The Extended Plane Wave Expansion Method in Three Dimensional Anisotropic Photonic Crystal

Young-Chung Hsu\textsuperscript{1}  
\textit{Department of Physics and Astronomy, Northwestern University, Evanston, Illinois 60201}

Ben-Yuan Gu\textsuperscript{2}  
\textit{Institute of Physics, Academia Sinica, P.O. Box 603, Beijing 100080, China}

In this paper, we extend the conventional plane wave expansion method in 3D anisotropic photonic crystal to be able to calculate the complex $k$ even if permittivity and permeability are complex numbers or the functions of $\omega$. There are some tricks in the derivation process, so we show the process in detail. Besides, we also provide an example for testing and explaining, and we also compare the results with the band structure derived from conventional plane wave expansion method, then we finally find that there is a good consistency between them.

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Recently, the researches of the properties of the photonic crystals (PCs) have aroused great interests, since the concept of the PCs has been proposed by Yablonovich and John\textsuperscript{[1,2,3]}. Briefly speaking, PCs are periodically structured electromagnetic media, generally processing photonic band gap (PBG). Most of the studies stress the PBG structures with the use of conventional plane-wave expanded (PWE) method\textsuperscript{[4,5]}. However, there are still many articles explore the influence of PCs with the use of conventional PWE method. So we have no qualms about the inaccuracy of the propagation modes between these two methods.

The system we discussed is periodically structured without charge $\rho$ and current $J$. Therefore, according to Maxwell Equation, the magnetic field $H(r)$ should obey

$$-(k + G) \times \epsilon^{-1}_G \cdot (k + G') \times H_{G'} = \omega^2 \mu_G \cdot H_{G'},$$

(1)

where

$$H(r) = \sum_G H_G e^{i(k + G) \cdot r},$$

$$\epsilon(r) = \sum_G \epsilon_G e^{iG \cdot r},$$

$$\mu(r) = \sum_G \mu_G e^{iG \cdot r},$$

$G$ and $G'$ are the reciprocal lattice vectors, $\omega$ and $k$ are the frequency and wave vector, $\epsilon(r)$ and $\mu(r)$ are the tensors of permittivity and permeability of which $\epsilon_G$ and $\mu_G$ are the Fourier expansion components, respectively.

Now, let us expand Eq.(1) directly through $\mathbf{\hat{x}}, \mathbf{\hat{y}}$ and $\mathbf{\hat{z}}$ directions.

\[ \hat{x}: \]

$$\left[(k + G)_y \epsilon^{-1}_{yz} (k + G')_z + (k + G)_z \epsilon^{-1}_{zy} (k + G')_y - (k + G)_y \epsilon^{-1}_{zx} (k + G')_y - (k + G)_z \epsilon^{-1}_{zy} (k + G')_y\right] H_x$$

$$+ \left[(k + G)_y \epsilon^{-1}_{xz} (k + G')_z + (k + G)_z \epsilon^{-1}_{zx} (k + G')_y - (k + G)_y \epsilon^{-1}_{xx} (k + G')_z - (k + G)_z \epsilon^{-1}_{xy} (k + G')_z\right] H_y$$

$$+ \left[(k + G)_y \epsilon^{-1}_{xy} (k + G')_y + (k + G)_z \epsilon^{-1}_{yy} (k + G')_z - (k + G)_y \epsilon^{-1}_{xy} (k + G')_y - (k + G)_z \epsilon^{-1}_{yx} (k + G')_y\right] H_z$$

