Vol 12 No 6, June 2003
1009-1963/2003/12(06)/0642-07

Chinese Physics

© 2003 Chin. Phys. Soc.
and IOP Publishing Ltd

Obtaining the band structure of a complicated photonic crystal by linear operations*

Wu Liang(吴 良)[a], Ye Zhuo(叶 卓)[a], and He Sai-Ling(何赛灵)[a,b]

[a] *State Key Laboratory for Modern Optical Instrumentation, Centre for Optical and Electromagnetic Research, Zhejiang University, Hangzhou 310027, China*

[b] *Department of Electromagnetic Theory, Royal Institute of Technology, S-100, 44 Stockholm, Sweden*

(Received 12 May 2002; revised manuscript received 23 February 2003)

Absolute band gaps can be created by lifting the degeneracy in the bands of a photonic crystal. To calculate the band structure of a complicated photonic crystal generated by e.g. symmetry breaking, general forms of all possible linear operations are presented in terms of matrices and a procedure to combine these operations is given. Other forms of linear operations (such as the addition, subtraction, and translation transforms) are also presented to obtain an explicit expression for the Fourier coefficient of the dielectric function in the plane-wave expansion method. With the present method, band structures for various complicated photonic crystals (related through these linear operations) can be obtained easily and quickly. As a numerical example, a large absolute band gap for a complicated photonic crystal structure of GaAs is found in the high region of normalized frequency.

Keywords: photonic crystal, plane-wave expansion method, linear operation, Fourier coefficients
PACC: 7115B

1. Introduction

Photonic crystals, which are in a periodic arrangement of dielectric or metallic materials, have attracted wide attention recently in both physics and engineering communities in view of their unique ability to control light propagation.[1−5] Many potential applications of photonic crystals rely on their photonic band gaps (PBGs). Thus, it is of great interest to design photonic crystals with an absolute band gap (as large as possible), particularly, for a given dielectric material. An absolute PBG in a two-dimensional case requires an overlap of the band gaps for the E- and H-polarizations. It is shown in previous work that degeneracy exists for simple cylinders in a two-dimensional lattice.[6,7] Absolute band gaps can be created by lifting the degeneracy. There are two ways to lift the degeneracy. One is to break the structure symmetry.[8−10] For example, the addition of a rod with a different size into the lattice unit cell can enlarge the absolute band gap.[10] The other is to change the dielectric distribution without breaking the symmetry.[11] In any way, it may result in a photonic crystal with a complicated dielectric distribution.

It is well known that the plane-wave expansion method (see e.g. Refs.[6,7,12,13]) is very useful in obtaining the band structures and studying the properties of photonic crystals. Fourier expansions of dielectric functions are required in the plane-wave expansion method. An explicit expression for the Fourier expansion coefficients of a dielectric function is desirable since a numerical Fourier transform is time-consuming and not effective in accuracy. However, it is not straightforward to obtain an explicit expression for the Fourier coefficients of the dielectric function for a complicated photonic crystal. Some specific examples were given very recently to simplify the calculation of the Fourier coefficients by linear operation.[14] This paper presents our independent work in a more general form including all the possible linear transforms which can be expressed in terms of matrices (we call it the first kind of linear transform). Rotation, scaling and reflection mentioned in Ref.[14] are only specific examples of our matrix expression. In an actual problem these fundamental transforms will appear more likely in a combined form. For this reason, we introduce a procedure to combine a series of linear transforms in the present paper. The verification of the matrix expression and the procedure are given in an elegant way. With the present general form, we can

*Project supported in part by the National Natural Science Foundation of China (Grant No 90101024).

conclude that the Fourier coefficients of a desired photonic crystal, which is obtained from a linear rotation in the real space, can be expressed by a corresponding rotation of the reciprocal vectors. This is still valid even when the linear rotation is not a unitary transform. In addition, we also include in the present paper the second kind of linear transform (such as the translation, addition, and subtraction transforms), which has no equivalent matrix expression. Note that the subtraction transform is not mentioned in Ref.[14].

It is expected that those linear operators of the two kinds can be used to generate complicated structures with large absolute band gaps. For example, both the chessboard lattice[15] and oblique elliptical pores[16,17] can open an absolute band gap when appropriate parameters are chosen (these structures can be obtained easily through the linear operations considered in the present paper). With the present general form of linear operations, band structures for various complicated photonic crystals can be obtained easily and quickly. As a numerical example, we construct a photonic crystal which cannot only demonstrate the validity of linear transform but also has a relatively big forbidden band located in a high region of normalized frequency in the corresponding band structure.

