# Degeneracy analysis for a supercell of a photonic crystal and its application to the creation of band gaps

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A method is introduced to analyze the degeneracy properties of the band structure of a photonic crystal by making use of supercells. The band structure associated with a supercell of a photonic crystal has degeneracies at the edge of the Brillouin zone if the photonic crystal has some kind of point group symmetry. The *E*-polarization and *H*-polarization cases have the same degeneracies for a two-dimensional (2D) photonic crystal. Two theorems on degeneracies in the band structure associated with the supercell are given and proved. These degeneracies can be lifted to create photonic band gaps by changing the translation group symmetry of the photonic crystal (the point group symmetry of the photonic crystal may remain unchanged), which consequently changes the transform matrix between the supercell and the smallest unit cell. The existence of photonic band gaps for many known 2D photonic crystals is explained through the degeneracy analysis. Some structures with large band gaps are also found through the present degeneracy analysis.

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## I. INTRODUCTION

Photonic crystals, which are periodic arrangements of dielectric or metallic materials, have attracted wide attention recently in both the physics and engineering communities in view of their unique ability to control light propagation [1–4]. Many potential applications of photonic crystals rely on their photonic band gaps (PBGs). It is thus of great interest to design photonic crystals with an absolute band gap as large as possible, particularly for a given dielectric material.

Two-dimensional (2D) photonic crystals have attracted special attention since they are easier to fabricate. Many 2D photonic crystals with large absolute band gaps have been found [5–7]. A rule of thumb based on the difference between the filling factors of the dielectric band and the air band (related to the distribution of the displacement field) can sometimes be used to explain the band gaps, particularly at low frequencies [3,8]. Because of the complication of the differential operators in electrodynamics [different field components are coupled to each other even if the permittivity $\varepsilon(\mathbf{r})$ is separable], it is difficult to obtain analytical (even approximate) solutions for the distribution of the displacement field (particularly at high frequencies). Therefore, many photonic crystals with large absolute band gaps cannot be explained or found by the rule of thumb [10,11,15].

Degeneracy lifting is another explanation for absolute band gaps and even a method to create band gaps [12–17]. The degeneracy can be lifted by, e.g., using hexagonal photonic structures [12], using anisotropic materials [13,14], breaking the space group symmetry [15,16], or changing the dielectric distribution without breaking the space group symmetry [17]. Both accidental and normal degeneracies can exist in a photonic band structure (see, e.g., [17]; this is different from an electronic system). To investigate the degeneracy properties of 2D photonic crystals, the *E* polarization and *H* polarization are usually considered separately as suggested in [12,18]. It is complicated to predict where the degeneracy appears and how to break the degeneracy.

In some cases, we do not have to rely on such an analysis. In the present paper, we introduce a method to create degeneracies first and then break them to create band gaps by studying the band structure associated with a supercell (instead of the unit cell as considered by others in the literature mentioned before). In the band structure associated with a supercell, we can analyze how degeneracies are formed and how to break them to create band gaps.

The point group symmetry of a photonic crystal is defined with respect to the point with the highest symmetry. For example, the point group symmetry is not changed by adding columns at the corners of the unit cell for the 2D photonic crystals considered in [15] (they belong to the same point group symmetry $C_{4v}$). We notice that the translation group symmetry does not change either. Thus the space group symmetry of the photonic crystal does not change at all although the smallest unit cell must include two rods after the additional rods are added. It may be hard to understand the degeneracy breaking for the *H* polarization at point **M** of the second and third bands (as shown in [15]) without careful analysis of the electromagnetic field distribution. However, if we study the band structure associated with a supercell, the lifting of the degeneracy and the creation of PBGs of such photonic crystals can be understood with some tricks even when the space group symmetry of the photonic crystal does not change. For the above example, the photonic crystal with additional columns at the corners can be treated as the result of changing the translation group symmetry (keeping the point group symmetry unchanged) from another photonic crystal with additional columns having the same size as the original column [as shown below in Fig. 3(a) for the square column case], which also belongs to $C_{4v}$ point group symmetry. The present method provides another view for understanding the idea of additional columns. Not surprisingly, many known photonic crystal structures such as the chessboard structure [19,20], a square lattice of square rods [11], and even a triangular air hole structure [3] can be somewhat understood from this point of view (cf. the numerical example associated with Figs. 3–6 below). By using such a degeneracy analysis associated with a supercell, some structures with large band gaps are also found in the present paper.

## II. THEOREMS FOR DEGENERACIES IN THE BAND STRUCTURE ASSOCIATED WITH A SUPER CELL

The unit cell we consider here refers to the smallest periodic region in a photonic crystal. If the periodic region includes more than one unit cell, e.g., two unit cells, it is called a supercell. First we want to study the relation between the band structure associated with the supercell and the original band structure (associated with the unit cell).

In general, we consider a three-dimensional (3D) photonic crystal with primitive lattice vectors $\mathbf{a_1}$, $\mathbf{a_2}$, and $\mathbf{a_3}$. The associated primitive reciprocal vectors $\mathbf{b_1}$, $\mathbf{b_2}$ and $\mathbf{b_3}$ are determined by

$$\mathbf{b}_i = 2\pi \frac{\sum_{j,k=1}^{3} \epsilon_{ijk} \mathbf{a}_j \times \mathbf{a}_k}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}, \tag{1}$$

where $\epsilon_{ijk}$ is the 3D Levi-Cività completely antisymmetric symbol. The complete set of reciprocal lattice vectors is written as $\{\mathbf{G}|\mathbf{G}=l_1\mathbf{b_1}+l_2\mathbf{b_2}+l_3\mathbf{b_3}\}$, where $(l_1,l_2,l_3)$ are integers. We denote the first Brillouin zone formed by these reciprocal lattice vectors $\{\mathbf{G}\}$ as zone A.

The primitive lattice vectors for a supercell are the linear combinations (with integer coefficients) of the primitive lattice vectors for the unit cell, i.e., $\mathbf{a}'_i=\Sigma_{j=1}^{3}N_{ij}\mathbf{a}_j$, $i,j=1,2,3$, where $N_{ij}$ are integers. The corresponding primitive reciprocal vectors for the supercell are determined by $\mathbf{b}'_i=2\pi(\Sigma_{j,k=1}^{3}\epsilon_{ijk}\mathbf{a}'_j\times\mathbf{a}'_k)/[\mathbf{a}'_1\cdot(\mathbf{a}'_2\times\mathbf{a}'_3)]$. The integers $N_{ij}$ form a $3\times3$ transform matrix with a positive determinant $\det(N)\equiv M>0$.

Since

$$\mathbf{b}_i \cdot \mathbf{a}'_j = 2\pi \frac{\sum_{m,n=1}^{3} \epsilon_{imn} \mathbf{a}_m \times \mathbf{a}_n}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \cdot \sum_{l=1}^{3} N_{jl}\mathbf{a}_l = 2\pi N_{ji} \tag{2}$$

it follows from $\mathbf{a}'_i\cdot\mathbf{b}'_j=2\pi\delta_{ij}$ that

$$\mathbf{b}_i = \sum_{j=1}^{3} N_{ji}\mathbf{b}'_j = \sum_{j=1}^{3} N_{ij}^{T}\mathbf{b}'_j, \tag{3}$$

where the superscript $T$ denotes the matrix transposition. The set of reciprocal lattice vectors associated with the supercell is $\{\mathbf{G}'|\mathbf{G}'=\Sigma_{j=1}^{3}n_j\mathbf{b}'_j\}$. Since $\mathbf{G}=\Sigma_{i=1}^{3}n_i\mathbf{b}_i=\Sigma_{i,j=1}^{3}n_iN_{ij}^{T}\mathbf{b}'_j$, one sees that $\{\mathbf{G}\}$ is a subset of $\{\mathbf{G}'\}$. Note that the elements of $\{\mathbf{G}\}$ and $\{\mathbf{G}'\}$ are the integer grid points (they do not fill any continuous space) formed by the corresponding reciprocal lattice vectors. We denote the first Brillouin zone formed by the reciprocal vectors $\{\mathbf{G}'\}$ as zone B.

*Lemma.* There exist a subset $\{\overline{\mathbf{G}}\}$ of $\{\mathbf{G}'\}$, which satisfies the following conditions.

(i) $\{\overline{\mathbf{G}}\}\subset\{\mathbf{G}'\}$ and $\{\overline{\mathbf{G}}\}\cap\{\mathbf{G}\}=\mathbf{0}$.