$$= -\omega^2 \left(\mu_{xx} H_x + \mu_{xy} H_y + \mu_{xz} H_z\right),$$

(2a)
\[ \hat{y} : \]
\[ \left[ (k + G)_z \epsilon_{zy}^{-1} (k + G')_z + (k + G)_x \epsilon_{zx}^{-1} (k + G')_y - (k + G)_x \epsilon_{zy}^{-1} (k + G')_y - (k + G)_x \epsilon_{zy}^{-1} (k + G')_z \right] H_x + \left[ (k + G)_z \epsilon_{zy}^{-1} (k + G')_x + (k + G)_x \epsilon_{zx}^{-1} (k + G')_z - (k + G)_x \epsilon_{zy}^{-1} (k + G')_z - (k + G)_x \epsilon_{zy}^{-1} (k + G')_x \right] H_y + \left[ (k + G)_z \epsilon_{zy}^{-1} (k + G')_y + (k + G)_x \epsilon_{zx}^{-1} (k + G')_y - (k + G)_x \epsilon_{zy}^{-1} (k + G')_x - (k + G)_x \epsilon_{zy}^{-1} (k + G')_y \right] H_z = -\omega^2 (\mu_{yx} H_x + \mu_{yy} H_y + \mu_{yz} H_z), \]

(2b)

\[ \hat{z} : \]
\[ \left[ (k + G)_z \epsilon_{zy}^{-1} (k + G')_z + (k + G)_y \epsilon_{yx}^{-1} (k + G')_y - (k + G)_y \epsilon_{zy}^{-1} (k + G')_y - (k + G)_y \epsilon_{zy}^{-1} (k + G')_z \right] H_x + \left[ (k + G)_z \epsilon_{zy}^{-1} (k + G')_x + (k + G)_y \epsilon_{yx}^{-1} (k + G')_z - (k + G)_y \epsilon_{zy}^{-1} (k + G')_z - (k + G)_y \epsilon_{zy}^{-1} (k + G')_x \right] H_y + \left[ (k + G)_z \epsilon_{zy}^{-1} (k + G')_y + (k + G)_y \epsilon_{yx}^{-1} (k + G')_y - (k + G)_y \epsilon_{zy}^{-1} (k + G')_x - (k + G)_y \epsilon_{zy}^{-1} (k + G')_y \right] H_z = -\omega^2 (\mu_{zx} H_x + \mu_{zy} H_y + \mu_{zz} H_z), \]

(2c)

where \( \epsilon_{ij} \) and \( \mu_{ij} \) are the abbreviations of \( \hat{\epsilon}_{G' \cdot i, j} \) and \( \hat{\mu}_{G' \cdot i, j} \), and \( H_1 \) is the abbreviation of \( H_{G', i} \). When \( k \) is provided, Eq.(2) becomes an eigenvalue problem in which the eigenvalue is \( \omega \) and is the conventional PWE method. Now, there comes up an interesting question that is whether \( k \) must be a vector of which the components are real numbers. The answer is "No", and we just need to do some modification on Eq.(2) to get the complex \( k \), because Eq.(2) is a 4 variables (\( k, x, y, z \)) component of Eq.(1), because \( \hat{\epsilon}_{G'} \) and its expansion type is

\[ \hat{\epsilon}_{G'} = \hat{\epsilon}_{A} \hat{G}_{1}, \]

and its expansion type is

\[ \hat{B}_1 H_{G, x} + \hat{C}_1 H_{G, x} + \hat{B}_2 \hat{C}_2 \left( \begin{array}{c} H_{G} \\ H_{G} \end{array} \right) = k_1 \tilde{A} \left( \begin{array}{c} \tilde{H}_{G_{1}, x} \\ \tilde{H}_{G_{1}, x} \end{array} \right), \]

(3)

where \( \tilde{A}, \hat{B}_1, \hat{B}_2, \hat{C}_1, \hat{C}_2 \) are \( 2N \times 2N, \quad 2N \times N, \quad 2N \times 2N, \quad 2N \times 2N \) and \( 2N \times 2N \) matrices and their elements will be illustrated in Appendix.

As regards the \( \tilde{x} \) component of Eq.(2), we can write in another form which is different from \( \tilde{y} \) and \( \tilde{z} \) components of Eq.(2). Thus the matrix form of Eq.(2a) is

\[ \left( \begin{array}{c} \tilde{E}_1 \tilde{E}_2 \\ H_G \end{array} \right) = \tilde{D} \left( \begin{array}{c} \tilde{H}_{G_{1}, x} \\ \tilde{H}_{G_{1}, x} \end{array} \right), \]

(4)

where \( \tilde{D}, \tilde{E}_1, \tilde{E}_2 \) are \( N \times 2N, \quad N \times N, \quad N \times 2N \) and their elements are also in Appendix.

