambda x}\cos z \end{bmatrix}$$

$$\omega = (1+\lambda^2)^{1/2}(1 - \frac{1-\lambda^2}{1+\lambda^2}D)^{1/2}\,.$$

Once we know the empty lattice bands and their splitting at symmetry points and along symmetry directions, it is not difficult to figure out the entire band structure. For example, the lowest three bands along $(1,0,0)$ axis could be

$$\begin{array}{lll} \Gamma - & \Delta_5 & -X_5' \\ & \Delta_5 & -X_5 \\ & / & \\ \Gamma_{25}' & & \\ & \backslash & \\ & \Delta_2' & -X_2'. \end{array}$$

Now, we come to discuss the photon modes at the corner of the cubic zone, *i.e.* the R point. The empty lattice state at $\omega = \sqrt{3}/2$ is sixteen fold degenerate. This state splits into the following modes due to the presence of the dielectric lattice.

$R_{15}(3)$

$$\begin{bmatrix} \hat{\mathbf{x}}\ 2\cos\frac{x}{2}\cos\frac{y}{2}\cos\frac{z}{2} + \hat{\mathbf{y}}\sin\frac{x}{2}\sin\frac{y}{2}\cos\frac{z}{2} \\ \qquad\qquad + \hat{\mathbf{z}}\sin\frac{x}{2}\cos\frac{y}{2}\sin\frac{z}{2} \\ \hat{\mathbf{x}}\ \sin\frac{x}{2}\sin\frac{y}{2}\cos\frac{z}{2} + \hat{\mathbf{y}}2\cos\frac{x}{2}\cos\frac{y}{2}\cos\frac{z}{2} \\ \qquad\qquad + \hat{\mathbf{z}}\cos\frac{x}{2}\sin\frac{y}{2}\sin\frac{z}{2} \\ \hat{\mathbf{x}}\ \sin\frac{x}{2}\cos\frac{y}{2}\sin\frac{z}{2}\ +\ \hat{\mathbf{y}}\cos\frac{x}{2}\sin\frac{y}{2}\sin\frac{z}{2} \\ \qquad\qquad + \hat{\mathbf{z}}\ 2\cos\frac{x}{2}\cos\frac{y}{2}\cos\frac{z}{2} \end{bmatrix}$$

$$\omega = \sqrt{3}/2(1 + A - B - C)^{1/2}$$

$R'_{15}(3)$

$$\begin{bmatrix} \hat{\mathbf{x}}\ \cos\frac{x}{2}\sin\frac{y}{2}\cos\frac{z}{2} - \hat{\mathbf{y}}\sin\frac{x}{2}\cos\frac{y}{2}\cos\frac{z}{2} \\ \hat{\mathbf{y}}\ \cos\frac{x}{2}\cos\frac{y}{2}\sin\frac{z}{2} - \hat{\mathbf{z}}\cos\frac{x}{2}\sin\frac{y}{2}\cos\frac{z}{2} \\ \hat{\mathbf{z}}\ \sin\frac{x}{2}\cos\frac{y}{2}\cos\frac{z}{2} - \hat{\mathbf{x}}\cos\frac{x}{2}\cos\frac{y}{2}\sin\frac{z}{2} \end{bmatrix}$$

$$\omega = \sqrt{3}/2(1 + \frac{5}{3}A + \frac{5}{3}B + C)^{1/2}$$

$R_{25}(3)$

$$\begin{bmatrix} -\hat{\mathbf{x}}\sin\frac{x}{2}\cos\frac{y}{2}\sin\frac{z}{2} + \hat{\mathbf{y}}\cos\frac{x}{2}\sin\frac{y}{2}\sin\frac{z}{2} \\ -\hat{\mathbf{y}}\sin\frac{x}{2}\sin\frac{y}{2}\cos\frac{z}{2} + \hat{\mathbf{z}}\sin\frac{x}{2}\cos\frac{y}{2}\sin\frac{z}{2} \\ -\hat{\mathbf{z}}\cos\frac{x}{2}\sin\frac{y}{2}\sin\frac{z}{2} + \hat{\mathbf{x}}\sin\frac{x}{2}\sin\frac{y}{2}\cos\frac{z}{2} \end{bmatrix}$$

