

# An Asymptotic Model of Three-Dimensional Photonic Crystal\*

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## Abstract

An asymptotic model of three-dimensional periodic dielectric structure (photonic crystal) containing cubic cavities separated by thin dielectric film is analyzed using perturbation techniques. Depending on the problem parameter, the model may exhibit an infinite number of gaps. Simple approximation of the spectral bands is suggested.

## 1 Introduction

We consider the propagation of electromagnetic waves in an infinite medium consisting of a periodic array of unit cubic cavities separated by dielectric planes of the thickness  $\delta$  of high dielectric constant  $\varepsilon$  (Fig. 1).

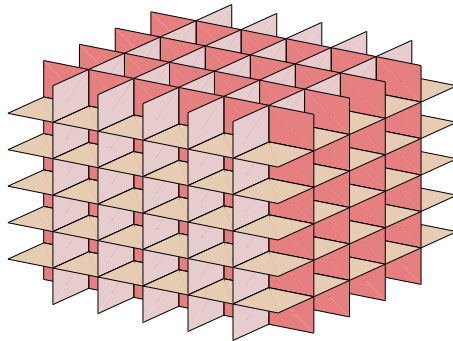


FIG. 1. A slab of three-dimensional photonic crystal composed of cubic air cavities separated by thin dielectric planes of high dielectric constant.

To ensure that nonzero electric energy can be stored in the dielectric, we impose the asymptotic condition

$$(1) \quad \varepsilon \rightarrow \infty \text{ as } \delta \rightarrow 0 \text{ while } \varepsilon\delta = \eta^{-1} \text{ is kept constant.}$$

For this model first introduced in [1] (see also [2]) it was shown that sufficiently small  $\eta$  produce narrow spectral bands about the eigenfrequencies of the cubic resonator with perfectly conducting walls. Hence, those  $\eta$  yield appreciable gaps. In this paper we investigate the asymptotic model further. We compute explicitly the first term of the asymptotics of spectrum branches and calculate numerically the bandgap bounds for finite values of the perturbation parameter. Numerical calculation of the bandgaps is a very

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challenging problem for the three-dimensional case [3], and the asymptotic model in hand might furnish insights into the theory of real photonic crystals.

We denote by  $Q_{\mathbf{m}}$  the periodic array of cubes obtained by translation of the unit cube  $Q_0$  by an integer-valued vector  $\mathbf{m}$ :  $Q_{\mathbf{m}} = Q_0 + \mathbf{m}$ ,  $\mathbf{m} \in \mathbb{Z}^3$ . Let also  $\Gamma$  be the union of the faces of the cubes  $Q_{\mathbf{m}}$ . Describing propagation of waves in the photonic crystal by Maxwell's equations, we will use stationary divergent-free potential  $\Psi(\mathbf{x})$  which is related to the electric induction field  $\mathbf{D}(\mathbf{x})$  through  $\mathbf{D}(\mathbf{x}) = \nabla \times \Psi(\mathbf{x})$ . The electric energy operator  $\mathcal{M}(\eta)$  can be represented as the sum of the air term  $\mathcal{M}_0$  and the energy  $\eta\mathcal{M}_1$  stored in the dielectric [1]

$$(2) \quad \mathcal{M}(\eta) = \mathcal{M}_0 + \eta\mathcal{M}_1,$$

where

$$(3) \quad (\mathcal{M}_0\Psi, \Psi) = \int_{\mathbb{R}^3 - \Gamma} |\nabla \times \Psi(\mathbf{x})|^2 d\mathbf{x},$$

$$(4) \quad (\mathcal{M}_1\Psi, \Psi) = \int_{\Gamma} |\mathbf{n}_+ \times \Psi_+(\mathbf{x}) + \mathbf{n}_- \times \Psi_-(\mathbf{x})|^2 dS$$

and  $\Psi(\mathbf{x})$  satisfies the following conditions

$$(5) \quad \nabla \cdot \Psi(\mathbf{x}) = 0, \quad \mathbf{x} \in \mathbb{R}^3 - \Gamma; \quad \mathbf{n}_{\pm} \cdot \Psi_{\pm}(\mathbf{x}) = 0, \quad \mathbf{x} \text{ in } \Gamma,$$

where  $\mathbf{n}_+ = -\mathbf{n}_-$  and  $\Psi_{\pm}$  are respectively the two opposite normal vectors to the surface  $\Gamma$  and the field in the adjacent to  $\Gamma$  areas.