From Eq.(4) we obtain

\[ H_{G, x} = -\tilde{E}_1^{-1} \tilde{E}_2 \tilde{H}_{G_{1}, x} + \tilde{E}_1^{-1} \tilde{D} \tilde{H}_{G_{1}, x}, \]

(5a)

\[ \tilde{H}_{G_{1}, x} = -\tilde{E}_1^{-1} \tilde{E}_2 \tilde{H}_{G_{1}, x} + k_{1} \tilde{E}_1^{-1} \tilde{D} \tilde{H}_{G_{1}, x}, \]

(5b)

where Eq.(5b) is the production of Eq.(5a) multiplied by \( k_{1} \). A combination of Eqs.(3) and (5) yields
$$k_x \tilde{H}_{G\perp} = \left[ \hat{A} - \hat{C}_1 \hat{E}_1^{-1} \hat{D} \right]^{-1} \left[ \left( \hat{B}_1 \hat{E}_1^{-1} \right) \left( -\hat{E}_2 : \hat{D} \right) + \left( \hat{C}_1 \hat{E}_1^{-1} \right) \left( 0 : -\hat{E}_2 \right) + \left( \hat{B}_2 \hat{C}_2 \right) \right] \left( \begin{array}{c} \hat{H}_{G\perp} \\ \hat{H}_{G\perp} \end{array} \right),$$

where $\tilde{F}$ is a $2N \times 4N$ matrix. Considering the equation above with $k_x \hat{H}_{G\perp} = \hat{H}_{G\perp}$, we finally have an equation

$$\left( \begin{array}{c} 0 : I \\ \ldots \\ F \end{array} \right) \left( \begin{array}{c} \hat{H}_{G\perp} \\ \hat{H}_{G\perp} \end{array} \right) = k_x \left( \begin{array}{c} \hat{H}_{G\perp} \\ \hat{H}_{G\perp} \end{array} \right),$$

which is an $k_x$ eigenvalue equation, and the order of eigenfunction $\left( \begin{array}{c} \hat{H}_{G\perp} \\ \hat{H}_{G\perp} \end{array} \right)$ is $4N$. In addition, $0$ and $I$ are $2N \times 2N$ zero matrix and identity matrix, alternatively.

For testing this method, we use an Intel centrino 1.4G, 512 MB RAM with matlab code published on mathworks website to run an isotropic simple cubic case in which the GaAs square rods — their widths are 0.4a, and $a$ is the lattice constant — cross together from the $\hat{x}$, $\hat{y}$ and $\hat{z}$ direction. The lattice constant, width of square rods and $\epsilon$ of GaAs are $a$, 0.4a and 11.43$\epsilon_0$, respectively.

We spent about 6 hours on getting Figs.(2b) and (2c) when using 729 {G} and taking 17 $k_y$ points from 0 to $\frac{\pi}{a}$ to accomplish the calculation. As regards Fig.(2a), it is the band structure which is derived from Eq.(2) and used to compare with our method. In Fig.(2a), we can find that $\omega = 0.2 \frac{\pi c}{a}$ is not located in band gap, so such kind of condition should also appeared in our method when we choose the same $\omega$ to plot the contour line or surface. Figure (2b) in which $\omega = 0.2 \frac{\pi c}{a}$, $k_z = 0$ and $k_y$ scanned from $-\frac{\pi}{a}$ to $\frac{\pi}{a}$ is the figure of real value solution of $k_x$ derived from Eq.(6). When Fig.(2a) compares with Fig.(2b), we will find out the width of contour in Fig.(2b) equals the width of $X \rightarrow \Gamma$ region in Fig.(2a).