2. General expressions for Fourier coefficients under linear operations

We consider a photonic crystal with dielectric function $\epsilon(\boldsymbol{r})$. From Maxwell's equations one can obtain the following eigenvalue equation

$$\nabla \times [\epsilon^{-1}(\boldsymbol{r})(\nabla \times \boldsymbol{H})] = \frac{\omega^2}{c^2}\boldsymbol{H}. \tag{1}$$

In the plane-wave expansion method, $\boldsymbol{H}$ and $\epsilon^{-1}(\boldsymbol{r})$ are expanded as

$$\boldsymbol{H}(\boldsymbol{r}) = \sum_G \boldsymbol{H}_G \exp[\mathrm{i}(\boldsymbol{k}+\boldsymbol{G})\cdot\boldsymbol{r}], \tag{2}$$

$$\epsilon^{-1}(\boldsymbol{r}) = \sum_G \bar{\epsilon}^{-1}(\boldsymbol{G})\exp(\mathrm{i}\,\boldsymbol{G}\cdot\boldsymbol{r}), \tag{3}$$

where $\boldsymbol{G}$ is the reciprocal lattice vector, and $\boldsymbol{k}$ is a Bloch wavevector.

For a two-component photonic crystal, one can write $\epsilon(\boldsymbol{r})$ in a unit cell in the following form:

$$\epsilon(\boldsymbol{r}) = \epsilon_1 + \Theta(\boldsymbol{r})(\epsilon_2 - \epsilon_1), \tag{4}$$

where ϵ_1, ϵ_2 are the permittivities for the background and inclusion media, respectively, and the step function $\Theta(\boldsymbol{r})$ describes the shape of the inclusion in the unit cell. To extend the integral of Fourier transform in a unit lattice to the whole space without changing the integral value, we extend the function $\Theta(\boldsymbol{r})$ to the whole space by setting its value to be 0 outside the unit lattice, i.e.,

$$\Theta(\boldsymbol{r}) = \begin{cases} 1, & \text{if } \boldsymbol{r} \text{ is inside the inclusion medium} \\ & S \text{ of a reference unit cell,} \\ 0, & \text{otherwise.} \end{cases} \tag{5}$$

The corresponding $\bar{\epsilon}^{-1}(\boldsymbol{G})$ is given by the following integral:

$$\begin{aligned} \bar{\epsilon}^{-1}(\boldsymbol{G}) &= \int_{\text{cell}} \epsilon^{-1}(\boldsymbol{r})\exp(-\mathrm{i}\,\boldsymbol{G}\cdot\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} \\ &= \int_{\text{cell}} \epsilon_1^{-1}\exp(-\mathrm{i}\,\boldsymbol{G}\cdot\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} + \frac{1}{V_{\text{cell}}}\int_S (\epsilon_2^{-1}-\epsilon_1^{-1})\exp(-\mathrm{i}\,\boldsymbol{G}\cdot\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} \\ &= \begin{cases} f\times\epsilon_2^{-1} + (1-f)\times\epsilon_1^{-1}, & \boldsymbol{G}=0, \\ (\epsilon_2^{-1}-\epsilon_1^{-1})\dfrac{1}{V_{\text{cell}}}\displaystyle\int_{-\infty}^{+\infty}\Theta(\boldsymbol{r})\exp(-\mathrm{i}\,\boldsymbol{G}\cdot\boldsymbol{r})\,\mathrm{d}\boldsymbol{r}, & \boldsymbol{G}\neq 0, \end{cases} \end{aligned} \tag{6}$$

where $f = \dfrac{V_S}{V_{\text{cell}}}$ is the filling fraction, i.e., the fraction of the total volume V_{cell} occupied by the volume V_S of the component ϵ_2 in the unit cell.

The linear operations considered in the present paper can be separated into two kinds. A linear operator of the first kind acts on the position vector $\boldsymbol{r}$ and can be expressed by a constant matrix. Linear operations of the second kind include translating, adding, etc., and they cannot be expressed by matrices.

