An Approximate Analytic Model for Evaluating the Photonic Band Structure of a 2-D Octagonal Photonic Quasicrystals

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***Abstract*— In this work, using perturbation technique we have developed an approximate analytic model for evaluating the band structure of a 2-D octagonal photonic quasicrystal (PQC). Although numerical techniques are being used for evaluating such band structures, developing a numerical model to the best of our knowledge this work is the first instance of reporting helps to understand the physical properties of the structure more easily. Use of perturbation technique can be beneficial in approximating the photonic band structures, in PQCs made with low-dielectric contrast materials, with high accuracy. To the best of our knowledge this work is the first instance of reporting the development of such an analytic model for octagonal PQCs. In addition, we have studied the effect of variations in the dielectric contrast on the photonic band structure.**

KEYWORDS: Photonic band structure, Perturbation theory, Photonic quasi-crystal (PQC), Pseudo-Brillouin zone (PBZ).

I. INTROCUCTION

Quasicrystals have inherent potentials that made them the subject of important theoretical developments in both solid-state physics and photonics engineering. They have neither true periodicity nor translational symmetry. However, their quasi-periodic structures exhibit long-range translational order and orientational symmetry [1]. Photonic quasicrystals (PQCs) are shown to enjoy from larger degrees of freedom in modifying optical properties, compared to the photonic crystals. In low dielectric contrast regime, PQCs due to their high level of rotational symmetry exhibit isotropic and complete photonic band gap [2-4]. Although PQCs and PC share many common features, concepts such as Brillouin zone and Bloch theorem are no longer valid in PQCs [5]. However, for analyzing PQC structures, Pseudo-Brillouin zone (PBZ) has already been developed [6].

To predict band structures of 2D-PQCs' various research groups have used different numerical techniques, such as finite difference time domain (FDTD) [7-11], finite element [12], multiple scattering [13], transfer matrix [14], and plane wave expansion [3,15] methods.

On the other hand, existence of the complete photonic band gap in PQC made of low dielectric contrast materials makes the use of perturbation technique beneficial in developing an approximate analytic model for evaluating their band structures with a relative accuracy. Such an approximation technique has already been employed by Ochiai and Sakoda [16] for obtaining an analytic model for evaluation of the band structure of a 2D-hexagonal PC. However, to the best of our knowledge this work is the first instance of reporting the use of perturbation technique for developing an approximate analytic model for evaluating the band structure of an 8-fold PQC structure. In implementing this technique, we have expanded the refractive index of the PQC

structure in terms of periodic functions and have also developed a PBZ for the quasicrystal. In addition, we have demonstrated how the photonic band structure and its corresponding gap can be affected by variations in the dielectric contrast.

The organization of this paper is as follows: Section II is dedicated to the development of the analytic model. In Section III, the numerical results and discussion are presented. Finally, this paper ends with a conclusion, in Section IV.

II. 2-D OCTAGONAL PHOTONIC QUASI-CRYSTALS

We consider a pillar-type octagonal-PQC made of dielectric rods of radii r in an air base with pitch size of a. The rods indices of refractions vary around an average value of n_0 in a quasi-periodic manner. The 2D-cross sectional view of this PQC is illustrated in Fig. 1. Values of all geometrical and physical parameters used in this paper are given in Table I.

Before developing our analytic model by use of the perturbation technique, we construct the refractive index for the octagonal-PQC structure in low contrast regime, first. Then, a pseudo-Brillouin zone (PBZ) for the structures is defined. At last, we use the perturbation technique to solve the wave equations.