(ii) There are $M$ elements in the set $\{\overline{\mathbf{G}}\}$ ($M$ is the determinant of the matrix $N$) and the difference of any two of them does not belong to $\{\mathbf{G}\}$, i.e., $(\overline{\mathbf{G}}_1-\overline{\mathbf{G}}_2)\notin\{\mathbf{G}\}$.

(iii) Any $\mathbf{G}'\in\{\mathbf{G}'\}$ can be expressed as

$$\mathbf{G}'=\overline{\mathbf{G}}+\mathbf{G}, \tag{4}$$

where $\mathbf{G}\in\{\mathbf{G}\},\overline{\mathbf{G}}\in\{\overline{\mathbf{G}}\}$.

The proof and a way to find the set $\{\overline{\mathbf{G}}\}$ are given in the Appendix.

If we define the addition of vectors as multiplication in group theory, we can take $\{\mathbf{G}'\}$ as a group and $\{\mathbf{G}\}$ as a subgroup. Then the vector $\mathbf{0}$ is the unit element of the group. From group theory, one knows that $\{\mathbf{G}'\}$ is the union of all the cosets of the set $\{\mathbf{G}\}$. The subset $\{\overline{\mathbf{G}}\}$ is used to give the cosets.

With these reciprocal vectors, each eigenstate of the electromagnetic field component $H_{\mathbf{k}}$ (with the wave vector $\mathbf{k}$ in the first Brillouin zone) in the photonic crystal can be expressed in terms of the following Bloch series [10]:

$$H_{\mathbf{k}}(\mathbf{r})=e^{i\mathbf{k}\cdot\mathbf{r}}\sum_{\mathbf{G}} H_{\mathbf{G}}e^{i\mathbf{G}\cdot\mathbf{r}}. \tag{5}$$

The field component $H_{\mathbf{k}}$ satisfies the following equation:

$$\Theta H_{\mathbf{k}}=\frac{\omega_{\mathbf{k}}^2}{c^2}H_{\mathbf{k}}, \tag{6}$$

where the operator $\Theta$ can be easily derived from Maxwell's equations, and $c$ is the speed of light.

For any wave vector $\mathbf{k}$ in the $\mathbf{k}$ space of a photonic crystal, one can find a wave vector in the first Brillouin zone that has the same eigenstate. The difference between the two wave vectors should be a reciprocal vector. Therefore, for any wave vector $\mathbf{k}$, there exists a $\mathbf{G}\in\{\mathbf{G}\}$ so that

$$\mathbf{k}_1=\mathbf{k}-\mathbf{G} \tag{7}$$

is in zone A (associated with the unit cell) and a $\mathbf{G}'\in\{\mathbf{G}'\}$ so that

$$\mathbf{k}_2=\mathbf{k}-\mathbf{G}' \tag{8}$$

is in zone B (associated with the supercell). We call $\mathbf{k}_1$ (in zone A) the counterpoint of $\mathbf{k}_2$ (in zone B) for the same photonic crystal. They denote the same eigenstate in the reciprocal vector spaces associated with the unit cell and the supercell, respectively.

For a fixed $\mathbf{k}_2\in B$, we define the set $\{\mathbf{K}_1|\mathbf{K}_1=\mathbf{k}_2+\overline{\mathbf{G}}$, for all $\overline{\mathbf{G}}\in\{\overline{\mathbf{G}}\}\}_{\mathbf{k}_2}$. Clearly, there are $M$ elements in $\{\mathbf{K}_1\}$. Since not all of these $M$ elements are in zone A, we can force each of them inside zone A by subtracting an appropriate reciprocal vector $\mathbf{G}_{\mathbf{K}_1}\in\{\mathbf{G}\}$. Thus, we define a set $\{\mathbf{k}_1|\mathbf{k}_1=\tilde{\mathbf{K}}_1\equiv\mathbf{K}_1-\mathbf{G}_{\mathbf{K}_1}$ in A for all $\mathbf{K}_1\in\{\mathbf{K}_1\}_{\mathbf{k}_2}\}_{\mathbf{k}_2}$. Obviously $\{\mathbf{k}_1\}_{\mathbf{k}_2}$ contains $M$ points inside zone A.

*Theorem 1*

(i) The $M$ elements in $\{\mathbf{k}_1\}_{\mathbf{k}_2}$ are the counterpoints of $\mathbf{k}_2$. They are $M$ different points in zone A.

(ii) All $M$ eigenstates with $M$ wave vectors in $\{\mathbf{k}_1\}_{\mathbf{k}_2}$ (associated with the unit cell) correspond to $M$ eigenstates with one wave vector $\mathbf{k}_2$ in zone B (associated with the supercell).

(iii) Each band in the band structure associated with the unit cell will split into $M$ bands in the band structure associated with the supercell.

*Proof.* For any wave vector $\mathbf{k}$ in $\mathbf{k}$ space, $\mathbf{k}_1$ and $\mathbf{k}_2$ are the counterpoints in zone A and zone B, respectively. From Eqs. (4), (7), and (8), one has

$$\mathbf{k}=\mathbf{k}_2+\mathbf{G}'=\mathbf{k}_1+\mathbf{G}, \tag{9}$$

$$\begin{aligned}\mathbf{k}_1&=\mathbf{k}_2+\mathbf{G}'-\mathbf{G}\\&=\mathbf{k}_2+\bar{\mathbf{G}}+\mathbf{G}_1-\mathbf{G}\\&\equiv\mathbf{k}_2+\bar{\mathbf{G}}+\mathbf{G}_2\\&=\mathbf{K}_1+\mathbf{G}_2.\end{aligned} \tag{10}$$

Since $\mathbf{k}_1$ is in zone $A$, it follows from the definition that $\mathbf{k}_1\in\{\mathbf{k}_1\}_{\mathbf{k}_2}$ (here $\mathbf{G}_{\mathbf{K}_1}=-\mathbf{G}_2$). Therefore, for any wave vector which has a counterpoint $\mathbf{k}_2$ in zone B, its counterpoint in zone A must belong to $\{\mathbf{k}_1\}_{\mathbf{k}_2}$. On the other hand, all the elements in $\{\mathbf{k}_1\}_{\mathbf{k}_2}$ for all possible $\mathbf{G}'$ (corresponding to all possible $\bar{\mathbf{G}}\in\{\bar{\mathbf{G}}\}$) in Eq. (10) are all counterpoints of $\mathbf{k}_2$. Therefore, the elements in the set $\{\mathbf{k}_1\}_{\mathbf{k}_2}$ are exactly all the counterpoints of $\mathbf{k}_2$.

Consider two different $\bar{\mathbf{G}}_1,\bar{\mathbf{G}}_2\in\{\bar{\mathbf{G}}\}$. Correspondingly, we have $\mathbf{K}_1=\mathbf{k}_2+\bar{\mathbf{G}}_1$ and $\mathbf{K}_2=\mathbf{k}_2+\bar{\mathbf{G}}_2$. From the definition we have $\tilde{\mathbf{K}}_1-\tilde{\mathbf{K}}_2=\mathbf{K}_1-\mathbf{G}_{\mathbf{K}_1}-(\mathbf{K}_2-\mathbf{G}_{\mathbf{K}_2})=\bar{\mathbf{G}}_1-\bar{\mathbf{G}}_2-(\mathbf{G}_{\mathbf{K}_1}-\mathbf{G}_{\mathbf{K}_2})$. Since $\bar{\mathbf{G}}_1-\bar{\mathbf{G}}_2\notin\{\mathbf{G}\}$ and $\mathbf{G}_{\mathbf{K}_1}-\mathbf{G}_{\mathbf{K}_2}\in\{\mathbf{G}\}$, we know that $\bar{\mathbf{G}}_1-\bar{\mathbf{G}}_2$ and $\mathbf{G}_{\mathbf{K}_1}-\mathbf{G}_{\mathbf{K}_2}$ are different, i.e., $\bar{\mathbf{G}}_1-\bar{\mathbf{G}}_2-(\mathbf{G}_{\mathbf{K}_1}-\mathbf{G}_{\mathbf{K}_2})\neq\mathbf{0}$, which immediately gives $\tilde{\mathbf{K}}_1-\tilde{\mathbf{K}}_2\neq\mathbf{0}$. This proves that $\tilde{\mathbf{K}}_1$ and $\tilde{\mathbf{K}}_2$ are two different points in zone A. Therefore, the elements in $\{\mathbf{k}_1\}_{\mathbf{k}_2}$ are $M$ different points.