2.1. Linear operations of the first kind

We assume that the linear operator T is a constant full rank matrix in a Cartesian coordinate system and is independent of time and position. Then

we have

$$\begin{aligned}\epsilon_T(\boldsymbol{r}) =&\epsilon(T\boldsymbol{r})\\ =&\epsilon_1+\Theta(T\boldsymbol{r})(\epsilon_2-\epsilon_1).\end{aligned}\tag{7}$$

The corresponding filling fraction is $f_T = f|T^{-1}|$, where T^{-1} is the inverse of T and $|T^{-1}|$ is the determinant of T^{-1}. Let $\hat{T}$ denote the corresponding operator acting on the Fourier coefficients in the $\boldsymbol{G}$ space. The Fourier coefficient for the transformed dielectric function becomes (cf. Eq.(6))

$$\begin{aligned}\bar{\epsilon}_T^{-1}(\boldsymbol{G}) \equiv&\hat{T}\bar{\epsilon}^{-1}(\boldsymbol{G})\\ =&\begin{cases} f_T\times\epsilon_2^{-1}+(1-f_T)\times\epsilon_1^{-1}, & \boldsymbol{G}=0,\\ (\epsilon_2^{-1}-\epsilon_1^{-1})\dfrac{1}{V_{\rm cell}}\displaystyle\int_{-\infty}^{+\infty}\Theta(T\boldsymbol{r})\exp(-\mathrm{i}\,\boldsymbol{G}\cdot\boldsymbol{r})\,\mathrm{d}\boldsymbol{r}, & \boldsymbol{G}\neq 0,\end{cases}\\ =&\begin{cases} f_T\times\epsilon_2^{-1}+(1-f_T)\times\epsilon_1^{-1}, & \boldsymbol{G}=0,\\ (\epsilon_2^{-1}-\epsilon_1^{-1})\dfrac{1}{V_{\rm cell}}|T^{-1}|\displaystyle\int_{-\infty}^{+\infty}\Theta(\boldsymbol{r}')\exp[-\mathrm{i}\,((T^{-1})^{\rm T}\boldsymbol{G})\cdot\boldsymbol{r}']\,\mathrm{d}\boldsymbol{r}', & \boldsymbol{G}\neq 0,\end{cases}\\ =&\begin{cases} |T^{-1}|f\times\epsilon_2^{-1}+(1-|T^{-1}|f)\times\epsilon_1^{-1}, & \boldsymbol{G}=0,\\ |T^{-1}|\bar{\epsilon}^{-1}((T^{-1})^{\rm T}\boldsymbol{G}), & \boldsymbol{G}\neq 0.\end{cases}\end{aligned}\tag{8}$$

The above equation gives the relation between the operator $\hat{T}$ in the $\boldsymbol{G}$ space and the corresponding operator T in the $\boldsymbol{r}$ space. From this equation, one can see that the Fourier coefficient of $\epsilon_T^{-1}(\boldsymbol{r})$ can be obtained from $\bar{\epsilon}^{-1}(\boldsymbol{G})$ by rotating its reciprocal lattice vector $\boldsymbol{G}$ to $(T^{-1})^{\rm T}\boldsymbol{G}$. Note that in the above procedure the lattice remains the same. If one wants to put the inclusions in a different lattice such as a triangular lattice, the reciprocal lattice vector $\boldsymbol{G}$ in an orthogonal lattice should be replaced by $\boldsymbol{G}'$ in the triangular lattice.

To make the paper more instructive, we illustrate the above linear operations and other linear operations with an interesting example in the two-dimensional (2D) case. We wish to transform the photonic crystal with a unit cell in a square lattice (the lattice constant is a) of Fig.1(a) to a photonic crystal with a unit cell of Fig.1(b) by a series of linear transforms. For this example, two simple operators of the first kind are needed, namely, the stretching operator $T_{\rm s}(R_1,R_2)$ (which stretches the inclusion R_1 times along the x-axis direction and R_2 times along the y-axis direction) and the rotation operator $T_{\rm r}(\alpha)$ (which rotates the inclusion with an angle of α in the clockwise direction). These two linear operators have the following forms in a 2D spatial coordinate system,

$$T_{\rm s}(R_1,R_2)=\begin{pmatrix}\dfrac{1}{R_1} & 0\\ 0 & \dfrac{1}{R_2}\end{pmatrix},$$

$$T_{\rm r}(\alpha)=\begin{pmatrix}\cos(-\alpha) & -\sin(-\alpha)\\ \sin(-\alpha) & \cos(-\alpha)\end{pmatrix}.$$