$$\omega = \sqrt{3}/2(1 - \frac{5}{3}A + \frac{5}{3}B - C)^{1/2}$$

$R'_{25}(3)$

$$\begin{bmatrix} \hat{\mathbf{x}}\ 2\sin\frac{x}{2}\sin\frac{y}{2}\sin\frac{z}{2} + \hat{\mathbf{y}}\cos\frac{x}{2}\cos\frac{y}{2}\sin\frac{z}{2} \\ \qquad + \hat{\mathbf{z}}\cos\frac{x}{2}\sin\frac{y}{2}\cos\frac{z}{2} \\ \hat{\mathbf{y}}\ 2\sin\frac{x}{2}\sin\frac{y}{2}\sin\frac{z}{2} + \hat{\mathbf{z}}\sin\frac{x}{2}\cos\frac{y}{2}\cos\frac{z}{2} \\ \qquad + \hat{\mathbf{x}}\cos\frac{x}{2}\cos\frac{y}{2}\sin\frac{z}{2} \\ \hat{\mathbf{z}}\ 2\sin\frac{x}{2}\sin\frac{y}{2}\sin\frac{z}{2} + \hat{\mathbf{x}}\cos\frac{x}{2}\sin\frac{y}{2}\cos\frac{z}{2} \\ \qquad + \hat{\mathbf{y}}\sin\frac{x}{2}\cos\frac{y}{2}\cos\frac{z}{2} \end{bmatrix}$$

$$\omega = \sqrt{3}/2(1 - A - B + C)^{1/2}$$

$R_{12}(2)$

$$\begin{bmatrix} \hat{\mathbf{x}}\sin\frac{x}{2}\cos\frac{y}{2}\cos\frac{z}{2} - \hat{\mathbf{y}}\cos\frac{x}{2}\sin\frac{y}{2}\cos\frac{z}{2} \\ -\hat{\mathbf{x}}\sin\frac{x}{2}\cos\frac{y}{2}\cos\frac{z}{2} - \hat{\mathbf{y}}\cos\frac{x}{2}\sin\frac{y}{2}\cos\frac{z}{2} \\ \qquad + \hat{\mathbf{z}}\ 2\cos\frac{x}{2}\cos\frac{y}{2}\sin\frac{z}{2} \end{bmatrix}$$

$$\omega = \sqrt{3}/2(1 - A - B + C)^{1/2}$$

$R'_{12}(2)$

$$\begin{bmatrix} -\hat{\mathbf{x}}\cos\frac{x}{2}\sin\frac{y}{2}\sin\frac{z}{2} + \hat{\mathbf{y}}\sin\frac{x}{2}\cos\frac{y}{2}\sin\frac{z}{2} \\ \hat{\mathbf{x}}\cos\frac{x}{2}\sin\frac{y}{2}\sin\frac{z}{2} + \hat{\mathbf{y}}\sin\frac{x}{2}\cos\frac{y}{2}\sin\frac{z}{2} \\ \qquad - \hat{\mathbf{z}}\ 2\sin\frac{x}{2}\sin\frac{y}{2}\cos\frac{z}{2} \end{bmatrix}$$

$$\omega = \sqrt{3}/2(1 + A - B - C)^{1/2}.$$

Thus, the $\omega = \sqrt{3}/2$ mode at R point splits into four states *i.e.*, $\omega = \sqrt{3}/2(1 - \frac{5}{3}A + \frac{5}{3}B - C)^{1/2}$ (3 modes), $\omega = \sqrt{3}/2(1 - A - B + C)^{1/2}$ (5 modes), $\omega = \sqrt{3}/2(1 + A - B - C)^{1/2}$ (5 modes), $\omega = \sqrt{3}/2(1 + \frac{5}{3}A + \frac{5}{3}B + C)^{1/2}$ (3 modes).