Let $H_{\mathbf{k}_1}$ be the eigenstate for a wave vector in the set $\{\mathbf{k}_1\}_{\mathbf{k}_2}$ associated with the unit cell. From Eqs. (5) and (10), one has

$$\begin{aligned}H_{\mathbf{k}_1}(\mathbf{r})&=e^{i\mathbf{k}_1\cdot\mathbf{r}}\sum_{\mathbf{G}}H_{\mathbf{G}}e^{i\mathbf{G}\cdot\mathbf{r}}\\&=e^{i(\mathbf{k}_2+\bar{\mathbf{G}}+\mathbf{G}_2)\cdot\mathbf{r}}\sum_{\mathbf{G}}H_{\mathbf{G}}e^{i\mathbf{G}\cdot\mathbf{r}}\\&=e^{i\mathbf{k}_2\cdot\mathbf{r}}\sum_{\mathbf{G}}H_{\mathbf{G}}e^{i(\mathbf{G}+\bar{\mathbf{G}}+\mathbf{G}_2)\cdot\mathbf{r}}\\&=e^{i\mathbf{k}_2\cdot\mathbf{r}}\sum_{\mathbf{G}'}H_{\mathbf{G}'}e^{i\mathbf{G}'\cdot\mathbf{r}}\equiv H'_{\mathbf{k}_2}(\mathbf{r}),\end{aligned} \tag{11}$$

where $H'_{\mathbf{k}_2}$ is the same eigenstate (with the same field distribution) but for the wave vector $\mathbf{k}_2$ in zone B (associated with the supercell). Therefore, all $M$ eigenstates with $M$ wave vectors in $\{\mathbf{k}_1\}_{\mathbf{k}_2}$ (associated with the unit cell) can be represented by $M$ eigenstates with one wave vector $\mathbf{k}_2$ in zone A (associated with the supercell). The $M$ points of $\mathbf{k}_1$ on any band in the band structure associated with the unit cell will be on $M$ bands for one $\mathbf{k}_2$ value in the band structure associated with the supercell. Generally speaking, one band in the band structure associated with the unit cell will split into $M$ bands (which may overlap partially and form degenerate eigenstates) in the band structure associated with the supercell. The theorem is thus proved.

*Theorem 2.* If a photonic crystal has some kind of point group symmetry, the eigenstates at the edge of the first Brillouin zone B will be degenerate in the band structure associated with the supercell. The degree of the degeneracy depends on both the determinant $M$ of the transform matrix $N$ and the point group symmetry of the photonic crystal.

*Proof.* For a wave vector $\mathbf{k}_2$ at the edge of zone B, in addition to $\mathbf{k}_1=\mathbf{k}_2+\mathbf{0}$ (corresponding to $\bar{\mathbf{G}}_1=\mathbf{0}$) being one of its counterpoints at the edge of zone B, it may have another counterpoint $\mathbf{k}'_1=\mathbf{K}_1-\mathbf{G}_{\mathbf{K}_1}$ (with $\mathbf{K}_1=\mathbf{k}_2+\bar{\mathbf{G}}_2$) located somewhere else at the edge of zone B. For nonzero $\bar{\mathbf{G}}$ only those points at the edge of zone B may have counterpoints still at the edge of zone B and the counterpoints for those points inside zone B will be outside zone B (but still inside A according to the definition of counterpoints; note that zone B is inside zone A). The wave vectors $\mathbf{k}_1$ and $\mathbf{k}'_1$ correspond to the same wave vector $\mathbf{k}_2$ in zone B associated with the supercell. Sometimes there exists a symmetric operation $\alpha$ (which can be represented by a matrix for coordinate transformation; then one has $\alpha^{-1}=\alpha^T$) and the associated operator $T(\alpha)$ [with $T(\alpha)f(\mathbf{r})=f(\alpha^{-1}\mathbf{r})$] for the photonic crystal such that $\alpha\mathbf{k}'_1=\mathbf{k}_1$ and $T(\alpha)\Theta(\mathbf{r})=\Theta(\alpha^{-1}\mathbf{r})T(\alpha)=\Theta(\mathbf{r})T(\alpha)$. Assume that $H_{\mathbf{k}_1}$ and $H_{\mathbf{k}'_1}$ are the eigenstates for these two wave vectors, i.e., $\Theta H_{\mathbf{k}_1}=\omega^2_{\mathbf{k}_1}/c^2H_{\mathbf{k}_1}$ and $\Theta H_{\mathbf{k}'_1}=\omega^{2\prime}_{\mathbf{k}1}/c^2H_{\mathbf{k}'_1}$. Since

$$T(\alpha)H_{\mathbf{k}'_1}(\mathbf{r})=H_{\mathbf{k}'_1}(\alpha^{-1}\mathbf{r})=H_{\alpha\mathbf{k}'_1}(\mathbf{r})=H_{\mathbf{k}_1}(\mathbf{r}), \tag{12}$$

we have

$$\begin{aligned}\Theta H_{\mathbf{k}_1}&=\Theta T(\alpha)H_{\mathbf{k}'_1}=T(\alpha)\Theta H_{\mathbf{k}'_1}=\frac{\omega^{2\prime}_{\mathbf{k}1}}{c^2}T(\alpha)H_{\mathbf{k}'_1}\\&=\frac{\omega^{2\prime}_{\mathbf{k}1}}{c^2}H_{\mathbf{k}_1},\end{aligned} \tag{13}$$

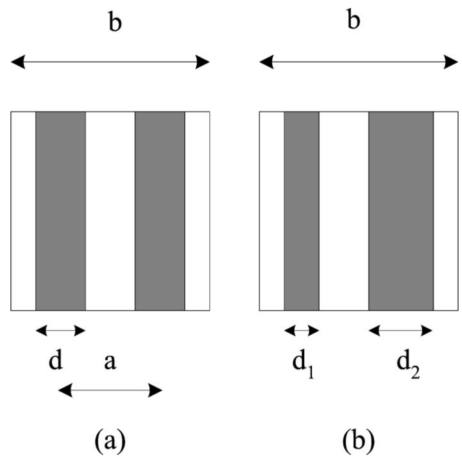


FIG. 1. A 1D photonic crystal consisting of alternating layers of two different materials. (a) The supercell (including two unit cells) of the photonic crystal. (b) The symmetry of the supercell is broken (by changing the widths of the two dielectric layers while keeping the positions of both unchanged) to form a unit cell for a new photonic crystal.

we have $\omega_{\mathbf{k}_1}=\omega_{\mathbf{k}_1'}$. Therefore, $H_{\mathbf{k}_1}$ and $H_{\mathbf{k}_1'}$ are two different eigenstates (for different wave vectors $\mathbf{k}_1$ and $\mathbf{k}_1'$) with the same eigenvalue. In the band structure associated with the supercell, these two eigenstates are located at two bands but have the same wave vector $\mathbf{k}_2$ and the same eigenvalue. Thus, they are degenerate states. Since we do not assume any specific form for $\Theta$ in the above proof, the theorem is valid in any dimensional space (and for any polarization in the 2D case).

In the next section, we will illustrate these degeneracy theorems with some numerical examples, use the degeneracy analysis to explain PBGs for some known 2D photonic crystals, and create large band gaps by breaking the symmetry properties of the photonic crystal.

### III. NUMERICAL RESULTS

First we give a one-dimensional example. Figure 1 is a 1D photonic crystal consisting of alternating layers of materials with two different dielectric constants ($\varepsilon_1=13$ and $\varepsilon_2=1$). We can select a periodic region (a supercell) to include two unit cells as shown in Fig. 1(a). The band structure associated with the unit cell and the band structure associated with the supercell (with $N=2$) are given in the same figure [Fig. 2(a)], where the frequency and the wave vector are normalized with the same constant $a=1$ in order to make them comparable. For this case, we have $\{G\}\equiv\{\overline{G}_1,\overline{G}_2\}=\{0,0.5(2\pi/a)\}$ and $M=2$. From Fig. 2(a) one sees that the eigenvalues (associated with the original unit cell) for the wave vectors outside the first Brillouin zone B (associated with the supercell) have their counterpoints in zone B in the band structure associated with the supercell. As expected, each band (solid line) associated with the unit cell corresponds to two bands (dashed lines) associated with the supercell. Since the center point of the supercell in Fig. 1(a) is mirror symmetric, one has $\alpha=-1$. At the edge of zone B, the two wave vectors $k_1'=0.25(2\pi/a)$ and $k_1=-0.25(2\pi/a)=\alpha k_1'$ correspond to the same wave vector $k_2=-0.25(2\pi/a)$ (note that $k_2+\overline{G}_1=k_1, k_2+\overline{G}_2=k_1'$). Thus, these two eigenstates are degenerate in the band structure associated with the supercell. Each eigenstate at $k=\pm 0.25(2\pi/a)$ is formed by two degenerate states in the band structure associated with the supercell. If one breaks the point group symmetry with respect to the center point of the supercell of the photonic crystal by changing the size of the inclusion medium, one obtains a new photonic crystal as shown in Fig. 1(b). Sine the resulting photonic crystal iss still mirror symmetric with respect to the center point of an inclusion layer, the symmetry breaking with respect to the center point of the supercell does not change the point group symmetry of the photonic crystal as a whole. However, the

