

Analytic approximation of spectra of thin-film three-dimensional photonic crystals

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Abstract

Based on the analytic perturbation theory we study spectra of three-dimensional photonic crystals formed by a periodic array of air cubes separated by a thin film of optically dense dielectric material. The dielectric is assumed to provide vanishing of the normal component of the magnetic field at its surface. The thickness δ of the dielectric component is assumed to be small, whereas its permittivity ε is large. The spectrum is studied for $\delta \rightarrow 0$ while $\varepsilon\delta = \eta^{-1}$ is kept constant. We find that the quadratic in η approximations to dispersion relations are very accurate for all values of η up to the point when all spectral gaps close down. Extensive numerical analysis of the obtained dispersion shows that the pattern of electromagnetic wave propagation varies from almost isotropic to extremely anisotropic depending on the frequency.

Key words. photonic crystal, electromagnetic waves, spectral bands and gaps, thin dielectric films, Maxwell's equations, periodic structure, dispersion surface

1 Introduction

For the last decade photonic crystals became one of important directions in the development on new optical and microwave materials. Three-dimensional photonic crystals is the most challenging case. There has been a considerable amount of publications in the recent years covering wide range of activities: from the new ideas in fabrication of the crystals and new ways to employ their properties in optical devices [6]-[10], [12], [13], [20], [21], [24], [25], [28], [30], [34], [41], [44]-[48], [50], to theoretical and computational studies, allowing accurate computation of the properties of photonic crystals [11], [31], [32], [42], [43], [49]. The computations of spectra and other characteristics play a significant role in the development and fabrication of electromagnetic materials based on photonic crystals (see the above references and the recent focus issue [35]).

In this paper we further develop the analytic perturbation theory analysis of spectra of thin-film three-dimensional photonic crystals (Figure 1) considered in [1].

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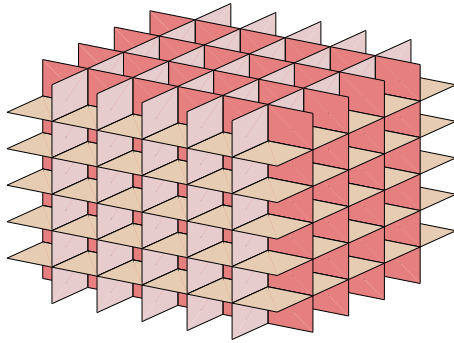


Figure 1: A slab of three-dimensional photonic crystal composed of cubic air cavities separated by thin dielectric plates of high dielectric constant.

As in [1] we study thin-film three-dimensional photonic crystals as an asymptotic model. Asymptotic models can provide valuable insights in physical phenomena in photonic crystals, and, on the other hand, can be treated analytically, [15], [17]-[19], [27], [40]. Photonic crystal in question consists of a periodic array of air cubes separated by a thin film of optically dense dielectric material (Figure 1). The relative thickness δ of the dielectric component is assumed to be small, whereas its permittivity ε is large. We consider the asymptotic situation when the thickness δ of the dielectric component tends to zero while its permittivity ε approaches infinity so that $\varepsilon\delta = \eta^{-1}$ is kept constant. We also assume that the normal component of the magnetic field vanishes at the surface of the optically dense dielectric film.

Propagation of electromagnetic waves in photonic crystal is described by Maxwell's equations

$$\begin{aligned}\nabla \times \mathbf{E} &= -\frac{1}{c} \frac{\partial \mathbf{B}}{\partial t}, & \nabla \times \mathbf{H} &= \frac{1}{c} \frac{\partial \mathbf{D}}{\partial t}, \\ \nabla \cdot \mathbf{D} &= 0, & \nabla \cdot \mathbf{B} &= 0,\end{aligned}$$

where

$$\mathbf{D} = \varepsilon \mathbf{E}, \quad \mathbf{B} = \mu \mathbf{H}.$$

Introducing potential

$$\mathbf{D}(\mathbf{x}, t) = \nabla \times \Phi(\mathbf{x}, t), \quad \mathbf{H}(\mathbf{x}, t) = \frac{1}{c} \frac{\partial \Phi(\mathbf{x}, t)}{\partial t}$$

Assuming temporal dependence of the electromagnetic field in the form $e^{-i\omega t}$, one can introduce divergent-free potential $\Psi(\mathbf{x})$ such that

$$\mathbf{D}(\mathbf{x}) = \nabla \times \Psi(\mathbf{x}), \quad \mathbf{H}(\mathbf{x}) = -\frac{i\omega}{c} \Psi(\mathbf{x}), \quad (1)$$

$$\nabla \cdot \Psi(\mathbf{x}) = 0, \quad \mathbf{n} \cdot \Psi(\mathbf{x}) \Big|_{\Gamma} = 0, \quad (2)$$

where c is the speed of light and Γ denotes the union of the cubes' faces having high dielectric constant ε .

In what follows we will use instead of \mathbf{x} dimensionless spatial variable $\xi_i = x_i/a$, where a is the dimension of the cubic cell, so inside the elementary cube

$$Q_0 = \{0 < \xi_i < 1, i = 1, 2, 3\}.$$

2 Variational formulation

Following to [1] we introduce the periodic array of cubes (see Figure 1):

$$Q_{\mathbf{m}} = Q_0 + \mathbf{m}, \quad \mathbf{m} \in \mathbb{Z}^3. \quad (3)$$

where \mathbb{Z}^3 is the lattice of integer-valued vectors.