**FIG. 1:** The schematic view of a cubic unit cell in which three GaAs square rods cross together from the $\hat{x}$, $\hat{y}$ and $\hat{z}$ direction. The lattice constant, width of square rods and $\epsilon$ of GaAs are $a$, 0.4a and 11.43$\epsilon_0$, respectively.

**FIG. 2:** The numerical results of Fig.1. (a) is the band structure derived from Eq.(2) and in which the bold line is the $\omega = 0.2 \frac{\pi c}{a}$ line. (b) and (c) are the equal frequency contour line of propagation modes in k space and the $\min(|\text{Im}(k_x)| \neq 0)$ vs. $k_y$ figure, alternatively. The circle in (b) denotes the incident light of which $\omega = 0.2 \frac{\pi c}{a}$, $k_z = 0$ and $k_y$ is scanned from $-\frac{\pi}{a}$ to $\frac{\pi}{a}$.

Besides, we can find that there are two propagation modes toward right when $k_y$ is a fixed number in Fig.(2b). These modes are similar to TE and TM modes in 2D isotropic PC, however, they can not be distinguished in 3D PC, we just plot them directly. Furthermore, $C_4^1$ sym-
metry exists in Fig.(2b) but not in the figure of real part of complex \( k_x \). The reason is the real number solutions of \( k_x \) are the \( k_x \) of the propagation modes which are the solutions of bulk system in which the \( C_4^1 \) symmetry exist. However, the above is not correct when \( k_x \) are complex numbers, because the complex means that there is an interface destroying the \( C_4^1 \) symmetry and facing \( \hat{x} \) direction in the system as well. Therefore, all the evanescent modes of which \( k_x \) are complex numbers just exist near the interface and their penetration depths correspond to 2\( \pi/|\text{Im}(k_x)| \neq 0 \) owing to \( \exp(ikx) = \exp(k_0x) \exp(k_x \bar{x}) \), where \( k_0 \) and \( k_x \) are the real and imaginary parts, respectively. The most remarkable one of the complex \( k_x \) relates to the longest penetration depth denoted as \( \lambda_{LPD}^I(k_y,k_x,\omega) \), because almost nothing but the propagation modes can exist in this system when the distance from the detecting position to the interface is larger than \( \lambda_{LPD}^I(k_y,k_x,\omega) \). Therefore, a semi-infinite system can be treated as two individual regions: surface and bulk regions, all the evanescent modes just exist in the surface region of which the width is \( \lambda_S \) defined as \( \text{max}(\lambda_{LPD}^S(k_y,k_z,\omega_0)) \), where \( \omega_0 \) is a fixed frequency. For a finite size PC, if the effect of corner is not important, \( \lambda_S \) decides the smallest size of PC. If the size is smaller than the smallest one, the system no longer can be treated as a periodic structured media. Figure(2c) is the figure of \( a/\lambda_{LPD}^S \) vs. \( k_y \) at \( \omega = 0.2 \frac{2\pi}{a} \). This figure indicates that the \( a/\lambda_{LPD}^S \) drops to zero quickly when \( k_y \) is located at the edge of contour in Fig.(2b). This kind of situation arises while the state located at the edge of contour changes from propagation mode to evanescent mode. Besides, because \( |k_y| \leq \frac{0.2}{a} \frac{2\pi}{a} \) when the incident light is a propagation mode in vacuum, we can find that \( a/\lambda_{LPD}^S > 0.7 \). Therefore, the longest penetration depth is \( a/0.7 \) for all incident light perpendicular to \( \hat{z} \) direction.

In conclusion, because Eq.(6) is a \( k_x \) eigenvalue equation when \( \omega, k_y \) and \( k_z \) are provided, the \( \omega \) can be a real number at any time, and \( \epsilon \) and \( \mu \) can be the function of \( \omega, k_y \) and \( k_z \) or complex tensors. In addition, since most of \( k_z \) are complex numbers, the minimum of \( \text{Im}(k_z) \neq 0 \) must exist, and this value will decide how large a PC is able to treated as a single crystal if the influence of corner is not important. Therefore, one of the issues we proceed to research is the influence of corner. We thank Prof. Ping Shen for his opinion to excite us to find out the 3D formula EPWE method.