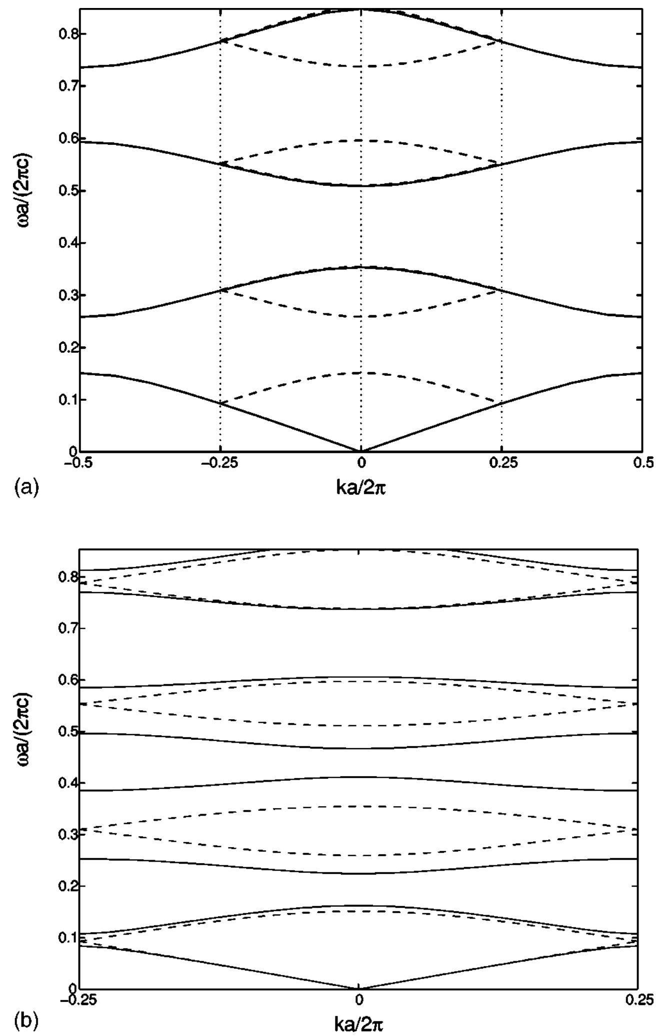


FIG. 2. The corresponding band structures of the 1D photonic crystals with $\varepsilon_1=13$, $\varepsilon_2=1$. (a) The solid lines are for the band structure associated with the unit cell and the dashed lines give the band structure associated with the supercell. Here we choose $b=2a$ and $d=0.5a$ for Fig. 1(a). (b) The solid lines give the band structure for a new photonic crystal with the unit cell shown Fig. 1(b) (here we choose $d_1=0.3a$ and $d_2=0.7a$). The dashed lines are for the band structure for Fig. 1(a) before the symmetry of the supercell is broken.

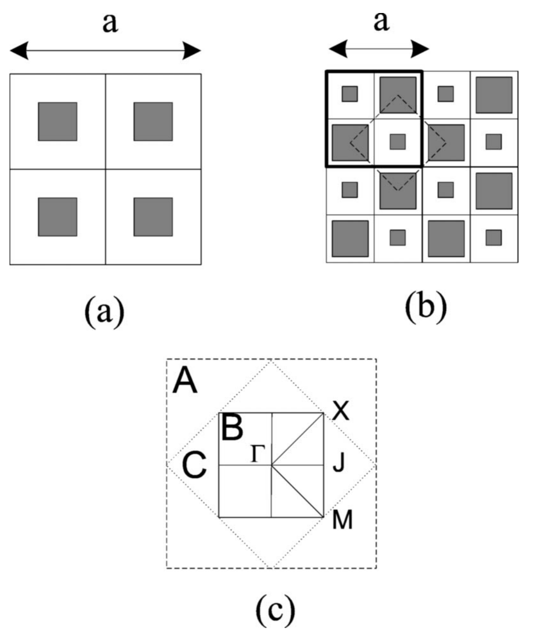


FIG. 3. The case for the square lattice of square dielectric rods. (a) The supercell including four unit cells. (b) The symmetry of the supercell is broken as two square rods increase in size and the other two rods decrease in size. The symmetry-broken supercell is marked by the thick solid lines. (c) The first Brillouin zone A (marked by the dashed lines) associated with the original unit cell and the first Brillouin zone B (marked by the solid lines) associated with the supercell of (a). The first Brillouin zone C associated with the new unit cell [marked by the dashed lines of (b)] of the new photonic crystal of (b) is marked by the dotted lines. $\Gamma,X,J,M$ are the symmetry points.

translation group symmetry changes due to the symmetry breaking, and this leads to a larger unit cell. The corresponding transform matrix between the supercell and the new unit cell changes from $N=2$ to $N=1$. The band structure is shown by the solid lines in Fig. 2(b), where one sees that the degeneracy disappears (since $M=1$ for this new photonic crystal and consequently there is only one counterpoint for each wave vector in the Brillouin zone) and more band gaps appear.

For the 2D case, if the dielectric inclusions have rectangular shapes, we can employ the plane wave expansion method with the inverse rule [21] to calculate the band structure. It is shown in [21,22] that this method with 225 plane waves can give more accurate results than a conventional plane wave expansion method with even 1681 plane waves. In our calculations, we use this method with 289 plane waves and the error in the band structure is less than 0.5%.

As an example, we choose $2\times2$ unit cells as the super cell. Then we have $N^T=\left(\begin{smallmatrix}2&0\\0&2\end{smallmatrix}\right)$, which corresponds to $\{\overline{\mathbf{G}}\}=\{0,\mathbf{b}_1',\mathbf{b}_2',\mathbf{b}_1'+\mathbf{b}_2'\}$ (see the Appendix for a derivation for a general case). Figure 3(a) shows a simple square lattice of square dielectric rods. Alumina is chosen as the dielectric medium and thus $\varepsilon=8.9$. The filling factor is set to $f=0.47$. Figure 4(a) gives the band structure associated with the supercell. Each band (associated with the unit cell) has split into four bands in the band structure associated with the

