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Photonic Crystal Devices Analysis Based on Perturbation Theory

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ABSTRACT

A novel approach for photonic crystals devices analysis, based on perturbation theory is reported. In this method the photonic crystal device is considered as the superposition of a parent lattice and a perturbing one. Then the solution is investigated in terms of the eigensolutions of the parent lattice. This way, one can easily obtain analytic expressions within the first order perturbation, describing the effects of different parameters on the eigensolutions of the structure. The perturbation theory employed in this work is typical of what is conventionally used in quantum mechanics literature. The proposed method is explicit, works fast, and does not involve complicated numerical calculations.

Although this approach can be used to obtain some rules of thumb about the eigensolutions of the device within the first order perturbation approximation, it can be further followed to higher order perturbation terms for acquiring any desired level of accuracy. Since the presented method is mostly formulated analytically, not much computational effort is required for analyzing complex structures. In this paper the approach is described in detail and some examples are given to show the usefulness of it.

Keywords: Perturbation Theory, Photonic Crystals, Analytic Solutions.

1. INTRODUCTION

Analysis and synthesis of photonic band gap devices requires reliable analysis methods. Band structure analysis of photonic crystal structures are mostly carried out by using the plane wave expansion (PWE) method[1], and the finite difference time domain (FDTD) approach[2]. PWE is the easiest and the most widely used approach; however, it suffers from poor convergence and numerical problems when analyzing photonic crystals with complicated unit cells. The problems become more severe when analysis of higher bands is concerned. FDTD is versatile and can be employed for analyzing different photonic band gap structures. However, FDTD analysis is time consuming. Also, none of the above mentioned methods yield much physical insight, because they are numerically implemented. Analytic expressions, even if approximate, not only can give physical insight into the problem, but also can be used for synthesis purposes. In this regard an approach is developed for obtaining band structure analytically for square lattices where separation of variables is possible[3]. Also, another method is developed for obtaining band structure by using the k.p perturbation approach[4,5]. In this method, eigenvalues and eigenfunctions at a single point in reciprocal lattice are used as initial point for starting the perturbation approach[4,5].

In this paper, a method based on perturbation theory[6,7] is introduced for analysis of photonic crystal structures. In this method, a complicated lattice can be considered as the superposition of a parent lattice and a perturbing lattice. The eigensolutions of the structure are investigated in terms of the eigensolutions of the parent lattice. The parent lattice can be chosen so that its eigensolutions are easily derived. Using the proposed approach, one can easily obtain analytic expressions within the first or the second order perturbations, describing the effects of different parameters on the solution. Through these expressions, it can be investigated that how different eigensolutions of the parent lattice contribute to form the band structure of the perturbed lattice. Also, one can pursue the perturbations to higher orders to obtain the solution with any desired level of accuracy. However, in most cases the first order perturbation provides an acceptable result which can be further accorded by using the second order perturbation.

In this report, the general explicit formulation is presented for the first order perturbation and the usefulness of the approach is demonstrated by applying it to analytic expressions of the band structure of a parent lattice[3] for obtaining the band structure of a lattice for which exact analytic expressions cannot be derived. The results are compared with those obtained by FDTD and PWE.

In section II, the perturbation formulation is discussed. In section III the results and examples are given. Conclusions are given in section IV.

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2. FORMULATION

2.1. Non-degenerate case

Any complicated photonic crystal structure can be considered as the superposition of a parent lattice and a perturbing lattice. Here, it is intended to obtain the eigensolutions of the overall structure in terms of the eigensolutions of the first lattice. The first lattice, called here parent lattice, can be chosen so that its eigensolutions are readily obtained. For TE polarization, the wave equation in a two-dimensional lattice reads as[8]:

$$\nabla^2 E_z = -\frac{\omega^2}{c^2}\varepsilon(x,y)E_z\,, \tag{1}$$

where $\varepsilon(x, y)$ is the permittivity of the photonic crystal structure. The permittivity profile can be considered as $\varepsilon_1+\varepsilon_2$, where ε_1 represents the permittivity profile of the parent lattice and ε_2 stands for the permittivity profile of the perturbing lattice. For example, the photonic crystal whose unit cell is shown in Fig.1 can be considered as the superposition of the two lattices shown in Fig.2. Then ε_1 and ε_2 correspond to Fig. 2a and Fig. 2b, respectively. The wave equation becomes:

$$\nabla^2 E_z = -\frac{\omega^2}{c^2}(\varepsilon_1+\varepsilon_2)E_z\,. \tag{2}$$