A. *Refractive index modeling*

A quasi-periodic function can be expressed as a sum of periodic functions whose periods are incommensurate (i.e. the ratios of the periods are irrational). Consider a series of N pillar-type octagonal-PCs of the same geometry whose rods are made from different materials that vary around the average value of n_0 in a 2D-periodic manner. However, the index periodicity from one PC to another varies irrationally. Hence, we can write the refractive index of the octagonal-PQC as a superposition of the refractive indices of the PCs with periodic indices:

$$n(\rho) = n_0 + \mu \sum_{i=1}^{N} n_i \cos(G_i \cdot \rho), \tag{1}$$

where ρ, μ, n_i, and G_i are the projection of r in x-y plane, the perturbing parameter, the amplitude of the periodic terms, and the reciprocal lattice vector of the i^{th} 2D-octagonal PQC, respectively. Values of the constants are also given in Table I. The reciprocal lattice vectors are defined as

$$G_i = \frac{2\pi}{a_i}\left(\cos\left(\frac{2\pi i}{N}\right), \sin\left(\frac{2\pi i}{N}\right)\right) \tag{2}$$

When $n_i << n_0$, perturbation theory can be used for developing band structure.

Table I Efficient parameters for modeling refractive index

Parameter	value
Background material refractive index	2.04
n_0	1.51
n_i	-0.065
a	260 *nm*
N	8

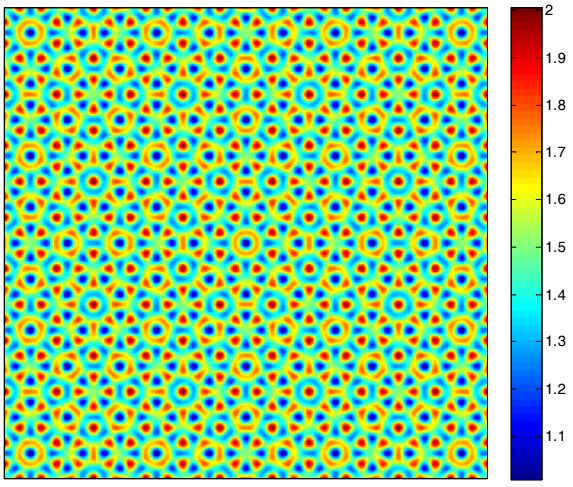

Fig. 1. Schematic representation of the top view of a pillar-type 8-fold PQC is illustrated. The rods indices of refractions vary in a 2D-quasi-periodic manner. The geometrical and physical parameters of the structure are given in Table I.

B. *Photonic Band Structure*

In order to evaluate photonic band structure Maxwell equations must be solved. Assuming

lossless and linear materials, we write the well known Maxwell equations

$$\nabla \times \left(\frac{1}{\varepsilon(\mathbf{r})} \nabla \times \mathbf{H}(\mathbf{r}) \right) = \frac{\omega^2}{c^2} \varepsilon(\mathbf{r}) \mathbf{H}(\mathbf{r}), \quad (3a)$$

$$\nabla \cdot \mathbf{H}(\mathbf{r}) = 0, \quad (3b)$$

$$\mathbf{E}(\mathbf{r}) = \frac{1}{\omega \varepsilon_0 \varepsilon(\mathbf{r})} \nabla \times \mathbf{H}(\mathbf{r}) \quad (3c)$$

where $\mathbf{H}(\mathbf{r})$, $\mathbf{E}(\mathbf{r})$, $\varepsilon(\mathbf{r})$, ε_0, ω, c, and $\mathbf{r}$ are the magnetic field, Electric field, dielectric constant, free space permittivity, the light radian frequency, speed of light in free space, and the position vector in a 3D coordinate system.

We identify the left side of the Eq. (3a) as operator $\boldsymbol{\Theta}$ acting on $\mathbf{H}(\mathbf{r})$ similar to eigenvalue equation. It should be mentioned that the operator $\boldsymbol{\Theta}$ is a Hermitian operator and thus the Maxwell equation is arranged as an eigenvalue problem for the magnetic field $\mathbf{H}(\mathbf{r})$ and then the $\mathbf{E}(\mathbf{r})$ can be calculated via Eq. (3c). For 2-D case, the eigenvalue equations are much simplified if the wavevector is parallel to the 2-D plane. In this case, the modes must be oscillatory in the z-direction; with no restrictions on the wavevector along this direction $\boldsymbol{k}_z$, because the system is homogeneous in that direction. By solving eigenvalue equation described by Eq. (3a), the eigenfrequencies and eigenfunctions of system are obtained.