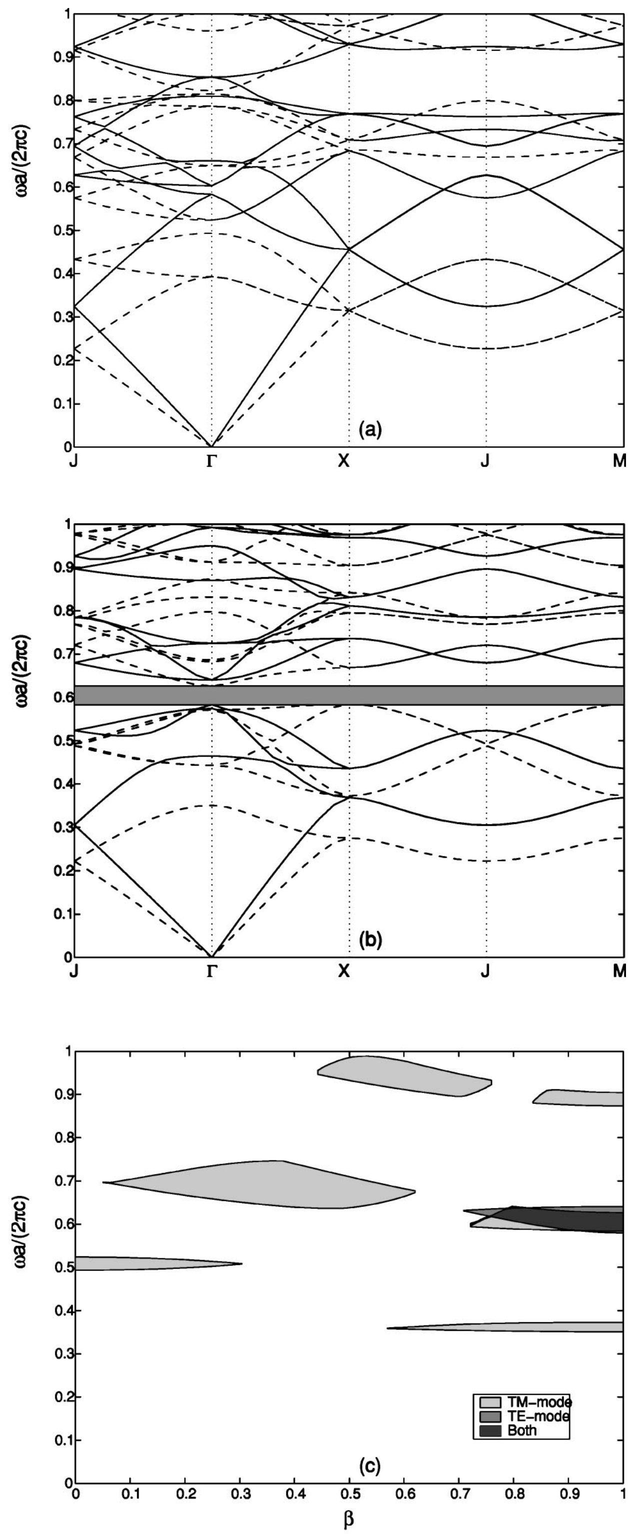


FIG. 4. The band structures associated with Fig. 3 for $f=0.47,\varepsilon=8.9$. The solid lines denote the $H$ polarization case and the dashed lines are for the $E$ polarization case. They are calculated by the plane wave expansion method (with the inverse rule) with 289 plane waves for (a) $\beta=0$, i.e., a simple square lattice of square rods; (b) $\beta=1$, i.e., the case of the chessboard. The absolute band gap $\Delta\omega/\omega_c=0.07$ appears at $\omega_c=0.605(2\pi c/a)$. (c) The band gap map for $0\leqslant\beta\leqslant1$.

supercell. The point group symmetry is $C_{4v}$. We use the two mirror symmetries $\alpha_1=\begin{pmatrix}-1 & 0\\ 0 & 1\end{pmatrix}$ and $\alpha_2=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$ to analyze the degeneracy here. The eigenstates with wave vectors at the four corners (e.g., points $X$ and $M$) of the Brillouin zone B have fourfold degeneracy and the eigenstates with wave vectors on two opposite edges are of twofold degeneracy under these two symmetry operations. Thus, in the band structure associated with the supercell one can see that there are four-fold degeneracies at the $X$ and $M$ points and there are also twofold accidental degeneracies for the four split bands (and thus one sees only three bands) in the region $\Gamma-X$. The $E$ polarization and the $H$ polarization have similar behaviors of degeneracy.

In the supercell, both the size and the position of the inclusions can be changed to break the point symmetry with respect to the center point of the supercell. Since the band structure is more sensitive to the inclusion size [9], the size of the inclusions will influence the band structure significantly. In our first example, the symmetry is broken as two square rods increase in size and the other two rods decrease in size in order to keep the filling factor $f=0.47$ unchanged. In the resulting photonic crystal shown in Fig. 3(b), the squares rotate through a 45° angle to form a chessboard structure in the new unit cell denoted by thickened lines in Fig. 3(b) after the symmetry is broken. The ratio of the side lengths between the smaller rods and the larger rods is $1-\beta$ with $0\leqslant\beta\leqslant1$. When $0<\beta<1$, it is just the case with the smaller square rods being added at the corners of the simple unit cell. When $\beta=1$, the side length of the smaller rods is 0 and only two larger rods exist in the supercell. The structure is exactly the chessboard structure reported in [20].

Since the symmetry with respect to the center point (which has the highest symmetry) of each square is still $C_{4v}$ for $0<\beta\leqslant1$ [see Fig. 3(b)], the point group symmetry of the photonic crystal is still $C_{4v}$. Similar to the 1D case, the symmetry breaking with respect to the center point of the supercell changes the translation symmetry of the photonic crystal. The corresponding transform matrix $N$ between the supercell and the unit cell changes from $N^T=\begin{pmatrix}2 & 0\\ 0 & 2\end{pmatrix}$ to $N^T=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$ as the unit cell changes to a larger one. Therefore, the degeneracies of the band structure associated with the supercell will also change. We take the chessboard ($\beta=1$) as an example to study its band structure [shown in Fig. 4(b)]. From Fig. 4(b) one sees clearly that some degeneracies (including the usual degeneracies at the edge of zone B and the accidental degeneracies for points at $\Gamma$-$X$) are lifted for both the $E$ polarization and the $H$ polarization. An absolute band gap appears where the degeneracies are lifted at the edge points of zone B. To understand this situation, after the unit cell of the photonic crystal in Fig. 3(b) changes to a larger one [denoted by the dashed line in Fig. 3(b)], the corresponding first Brillouin zone of this new photonic crystal is denoted as zone C in Fig. 3(c). The transform matrix between zone C and zone A is $N^T=\begin{pmatrix}1 & 1\\ -1 & 1\end{pmatrix}$, which corresponds to $M=\det(N^T)=2,\{\overline{\mathbf{G}}\}=\{0,\overline{\mathbf{b}}_2'\}=\{0,\mathbf{b}_2'\}$ according to the Appendix. For the point group symmetry of $C_{4v}$, we can analyze the degeneracy with the two mirror symmetry operators $\alpha_3=\alpha_1$ and $\alpha_4=\alpha_2$. The eigenstates with two wave vectors on the two opposite edges in the Brillouin zone B are twofold degenerate states under these two symmetry operations. The degeneracy becomes only twofold at points $X$ and $M$ now (as compared to the fourfold degeneracy in the band structure associated with the supercell) since $|N^T|=2$ here. Therefore, the degeneracies must disappear at the $X$ and $M$ points and each group of four bands in Fig. 4(a) breaks at points $X$ and $M$ to form two groups with two bands in each group [see Fig. 4(b)]. An absolute band gap $\Delta\omega/\omega_c=0.070$ appears at the midfrequency (of the band gap) $\omega=\omega_c=0.605(2\pi c/a)$. The large absolute band gaps can be explained by the present theory of supercells.

Figure 4(c) is the corresponding gap map when $\beta$ increases from 0 to 1. The situation is similar to the case considered in [15] (the only difference is that here we use square dielectric rods instead of round air holes). To make a map for the actual procedure of degeneracy breaking, we take $\beta$ as the varying parameter. A photonic crystal with additional smaller squares ($0<\beta<1$; we call it case 2) is considered in [15] as a result of adding the smaller squares to corners of the square lattice of the square rods ($\beta=1$; we call it case 3). Here, we take both case 2 and case 3 as the results of changing the translation symmetry of the photonic crystal when the additional square is of equal size ($\beta=0$; we call it case 1). They have the same degeneracy breaking properties as the chessboard structure mentioned above. Thus, large absolute band gaps can be expected by choosing an appropriate value of $\beta$. When $\beta\geqslant0.76$, an absolute band gap appears around $\omega=0.6(2\pi c/a)$. It is more useful to use $\Delta\omega/\omega_c$ to describe the PBGs due to the scaling property of a photonic crystal. In the band structure associated with the supercell, $\Delta\omega/\omega_c$ remains almost unchanged. A maximum $\Delta\omega/\omega_c=0.071$ occurs when $\beta=0.93$.

Following the same procedure, from the chessboard photonic crystal shown in Fig. 5(a) we can obtain a photonic crystal formed with square dielectric rods of two different sizes [see Fig. 5(b)]. The ratio of the side lengths between the smaller rods and the larger rods is $1-\beta$ with $0\leqslant\beta\leqslant1$. Figure 6 gives the gap map when the filling ratio is fixed to $f=0.35$ with $0\leqslant\beta\leqslant1$ and the inclusion material has a dielectric constant $\varepsilon=11.4$. From Fig. 6, one sees that there is no absolute band gap for the chessboard case (when $\beta=0$) in the frequency range of $0\leqslant\omega\leqslant2\pi c/a$. When $\beta=1$, the structure becomes a simple square lattice of square rods of the same size [see Fig. 5(c)], which has an absolute band gap $\Delta\omega/\omega_c=0.0453$ with the midfrequency $\omega_c=0.7231(2\pi c/a)$. It is thus not surprising that with appropriate parameters an absolute photonic band gap exists for the 2D square lattice of square dielectric rods as considered in [11]. The maximal gap of $\Delta\omega/\omega_c=0.0717$ (much larger than in the case of inclusions with a single size) occurs at $\omega=\omega_c=0.7449(2\pi c/a)$ when the ratio of the size lengths for the two inclusion rods is $\beta=0.31$.