The eigenvalues are defined as $W=\frac{\omega^2}{c^2}$ for convenience. Also, a new parameter, λ, representing the strength of perturbation, is introduced. When λ=0, there is not any perturbation and the photonic crystal structure transforms to the parent lattice, when λ=1, the perturbation fully "turns on". In the same manner as what is conventionally done in the analysis of an ordinary photonic crystal, E_z are classified according to the number of bands to which they correspond and the values of κ they take[8]. Henceforth, eigenfunctions are shown as $E_{zm\boldsymbol{\kappa}}$, where m is the number of bands and $\boldsymbol{\kappa}$ is the Bloch wavevector. Thus, Eq. (2) becomes:

$$\nabla^2 E_{zm\kappa} = -W_m(\varepsilon_1+\lambda\varepsilon_2)E_{zm\kappa}\,. \tag{3}$$

Each eigenvalue, W_m, and eigenfunction, $E_{zm\boldsymbol{\kappa}}$, in the perturbed system, can be expanded as a power series of λ :

$$W_m = W_m^{(0)} + \lambda W_m^{(1)} + \lambda^2 W_m^{(2)} + \ldots, \tag{4}$$

$$E_{zm\boldsymbol{\kappa}} = E_{zm\boldsymbol{\kappa}}^{(0)} + \lambda E_{zm\boldsymbol{\kappa}}^{(1)} + \lambda^2 E_{zm\boldsymbol{\kappa}}^{(2)} + \ldots, \tag{5}$$

where $W_m^{(k)}$ and $E_{zm\boldsymbol{\kappa}}^{(k)}$ are kth-order perturbation terms of mth eigenfrequency and eigenfunction respectively.

After substituting the above expansions in Eq. (3) and equating respective coefficients of each power of λ in both sides, a set of equations is obtained:

$$\nabla^2 E_{zm\boldsymbol{\kappa}}^{(0)} = -W_m^{(0)}\varepsilon_0 E_{zm\boldsymbol{\kappa}}^{(0)}\,. \tag{6a}$$

$$\nabla^2 E_{zm\boldsymbol{\kappa}}^{(1)} = -W_m^{(0)}\varepsilon_0 E_{zm\boldsymbol{\kappa}}^{(1)} - W_m^{(1)}\varepsilon_0 E_{zm\boldsymbol{\kappa}}^{(0)} - W_m^{(0)}\varepsilon_1 E_{zm\boldsymbol{\kappa}}^{(0)}\,. \tag{6b}$$

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Eq. (6a) corresponds to the zeroth order perturbation and indicates that the zeroth order perturbed eigenvalues and eigenfunctions are merely eigensolutions of the first (parent) lattice, i.e.

$$W_m^{(0)} = \frac{{\omega^u}_m^2(\boldsymbol{\kappa})}{c^2}\,. \tag{7}$$

$$E_{zm\boldsymbol{\kappa}}^{(0)}(\boldsymbol{r}) = E_{zm\boldsymbol{\kappa}}^{u}(\boldsymbol{r})\,. \tag{8}$$

In these equations, the superscript u stands for unperturbed and refers to the unperturbed lattice or the parent lattice.
First order perturbed eigenfunctions are expanded in terms of the eigensolutions of the first lattice as:

$$E_{zm\boldsymbol{\kappa}}^{(1)}(\boldsymbol{r}) = \sum_n a_n^{(1)} E_{zm\boldsymbol{\kappa}}^{(0)}(\boldsymbol{r})\,. \tag{9}$$

After substituting Eq. (9) in Eq. (6b), and projecting the resultant equation on $E_{zm\boldsymbol{\kappa}}^{(0)*}$, an expression for the first order perturbed eigenvalue is obtained as:

$$W_m^1 = -W_m^0 \int_V \varepsilon_1(r) d^2\mathbf{r} \left| E_{zm\boldsymbol{\kappa}}^{(0)}(\mathbf{r}) \right|^2 , \tag{10}$$

where V stands for the volume of the parent photonic crystal. For obtaining Eq. (10) the orthonormality relation is used which reads as:

$$\int_V d^2\mathbf{r} \varepsilon_0(r) E_{zm\boldsymbol{\kappa}}^{(0)}(\mathbf{r}) E_{zp\boldsymbol{\kappa}}^{(0)*}(\mathbf{r}) = \delta_{np} , \tag{11}$$

Here, δ_{np} is the Kronecker delta. Since both eigenfunctions are chosen from the same Bloch wavevectors, $\delta(\boldsymbol{\kappa}-\boldsymbol{\kappa}')$ is not required.