Along the body-diagonal of the cubic zone, *i.e.* Λ axis, the lowest empty lattice band remains doubly degenerate and transforms according to Λ_3 irreducible representation. The next six fold degenerate band splits into four bands. When interaction with other bands is neglected, these bands behave as follows:

$\Lambda_1(1)$

$$\mathrm{e}^{i(\lambda x+\lambda y+\lambda z)}\left[\hat{\mathbf{x}}\left(\lambda\mathrm{e}^{-ix} + \frac{1-\lambda}{2}\mathrm{e}^{-iy} + \frac{1-\lambda}{2}\mathrm{e}^{-iz}\right) + \hat{\mathbf{y}}\left(\frac{1-\lambda}{2}\mathrm{e}^{-ix} + \lambda\mathrm{e}^{-iy} + \frac{1-\lambda}{2}\mathrm{e}^{-iz}\right) + \hat{\mathbf{z}}\left(\frac{1-\lambda}{2}\mathrm{e}^{-ix} + \frac{1-\lambda}{2}\mathrm{e}^{-iy} + \lambda\mathrm{e}^{-iz}\right)\right]$$

$$\omega = (3\lambda^2 - 2\lambda + 1)^{1/2}(1 - B)^{1/2}$$

$\Lambda_2(1)$

$$\mathrm{e}^{i(\lambda x+\lambda y+\lambda z)}\left[\hat{\mathbf{x}}(\mathrm{e}^{-iy} - \mathrm{e}^{-iz}) + \hat{\mathbf{y}}(\mathrm{e}^{-iz} - \mathrm{e}^{-ix}) + \hat{\mathbf{z}}(\mathrm{e}^{-ix} - \mathrm{e}^{-iy})\right]$$

$$\omega = (3\lambda^2 - 2\lambda + 1)^{1/2}(1 - \frac{3\lambda^2 - 2\lambda - 1}{3\lambda^2 - 2\lambda + 1}B)^{1/2}$$

$\Lambda_3(2)$

$$\begin{bmatrix} \mathrm{e}^{i(\lambda x+\lambda y+\lambda z)}[\hat{\mathbf{x}}(\mathrm{e}^{-iy} + \mathrm{e}^{-iz}) - \hat{\mathbf{y}}\mathrm{e}^{-iz} - \hat{\mathbf{z}}\mathrm{e}^{-iy}] \\ \mathrm{e}^{i(\lambda x+\lambda y+\lambda z)}[\hat{\mathbf{x}}(\mathrm{e}^{-iy} - \mathrm{e}^{-iz}) + \hat{\mathbf{y}}(2\mathrm{e}^{-ix} + \mathrm{e}^{-iz}) \\ \qquad - \hat{\mathbf{z}}(2\mathrm{e}^{-ix} + \mathrm{e}^{-iy})] \end{bmatrix}$$

$$\omega = (3\lambda^2 - 2\lambda + 1)^{1/2}(1 + \frac{1}{2}\frac{3\lambda^2 - 2\lambda - 1}{3\lambda^2 - 2\lambda + 1}B)^{1/2}$$

$\Lambda_3(2)$

$$\begin{bmatrix} \mathrm{e}^{i(\lambda x+\lambda y+\lambda z)} \\ [\hat{\mathbf{x}}\ (\lambda\mathrm{e}^{-ix} - \frac{1-\lambda}{4}\mathrm{e}^{-iy}) - \frac{1-\lambda}{4}\mathrm{e}^{-iz}) + \hat{\mathbf{y}}(\frac{1-\lambda}{2}\mathrm{e}^{-ix} \\ \qquad -\frac{\lambda}{2}\mathrm{e}^{-iy} - \frac{1-\lambda}{4}\mathrm{e}^{-iz}) + \hat{\mathbf{z}}(\frac{1-\lambda}{2}\mathrm{e}^{-ix} \\ \qquad\qquad -\frac{1-\lambda}{4}\mathrm{e}^{-iy} - \frac{\lambda}{2}\mathrm{e}^{-iz})] \\ \mathrm{e}^{i(\lambda x+\lambda y+\lambda z)} \\ [\hat{\mathbf{x}}\ (\frac{1-\lambda}{4}\mathrm{e}^{-iy} - \frac{1-\lambda}{4}\mathrm{e}^{-iz}) + \hat{\mathbf{y}}(\frac{\lambda}{2}\mathrm{e}^{-iy} - \frac{1-\lambda}{4}\mathrm{e}^{-iz}) \\ \qquad\qquad + \hat{\mathbf{z}}(\frac{1-\lambda}{4}\mathrm{e}^{-iy} - \frac{\lambda}{2}\mathrm{e}^{-iz})] \end{bmatrix}$$