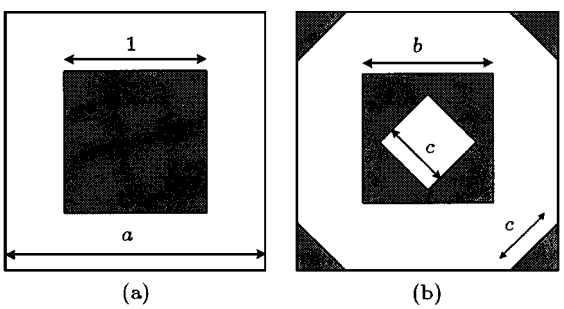


Fig.1. An example for illustrating the linear operations. (a) A unit cell of a simple photonic crystal with a unit square rod as the inclusion. (b) A unit cell of a complicated photonic crystal, whose band structure can be obtained easily from the Fourier coefficient for Fig.1(a) through a series of linear operations.

For a chessboard with equal side length c, we can set $R_1 = R_2 = c$ and $\alpha = \pi/4$. The chessboard can be easily obtained from a simple unit square $\epsilon_{\rm s}(\boldsymbol{r})$ by two consecutive operations $T_{\rm s}$ and $T_{\rm r}$, i.e.,

$$\epsilon_{\rm c}(\boldsymbol{r})=\epsilon_{\rm s}(T_{\rm c}\boldsymbol{r})=\epsilon_{\rm s}(T_{\rm s}T_{\rm r}\boldsymbol{r}),\tag{9}$$

where

$$\begin{aligned}T_{\rm c}(c)=&\begin{pmatrix}\dfrac{1}{c} & 0\\ 0 & \dfrac{1}{c}\end{pmatrix}\times\begin{pmatrix}\cos(-\pi/4) & -\sin(-\pi/4)\\ \sin(-\pi/4) & \cos(-\pi/4)\end{pmatrix}\\ =&\begin{pmatrix}\cos(\pi/4)\dfrac{1}{c} & \sin(\pi/4)\dfrac{1}{c}\\ -\sin(\pi/4)\dfrac{1}{c} & \cos(\pi/4)\dfrac{1}{c}\end{pmatrix}.\end{aligned}$$

When performing a series of linear operations of the first kind on the unit cell in a physical order of T_1,

then T_2, $\cdots$ and finally T_n, one should represent the associated matrix with $T = T_1 T_2 \cdots T_n$ (attention should be paid to the reverse order of the matrices). This is because $\epsilon^{(1)}(\boldsymbol{r}) = \epsilon(T_1\boldsymbol{r})$, $\epsilon^{(2)}(\boldsymbol{r}) = \epsilon^{(1)}(T_2\boldsymbol{r}) = \epsilon(T_1(T_2\boldsymbol{r})) = \epsilon(T_1T_2\boldsymbol{r})$, $\cdots$ Note that linear operators expressed by matrices act on the unit cell only through acting on position vector $\boldsymbol{r}$.

One can easily find the following explicit Fourier coefficient for a square lattice of unit square inclusions,

$$\bar{\epsilon}_{\mathrm{s}}^{-1}(\boldsymbol{G}) = \begin{cases} f \times \epsilon_2^{-1} + (1-f) \times \epsilon_1^{-1}, & \boldsymbol{G} = 0, \\ (\epsilon_2^{-1} - \epsilon_1^{-1}) f \dfrac{\sin(G_x/2)}{G_x/2} \dfrac{\sin(G_y/2)}{G_y/2}, & \boldsymbol{G} \neq 0, \end{cases} \tag{10}$$

where $f = 1/a^2$. Thus, it follows from Eq.(8) that

$$\bar{\epsilon}_{\mathrm{c}}^{-1}(\boldsymbol{G}) \equiv \hat{T}_{\mathrm{c}} \bar{\epsilon}_{\mathrm{s}}^{-1}(\boldsymbol{G}) = \begin{cases} c^2 f \times \epsilon_2^{-1} + (1-c^2 f) \times \epsilon_1^{-1}, & \boldsymbol{G} = 0, \\ (\epsilon_2^{-1} - \epsilon_1^{-1}) c^2 f \dfrac{\sin(G_x^T/2)}{G_x^T/2} \dfrac{\sin(G_y^T/2)}{G_y^T/2}, & \boldsymbol{G} \neq 0, \end{cases} \tag{11}$$

where $\boldsymbol{G}^T \equiv G_x^T \hat{\boldsymbol{x}} + G_y^T \hat{\boldsymbol{y}} = (T_{\mathrm{c}}^{-1}(c))^{\mathrm{T}} \boldsymbol{G} = \left(\dfrac{\sqrt{2}}{2} c G_x + \dfrac{\sqrt{2}}{2} c G_y \right) \hat{\boldsymbol{x}} + \left(-\dfrac{\sqrt{2}}{2} c G_x + \dfrac{\sqrt{2}}{2} c G_y \right) \hat{\boldsymbol{y}}$.