Within the first order perturbation, the normalized eigenfrequencies are thus obtained by substituting Eq. (10) in Eq. (4) and setting λ=1:

$$\Omega_m(\boldsymbol{\kappa}) = \Omega_m^0(\boldsymbol{\kappa}) \sqrt{1 - \int_V d^2\mathbf{r} \varepsilon_1(r) \left| E_{zm\boldsymbol{\kappa}}^{(0)}(\mathbf{r}) \right|^2} . \tag{12}$$

The normalized eigenfrequency is defined as $\Omega_m = \dfrac{\omega_m L}{c}$, where L is the lattice constant. From Eq. (12) it can be seen how the eigenfunctions and eigenfrequencies of the parent lattice contribute to form the band structure of the perturbed lattice. Eq. (12) is not valid for degenerate bands and another scheme, described in the next section, need to be adopted.

2.2. Degenerate Case

When the eigensolutions of the parent lattice are degenerate, the perturbation theory introduced in the last section requires modification. In this case, more than one eigenfunction correspond to each eigenvalue, and any linear combination of these can be used for the parent lattice eigenfunctions. This ambiguity is resolved by adopting an appropriate scheme[6]. The eigenfunction corresponding to the degenerate band is expanded as a linear combination of orthonormal degenerate eigenfunctions:

$$E_{zm\boldsymbol{\kappa}}^{(0)}(\mathbf{r}) = C_\alpha E_\alpha^{(0)}(\mathbf{r}) + C_\beta E_\beta^{(0)}(\mathbf{r}) , \tag{13}$$

C_α and C_β are the expansion coefficients which will be determined later. After substituting Eq. (13) in Eq. (6b) and projecting the resultant equation on the bases of the degenerate space, i.e. $E_\alpha^{(0)}$ and $E_\beta^{(0)}$, an eigenvalue equation is obtained:

$$[A] \begin{bmatrix} C_\alpha \\ C_\beta \end{bmatrix} = -W_m^1 \begin{bmatrix} C_\alpha \\ C_\beta \end{bmatrix} , \tag{14}$$

where $[A]$ is a matrix whose elements are obtained as:

$$A_{11} = W_m^{(0)} \int_V d^2\mathbf{r} \varepsilon_1(\mathbf{r}) \left| E_\alpha^{(0)}(\mathbf{r}) \right|^2 . \tag{15a}$$

$$A_{22} = W_m^{(0)} \int_V d^2\mathbf{r} \varepsilon_1(\mathbf{r}) \left| E_\beta^{(0)}(\mathbf{r}) \right|^2 . \tag{15b}$$

$$A_{12} = A_{21}^* = W_m^{(0)} \int_V d^2\mathbf{r} \varepsilon_1(\mathbf{r}) E_\alpha^{(0)}(\mathbf{r}) E_\beta^{(0)*}(\mathbf{r}) . \tag{15c}$$

From Eq. (14), it can be readily shown that there are two values for W_m^1 corresponding to the two eigenvalues of matrix $[A]$. The two values for W_m^1 are proportional to $-W_m^0$, as in the non-degenerate case. Therefore the degeneracy may be resolved after applying the perturbation method to degenerate bands.