To reduce the infinite periodic problem to a finite cell  $K$ , we introduce the Floquet-Bloch transform

$$(6) \quad \Psi(\mathbf{k}, \mathbf{x}) = \sum_{\mathbf{m} \in \mathbb{Z}^3} \Psi(\mathbf{x} + \mathbf{m})e^{-i\mathbf{k} \cdot \mathbf{m}}, \quad \mathbf{x} \in Q_0, \quad \mathbf{k} \in K,$$

where  $K = [-\pi, \pi]^3$  is the Brillouin zone. This transform decomposes operator  $\mathcal{M}$  into the fibers  $M(\mathbf{k}, \eta)$  [4], [5]

$$(7) \quad (\mathcal{M}\Psi)(\mathbf{k}, \eta) = M(\mathbf{k}, \eta)\Psi(\mathbf{k}, \eta).$$

The fiber  $M(\mathbf{k}, \eta)$  here is a self-adjoint operator in the Hilbert space  $L^2(Q_0)$

$$(8) \quad M(\mathbf{k}, \eta) = M_0 + \eta M_1(\mathbf{k}), \quad \text{where}$$

$$(9) \quad (M_0\Psi, \Psi) = \int_{Q_0} |\nabla \times \Psi(\mathbf{x})|^2 d\mathbf{x}, \quad \nabla \cdot \Psi(\mathbf{x}) = 0, \quad \mathbf{n} \cdot \Psi(\mathbf{x}) \Big|_{\Gamma} = 0.$$

Operator  $M_0$ , given by (9), corresponds to a single cubic cavity with perfectly conducting walls whose eigenvalues have the form

$$(10) \quad \xi = \frac{\omega^2}{c^2} = \pi^2 (p_1^2 + p_2^2 + p_3^2) = \pi^2 \mathbf{p}^2,$$

where  $\mathbf{p}$  is an integer-valued nonzero index vector, which may have at most one zero component,  $\omega$  is the frequency of electromagnetic wave, and  $c$  is the speed of light. In what follows we will distinguish identical eigenvalues corresponding to different sets of indices  $p_1, p_2, p_3$  as well as eigenvalues of multiplicity two (when all  $p_i > 0$ ,  $i = 1, 2, 3$ ).

The operator  $M_1(\mathbf{k})$  is defined by the quadratic form [1]

$$(11) \quad (M_1(\mathbf{k})\Psi, \Psi) = \sum_{j=1}^3 \int_{\gamma_j} \left| \mathbf{e}_j \times \left[ \Psi(\mathbf{x}) - e^{i\mathbf{k}j} \Psi(\mathbf{x} + \mathbf{e}_j) \right] \right|^2 dS,$$

where  $\gamma_j$  are the faces of the unit cube  $Q_0$  that are determined by the intersection  $\gamma_j = \Gamma_0 \cap \{x_j = 0\}$ ,  $j = 1, 2, 3$  and  $\mathbf{e}_j$  are the vectors of the standard basis.

According the Floquet-Bloch theory, the spectrum  $\sigma(\mathcal{M})$  of the operator  $\mathcal{M}$  is the union of spectra  $\sigma(M(\mathbf{k}, \eta))$  as  $\mathbf{k}$  runs the Brillouin zone  $K = [-\pi, \pi]^3$ . To calculate efficiently the spectrum  $\sigma(M(\mathbf{k}, \eta))$  we observe that operator  $M_0$  has a compact resolvent and that  $M_1(\mathbf{k})$  is compact relatively to  $M_0$  [1], i.e., the operator

$$(12) \quad \mathfrak{M}(\mathbf{k}) = M_0^{-1/2} M_1(\mathbf{k}) M_0^{-1/2}$$

is compact. This allows to treat  $\eta M_1(\mathbf{k})$  in (8) as a small perturbation of  $M_0$  for  $\eta \ll 1$ .

From the properties of  $M_1$  it follows that

- (i) Operator  $M(\mathbf{k}, \eta)$  has a compact resolvent, the spectrum  $\sigma(M(\mathbf{k}, \eta))$  is discrete.
- (ii) Spectrum  $\sigma(M(\mathbf{k}, \eta))$  approaches  $\sigma(M_0)$  (10) uniformly in  $\mathbf{k}$  as  $\eta \rightarrow 0$ . In particular, for small  $\eta$  there must be gaps in the spectrum of the original operator  $\mathcal{M}$  [1], [2].
- (iii) Spectral bands of  $M(\mathbf{k}, \eta)$  lie above the corresponding point spectrum (10) of unperturbed operator  $M_0$  since  $M_0 \leq M(\mathbf{k}, \eta)$ .

## 2 Matrix form of the energy operator

Matrix representation  $\mathcal{M}_0$  of the operator  $M_0$  in the eigenbasis  $\{\Psi_p(\mathbf{x})\}$ ,  $p = 1, 2, \dots$ , has diagonal form

$$(13) \quad \mathcal{M}_0 = \text{diag}(\Lambda_1, \Lambda_2, \dots),$$

where  $\Lambda_i$ ,  $i = 1, 2, \dots$ , is a diagonal matrix with  $\xi_i = \pi^2 \mathbf{p}^2$  on its diagonal (10). The order of the matrix  $\Lambda_i$  equals the multiplicity of the eigenvalue  $\xi_i$ .