1) Pseudo-Brillouin zone: In the case of 2-D photonic crystal, the system has discrete translational symmetry in the *x*-y plane. So by applying Bloch's theorem, one can focus on the value of in-plane wavevector $\boldsymbol{k}_{\|}$ that are in the Brillouin zone.

Unfortunately, for quasiperiodic systems, Brillouin zone in the usual sense does not exist. In these systems, the reciprocal lattice vectors of a quasiperiodic structure densely fill all reciprocal space. However, it is often useful to choose a subset of basic reciprocal lattice vectors that corresponds to the relatively intense spots in the diffraction pattern. In addition, although quasicrystals do not possess a Brillouin zone, it is possible to construct an analogue called the pseudo-Brillouin zone which is defined by lines bisecting the basic reciprocal lattice vectors [3, 6]. Diffraction pattern of 2-D 8-fold photonic quasicrystal is calculated and it is illustrated in Fig. 2. The first pseudo-Brillouin zone boundary is halfway between the origin and the strongest diffraction peaks and it is indicated in Fig. 2. by white octagon.

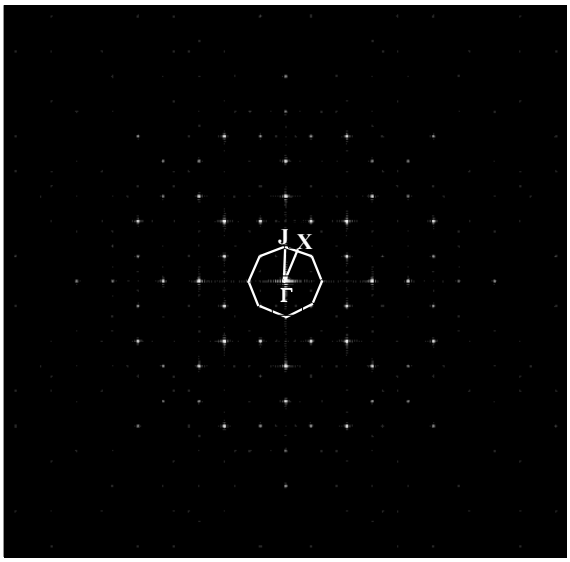

Fig. 2. Reciprocal lattice of 2-D 8-fold photonic quasicrystal, the first pseudo-Brillouin zone is indicated by white octagon

By defining pseudo-Brillouin zone for quasicrystal, one pays attention to the values of $\boldsymbol{k}_{\|}$ in to this zone. The label n (band number) is used to label the modes in order of increasing frequency. Indexing the modes of quasicrystal by $\boldsymbol{k}_z$ and $\boldsymbol{k}_{\|}$ and n, they take the familiar form of Bloch states.

$$\mathbf{H}_{(n,k_z,k_{\|})}(\mathbf{r}) = e^{ik_{\|}\rho} e^{ik_z z} u_{(n,k_z,k_{\|})}(\rho). \quad (4)$$

In this equation, ρ is the projection of $\mathbf{r}$ in the *x*-y plane and $u(\rho)$ is a profile of modes. In this paper, we mainly restrict ourselves to in-plane ($\boldsymbol{k}_z$=0) propagation. Right now, perturbation method is considered to solve the Maxwell equation.

2) Perturbation theory: perturbation theory is an efficient method to evaluate band structure

of this system duo to small variation of dielectric constant which is considered as a small perturbation to homogeneous media. The idea is to begin with the modes of idealized homogeneous medium (as an unperturbed system), and using analytical tools to approximately evaluate the effect of small changes in the dielectric function (as a profile of quasiperiodic function) on the modes and their frequencies. For many realistic problems, the error in this approximation is negligible. The derivation of perturbation theory for Hermitian eigen problem is straightforward and is covered in many texts on quantum mechanics [18-19]. Suppose a Hermitian operator Θ is altered by a small amount ΔΘ. The resulting eigenvalues and eigenvectors of the perturbed operator can be written as series expansions, in terms that depend on increasing powers of the perturbation strength ΔΘ. The resulting equation can be solved order-by-order using only the eigenmodes of the unperturbed operator. Now, we briefly review this method according to our system. The Eq. (3) for TM polarization and 2-D case is considered.