3. EXAMPLES AND RESULTS

In order to verify the presented method, a photonic crystal whose unit cell is shown in Fig. 1, is analyzed. This structure cannot be analyzed analytically because the separation of variables along the Cartesian coordinates is not possible. However, this photonic crystal can be considered as the superposition of two other lattices shown in Fig. 2a and Fig. 2b. It has been shown that the band structure of the photonic crystal in Fig. 2a can be calculated analytically[3]. Thanks to the coincidence of the geometry with the coordinate system, this is accomplished by decomposing the problem into two one-dimensional crystals shown in Fig. 3. Thus, the eigenfunctions can be considered as:

$$E^{(0)}_{zm\boldsymbol{\kappa}}(x,y)=\Psi(x)\Lambda(y) \tag{16}$$

Each of ψ and Λ satisfy a wave equation separately and therefore the band structure and eigenfunctions can be obtained analytically[3]:

$$\cos(\kappa_x L)=\cos(k_b t)\cos[k_a(L-t)]-\frac{k_a^2+k_b^2}{2k_a k_b}\sin(k_b t)\sin[k_a(L-t)], \tag{17a}$$

$$\cos(\kappa_y L)=\cos(k_d t)\cos[k_c(L-t)]-\frac{k_c^2+k_d^2}{2k_c k_d}\sin(k_d t)\sin[k_c(L-t)], \tag{17b}$$

in which $k_a=\frac{\omega}{c}\sqrt{\frac{\varepsilon_b}{2}+\beta}$, $k_c=\frac{\omega}{c}\sqrt{\frac{\varepsilon_b}{2}-\beta}$, $k_b=\frac{\omega}{c}\sqrt{\varepsilon_a-\frac{\varepsilon_b}{2}+\beta}$, and $k_d=\frac{\omega}{c}\sqrt{\varepsilon_a-\frac{\varepsilon_b}{2}-\beta}$. β is a separation constant.

It should be noted that ε_p may be positive or negative, according to the relative values of ε_a and ε_b. Since the eigenfunctions are easily obtained analytically, the integrals in Eq. (12) and Eqs.(15) can be calculated analytically reducing the computation load. Also, the integration is limited to the central patch of Fig. 2b, because the permittivities of all the other areas in the perturbing lattice are zero.

As the first example, a photonic crystal with the following parameters is analyzed:

ε_b =1, ε_a =5, t =L/3.

For this structure ε_p=-4. The band structure for the parent lattice is calculated using the exact analytic formulas of Eqs.(17), the PWE method, and the FDTD approach. The results are shown in Fig. 4. PWE results are obtained by keeping 16 harmonics and those of FDTD are obtained after 2^{13} time steps. It can be seen that the results of the three methods agree well for the first band; however, for the second and the third bands the PWE results degrade. This is due to the fact that the convergence of the PWE results for higher bands is slow, and this requires increasing the number of harmonics, which in turn results in numerical errors. Another point is that the PWE method cannot predict the degeneracy of the second band in ΓM direction correctly because of numerical errors in estimating the eigenvalues. This mentioned degeneracy in ΓM direction arises from the fact that the two cones centered on Γ_2 and Γ_3 meet along the ΓM direction in the first Brillouin zone for each frequency. This is schematically shown in Fig. 5.

After applying perturbation, the band structure for the perturbed lattice, shown in Fig. 1, is depicted in Fig. 6. In this figure the band structure of the unperturbed lattice (the parent lattice) is also shown. From this figure, one can see how the first order perturbation moves and reshapes the bands for the perturbed lattice. Also, the degenerate band in ΓM direction is split after applying the perturbation. The results agree well with the FDTD results, justifying the proposed approach. In Fig. 7 the perturbed lattice band structure obtained by using the proposed method is compared with the results of the PWE, where the agreement of the results is observed.

Another example is a photonic crystal of the same structure as what is shown in Fig. 1, with the following parameters:

ε_b =5, ε_a =1, t =L/3.

For this structure ε_p=4. This photonic crystal exhibits a full gap. The band structure of this photonic crystal together with the band structure of its parent lattice is shown in Fig. 8, where the FDTD results justify the calculated band structure.

In Fig. 9, the perturbed lattice band structure computed by using the proposed approach is compared with the results of the PWE approach obtained by keeping 16 harmonics. It can be seen that the perturbation approach within the first order approximation, computes the band structure and consequently the band gap more precisely.