The spectrum of the periodic medium can be found with the help of the stationary values of the quadratic form [1]

$$\mathcal{M}(\eta) = \mathcal{M}_0 + \eta\mathcal{M}_1, \quad (4)$$

where

$$(\mathcal{M}_0\Psi, \Psi) = \int_{3-\Gamma} |\nabla \times \Psi(\boldsymbol{\xi})|^2 d\boldsymbol{\xi}, \quad (5)$$

$$(\mathcal{M}_1\Psi, \Psi) = \int_{\Gamma} |\mathbf{n}_+ \times \Psi_+(\boldsymbol{\xi}) + \mathbf{n}_- \times \Psi_-(\boldsymbol{\xi})|^2 dS, \quad (6)$$

and $\Psi(\boldsymbol{\xi})$ satisfies the following conditions

$$\nabla \cdot \Psi(\boldsymbol{\xi}) = 0, \quad \boldsymbol{\xi} \in \mathbb{R}^3 - \Gamma; \quad (7)$$

$$\mathbf{n}_{\pm} \cdot \Psi_{\pm}(\boldsymbol{\xi}) = 0, \quad \boldsymbol{\xi} \in \Gamma, \quad (8)$$

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

The problem is then reduced from the infinite domain to a finite cell K using the Floquet-Bloch transform

$$\Psi(\mathbf{k}, \boldsymbol{\xi}) = \sum_{\mathbf{m} \in \mathbb{Z}^3} \Psi(\boldsymbol{\xi} + \mathbf{m}) e^{-i\mathbf{k} \cdot \mathbf{m}}, \quad \boldsymbol{\xi} \in Q_0, \quad \mathbf{k} \in K, \quad (9)$$

where the quasimomentum \mathbf{k} belongs to the Brillouin zone $K = [-\pi, \pi]^3$. Quadratic form (4) is transformed into

$$M(\mathbf{k}, \eta) = M_0 + \eta M_1(\mathbf{k}). \quad (10)$$

A self-adjoint operator M_0 corresponds to a single cubic cavity with perfectly conducting walls and is defined by the extreme values of the quadratic form

$$\int_{Q_0} |\nabla \times \Psi(\boldsymbol{\xi})|^2 d\boldsymbol{\xi} = (M_0\Psi, \Psi), \quad (11)$$

$$\nabla \cdot \Psi(\boldsymbol{\xi}) = 0, \quad (12)$$

$$\mathbf{n} \cdot \Psi(\boldsymbol{\xi}) \Big|_{\Gamma_0} = 0, \quad (13)$$

while the perturbation operator $M_1(\mathbf{k})$ is given by

$$(M_1(\mathbf{k})\Psi, \Psi) = \sum_{j=1}^3 \int_{\gamma_j} |\mathbf{e}_j \times [\Psi(\boldsymbol{\xi}) - e^{ik_j} \Psi(\boldsymbol{\xi} + \mathbf{e}_j)]|^2 dS, \quad (14)$$

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

Properties of operator (10) are analysed in [1].

3 Perturbation analysis

For matrix representation of the operator $\mathcal{M}(\mathbf{k}, \eta)$ (10) we use, as in [1], the basis of the eigenfunctions $\Psi(\boldsymbol{\xi})$ of a unit cubic cavity $Q_0 : 0 < \xi_i < 1, i = 1, 2, 3$ with perfectly conducting walls

$$\Psi_{\mathbf{p}}(\boldsymbol{\xi}) = \begin{pmatrix} A_{p,1} \sin(\pi p_1 \xi_1) \cos(\pi p_2 \xi_2) \cos(\pi p_3 \xi_3) \\ A_{p,2} \cos(\pi p_1 \xi_1) \sin(\pi p_2 \xi_2) \cos(\pi p_3 \xi_3) \\ A_{p,3} \cos(\pi p_1 \xi_1) \cos(\pi p_2 \xi_2) \sin(\pi p_3 \xi_3) \end{pmatrix}, \quad (15)$$

where $\mathbf{A}_{\mathbf{p}} = (A_{p,1}, A_{p,2}, A_{p,3})$ is a real polarization vector corresponding to an integer-valued nonzero index-vector $\mathbf{p} = (p_1, p_2, p_3)$. In this basis representation (10) has the form

$$\mathcal{M} = \mathcal{M}_0 + \eta \mathcal{M}_1, \quad (16)$$

where \mathcal{M}_0 is a real diagonal matrix and \mathcal{M}_1 is a hermitian matrix. Entries of \mathcal{M}_0 are the eigenfrequencies of the unit cavity subject to the conditions (12)-(13)

$$2\pi^2, 3\pi^2, 5\pi^2, 6\pi^2, 8\pi^2, 9\pi^2, 10\pi^2, \dots, \quad (17)$$

where the multiplicity of the eigenvalues must also be taken into account.

To find analytic approximation of the perturbed spectrum, we transform matrix \mathcal{M} to a unitary equivalent matrix \mathcal{X} using a similarity transformation [3]. Matrix \mathcal{X} has the same spectrum as \mathcal{M} and must be block-diagonal whose block dimensions are identical to those of matrix \mathcal{M}_0 . Thus, instead of infinite-dimensional linear perturbation we obtain an infinite series of finite-dimensional perturbations

$$\begin{aligned} \mathcal{X} &= \text{diag} \{X^{(1)}, X^{(2)}, \dots\} = e^{-\mathcal{S}(\eta)} \mathcal{M} e^{\mathcal{S}(\eta)} \\ &= \mathcal{M}_0 + \eta \mathcal{X}_1 + \eta^2 \mathcal{X}_2 + \dots, \end{aligned} \quad (18)$$

where $\mathcal{S}(\eta) = \eta S_1 + \eta^2 S_2 + \dots$, and matrices $S_j, j = 1, 2, \dots$, do not depend on η .