A triangular lattice of air columns [see Fig. 7(b)] has been found to have a large absolute band gap. The rule of thumb [2] can be employed to give a reasonable explanation. Here we explain how a gap appears from the viewpoint of the changes of translation symmetry. Although the triangular lattice has high symmetry, it can be viewed as the result of

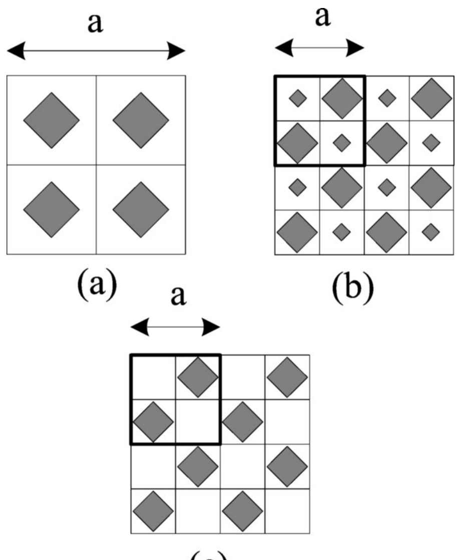


FIG. 5. The case of the chessboard structure. (a) The supercell including four unit cells. (b) The symmetry of the supercell is broken when two square rods increase in size and the other two square rods decrease in size. (c) The photonic crystal when the size of the smaller square rods becomes zero. The structure becomes a simple square lattice of square rods.

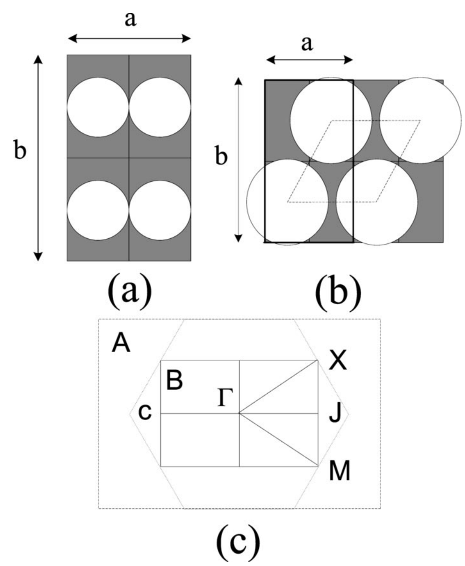


FIG. 7. The case for a rectangular lattice of air holes. The ratio of the two side lengths is $\sqrt{3}$. (a) The supercell including four unit cells. (b) The symmetry of the supercell is broken when two diagonal air holes are reduced in size to zero and the other two diagonal air holes increase in size. The symmetry-broken supercell is marked by the thick solid lines. (c) The first Brillouin zone A (marked by the dashed lines) associated with the original unit cell and the first Brillouin zone B (marked by the solid lines) associated with the supercell of (a). The first Brillouin zone C associated with the new unit cell [marked by the dashed lines of (b)] of the new photonic crystal of (b) is marked by the dotted lines. $\Gamma, X, J, M$ are the symmetry points.

symmetry breaking from a supercell of another photonic crystal shown in Fig. 7(a). From Figs. 8(a) and 8(b) we can see clearly how the degeneracies are lifted at the edge points $X$ and $M$ [cf. Fig. 7(c)] and an absolute band gap is created in the band structure associated with the supercell when the symmetry of the supercell is broken.

As a final numerical example, we break the symmetry of the supercell shown in Fig. 9(a) by changing both sizes (for all nine square rods) and positions (except for the central square rod) of the square rods, but with the dielectric filling factor $f$ fixed. Figure 9(b) is the resulting structure. The band structure with parameters $p_1=0.194a, p_2=0.236a, p_3=0.374, f=0.5132$ is shown in Fig. 10. From this figure one sees that the degeneracies are lifted at the edge points and two absolute band gaps are created at higher normalized frequencies, namely, a large gap $\Delta\omega_1=0.072(2\pi c/a)$ at $\omega_c=1.291(2\pi c/a)$ and another gap $\Delta\omega_2=0.043$ at $\omega_c=1.142(2\pi c/a)$. Note that it is easier to fabricate a photonic crystal with the absolute band gap occurring at a higher normalized frequency.

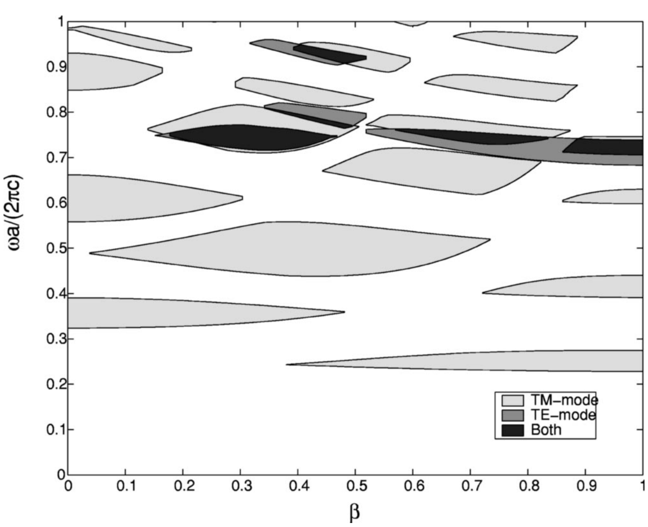


FIG. 6. The gap map for Fig. 5 with $0 \leqslant \beta \leqslant 1$ ($1-\beta$ is the side length ratio of the smaller squares to the larger ones).

## IV. CONCLUSION

In the present paper, we have presented a method of explaining or creating photonic band gaps through analyzing the degeneracy of the band structure associated with a supercell. The band structure associated with a supercell of a photonic crystal has degeneracies at the edge of the first Brillouin zone if the photonic crystal has some kind of point group symmetry. We analyzed these degeneracies and presented two theorems on degeneracies in the band structure associated with the supercell. These theorems and the analysis are valid in any dimensional space (and for any polarization in the 2D case) and do not require investigation of the field distribution. Photonic band gaps can be created through lifting these degeneracies by changing the translation group symmetry of the photonic crystal, which consequently changes the transform matrix between the supercell and the smallest unit cell. Many numerical examples have been given in the present paper to illustrate this. In the 2D case,

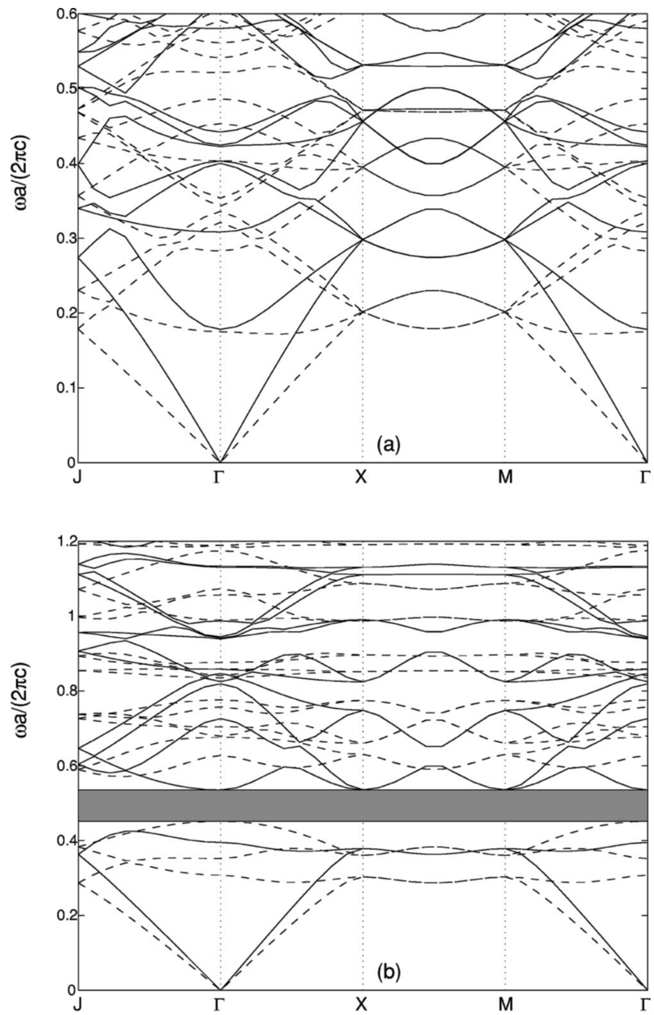


FIG. 8. Band structures calculated with the plane wave expansion method (with 961 plane waves). The relative permittivity for the background medium is $\varepsilon = 13$. The solid lines denote the *H*-polarization case and the dashed lines are for the *E*-polarization case. (a) The band structure associated with the supercell of Fig. 7(a). The radius of the air holes is $r = 0.5a$. (b) The band structure associated with the symmetry-broken supercell [marked by the thick solid line in Fig. 7(b)]. The filling factor is $f = 0.836$. The absolute band gap $\Delta\omega/\omega_c = 0.169$ appears at midfrequency $\omega_c = 0.4936(2\pi c/a)$.

the *E* polarization and the *H* polarization have the same properties of degeneracies. The existence of photonic band gaps for many known 2D photonic crystals has been explained through a degeneracy analysis of the band structure associated with the supercell. Some photonic crystal structures with large or multiple band gaps have also been found by breaking the symmetry of the supercell.