In order to transform the photonic crystal of Fig.1(a) to the photonic crystal of Fig.1(b), several linear operations of the second kind are required.

2.2. Linear operators of the second kind

Unlike the linear operators (of the first kind) T_{s} and T_{c}, the linear operators of the second kind do not take matrix forms. Thus Eq.(8) is not suitable any longer. In the following, two examples are given to obtain the Fourier coefficients expression under the operators of the second kind.

Consider the adding operation. Since Fourier transform is a linear transform, Fourier coefficients can be added directly to describe the Fourier transform for additive objects. For two photonic crystals with the same lattice, we can define the following adding operation (denoted by $\oplus$).

$$\epsilon_a(\boldsymbol{r}) = \epsilon_1(\boldsymbol{r}) + \epsilon_2(\boldsymbol{r}), \tag{12}$$

$$\bar{\epsilon}_a^{-1}(\boldsymbol{G}) \equiv \bar{\epsilon}_1^{-1}(\boldsymbol{G}) \oplus \bar{\epsilon}_2^{-1}(\boldsymbol{G}) = \begin{cases} f \times \epsilon_2^{-1} + (1-f) \times \epsilon_1^{-1}, & \boldsymbol{G} = 0, \\ \bar{\epsilon}_1^{-1}(\boldsymbol{G}) + \bar{\epsilon}_2^{-1}(\boldsymbol{G}), & \boldsymbol{G} \neq 0, \end{cases} \tag{13}$$

where f is the filling fraction of the new photonic crystal. If the inclusions of the two photonic crystals have no overlapping part, one has $f = f_1 + f_2$, where f_1 and f_2 are the filling fractions for the two photonic crystals (to be added together).

If one chooses $\epsilon_2' = \epsilon_1 - \epsilon_2$ for the inclusion medium and $\epsilon_1' = 0$ for the background medium, one can obtain a negative chessboard. Thus, we define the following negative linear operation (denoted by T_{n}),

$$\begin{aligned} \epsilon_{\mathrm{n}}(\boldsymbol{r}) = T_{\mathrm{n}}(\epsilon(\boldsymbol{r})) &= \epsilon_1' + \Theta(\boldsymbol{r})(\epsilon_2' - \epsilon_1') \\ &= 0 + \Theta(\boldsymbol{r})(\epsilon_1 - \epsilon_2), \end{aligned} \tag{14}$$

$$\bar{\epsilon}_{\mathrm{n}}^{-1}(\boldsymbol{G}) \equiv \hat{T}_{\mathrm{n}}(\bar{\epsilon}^{-1}(\boldsymbol{G})) = \begin{cases} f \times (\epsilon_1^{-1} - \epsilon_2^{-1}), & \boldsymbol{G} = 0, \\ (\epsilon_1^{-1} - \epsilon_2^{-1}) \dfrac{1}{V_{\mathrm{cell}}} \\ \times \displaystyle\int_{-\infty}^{+\infty} \Theta(\boldsymbol{r}) \exp(-\mathrm{i}\,\boldsymbol{G} \cdot \boldsymbol{r})\, \mathrm{d}\boldsymbol{r}, & \boldsymbol{G} \neq 0. \end{cases} \tag{15}$$

When we add a negative chessboard to an object, the object loses the chessboard part.

The final operator to be discussed is the translating operator (denoted by T_{t}), which gives the Fourier coefficients for $\epsilon(\boldsymbol{r} - \Delta\boldsymbol{r})$. According to the properties of Fourier transform, we have

$$\epsilon'(\boldsymbol{r}) = T_{\mathrm{t}}(\epsilon(\boldsymbol{r})) = \epsilon(\boldsymbol{r} - \Delta\boldsymbol{r}), \tag{16}$$

$$\begin{aligned} \bar{\epsilon}'^{-1}(\boldsymbol{G}) \equiv& \hat{T}_{\mathrm{t}}(\Delta\boldsymbol{r})(\bar{\epsilon}^{-1}(\boldsymbol{G})) \\ =& \bar{\epsilon}^{-1}(\boldsymbol{G}) \exp(\mathrm{i}\,\boldsymbol{G} \cdot \Delta\boldsymbol{r}). \end{aligned} \tag{17}$$