Transformation (18) is given by Hausdorff's representation

$$\mathcal{X} = e^{-\mathcal{S}} \mathcal{M} e^{\mathcal{S}} = \mathcal{M} + [\mathcal{M}, \mathcal{S}] + \frac{1}{2!} [[\mathcal{M}, \mathcal{S}], \mathcal{S}] + \frac{1}{3!} [[[\mathcal{M}, \mathcal{S}], \mathcal{S}], \mathcal{S}] + \dots, \quad (19)$$

where the brackets denote the commutator of two matrices

$$[\mathcal{A}, \mathcal{B}] = \mathcal{A}\mathcal{B} - \mathcal{B}\mathcal{A}. \quad (20)$$

Substituting (16)-(18) into (19) and equating the terms of like power in η we obtain expressions of matrices \mathcal{X}_j in (18)

$$\mathcal{X}_1 = [\mathcal{M}_0, i\mathcal{S}_1] + \mathcal{M}_1, \quad (21)$$

$$\mathcal{X}_2 = [\mathcal{M}_0, \mathcal{S}_2] + [\mathcal{M}_1, \mathcal{S}_1] + \frac{1}{2!} [[\mathcal{M}_0, \mathcal{S}_1], \mathcal{S}_1], \quad (22)$$

$$\begin{aligned} \mathcal{X}_3 &= [\mathcal{M}_0, \mathcal{S}_3] + [\mathcal{M}_1, \mathcal{S}_2] + \frac{1}{2!} ([[\mathcal{M}_0, \mathcal{S}_1], \mathcal{S}_2] + [[\mathcal{M}_0, \mathcal{S}_2], \mathcal{S}_1] + [[\mathcal{M}_1, \mathcal{S}_1], \mathcal{S}_1]) \\ &+ \frac{1}{3!} [[[\mathcal{M}_0, \mathcal{S}_1], \mathcal{S}_1], \mathcal{S}_1], \dots \end{aligned} \quad (23)$$

In order to find expansion (21) explicitly [3] we extract from \mathcal{M}_1 the block-diagonal matrix $\bar{\mathcal{M}}_1$ whose block dimensions are identical to those of \mathcal{M}_0 and denote by $\overset{\circ}{\mathcal{M}}_1$ the remainder

$$\mathcal{M}_1 = \bar{\mathcal{M}}_1 + \overset{\circ}{\mathcal{M}}_1. \quad (24)$$

Then we have from (21)

$$\mathcal{X}_1 = [\mathcal{M}_0, \mathcal{S}_1] + \bar{\mathcal{M}}_1 + \overset{\circ}{\mathcal{M}}_1. \quad (25)$$

Hermitian matrix \mathcal{X}_1 must have the same block-diagonal form as $\bar{\mathcal{M}}_1$, while matrix \mathcal{S}_1 satisfies the equation

$$[\mathcal{M}_0, \mathcal{S}_1] + \overset{\circ}{\mathcal{M}}_1 = 0. \quad (26)$$

Thus, \mathcal{S}_1 is chosen in such a way to annihilate off-block-diagonal terms in (25). Solution of (26) in block form is

$$(S_1)_{ik} = -\frac{(\overset{\circ}{\mathcal{M}}_1)_{ik}}{\lambda_i - \lambda_k}, \quad i \neq k, \quad i, k = 1, 2, \dots,$$

while diagonal blocks of \mathcal{S}_1 are zeros. Higher order matrices $\mathcal{S}_j, j = 2, 3, \dots$, can be obtained recurrently. Finally, first two terms in the expansion (18) are

$$\mathcal{X}_1 = \text{diag } \mathcal{M}_1 = \bar{\mathcal{M}}_1, \quad (27)$$

$$\mathcal{X}_2 = \frac{1}{2} \text{diag } [\overset{\circ}{\mathcal{M}}_1, \mathcal{S}_1]. \quad (28)$$

Elements of matrix \mathcal{X}_1 are computed exactly, while those of \mathcal{X}_2 involve truncation errors. Below we describe the blocks of matrix \mathcal{X} in (18). Quadratic approximation terms are obtained through truncation of (28) to the order 222 .

The first block corresponding to the eigenvalue $\lambda = 2\pi^2$ has the form

$$\begin{aligned} X^{(1)} &= 2\pi^2 I + 2\eta \begin{pmatrix} q_1(k_1, k_2, k_3), 0, 0 \\ 0, q_1(k_2, k_3, k_1), 0 \\ 0, 0, q_1(k_3, k_1, k_2) \end{pmatrix} \\ &+ \eta^2 \begin{pmatrix} p_1(k_1, k_2, k_3), \frac{4}{\pi^2} \sin k_1 \sin k_2, \frac{4}{\pi^2} \sin k_1 \sin k_3 \\ \frac{4}{\pi^2} \sin k_1 \sin k_2, p_1(k_2, k_3, k_1), \frac{4}{\pi^2} \sin k_2 \sin k_3 \\ \frac{4}{\pi^2} \sin k_1 \sin k_3, \frac{4}{\pi^2} \sin k_2 \sin k_3, p_1(k_3, k_1, k_2) \end{pmatrix} + O(\eta^3), \end{aligned} \quad (29)$$

where

$$q_1(x, y, z) = -\cos x + \cos y + \cos z + 3, \quad (30)$$

$$\begin{aligned} p_1(k_1, k_2, k_3) &= 0.6800 \cos^2 k_1 + 0.5068 \cos k_1 + 0.1434 \cos^2 k_2 \\ &- 0.2475 \cos k_2 + 0.1434 \cos^2 k_3 - 0.2475 \cos k_3 - 1.968. \end{aligned} \quad (31)$$