$$\omega = (3\lambda^2 - 2\lambda + 1)^{1/2}(1 + \frac{1}{2}B)^{1/2}.$$

From the results above, we conclude that the lowest three bands along Λ-axis could be

$$\begin{array}{ccccc} \Gamma & - & \Lambda_3 & - & R_{12} \\ & & \Lambda_3 & & \\ & / & & \backslash & \\ \Gamma'_{25} & & & & R'_{25} \\ & \backslash & & / & \\ & & \Lambda_1 & & \end{array} .$$

4 Remarks

As is known, the nearly-plane-wave method, when applied to electrons in a crystal, often gives us powerful insight into the electronic band structure. In the form of semi-empirical pseudopotential approach, the method even produces quantitatively meaningful results. When applied to photons, since the condition (3.2) for the validity of the method can be more easily satisfied than the weak potential assumption in the electron case, the method is expected to work better here. On the other hand, there is a problem with the convergence of the plane wave method. As can be seen from (3.1) and (2.1), the coupling between larger and larger reciprocal lattice vectors does not decrease very rapidly. These higher band interactions should be included, perhaps by using techniques of perturbation theory or by numerical procedures, if one wants to obtain quantitatively meaningful results. We have numerically calculated the band structure by including a large number of plane waves in the expansion in (2.5). In the Appendix we compare the numerical results with the approximate results obtained in the previous Section. In any case, the splittings of degenerate modes at symmetry points and along symmetry directions obtained here are based on group theory; they remain qualitatively correct. Therefore, we may draw certain conclusions from these results, especially in regard to questions like how to manufacture a photonic gap which extends to the entire Brillouin zone.

For this problem, one would first look at the symmetry of the dielectric lattice. For example, in a simple cubic lattice studied here, it seems impossible to get a full gap between the second and the third band because the two bands will always touch each other at the Γ-point. This is because that the split modes of $\omega = 1$ degenerate state at Γ are all 3-fold degenerate, as discussed in Section 3. To lift this degeneracy, one must distort the cubic lattice into, say, a tetragonal lattice. In a simple cubic lattice, it looks more hopeful to obtain a full gap between the first and the second band. But whether this can be realized depends on two factors. First, the lowest split state of $\omega = \sqrt{3}/2$ degenerate mode at R should be only doubly degenerate, *i.e.*, having either R'_{12} or R_{12} symmetry, instead of belonging to other symmetry with 3-fold degeneracy. Second, this lowest split state at R must lie below the upper split mode of $\omega = 1/2$ state at X so that the gaps at R and at X may coincide. Since $\omega = \sqrt{3}/2$ state and $\omega = 1/2$ state are widely separated, in the sense that their difference is an appreciable fraction of their frequency, the second requirement may not be easy to achieve unless the lattice has very high dielectric contrast.

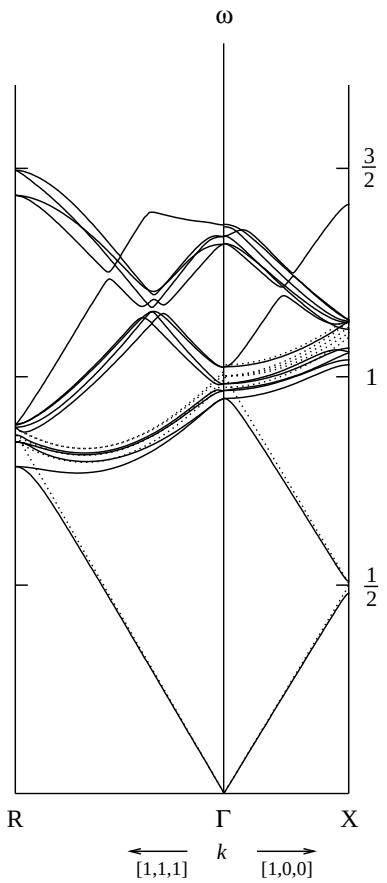

Fig. 2. Photonic band structure for the simple cubic lattice of Section 3 with $\epsilon_1 = 2$, $\epsilon_2 = 1$, and frequency in units of $c\sqrt{\left(\frac{1}{\epsilon}\right)_{000}}\frac{2\pi}{a}$. The solid lines were determined numerically using $N = 587$ plane waves, while the dotted lines represent the lowest band approximation considered in the text.