$$-\left(\frac{\partial}{\partial x}\frac{1}{\varepsilon(\rho)}\frac{\partial}{\partial x}+\frac{\partial}{\partial y}\frac{1}{\varepsilon(\rho)}\frac{\partial}{\partial y}\right)\mathbf{H}_z(\rho)=\frac{\omega^2}{c^2}\mathbf{H}_z(\rho),$$
$$\Theta^{(2)}\mathbf{H}_z(\rho)\equiv\frac{\omega^2}{c^2}\mathbf{H}_z(\rho), \tag{5}$$

where superscript (2) denotes the 2-D operator. Then, by substituting Eq. (4) in this equation and assuming the in-plane propagation ($\boldsymbol{k_z}$=0), the 2-D operator can be written as,

$$\Theta^{(2)}u_{(n,k_\parallel)}(\rho)\equiv\frac{\omega^2}{c^2}u_{(n,k_\parallel)}(\rho),$$
$$\Theta^{(2)}=-\left(\frac{1}{\varepsilon(\rho)}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)+\frac{\partial}{\partial x}\frac{1}{\varepsilon(\rho)}\frac{\partial}{\partial x}+\frac{\partial}{\partial y}\frac{1}{\varepsilon(\rho)}\frac{\partial}{\partial y}-{k_\parallel}^2\right), \tag{6}$$

where in this notation the subscript *n* and $\boldsymbol{k}_\parallel$ denotes the band number and corresponding $\boldsymbol{k}_\parallel$ in the pseudo-Brillion zone. After that, according to Eq. (1), $\varepsilon^{-1}(\rho)$ is expanded and substituted into the 2-D eigenvalue problem given by Eq. (6). The unperturbed Hermitian operator $\hat{\Theta}^{(2)}$ and the perturbation operator $\Delta\hat{\Theta}^{(2)}$ are obtained as follows,

$$\left(\hat{\Theta}^{(2)}+\Delta\hat{\Theta}^{(2)}\right)u'_{(n,k_\parallel)}(\rho)\equiv\Omega'_{(n,k_\parallel)}u'_{(n,k_\parallel)}(\rho),$$
$$\hat{\Theta}^{(2)}\equiv-\left(\frac{1}{n_0^2}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)-{k_\parallel}^2\right),$$
$$\Delta\hat{\Theta}^{(2)}\equiv 2n_0\sum_{i=1}^{N}n_i\cos(G_i.\rho)\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)$$
$$+\frac{\partial}{\partial x}\left(2n_0\sum_{i=1}^{N}n_i\cos(G_i.\rho)\right)\frac{\partial}{\partial x}+\frac{\partial}{\partial y}\left(2n_0\sum_{i=1}^{N}n_i\cos(G_i.\rho)\right)\frac{\partial}{\partial y},$$

(7)

where $u'_{(n,k_\parallel)}(\rho)$ and $\Omega'_{(n,k_\parallel)}=\frac{\omega^2}{c^2}$ are the eigenvectors and eigenfrequencies of the perturbed operator. They can be written as series expansion,

$$u'_{(n,k_\parallel)}(\rho)=u^{(0)}_{(n,k_\parallel)}(\rho)+\mu u^{(1)}_{(n,k_\parallel)}(\rho),$$
$$\Omega'_{(n,k_\parallel)}=\Omega^{(0)}_{(n,k_\parallel)}+\mu\Omega^{(1)}_{(n,k_\parallel)}, \tag{8}$$

where the superscripts denote the order of eigenfrequencies and eigenvectors corrections. Now, perturbed eigenfrequencies and eigenvectors given by Eq. (8) is substituted into the Eq. (6). Then, terms are collected and factorized order-by-order in μ. For the zeroth order in μ (i.e. O (1)), the unperturbed system is considered, which can be solved by different methods such as finite difference method and eigenvectors and eigenvalues $u^{(0)}_{(n,k_\parallel)}(\rho)$, $\Omega^{(0)}_{(n,k_\parallel)}$ can be obtained. For the first order, O (μ), is obtained as

$$\hat{\Theta}^{(2)}u^{(1)}_{(n,k_\parallel)}(\rho)+\Delta\hat{\Theta}^{(2)}u^{(0)}_{(n,k_\parallel)}(\rho)=\Omega^{(0)}_{(n,k_\parallel)}u^{(1)}_{(n,k_\parallel)}(\rho)+\Omega^{(1)}_{(n,k_\parallel)}u^{(0)}_{(n,k_\parallel)}(\rho).$$