The second block which defines perturbation of the eigenvalue $\lambda = 3\pi^2$ is

$$\begin{aligned} X^{(2)} &= 3\pi^2 I + 2\eta \begin{pmatrix} 2 \cos k_1 + \cos k_2 + \cos k_3 + 4, & -\frac{\sqrt{3}}{3}[\cos k_2 - \cos k_3] \\ -\frac{\sqrt{3}}{3}[\cos k_2 - \cos k_3], & 2 \cos k_1 + \cos k_2 + \cos k_3 + 4 \end{pmatrix} \\ &+ \eta^2 \begin{pmatrix} p_2(k_1, k_2, k_3), & q_2(k_2, k_3) \\ q_2(k_2, k_3), & s_2(k_1, k_2, k_3) \end{pmatrix} + O(\eta^3), \end{aligned} \quad (32)$$

where

$$\begin{aligned} p_2(k_1, k_2, k_3) &= -0.4322 \cos^2 k_1 - 0.5400 \cos k_1 - 0.05108 \cos^2 k_2 \\ &- 0.2492 \cos k_2 - 0.05108 \cos^2 k_3 - 0.2492 \cos k_3 - 0.5041, \end{aligned} \quad (33)$$

$$q_2(k_2, k_3) = 0.2199(\cos^2 k_2 - \cos^2 k_3) + 0.1680(\cos k_2 - \cos k_3), \quad (34)$$

$$\begin{aligned} s_2(k_1, k_2, k_3) &= 0.07595 \cos^2 k_1 - 0.1521 \cos k_1 - 0.3050 \cos^2 k_2 \\ &- 0.4431 \cos k_2 - 0.3050 \cos^2 k_3 - 0.4431 \cos k_3 - 0.5042. \end{aligned} \quad (35)$$

The third block in (18) for the eigenvalue $\lambda = 5\pi^2$ is defined by the matrix

$$\begin{aligned} X^{(3)} &= 5\pi^2 I + 2\eta \begin{pmatrix} q_3(k_1, k_2, k_3), & 0, & 0, & 0, & 0, & 0 \\ 0, & q_3(k_1, k_3, k_2), & 0, & 0, & 0, & 0 \\ 0, & 0, & q_3(k_2, k_1, k_3), & 0, & 0, & 0 \\ 0, & 0, & 0, & q_3(k_3, k_1, k_2), & 0, & 0 \\ 0, & 0, & 0, & 0, & q_3(k_2, k_3, k_1), & 0 \\ 0, & 0, & 0, & 0, & 0, & q_3(k_3, k_2, k_1) \end{pmatrix} \\ &+ \eta^2 \begin{pmatrix} p_3(k_1, k_2, k_3), & r_3(k_2, k_3), & r_3(k_1, k_2), & 0, & 0, & s_3(k_1, k_3) \\ r_3(k_2, k_3), & p_3(k_1, k_3, k_2), & 0, & r_3(k_1, k_3), & s_3(k_1, k_2), & 0 \\ r_3(k_1, k_2), & 0, & p_3(k_2, k_1, k_3), & s_3(k_2, k_3), & r_3(k_1, k_3), & 0 \\ 0, & r_3(k_1, k_3), & s_3(k_2, k_3), & p_3(k_3, k_1, k_2), & 0, & r_3(k_1, k_2) \\ 0, & s_3(k_1, k_2), & r_3(k_1, k_3), & 0, & p_3(k_2, k_3, k_1), & r_3(k_2, k_3) \\ s_3(k_1, k_3), & 0, & 0, & r_3(k_1, k_2), & r_3(k_2, k_3), & p_3(k_3, k_2, k_1) \end{pmatrix} + O(\eta^3), \end{aligned} \quad (36)$$

where

$$q_3(k_1, k_2, k_3) = -\cos k_1 + 0.4 \cos k_2 - 1.6 \cos k_3 + 3, \quad (37)$$

$$\begin{aligned} p_3(k_1, k_2, k_3) &= 0.6796 \cos^2 k_1 + 0.5065 \cos k_1 + 0.03162 \cos^2 k_2 \\ &- 0.07939 \cos k_2 - 0.02503 \cos^2 k_3 + 0.2034 \cos k_3 - 1.475, \end{aligned} \quad (38)$$

$$r_3(k_1, k_2) = 0.1621 \sin k_1 \sin k_2, \quad (39)$$

$$s_3(k_1, k_2) = 0.1621(1 + \cos k_1 \cos k_2 - \cos k_1 - \cos k_2). \quad (40)$$