4. CONCLUSIONS

A method based on the perturbation theory for analyzing photonic crystal structures has been proposed. In this method, a complicated photonic crystal structure is considered as a superposition of a parent lattice, for which the eigensolutions are readily known, and a perturbing lattice. Then the solution is sought in terms of the eigensolutions of the parent lattice. Both the degenerate and non-degenerate cases are discussed. Since, in many cases, the calculations can be carried out analytically, the proposed approach is fast and does not suffer from numerical errors during implementation. Also, within the first order approximation, one can obtain approximate analytic expressions for the band structure, which are useful for obtaining a physical insight and can be used for synthesis purposes. The PWE method, while being a popular approach, does not yield satisfactory results for complicated structures. Also, FDTD being a versatile approach is computationally intensive and does not yield much physical insight into the problem. The proposed method, however, can be used for analyzing different structures wherever appropriate parent lattice can be chosen.

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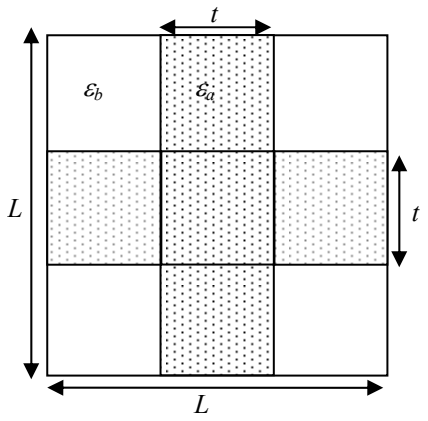

Fig.1. Unit cell of a photonic crystal.

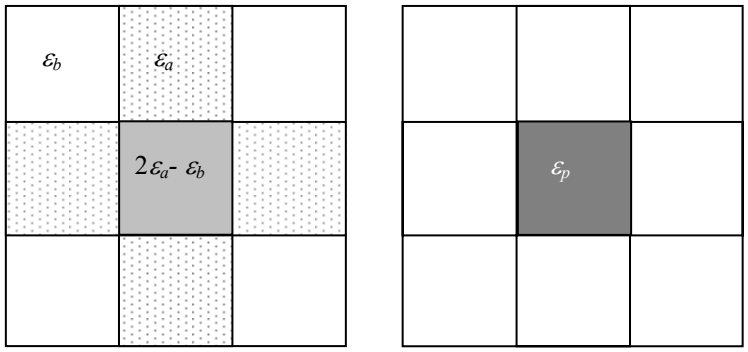

Fig. 2. (a) The parent lattice: $\varepsilon_1(x,y)$. (b) The perturbing lattice: $\varepsilon_2(x,y)$.

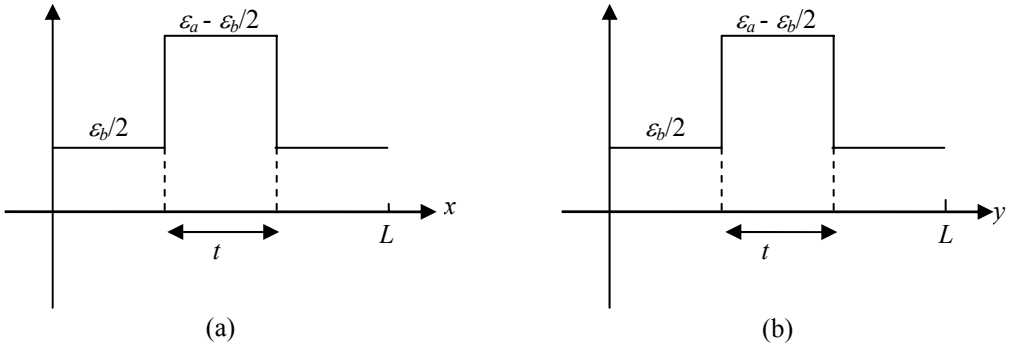

Fig.3. (a) permittivity profile of the photonic crystal of Fig. 2a in x direction.
(b) permittivity profile of the photonic crystal in y direction.