3. Numerical results

It is obvious that the unit cell of Fig.1(b) (i.e., Fig.2(d)) can be obtained by adding together the three unit cells given by Figs.2(a)–2(c). Therefore, starting from the explicit Fourier coefficient $\bar{\epsilon}_{\mathrm{s}}^{-1}(\boldsymbol{G})$ for a simple photonic crystal with a unit square inclusion (cf. Eq. (10)), we obtain the following explicit Fourier coefficient $\bar{\epsilon}^{-1}(\boldsymbol{G})$ for the photonic crystal with a unit cell of Fig.2(d) through a series of linear operations

$$\bar{\epsilon}^{-1}(\boldsymbol{G}) = \hat{T}_{\mathrm{t}}(\Delta\boldsymbol{r})(\hat{T}_{\mathrm{c}}(c)\bar{\epsilon}_{\mathrm{s}}^{-1}(\boldsymbol{G})) \oplus \hat{T}_{\mathrm{s}}(b,b)\bar{\epsilon}_{\mathrm{s}}^{-1}(\boldsymbol{G}) \oplus \hat{T}_{\mathrm{n}}(\hat{T}_{\mathrm{c}}(c)\bar{\epsilon}_{\mathrm{s}}^{-1}(\boldsymbol{G})), \tag{18}$$

$$= \begin{cases} f \times \epsilon_2^{-1} + (1-f) \times \epsilon_1^{-1}, & \boldsymbol{G} = 0, \\ (\epsilon_2^{-1} - \epsilon_1^{-1}) \left(f \dfrac{\sin(G_x b/2)}{G_x b/2} \dfrac{\sin(G_y b/2)}{G_y b/2} + c^2/a^2 \dfrac{\sin(G_x^T/2)}{G_x^T/2} \dfrac{\sin(G_y^T/2)}{G_y^T/2} \times (S-1) \right), & \boldsymbol{G} \neq 0, \end{cases} \tag{19}$$

where $f = b^2/a^2 - c^2/a^2 + c^2/a^2 = b^2/a^2, S = \exp(-\mathrm{i}\boldsymbol{G} \cdot \Delta\boldsymbol{r})$, and $\hat{T}_{\mathrm{s}}(b,b)$ is related to $T_{\mathrm{s}}(b,b)$ through Eq.(8). Note that there are three additive terms on the right-hand side of Eq.(18). The first, second and third additive terms correspond to the unit cells of Fig.2(b), Fig.2(a) and Fig.2(c), respectively.

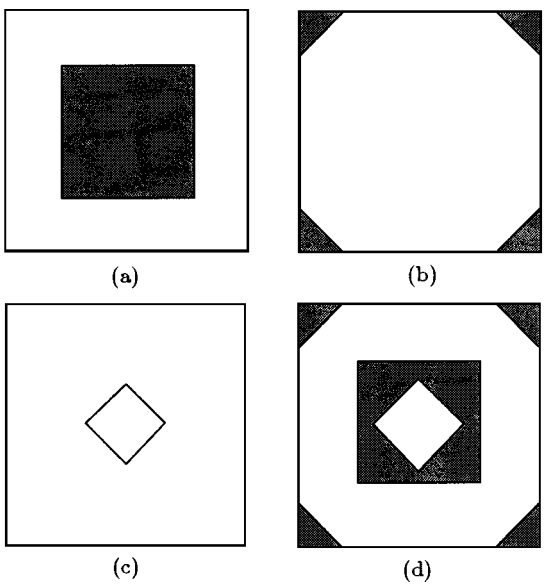


Fig.2. Series of linear operations required for obtaining the unit cell of Fig.1(b) from a unit cell of a unit square rod. The transformed unit cell corresponds to (a) linear operation $T_{\mathrm{s}}(b,b)$; (b) linear operation $T_{\mathrm{t}}(\Delta r)T_{\mathrm{c}}(c)$ with $\Delta r = (a/2, a/2)$; (c) linear operation $T_{\mathrm{n}}T_{\mathrm{c}}(c)$; (d) the consecutive additive operation of (a), (b) and (c).