The fourth block in (18) corresponding to perturbation of the eigenvalue $\lambda = 6\pi^2$ has the form defined by the matrix

$$\begin{aligned}
X^{(4)} = & 6\pi^2 I + 2\eta \begin{pmatrix} q_4(k_1, k_2, k_3), -r_4(k_2, k_3), 0, 0, 0, 0 \\ -r_4(k_2, k_3), s_4(k_1, k_2, k_3), 0, 0, 0, 0 \\ 0, 0, q_4(k_1, k_3, k_2), r_4(k_2, k_3), 0, 0 \\ 0, 0, r_4(k_2, k_3), s_4(k_1, k_3, k_2), 0, 0 \\ 0, 0, 0, 0, q_4(k_2, k_3, k_1), -r_4(k_1, k_3) \\ 0, 0, 0, 0, -r_4(k_1, k_3), s_4(k_2, k_3, k_1) \end{pmatrix} \\
+ & \eta^2 \begin{pmatrix} p_4(k_1, k_2, k_3), u_4(k_2, k_3), \alpha_1 t_4(k_2, k_3), \alpha_2 t_4(k_2, k_3), -\alpha_3 t_4(k_1, k_3), \alpha_4 t_4(k_1, k_3) \\ u_4(k_2, k_3), v_4(k_1, k_2, k_3), -\alpha_2 t_4(k_2, k_3), -\beta_1 t_4(k_2, k_3), \beta_2 t_4(k_1, k_3), -\beta_3 t_4(k_1, k_3) \\ \alpha_1 t_4(k_2, k_3), -\alpha_2 t_4(k_2, k_3), p_4(k_1, k_3, k_2), u_4(k_3, k_2), \alpha_3 t_4(k_1, k_3), -\alpha_4 r_4(k_1, k_2) \\ \alpha_2 t_4(k_2, k_3), -\beta_1 t_4(k_2, k_3), u_4(k_3, k_2), v_4(k_1, k_3, k_2), \alpha_4 t_4(k_1, k_2), -\gamma_1 t_4(k_1, k_2) \\ -\alpha_3 t_4(k_1, k_3), \beta_2 t_4(k_1, k_3), \alpha_3 t_4(k_1, k_3), \alpha_4 t_4(k_1, k_2), p_4(k_2, k_3, k_1), u_4(k_3, k_1) \\ \alpha_4 t_4(k_1, k_3), -\beta_3 t_4(k_1, k_3), -\alpha_4 r_4(k_1, k_2), -\gamma_1 t_4(k_1, k_2), u_4(k_3, k_1), v_4(k_2, k_3, k_1) \end{pmatrix} \\
+ & O(\eta^3), \tag{41}
\end{aligned}$$

where

$$q_4(k_1, k_2, k_3) = 2 \cos k_1 + 0.4 \cos k_2 - 1.6 \cos k_3 + 4, \tag{42}$$

$$r_4(k_1, k_2) = \frac{2\sqrt{6}}{15}(\cos k_1 + \cos k_2), \tag{43}$$

$$s_4(k_1, k_2, k_3) = \frac{1}{3} \cos k_1 + \frac{29}{15} \cos k_2 - \frac{26}{15} \cos k_3 + 4, \tag{44}$$

$$\begin{aligned}
p_4(k_1, k_2, k_3) = & -0.4322 \cos^2 k_1 - 0.5402 \cos k_1 + 0.004458 \cos^2 k_2 \\
& - 0.08128 \cos k_2 - 0.01394 \cos^2 k_3 + 0.04201 \cos k_3 - 0.2219, \tag{45}
\end{aligned}$$

$$t_4(k_1, k_2) = \sin k_1 \sin k_2, \tag{46}$$

$$\begin{aligned}
u_4(k_1, k_2) = & 0.08915 \cos^2 k_1 + 0.09369 \cos k_1 \\
& - 0.04691 \cos^2 k_2 - 0.1446 \cos k_2 + 0.1961, \tag{47}
\end{aligned}$$

$$\begin{aligned}
v_4(k_1, k_2, k_3) = & 0.02266 \cos^2 k_1 - 0.06222 \cos k_1 - 0.4140 \cos^2 k_2 \\
& - 0.5212 \cos k_2 - 0.03310 \cos^2 k_3 - 0.01701 \cos k_3 - 0.1419, \tag{48}
\end{aligned}$$

$$\alpha_1 = 0.09604, \alpha_2 = 0.1274, \alpha_3 = 0.1440, \alpha_4 = 0.1176, \tag{49}$$

$$\beta_1 = 0.09405, \beta_2 = 0.06857, \beta_3 = 0.1061 \tag{50}$$

$$\gamma_1 = 0.04602 \tag{51}$$

Expansion of the fifth block corresponding to the eigenvalue $\lambda = 8\pi^2$ has the form

$$\begin{aligned}
X^{(5)} = & 8\pi^2 I + 2\eta \begin{pmatrix} q_5(k_1, k_2, k_3), 0, 0 \\ 0, q_5(k_1, k_2, k_3), 0 \\ 0, 0, q_5(k_1, k_2, k_3) \end{pmatrix} \\
+ & \eta^2 \begin{pmatrix} p_5(k_1, k_2, k_3), r_5(k_1, k_2), r_5(k_1, k_3) \\ r_5(k_1, k_2), p_5(k_2, k_3, k_1), r_5(k_2, k_3) \\ r_5(k_1, k_3), r_5(k_2, k_3), p_5(k_3, k_1, k_2) \end{pmatrix} + O(\eta^3), \tag{52}
\end{aligned}$$

where

$$q_5(k_1, k_2, k_3) = -\cos k_1 - \cos k_2 - \cos k_3 + 3, \quad (53)$$

$$p_5(k_1, k_2, k_3) = 0.6797 \cos^2 k_1 + 0.5065 \cos k_1 + 0.03742 \cos^2 k_2 \\ + 0.1080 \cos k_2 + 0.03742 \cos^2 k_3 + 0.1080 \cos k_3 - 1.478, \quad (54)$$

$$r_5(k_1, k_2) = 0.1013(\cos k_1 \cos k_2 - \cos k_1 - \cos k_2 + 1) \quad (55)$$