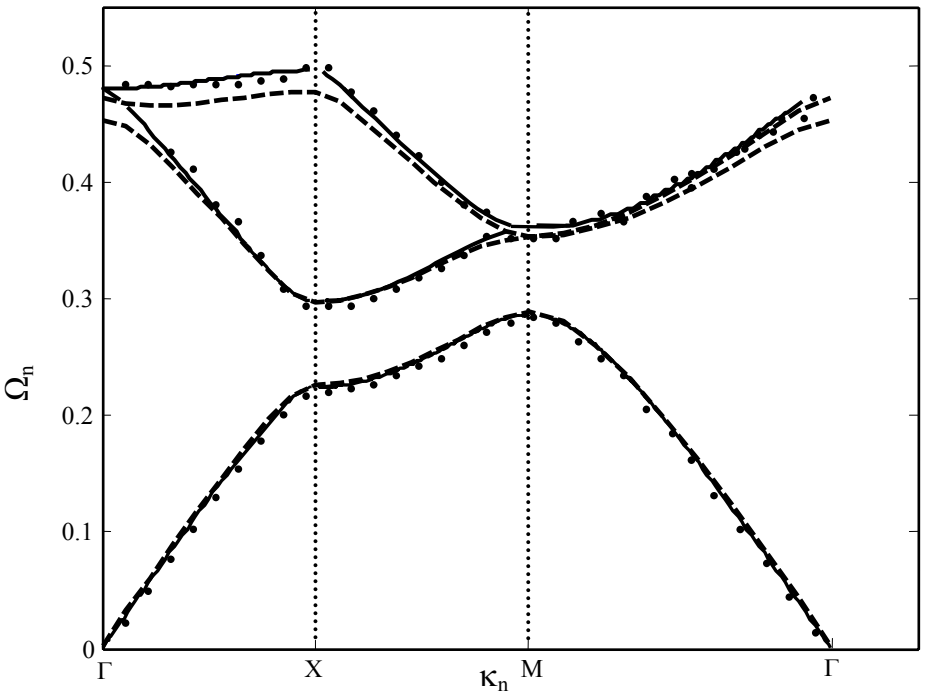

Fig.4. Band structure of the unperturbed lattice shown in Fig. 2a with (ε_b =1, ε_a =5, t =L/3). Solid lines: exact analytic solution. Dashed lines: PWE by keeping 16 harmonics. Dots: FDTD after 2^{13} time steps.

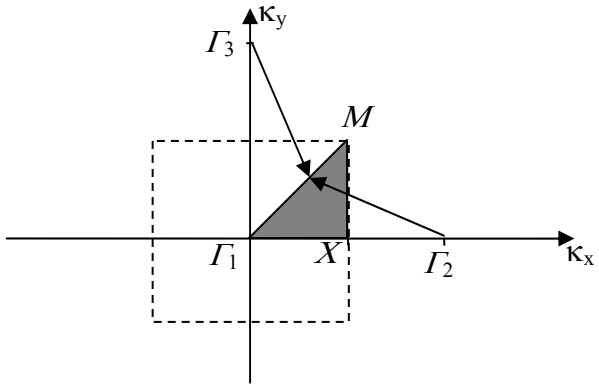

Fig.5. Irreducible Brillouin zone, the two light cones centered on Γ_2 and Γ_3, intersect along the ΓM direction with the same κs at each frequency.