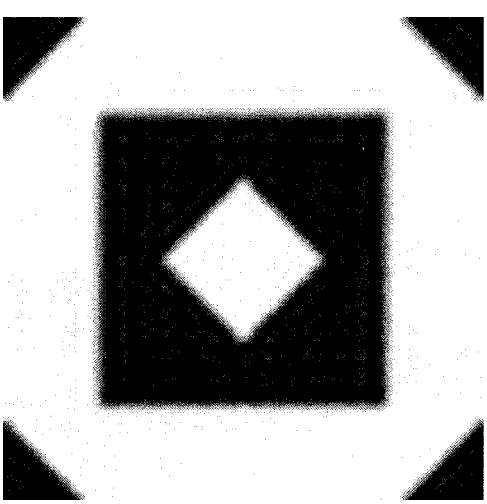


Fig.3. The image of the numerical inverse Fourier transform of the data given by expression (19).

For numerical calculation, we choose $\epsilon_1 = 1$, $\epsilon_2 = 11.4$ (the relative permittivity for GaAs), $b = 0.6a, c = 0.24a, f = 0.36, \Delta\boldsymbol{r} = (a/2, a/2)$. In order to check numerically whether the explicit expression (19) really corresponds to Fourier transform of a unit cell of Fig.1(b), we take a numerical inverse Fourier transform of the data given by expression (19). A total of 20 lattice reciprocal vectors and 100×100 mesh grid points are used to obtain the inverse Fourier transform (cf. Eq.(3)). The numerical results (i.e., the image of the unit cell) are presented in Fig.3, where one sees that the image is indeed the unit cell of Fig.1(b) that we wish to have (the small ripples in Fig.3 are mainly due to errors of numerical inverse Fourier transform). Note that one does not need to perform any numerical Fourier transform or its inverse in the calculation of the band structure of the photonic crystal.

The explicit Fourier coefficients given by Eq.(19) are used to calculate the band structure of the photonic crystal with a unit cell of Fig.1(b). 961 plane waves are used in the plane-wave expansion method and the calculated band structures are shown in Fig.4. The band structures for the E- and H-polarizations are given by the solid and dashed curves, respectively. From this figure, one sees that a large absolute band gap with $\Delta\omega = 0.048(2\pi c_0/a)$ is created around $\omega = 1.048(2\pi c_0/a)$, where c_0 is the speed of light in vacuum. We know that a square lattice of square GaAs rods with the same filling fraction (i.e., the side length $b = 0.6a$) does not have any absolute band gap. It has been shown that the maximum complete band gap for a square lattice of air holes in GaAs is $0.0188(2\pi c_0/a)$.[10] The absolute band gap found in the present paper is nearly 2.6 times larger than that maximum gap value, and is also about 37% larger than the maximum gap value $(0.035(2\pi c_0/a))$ for a square lattice of anisotropic inclusions.[18] What is more interesting is that the present absolute band gap is in a quite high frequency region. For a specific application a photonic device works at a fixed frequency or in a fixed frequency range (e.g., a wavelength around 1.55 μm is used in modern optical communication). On the other hand, one knows that it is easier to fabricate a photonic device with a larger size (i.e., with a larger lattice constant a for a PBG device). For a given filling fraction, the feature scales with the lattice constant a. Therefore, for two different photonic crystals possessing absolute band gaps of similar width, it is easier to fabricate one with the absolute band gap occurring at the higher normalized frequency $\omega(a/2\pi c_0)$ (corresponding to a larger value of a).