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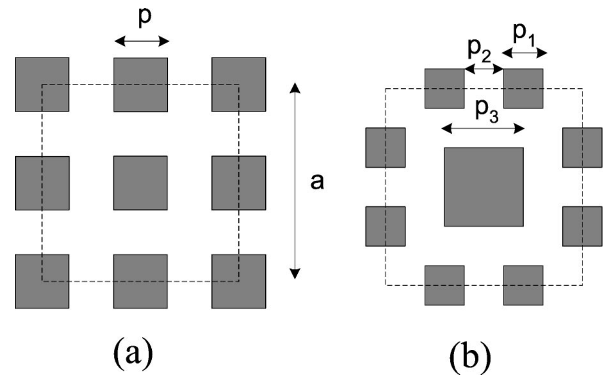


FIG. 9. Symmetry breaking of a supercell by changing both the sizes and positions of the inclusions. (a) The supercell including four unit cells. (b) The symmetry of the supercell is broken when both the sizes (for all nine square rods) and the positions (except for the central square rod) of the square rods are changed (but with the dielectric filling factor *f* fixed).

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## APPENDIX THE PROOF OF THE LEMMA AND A METHOD TO FIND THE SET $\{\overline{\mathbf{G}}\}$

We can take three kinds of primary transformations for the integer matrix $N$ while keeping the absolute value of $\det(N)$ unchanged. The first transformation is to multiply a column or row by $\pm 1$. The second transformation is to interchange two columns or rows. The third transformation is to add one column or row to $k$ times another column or row

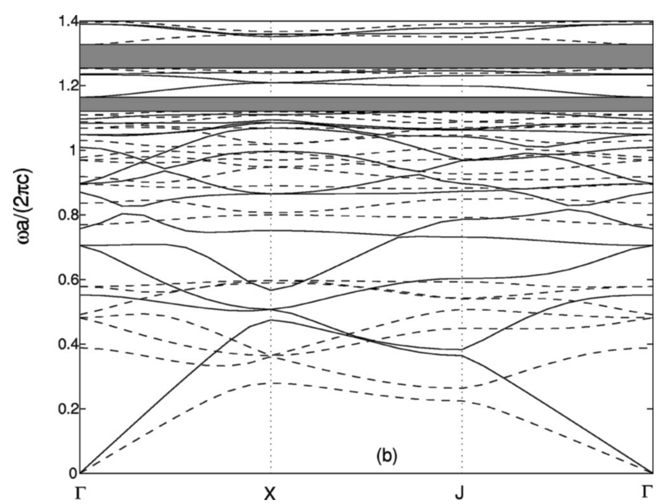


FIG. 10. The band structure associated with the symmetry-broken supercell shown in Fig. 9(b) with $f = 0.5132$ and $\varepsilon = 11.4$. The solid lines denote the *H* polarization case and the dashed lines are for the *E* polarization case. The other parameters are $p_1 = 0.194a$, $p_2 = 0.236a$, $p_3 = 0.374a$. Through the symmetry breaking of the supercell, one obtains a band structure with two absolute band gaps, namely, one gap $\Delta\omega_1 = 0.0724$ at $\omega_1 = 1.2905(2\pi c/a)$, and another gap $\Delta\omega_2 = 0.0427$ at $\omega_2 = 1.1424(2\pi c/a)$.

($k$ is an integer). Each primary transformation can be expressed with a left or right multiplication of the matrix $N$ by an integer matrix. Furthermore, the determinants of these integer matrices (associated with these primary transformations) are 1 and their inverses are also integer matrices. Under these primary transformations [23], the determinant of the matrix is kept unchanged and the resulted matrix $N'$ is still an integer matrix.

Here we give a specific procedure for obtaining a diagonal matrix $N'=D$ by taking these transformations. First, we interchange the column or the row with the second kind of transformation to make $N_{11}$ the minimal among $N_{1i}$ and $N_{i1}$, $i=1,2,3$. Then we make $N_{11}$ positive (if it is negative) with the first kind of transformation. If all the integers $N'_{1i}$ and $N'_{i1}$ $(i=1,2,3)$ are divisible by $N'_{11}$, we can make all $N'_{1i}$ and $N'_{i1}$ (except $N'_{11}$) zero by using the third kind of transformation. If any of $N'_{1i}$ or $N'_{i1}$ is not divisible by $N'_{11}$, its column or row can be subtracted from $k$ times $N_{11}$ so that the remaining component at the $N'_{1i}$ or $N'_{i1}$ position becomes smaller than $N'_{11}$. The column or row is then interchanged with the first column or the first row (with $N_{11}$) to make $N'_{11}$ smaller. This can be done repeatedly until all $N'_{1i}$ and $N'_{i1}$ are divisible by $N'_{11}$ or $N'_{11}=1$. Then we can make all $N'_{1i}$ and $N'_{i1}$ but $N'_{11}$ zero. Applying a similar method to $N'_{22}$, we can make $N'_{23}=N'_{32}=0$. Therefore, the integer matrix $N^T$ is diagonalized as

$$N^T=P^{-1}DQ, \tag{A1}$$

$$D=\begin{pmatrix} d_1 & 0 & 0 \\ 0 & d_2 & 0 \\ 0 & 0 & d_3 \end{pmatrix},$$

where $D$, $P^{-1}$, $Q$ are all integer matrices. Here $P^{-1}$ is the inverse of $P$ and $\det(P^{-1})=\det(Q)=1$. Thus, we have $\det(D)=d_1d_2d_3=\det(N^T)=M$.

From Eq. (5) we have

$$\mathbf{b}_i=\sum_{j=1}^{3} N^T_{ij}\mathbf{b}'_j=\sum_{j=1}^{3} (P^{-1}DQ)_{ij}\mathbf{b}'_j\,. \tag{A2}$$

We can define two other basic vectors $\overline{\mathbf{b}}$ and $\overline{\mathbf{b}'}$ by $\overline{\mathbf{b}}_i=\Sigma_{j=1}^{3}P_{ij}\mathbf{b}_j$ and $\overline{\mathbf{b}}'_i=\Sigma_{j=1}^{3}Q_{ij}\mathbf{b}'_j$. Below we find $\{\overline{\mathbf{G}}\}$ in terms of the vectors $\overline{\mathbf{b}}'_i$. It follows from Eq. (14) that

$$\overline{\mathbf{b}}_i=\sum_{j=1}^{3} D_{ij}\overline{\mathbf{b}}'_j=\sum_{j=1}^{3} \delta_{ij}d_j\overline{\mathbf{b}}'_j\,. \tag{A3}$$

Since

$$\sum_{i=1}^{3} n_i\mathbf{b}_i=\sum_{i,j=1}^{3} n_iP^{-1}{}_{ij}\overline{\mathbf{b}}_j=\sum_{j=1}^{3} n'_j\overline{\mathbf{b}}_j\in\left\{\sum_{i=1}^{3} n_i\overline{\mathbf{b}}_i\right\}, \tag{A4}$$

$$\sum_{i=1}^{3} n_i\overline{\mathbf{b}}_i=\sum_{i,j=1}^{3} n_iP_{ij}\mathbf{b}_j=\sum_{j=1}^{3} n'_j\mathbf{b}_j\in\left\{\sum_{i=1}^{3} n_i\mathbf{b}_i\right\}, \tag{A5}$$

we see that the set $\{\Sigma_{i=1}^{3}n_i\overline{\mathbf{b}}_i\}=\{\Sigma_{i=1}^{3}n_i\mathbf{b}_i\}$ ($n_i,n'_i$ are arbitrary integers). Similarly, we can show that

$$\left\{\sum_{i=1}^{3} n_i\overline{\mathbf{b}}'_i\right\}=\left\{\sum_{i=1}^{3} n_i\mathbf{b}'_i\right\}. \tag{A6}$$

Therefore, the sets $\{\mathbf{G}\}$ and $\{\mathbf{G}'\}$ can be written as $\{\mathbf{G}|\mathbf{G}=\Sigma_{i=1}^{3}n_i\overline{\mathbf{b}}_i=\Sigma_{j=1}^{3}n_id_i\overline{\mathbf{b}}'_i\}$ and $\{\mathbf{G}'|\mathbf{G}'=\Sigma_{i=1}^{3}n_i\overline{\mathbf{b}}'_i\}$.