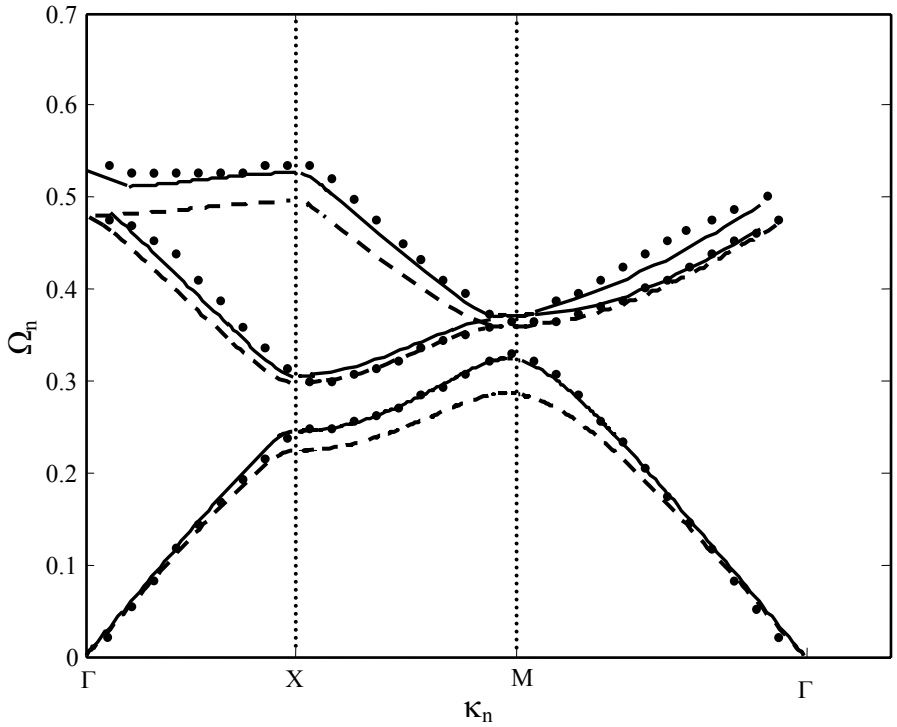

Fig.6. Band structure of the photonic crystal shown in Fig. 1 with (ε_b =1, ε_a =5, t =L/3). Solid lines: perturbed lattice band structure obtained by the proposed approach. Dashed lines: unperturbed lattice results. Dots: FDTD results for the perturbed lattice after 2^{13} time steps.

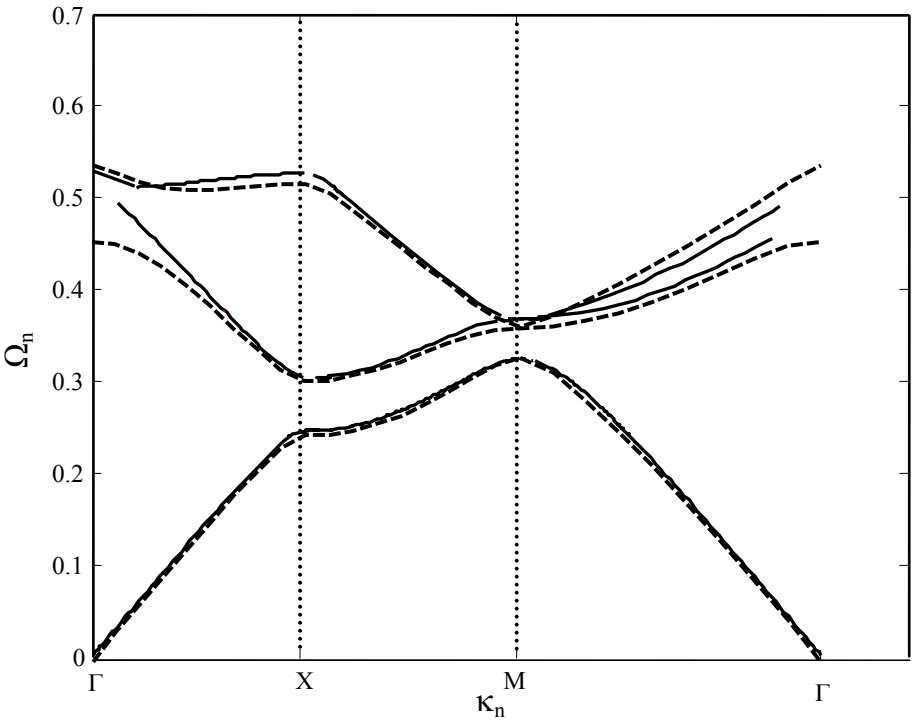

Fig.7. Band structure of the photonic crystal shown in Fig. 1 with (ε_b =1, ε_a =5, t =L/3). Solid lines: perturbed lattice band structure obtained by the proposed approach. Dashed lines: PWE results by keeping 16 harmonics.