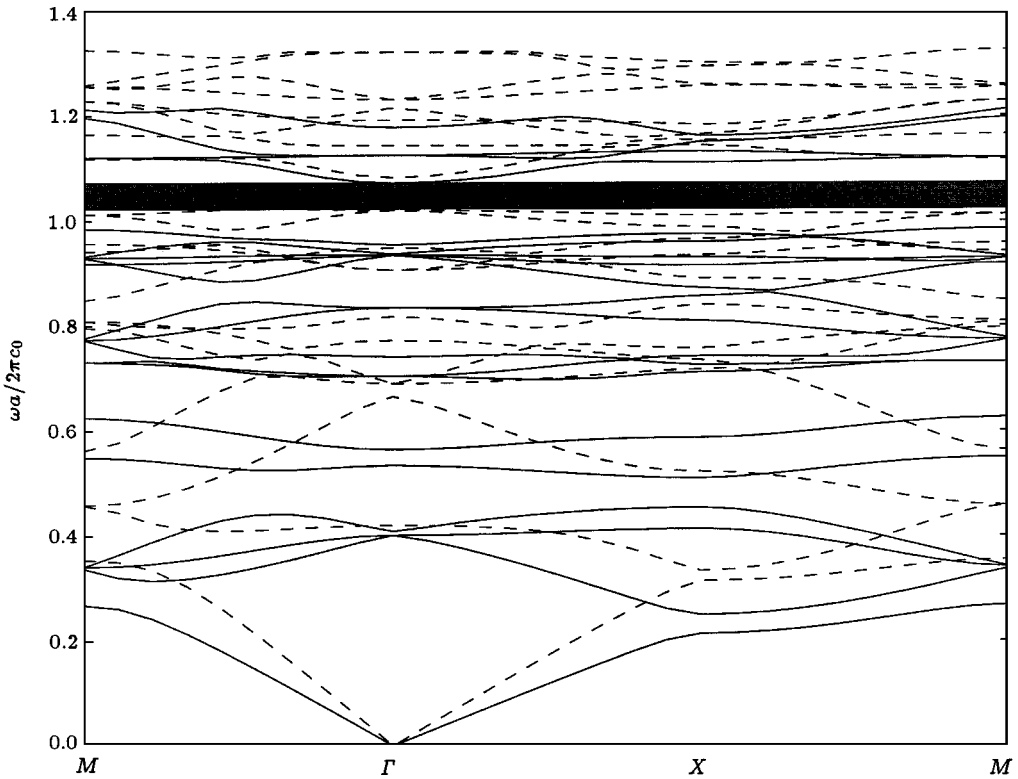


Fig.4. The band structure for the complicated photonic crystal shown in Fig.1(b). Explicit expression (19) for Fourier coefficients is used in the plane-wave expansion method. The band structures for the TE- and TM-mode are given by the solid and dashed curves, respectively.

4. Conclusions

In summary, linear operations have been divided into two categories in the present paper depending on whether they can be expressed in terms of matrices. We have presented the general forms of linear operators which can be expressed in terms of matrices as well as three kinds of linear operators which cannot be expressed with matrices. With the present method, band structures for various complicated photonic crystals (related through these linear operators) can be obtained easily and quickly. To find a manufacturable photonic crystal with a large absolute band gap in the desired frequency region, one usually needs to perform many calculations with a conventional method.[10] With the help of the explicit expression for the Fourier coefficient $\bar{\epsilon}^{-1}(\boldsymbol{G})$ derived in the present paper, the parameters for the introduced linear operations can be optimized quickly to obtain an optimal design of photonic crystals. As a numerical example, a large absolute band gap for a complicated photonic crystal of square lattice of GaAs inclusions has been found in a high region of the normalized frequency.

References

[1] Yablonovitch E 1987 *Phys. Rev. Lett.* **58** 2059

[2] Joannopoulos J D, Mead R D and Winn J N 1995 *Photonic Crystals: Molding the Flow of Light* (Princeton, NJ: Princeton University Press)

[3] Soukoulis C M 1995 *Photonic Band Gaps and Localization, Proceedings of the NATO ARW* (New York: Plenum)

[4] Joannopoulos J D, Villeneuve P and Fan S 1997 *Nature* **386** 143

[5] Xie S Y, Lin Z X and Wu X 1999 *Acta Phys. Sin.* **48** 1459 (in Chinese)

[6] Ho K M, Chan C T and Soukoulis C M 1990 *Phys. Rev. Lett.* **65** 3152

[7] Plihal M and Maradudin A A 1991 *Phys. Rev.* B **44** 8565

[8] Villeneuve P R and Piché M 1992 *Phys. Rev.* B **46** 4969

[9] Cassagne D, Jouanin C and Bertho D 1995 *Phys. Rev.* B **52** 2217

[10] Anderson C M and Giapis K P 1996 *Phys. Rev. Lett.* **77** 2949

[11] Zhang X D and Zhang Z Q 2000 *Phys. Rev.* B **61** 9847

[12] Villeneuve P R and Piché M 1992 *Phys. Rev.* B **46** 4969

[13] Shen L F, He S L and Wu L 2002 *Acta Phys. Sin.* **51** 1133 (in Chinese)

[14] Luan P G and Ye Z 2001 *Preprint* arXiv:cond-mat/0105428

[15] Agio M and Andreani L C 2000 *Phys. Rev.* B **61** 15519

[16] Hillebrand R and Hergert W 2000 *Solid State Commun.* **115** 227

[17] Zhuang F *et al* 2002 *Acta Phys. Sin.* **51** 355 (in Chinese)

[18] Li Z Y, Gu B Y and Yang G Z 1998 *Phys. Rev. Lett.* **81** 2574