Since any integer $n_i$ can be written as $n_i=l_id_i+m_I$ with $0\leqslant m_i\leqslant d_i-1$, we see that the set $\{\overline{\mathbf{G}}|\overline{\mathbf{G}}=\Sigma_{i=1}^{3}m_i\overline{\mathbf{b}}'_i,m_i=0,\ldots,d_i-1\}$. Obviously, we have $\{\overline{\mathbf{G}}\}\cap\{\mathbf{G}\}=\mathbf{0}$ and there are $d_1d_2d_3=M$ possible combinations of $(m_1,m_2,m_3)$ for $\overline{\mathbf{G}}$ (i.e., the set $\{\overline{\mathbf{G}}\}$ has $M$ elements). Also, for any two of them, e.g., $\overline{\mathbf{G}}_1=\Sigma_{i=1}^{3}m_i\overline{\mathbf{b}}'_i$, $\overline{\mathbf{G}}_2=\Sigma_{i=1}^{3}m'_i\overline{\mathbf{b}}'_i$, $0\leqslant m_i\leqslant d_i-1$, $0\leqslant m'_i\leqslant d_i-1$, the difference $\overline{\mathbf{G}}_1-\overline{\mathbf{G}}_2=\Sigma_{i=1}^{3}m_i\overline{\mathbf{b}}'_i-\Sigma_{i=1}^{3}m'_i\overline{\mathbf{b}}'_i=\Sigma_{i=1}^{3}(m_i-m'_i)\overline{\mathbf{b}}'_i$ does not belong to $\{\mathbf{G}\}$ since $0\leqslant|m_i-m'_i|\leqslant d_i-1$.

Obviously, any $\mathbf{G}'\in\{\mathbf{G}'\}$ can be written as

$$\mathbf{G}'=\sum_{i=1}^{3} n_i\overline{\mathbf{b}}'_i=\sum_{i=1}^{3} (l_id_i\overline{\mathbf{b}}'_i+m_i\overline{\mathbf{b}}'_i)$$

$$=\mathbf{G}+\overline{\mathbf{G}}, \tag{A7}$$

where $\mathbf{G}\in\{\mathbf{G}\}$ and $\overline{\mathbf{G}}\in\{\overline{\mathbf{G}}\}$.

As a numerical example in the 2D case, we can consider the supercell indicated by the thick line in Fig. 3(b) where the unit cell is indicated by the dashed line (the supercell includes two unit cells). Obviously, we have $\mathbf{a}'_1=\mathbf{a}_1+\mathbf{a}_2$ and $\mathbf{a}'_2=\mathbf{a}_1-\mathbf{a}_2$. Then we have $N^T=\left(\begin{smallmatrix}1&1\\-1&1\end{smallmatrix}\right)$. Following the above procedure, we obtain $N^T=\left(\begin{smallmatrix}1&1\\-1&1\end{smallmatrix}\right)=\left(\begin{smallmatrix}1&0\\1&1\end{smallmatrix}\right)\left(\begin{smallmatrix}1&0\\0&2\end{smallmatrix}\right)\times\left(\begin{smallmatrix}1&-1\\0&1\end{smallmatrix}\right)$, $D=\left(\begin{smallmatrix}1&0\\0&2\end{smallmatrix}\right)$, $P^{-1}=\left(\begin{smallmatrix}1&0\\1&1\end{smallmatrix}\right)$, $\left(\begin{smallmatrix}1&-1\\0&1\end{smallmatrix}\right)$, $P=\left(\begin{smallmatrix}1&0\\-1&1\end{smallmatrix}\right)$, $Q^{-1}=\left(\begin{smallmatrix}1&1\\0&1\end{smallmatrix}\right)$. Therefore, we have $d_1=1, d_2=2$, and $\{\overline{\mathbf{G}}\}=\{0,\overline{\mathbf{b}}'_2\}=\{0,\mathbf{b}'_2\}$. Since $\overline{\mathbf{G}}_1-\overline{\mathbf{G}}_2=\mathbf{b}'_2$ in this special example and we have the general form for $\mathbf{G}=n_1\mathbf{b}_1+n_2\mathbf{b}_2=n_1(\mathbf{b}'_1+\mathbf{b}'_2)+n_2(-\mathbf{b}'_1+\mathbf{b}'_2)=(n_1-n_2)\mathbf{b}'_1+(n_1+n_2)\mathbf{b}'_2$, $\overline{\mathbf{G}}_1-\overline{\mathbf{G}}_2\in\{\mathbf{G}\}$ will end up with $n_1=n_2=1/2$ which is contradictory to the requirement that $n_1$ and $n_2$ are integers. Therefore, for this special example we also see that $\overline{\mathbf{G}}_1-\overline{\mathbf{G}}_2\notin\{\mathbf{G}\}$.

[1] E. Yablonovitch, Phys. Rev. Lett. **58**, 2059 (1987).
[2] J. D. Joannopoulos, R. D. Mead, and J. N. Winn, *Photonic Crystals: Molding the Flow of Light* (Princeton University Press, Princeton, NJ, 1995).
[3] *Photonic Band Gaps and Localization*, Proceedings of the NATO ARW, edited by C. M. Soukoulis (Plenum Press, New York, 1993).
[4] J. D. Joannopoulos, P. Villeneuve, and S. Fan, Nature (London) **386**, 143 (1997).
[5] R. Padjen, J. M. Gérard, and J. Y. Marzin, J. Mod. Opt. **41**, 295 (1994).
[6] K. M. Ho, C. T. Chan, and C. M. Soukoulis, Phys. Rev. Lett. **65**, 3152 (1990).
[7] M. Qiu and S. L. He, J. Opt. Soc. Am. B **17**, 1027 (2000).
[8] R. D. Meade, K. D. Brommer, A. M. Rappe, and J. D. Joannopoulos, Appl. Phys. Lett. **61**, 495 (1992).
[9] Z. Y. Li and Z. Q. Zhang, Phys. Rev. B **62**, 1516 (2000).
[10] P. R. Villeneuve and M. Piche, Phys. Rev. B **46**, 4973 (1992).
[11] C. S. Kee, J. E. Kim, and H. Y. Park, Phys. Rev. E **56**, 6291 (1997).
[12] D. Cassagne, C. Jouanin, and D. Bertho, Phys. Rev. B **53**, 7134 (1996).
[13] I. H. H. Zabel and D. Stroud, Phys. Rev. B **48**, 5004 (1993).
[14] Z. Y. Li, B. Y. Gu, and G. Z. Yang, Phys. Rev. Lett. **81**, 2574 (1998).
[15] C. M. Anderson and K. P. Giapis, Phys. Rev. Lett. **77**, 2949 (1996).
[16] C. M. Anderson and K. P. Giapis, Phys. Rev. B **56**, 7313 (1997).
[17] X. Zhang and Z. Q. Zhang, Phys. Rev. B **61**, 9847 (2000).
[18] F. Bassani and G. Pastori-Parravicini, *Electronic States and Optical Transitions in Solids* (Pergamon, Oxford, 1975).
[19] M. Plihal and A. A. Maradudin, Phys. Rev. B **44**, 8565 (1991).
[20] M. Agio and L. C. Andreani, Phys. Rev. B **61**, 15519 (2000).
[21] P. Lalanne, Phys. Rev. B **58**, 9801 (1998).
[22] L. F. Shen and S. L. He, J. Opt. Soc. Am. A **19**, 1021 (2002).
[23] *Linear Algebra and Matrix Theory*, edited by Evar D. Nering (Wiley, New York, 1963).