I. APPENDIX

The \( \epsilon_{ij} \) shown as below is the abbreviation of \( \mathbf{G} \). G.\( i,j \).

\[
A = \begin{pmatrix}
\epsilon_{xx}^{-1} & -\epsilon_{xy}^{-1} & -\epsilon_{xz}^{-1} \\
-\epsilon_{yx}^{-1} & \epsilon_{yy}^{-1} & -\epsilon_{yz}^{-1} \\
-\epsilon_{zx}^{-1} & -\epsilon_{zy}^{-1} & \epsilon_{zz}^{-1}
\end{pmatrix}
\]

\[
B_{1,11} = \epsilon_{xx}^{-1}(k + G')y + \epsilon_{xy}^{-1}(k + G')z - \epsilon_{yx}^{-1}(k + G')y - \epsilon_{yy}^{-1}(k + G')z - \epsilon_{xy}^{-1}(k + G')y - \epsilon_{yy}^{-1}(k + G')z
\]

\[
B_{1,21} = \epsilon_{xx}^{-1}(k + G')y + \epsilon_{xy}^{-1}(k + G')z - \epsilon_{yx}^{-1}(k + G')y - \epsilon_{yy}^{-1}(k + G')z
\]

\[
B_{2,11} = \epsilon_{xx}^{-1}(k + G')y + \epsilon_{xy}^{-1}(k + G')z - \epsilon_{yx}^{-1}(k + G')y - \epsilon_{yy}^{-1}(k + G')z
\]

\[
C_{1,11} = \epsilon_{xx}^{-1}(k + G')y - \epsilon_{xy}^{-1}(k + G')z
\]

\[
C_{1,21} = \epsilon_{yy}^{-1}(k + G')y - \epsilon_{yx}^{-1}(k + G')y
\]

\[
C_{2,11} = \epsilon_{xx}^{-1}(k + G')z - \epsilon_{yx}^{-1}(k + G')y - \epsilon_{xz}^{-1}(G_x + G')z
\]

\[
C_{2,12} = \epsilon_{yy}^{-1}(k + G')z - \epsilon_{yx}^{-1}(k + G')y - \epsilon_{xz}^{-1}(k + G')y
\]

\[
D_{11} = (k + G)z \epsilon_{yy}^{-1} - \epsilon_{yx}^{-1}G_x + \epsilon_{yz}^{-1}G_y
\]

\[
D_{12} = (k + G)z \epsilon_{yx}^{-1} - \epsilon_{yy}^{-1}G_x + \epsilon_{yz}^{-1}G_y
\]

\[
E_1 = (k + G)_y \epsilon_{yy}^{-1}(k + G')z + (k + G)_z \epsilon_{yz}^{-1}(k + G')y - (k + G)_y \epsilon_{yy}^{-1}(k + G')z + (k + G)_z \epsilon_{yz}^{-1}(k + G')y + \epsilon_{yx}^{-1}(k + G')z - \epsilon_{yy}^{-1}(k + G')y
\]

\[
E_{2,11} = (k + G)_y \epsilon_{yy}^{-1}G_x + (k + G)_z \epsilon_{yz}^{-1}G_y - (k + G)_y \epsilon_{yy}^{-1}G_x + \epsilon_{yx}^{-1}G_y + \epsilon_{yx}^{-1}G_x + \epsilon_{yy}^{-1}G_y
\]

\[
E_{2,12} = (k + G)_z \epsilon_{yx}^{-1}G_x + (k + G)_y \epsilon_{yy}^{-1}G_y - (k + G)_z \epsilon_{yx}^{-1}G_x + \epsilon_{yx}^{-1}G_y + \epsilon_{yx}^{-1}G_x + \epsilon_{yy}^{-1}G_y
\]

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