And finally we give here expansion of the sixth block in (18) corresponding to the eigenvalue $\lambda = 9\pi^2$

$$X^{(6)} = 9\pi^2 I + 2\eta \begin{pmatrix} q_6(k_1, k_2, k_3), p_4(k_2, k_3), 0, 0, 0, 0 \\ p_6(k_2, k_3), r_6(k_1, k_2, k_3), 0, 0, 0, 0 \\ 0, 0, q_6(k_2, k_3, k_1), p_6(k_3, k_1), 0, 0 \\ 0, 0, p_6(k_3, k_1), r_6(k_2, k_3, k_1), 0, 0 \\ 0, 0, 0, 0, q_6(k_3, k_1, k_2), r_6(k_1, k_2) \\ 0, 0, 0, 0, r_6(k_1, k_2), r_6(k_3, k_1, k_2) \end{pmatrix} \\ + \eta^2 \begin{pmatrix} t_6(k_1, k_2, k_3), u_6(k_2, k_3), \alpha_5 s_6(k_1, k_2), -\alpha_6 s_6(k_1, k_2), \alpha_5 s_6(k_1, k_2), \alpha_6 s_6(k_1, k_3) \\ u_6(k_2, k_3), v_6(k_1, k_2, k_3), \alpha_6 s_6(k_1, k_2), \beta_4 s_6(k_1, k_2), -\alpha_6 s_6(k_1, k_3), \beta_4 s_6(k_1, k_3) \\ \alpha_5 s_6(k_2, k_3), \alpha_6 s_6(k_2, k_3), t_6(k_1, k_3, k_2), u_6(k_3, k_1), \alpha_5 s_6(k_2, k_3), -\alpha_6 r_6(k_2, k_3) \\ -\alpha_6 s_6(k_1, k_2), \beta_4 s_6(k_1, k_2), u_6(k_3, k_1), v_6(k_2, k_3, k_1), \alpha_6 s_6(k_2, k_3), \beta_4 s_6(k_2, k_3) \\ \alpha_5 s_6(k_1, k_2), -\alpha_6 s_6(k_1, k_3), \alpha_5 s_6(k_2, k_3), \alpha_6 s_6(k_2, k_3), t_6(k_3, k_1, k_2), u_6(k_1, k_2) \\ \alpha_6 s_6(k_1, k_3), \beta_4 s_6(k_1, k_3), -\alpha_6 r_6(k_2, k_3), \beta_4 s_6(k_2, k_3), u_6(k_1, k_2), v_6(k_3, k_1, k_2) \end{pmatrix} \\ + O(\eta^3), \quad (56)$$

where

$$q_6(k_1, k_2, k_3) = 2 \cos k_1 - \cos k_2 - \cos k_3 + 4, \quad (57)$$

$$p_6(k_1, k_2) = \frac{1}{3}(\cos k_1 - \cos k_2), \quad (58)$$

$$r_6(k_1, k_2) = \frac{1}{9}(2 \cos k_1 - 17 \cos k_2 - 17 \cos k_3) + 4, \quad (59)$$

$$t_6(k_1, k_2, k_3) = -0.4321 \cos^2 k_1 - 0.5404 \cos k_1 - 0.02477 \cos^2 k_2 \\ + 0.06883 \cos k_2 + 0.02477 \cos^2 k_3 + 0.06883 \cos k_3 - 0.2952, \quad (60)$$

$$s_6(k_1, k_2) = \sin k_1 \sin k_2, \quad (61)$$

$$u_6(k_1, k_2) = 0.03205(\cos^2 k_1 - \cos^2 k_2) + 0.06794(\cos k_1 - \cos k_2) \quad (62)$$

$$v_6(k_1, k_2, k_3) = 0.01041 \cos^2 k_1 - 0.03519 \cos k_1 - 0.06069 \cos^2 k_2 \\ - 0.1124 \cos k_2 - 0.06069 \cos^2 k_3 - 0.1124 \cos k_3 + 0.3004, \quad (63)$$

$$\alpha_5 = 0.1801, \alpha_6 = 0.06003, \beta_4 = 0.02001 \quad (64)$$

$$(65)$$

Figure 2 shows dependence of the spectral bands of $\lambda = \omega^2 a^2 / c^2$ calculated numerically (shaded areas enclosed by solid lines) on the perturbation parameter $\eta = (\varepsilon \delta)^{-1}$. The eigenvalues were calculated through truncation of the matrix \mathcal{M} to the order 2273 yielding 138 distinct eigenvalues of the greatest multiplicity 48. The computations were carried out on the SGI

Origin 2000 parallel computer on a uniform $10 \times 10 \times 10$ grid over the reduced Brillouin zone. Dashed lines denote the upper bounds of the bands in the quadratic approximation. The latter agrees closely with the numerical bounds to the point of closing the gaps.