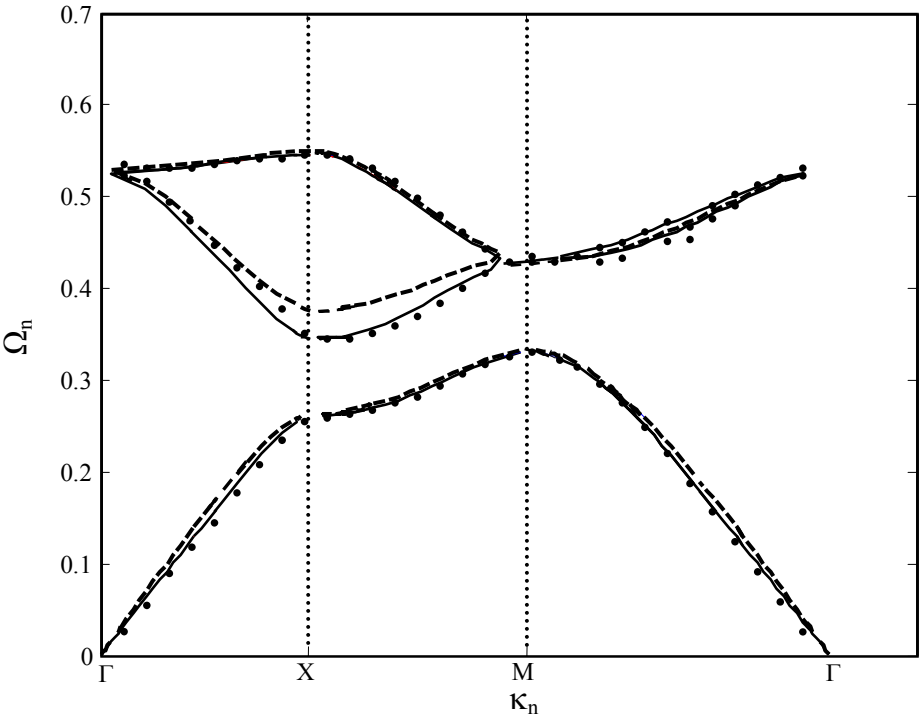

Fig.8. Band structure of the photonic crystal shown in Fig. 1 with (ε_b =5, ε_a =1, t =L/3). Solid lines: perturbed lattice band structure obtained by the proposed approach. Dashed lines: unperturbed lattice results. Dots: FDTD results for the perturbed lattice after 2^{13} time steps.

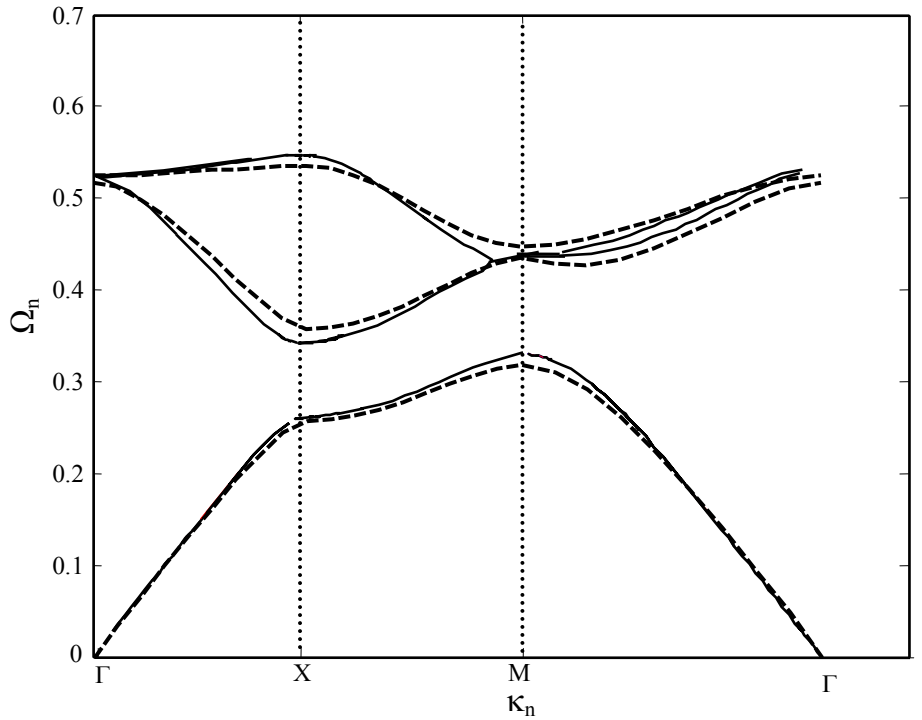

Fig.9. Band structure of the photonic crystal shown in Fig. 1 with (ε_b =5, ε_a =1, t =L/3). Solid lines: perturbed lattice band structure obtained by the proposed approach. Dashed lines: PWE results by keeping 16 harmonics.