(9)

When, Eq. (9) is multiplied by $u^{*(0)}_{(n,k_\parallel)}(\rho)$ and is integrated over the surface of crystal, $\Omega^{(1)}_{(n,k_\parallel)}$ is obtained.

$$\Omega^{(1)}_{(n,k_\parallel)}=\frac{\iint u^{*(0)}_{(n,k_\parallel)}(\rho)\Delta\hat{\Theta}^{(2)}u^{(0)}_{(n,k_\parallel)}(\rho)d\rho}{\iint\left|u^{(0)}_{(n,k_\parallel)}(\rho)\right|^2 d\rho}. \tag{10}$$

It can also be found the correction to the eigenvector by multiplying Eq. (10) to another mode at a different band, *m*.

3) Degenerate perturbation theory: It must be noticed that if there are degeneracy in the

eigenfrequency of unperturbed system, that it means any two zeroth order eigenvectors had the same frequency, the perturbation theory developed before is no longer valid. In this case, the degenerate perturbation theory can be used to identify the eigenfrequency of perturbed system. This theory is covered in some text book [18-19] and it is briefly reviewed here.

According to degenerate perturbation theory, the eigenfrequencies of degenerate state is obtained by solving the following equation,

$$\sum_{m=1}^{g}\left(M_{pm}-\Omega^{(1)}_{(n,k_{\|})}\delta_{mp}\right)a_m^{\alpha}=0, \tag{11}$$

where a_m^{α} is the coefficients of degenerate eigenfunction expansion and M_{mn} is mean value of 2-D operator between degenerate states [18].

For example, if there is a two-fold degeneracy between the modes of the first and second bands, the degeneracy is lifted in the first order perturbation. The eigenvalue equation in the first order perturbation is given by

$$\begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix}\begin{bmatrix} a_1^{\alpha} \\ a_2^{\alpha} \end{bmatrix}=\Omega^{(1)}_{(0,k_{\|})}\begin{bmatrix} a_1^{\alpha} \\ a_2^{\alpha} \end{bmatrix} \tag{12}$$

The lifted modes can be given by:

$$\Omega^{(1)}_{(0,k_{\|})}=\frac{1}{2}(M_{11}+M_{22})+\sqrt{(M_{11}-M_{22})^2+4|M_{12}|^2},\quad \text{for upper eigenfrequency} \tag{13}$$
$$\Omega^{(1)}_{(0,k_{\|})}=\frac{1}{2}(M_{11}+M_{22})+\sqrt{(M_{11}-M_{22})^2+4|M_{12}|^2},\quad \text{for lower eigenfrequency}$$

When there is a three-fold degeneracy between the first three modes, where lifted in the first order perturbation. The eigenvalue equation is given by

$$\begin{bmatrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{31} & M_{33} \end{bmatrix}\begin{bmatrix} a_1^{\alpha} \\ a_2^{\alpha} \\ a_3^{\alpha} \end{bmatrix}=\Omega^{(1)}_{(0,k_{\|})}\begin{bmatrix} a_1^{\alpha} \\ a_2^{\alpha} \\ a_3^{\alpha} \end{bmatrix} \tag{14}$$

Thus the eigenfrequencies can be found by solving this equation. For higher degeneracy order, the similar approach can be used.