Large number of spectral points in the Brillouin zone allows to plot dispersion (equifrequency) surfaces. Figure 3 shows dispersion surfaces in the first band for the value of perturbation parameter $\eta = 0.5$ while the quasimomentum \mathbf{k} runs the Brillouin zone $[-\pi, \pi]^3$. Each point on the dispersion surfaces corresponds to a propagating wave whose direction of propagation is perpendicular to the surface. Near the band edges (figs. 3a and 3l) the surfaces have spherical shape, that corresponds to isotropic wave propagation. However, inside the band the photonic crystal is strongly anisotropic. Dispersion surfaces of the second band for $\eta = 0.5$ are shown in figure 4.

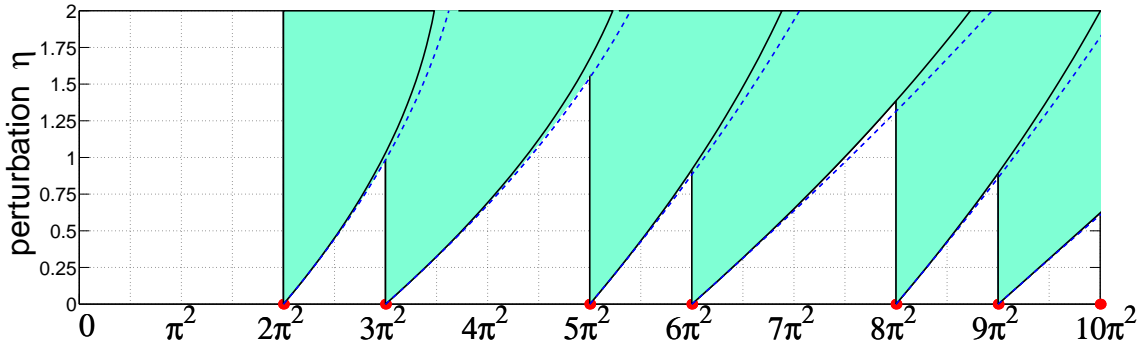


Figure 2: Dependence of the spectral bands of the photonic crystal calculated numerically (shades areas enclosed by solid curves) on the perturbation parameter $\eta = (\varepsilon\delta)^{-1}$. Dashed lines denote the upper bounds of the bands in quadratic approximation.