Since elements  $[\mathcal{M}_1]_{pq}$  of matrix  $\mathcal{M}_1 = \mathcal{M}_1(\mathbf{k})$  are defined by the components of vectors  $\mathbf{p}$  and  $\mathbf{q}$ , they have natural vectorial enumeration. From inspection of matrix elements  $[\mathcal{M}_1]_{pq}$  which can be calculated explicitly one can derive the following properties of  $\mathcal{M}_1$  and its elements.

- (i)  $\mathcal{M}_1$  is a sparse matrix. For fixed  $\mathbf{p}$  the element  $[\mathcal{M}_1]_{pq}$  is nonzero if and only if  $(\mathbf{p} - \mathbf{q})$  parallel to  $\mathbf{e}_i$ ,  $i = 1, 2, 3$ , i.e.,  $\mathbf{q}$  belongs to the line passing through  $\mathbf{p}$  and parallel to one of the coordinate axes.
- (ii) Any nonzero matrix element  $[\mathcal{M}_1]_{pq}$  vanishes when  $\mathbf{k} = \frac{\pi}{2}(1 - (-1)^{p_1}, 1 - (-1)^{p_2}, 1 - (-1)^{p_3})$  or  $\mathbf{k} = \frac{\pi}{2}(1 - (-1)^{q_1}, 1 - (-1)^{q_2}, 1 - (-1)^{q_3})$ .
- (iii)  $\max_{\mathbf{k}} \left| [\mathcal{M}_1]_{pp} \right| = 4(4 - \delta_{p_1,0} - \delta_{p_2,0} - \delta_{p_3,0})$ . If the eigenvector  $\Psi_p$  admits two polarizations (no zeros among  $p_i$ ,  $i = 1, 2, 3$ ), then  $\max_{\mathbf{k}} \left| [\mathcal{M}_1]_{pp} \right| = 16$ . Otherwise  $\max_{\mathbf{k}} \left| [\mathcal{M}_1]_{pp} \right| = 12$ .

The entries of  $\mathcal{M}_1$  have natural three-dimensional indices. In order to rearrange them in a two-dimensional matrix we enumerate three-dimensional indices according to their proximity to the origin.

Thus, calculation of the eigenvalues of the operator  $M(\mathbf{k}, \eta)$  (8) is reduced to calculation of the eigenvalues of the infinite matrix  $\mathcal{M}_0 + \eta \mathcal{M}_1$ .

TABLE 1  
*Quadratic approximation of the first ten upper bounds of the spectral bands.*

# of band	upper bound approximation	# of band	upper bound approximation
1	$2\pi^2 + 12\eta - 2.01\eta^2$	6	$9\pi^2 + 16\eta - 0.30\eta^2$
2	$3\pi^2 + 16\eta - 2.31\eta^2$	7	$10\pi^2 + 12\eta - 0.97\eta^2$
3	$5\pi^2 + 12\eta - 1.29\eta^2$	8	$11\pi^2 + 12\eta - 1.28\eta^2$
4	$6\pi^2 + 16\eta - 1.43\eta^2$	9	$12\pi^2 + 12\eta - 0.82\eta^2$
5	$8\pi^2 + 12\eta - 1.08\eta^2$	10	$13\pi^2 + 12\eta - 1.00\eta^2$

### 3 Calculation of the spectrum

We employ perturbation techniques for the spectral analysis of the matrix  $\mathcal{M}$  given by (8)

$$(14) \quad \mathcal{M} = \mathcal{M}_0 + \eta\mathcal{M}_1,$$

where  $\mathcal{M}_0$  is block-diagonal matrix and  $\eta$  is a small parameter. For computation of highly degenerate spectrum of matrix  $\mathcal{M}$  we use the approach outlined in [6]. Using a similarity transformation, we transform matrix  $\mathcal{M}$  to a unitary equivalent matrix  $\mathcal{X}$  that has the same block-diagonal form  $\mathcal{X} = \text{diag} \{X^{(1)}, X^{(2)}, \dots\}$  as the unperturbed matrix  $\mathcal{M}_0$ :

$$(15) \quad \mathcal{X} = e^{-S(\eta)} \mathcal{M} e^{S(\eta)} = \mathcal{M}_0 + \eta\mathcal{X}_1 + \eta^2\mathcal{X}_2 + \dots,$$

$$(16) \quad S = \eta S_1 + \eta^2 S_2 + \dots,$$

where matrices  $S_j$ ,  $j = 1, 2, \dots$ , do not depend on  $\eta$  and  $\mathcal{X}_1, \mathcal{X}_2, \dots$  are diagonal block-matrices whose block dimensions coincide with those of matrix  $\mathcal{M}_0$ . The perturbation is then partitioned into the blocks corresponding to the distinct eigenvalues. Thus, instead of infinite-dimensional perturbation  $\mathcal{M}_1$  we obtain an infinite series of independent finite-dimensional perturbations for each of the blocks. In the case of our problem the linear perturbation term  $\mathcal{X}_1$  is calculated exactly. Calculation of the higher-order matrices involves truncation error.