III. Numerical Results and Discussion

In this section, we present the numerical results obtained from the analytical model developed in Section II. At first, to demonstrate how accurate our approximate analytical model is, we present the numerical results on the band structure of 2-D hexagonal photonic crystal calculated from this model developed in Section II using the perturbation technique. Then, we compare these results with those obtained from the well-known plane wave expansion (PWE) numerical method. The hexagonal photonic crystal under study is composed of array of 10×10 rods in an air background with geometrical and physical parameter given in Table II. Figure 3 illustrates this comparison. The solid lines represent the numerical values obtained from Eqs. (10) or (11), as described in Section II. The dotted lines demonstrate the numerical values obtained from the PWE numerical method.

Table II Efficient parameters for simulation Fig. 3.

Parameter	value
Background material refractive index	1.7
n_0	1.48
n_i	-0.08
a (nm)	260
N	6

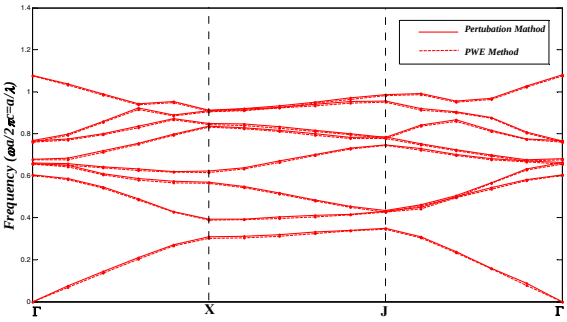

Fig. 3. Comparison the band structure for a2D-pillar hexagonal PhC evaluated by perturbation theory (solid lines) with those obtained from PWE numerical method (dotted lines).

A careful inspection of this comparison shows that the error incurred by the approximation through the perturbation technique is an overestimation of about 2-3%, in comparison

to the more accurate PWE numerical method. Knowing this reasonable error, we use our developed approximate analytic model to evaluate band structure for the 2-D 8-fold PQC of Fig. 1.

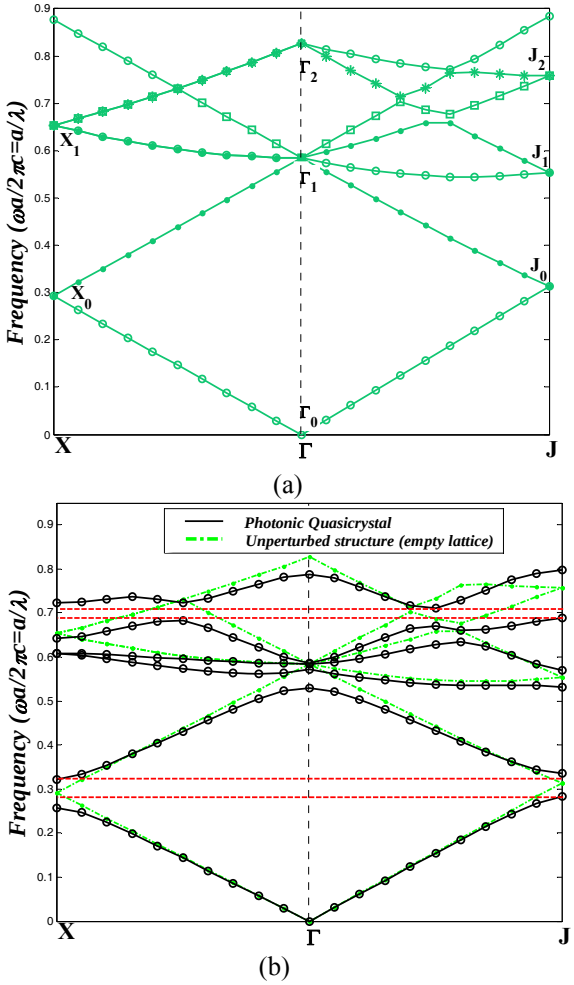

Fig. 4. (a) Band structure of unperturbed structure (empty lattice). (b) Band structure of considered 2-D 8-fold PQC (solid line) and the empty lattice (dashed line).