This brings us to discuss a F.C.C. dielectric lattice structure. Comparing with simple cubic lattice, the Brillouin zone, as a truncated octahedron, is closer to being a sphere. The distances of X, L, and W points from the center of the zone do not differ that much. As a result, the first empty lattice band states at these points are close to each other in frequency. Specifically, the first empty lattice state has frequency $\omega = 1$ at X, $\omega = \sqrt{3}/2$ at L and $\omega = \sqrt{5}/2$ at W. Unlike in the simple cubic structure the frequency difference between any two state here is a small fraction of the frequency itself. All these degenerate states split due to lattice scattering with the gap proportional to $\left(\frac{1}{\epsilon}\right)_{200}$ at X and W, and to $\left(\frac{1}{\epsilon}\right)_{111}$ at L. So long as these Fourier coefficients do not vanish, gaps will open up at these symmetry points. When the size of the gaps become comparable to the frequency difference between the empty lattice states, the gaps are likely to coincide. This is the essential reason why all calculations in photonic bands leads to the conclusion that gaps exist in F.C.C. and diamond

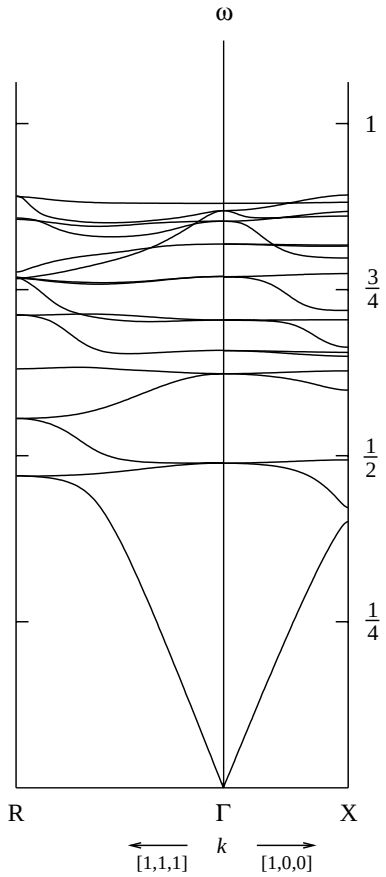

Fig. 3. Photonic band structure for $\epsilon_1 = 16, \epsilon_2 = 1$,and frequency in units of $c\sqrt{\left(\frac{1}{\epsilon}\right)_{000}}\frac{2\pi}{a}$. The bands were determined numerically using $N = 1503$ plane waves.

structure. We shall, in a future publication, elaborate in detail what factors in a dielectric lattice would make it favorable for obtaining a full photonic gap.

Appendix

In order to check whether our results based on the empty lattice band structure are quantitatively meaningful, we have performed a numerical calculation of the photonic bands by including a large number of plane waves in the expansion in (2.5). This has been done for two cases, one for lattice with low dielectric contrast and one with high dielectric contrast. In each case, we have included enough number of plane waves to achieve convergence. The numerical results are compared with those obtained using the approximations described in Section 3. For low dielectric contrast the comparison is presented in Figure 2 and for high dielectric contrast in Figure 3. As expected, the agreement is quite good for low dielectric contrast. In fact, the agreement is very good for the case with dielectric ratio $\epsilon_2/\epsilon_1 = 1.1$, but we do not show this case here because for the most part it is hard to distinguish the two sets of results. On the other hand there are noticeable deviations between the two sets of results for high dielectric contrast case in Figure 3. It is noted that in the present model, the lowest state at R is triply degenerate so there is no gap between the first and the second band.

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