It can be shown that if all indices of the eigenvalue  $\xi$  are positive then the linearized upper bound of its band has the form  $\xi + 16\eta$ . Otherwise, when the eigenvalue  $\xi$  has zero index, its upper bound of the spectral band in linear approximation is  $\xi + 12\eta$ . Quadratic approximations of the first ten upper bounds of spectral bands are given in Table 1.

### 4 Numerical results

Figure 2 shows dependence of the spectral bands of  $\xi = \omega^2/c^2$  calculated numerically (shaded areas) on the perturbation parameter  $\eta = (\varepsilon\delta)^{-1}$ . The eigenvalues were calculated through truncation of matrix  $\mathcal{M}$  to the order 2273 which contains 138 distinct eigenvalues of the greatest multiplicity 48. Dotted lines indicate the upper bound of the bands. Dashed lines denote the upper bound of the bands in the linear approximation, while solid lines correspond to the quadratic approximation (see Table 1). The latter agrees closely with

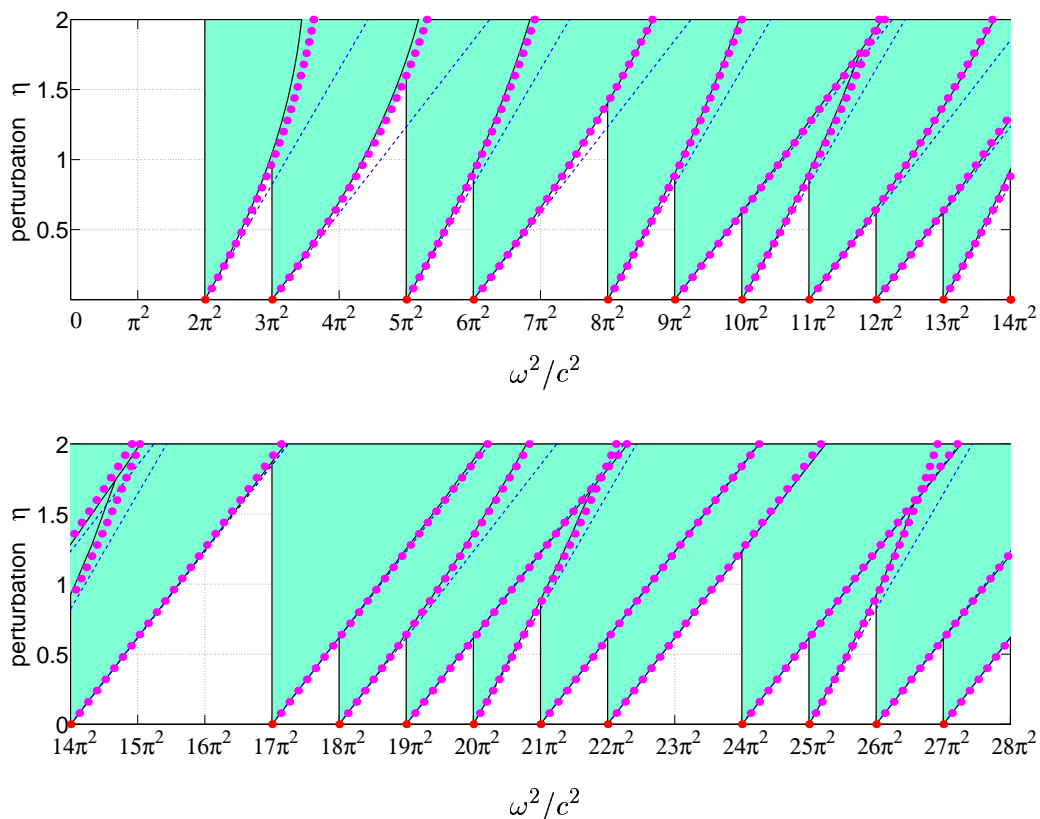


FIG. 2. Dependence of the spectral bands of photonic crystal calculated numerically (shades areas) on the perturbation parameter  $\eta = (\varepsilon\delta)^{-1}$ . Dashed lines denote the upper bound of the bands in linear approximation calculated explicitly. Solid lines correspond to quadratic approximation.

the numerical bound to the point of closing the gaps ( $\eta \approx 2$ ). Figure 2 also suggests that that for high frequencies the linear approximation gives good estimations of spectral gaps.

## References

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