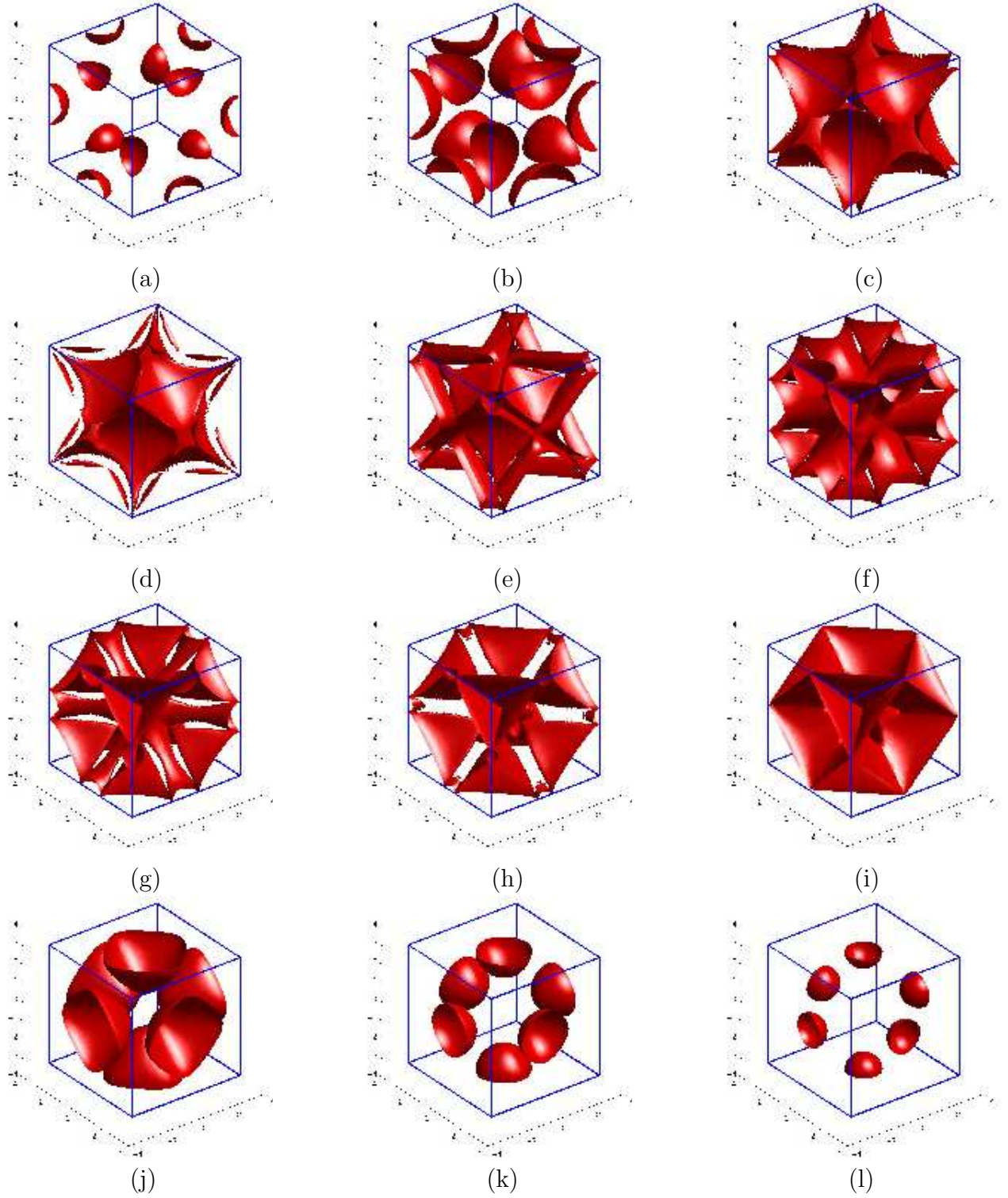


Figure 3: Dispersion (equipfrequency) surfaces of the first band while traversing it at $\eta = (\varepsilon\delta)^{-1} = 0.5$. The values of $\omega^2 a^2 / c^2$ are 20.1, 20.7, 21.3, 21.5, 21.8, 22.6, 23.1, 23.3, 23.4, 23.8, 24.5, 24.9 corresponding to figures (a)–(l), respectively. One Brillouin zone $[-\pi, \pi]^3$ is shown.

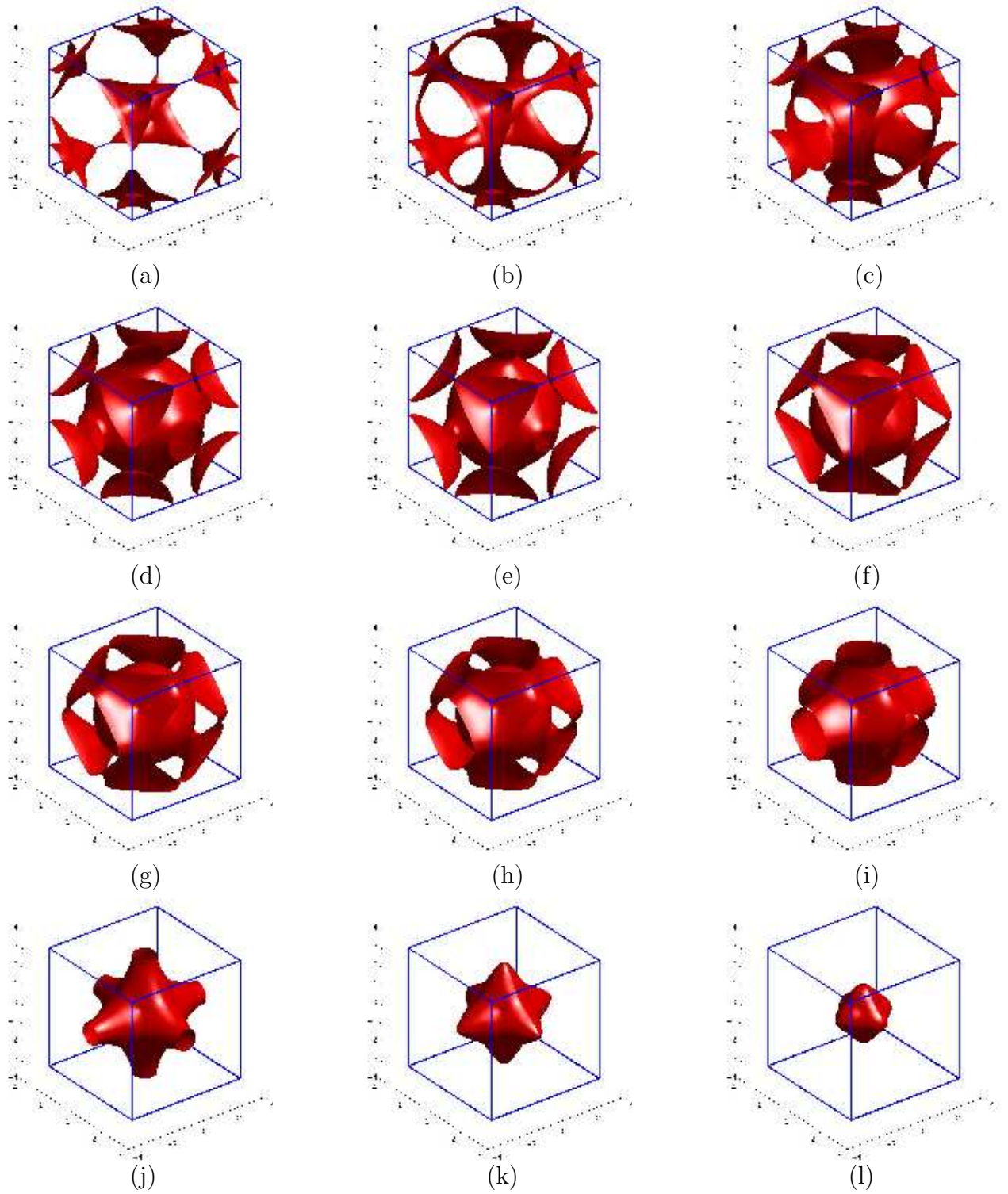


Figure 4: Dispersion(equifrequency) surfaces of the second band while traversing it at $\eta = (\varepsilon\delta)^{-1} = 0.5$. The values of $\omega^2 a^2 / c^2$ are 30.8, 31.1, 32.0, 32.9, 33.2, 33.5, 33.8, 34.1, 34.7, 35.6, 35.9, 36.5 corresponding to figures (a)–(l), respectively. One Brillouin zone $[-\pi, \pi]^3$ is shown.

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