The band structure for the unperturbed structure (empty lattice) that is evaluated from zeroth order equation of perturbation method is shown in Fig. 4(a). As indicated in Fig. 4-a, there are some points with high symmetry which the eigenfrequency of unperturbed operator is degenerated (i.e. they have different eigenvector with equal eigenfrequency). The correction of eigenfrequency of perturbed operator in these cases can be obtained using degenerate perturbation theory that is briefly reviewed in section II. In other points of this figure that there is not degeneracy, correction of eigenfrequency can be calculated using Eq. (10) described in the previous section.

At the X_0 point where there is a two-fold degeneracy between the modes of the first and second bands, eigenfrequencies is calculated using Eq. (13). Also there is a three-fold degeneracy at the X_1 point which is obtained based on Eq. (14). The four-fold degeneracy at the Γ_1 point is lifted in the same way. Finally, we can calculate the correction of eigenfrequency in all points of the band structure of unperturbed system. Now, the band structure of 2-D 8-fold photonic quasicrystal is illustrated in Fig. 4-b.

Table III Efficient parameters for modeling refractive index

Background material refractive index	n_0	n_i
2.04	1.510	-0.065
2.10	1.560	-0.070
2.20	1.595	-0.077
2.30	1.670	-0.085
2.40	1.750	-0.090
2.50	1.800	-0.100
2.60	1.850	-0.110
2.70	1.900	-0.115
2.80	1.950	-0.117
2.90	1.970	-0.125

According to Fig.4-b, the relative photonic band gap between two bands is defined as

$$\text{Gap} = \frac{\Delta\omega}{\omega_0} = \frac{\min\limits_{k_{\|}\in P-BZ} : \{\omega_h(k_{\|})\} - \max\limits_{k_{\|}\in P-BZ} : \{\omega_l(k_{\|})\}}{\min\limits_{k_{\|}\in P-BZ} : \{\omega_h(k_{\|})\} + \max\limits_{k_{\|}\in P-BZ} : \{\omega_l(k_{\|})\}} \quad (15)$$

where the minima and maxima are taken over all k|| on the pseudo-Brillouin zone (P-BZ), and ω_l and ω_h are bands just below and just above the complete gap. As shown in Fig. 4.b, there are two gaps between first and second bands and between fifth and sixth bands which by increasing dielectric contrast, gap size will be broaden and mid frequency of these gaps shifted to small frequencies. Also, another gap between second and third bands will be appeared. The corresponding effect of dielectric contrast variation on the relative band gap and mid frequency is shown in Fig. 5

and the efficient parameters for modeling refractive index are listed in table III. Narrower photonic band gap in higher frequencies as a result of decrement in dielectric contrast is obtained.

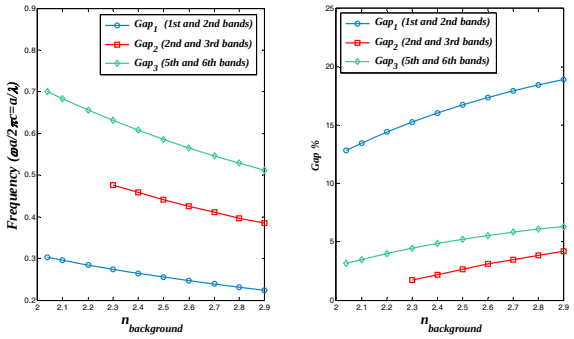

Fig. 5. Mid frequency of band gap versus background material index (Left) and relative photonic band gap versus background material index (Right) for considered 2-D 8-fold PQC.

IV. CONCLUSION

As conclusion, it should be pointed out that pseudo-Brillouin zone was defined for evaluation of the band structure for quasicrystals and consequently the Bloch theory was applied to quasicrystals. Then, we have calculated the band structure of 2-D 8-fold photonic quasicrystal by using perturbation method. It was shown that using first order perturbation theory band structure (eigenfrequencies) can be obtained. As we know, in quasicrystals complete band gap can be observed in low dielectric contrasts, so developing perturbation theory based band solver is interesting. Also, we used degenerate perturbation theory for points with high symmetry to extract precision band structure. Narrower photonic band gap in higher frequencies as a result of decrement in dielectric contrast is obtained. Finally, the proposed method is semi-analytic and presents a conceptual view for applied designer.

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