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Doubly-Periodic Photonic Crystals: Spectral Problems Analysis

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Abstract—The present work is devoted to the clarification of the conditions necessary for step-by-step justification of the possibility of reduction of the homogeneous system of linear algebraic equations for the spectral problems of 2-D photonic crystals by the plane waves method. The issues related to the algorithms and the numerical solutions of these spectral problems are analyzed. The possibility of analytical regularization is investigated, and the ways to improve the convergence of the obtained results are identified.

1. INTRODUCTION

The problem discussed in this paper appeared long time ago in the theory of 2-D and 3-D photonic crystals [1, 2]. It is associated with the misconvergence or instability of computational schemes which are often observed while implementing the standard algorithms for the spectra calculation of free oscillations of the electromagnetic field in such periodic structures and the spectra of their eigenwaves [2, 3]. This refers to the grid technique algorithms in the frequency domain and to the so-called 'the plane waves method'. The algorithms of the time-domain methods are without such drawbacks, and they permit one to calculate accurately all spectral characteristics of particularly any opened and closed resonant structures (complex eigenfrequencies, configuration and the Q-factor of free oscillations of the field) related to the selected finite frequency band [4–7].

A reason causing the mentioned breakdowns can be the lack of smoothness of the function describing the material parameters of the crystals, and this phenomenon may be eliminated by increasing the smoothness artificially. Sometimes it is possible to recover the stability and convergence of the scheme in this way [3]. However, there is an open question: do the data, to which the convergence is observed, provide the exact solution of the problem? The point is that the implemented algorithms are conceptually reduced to the substitution of some 'exact' infinite homogeneous system of linear algebraic equations $A(k)x = 0$ ($A(k)$ is the finite matrix-function of the complex spectral parameter k) by their finite dimensional analogue $A_N(k)x_N = 0$ as well as to the solution of the dispersion equation $\det A_N(k) = 0$, i.e., to the the definition of such values $k = \bar{k}_N$, for which the system $A_N(k)x_N = 0$ has a nontrivial solution. However, one can guarantee the convergence $x_N \to x$, $\bar{k}_N \to \bar{k}$, $N \to \infty$ (x is the nontrivial solution of the problem $A(k)x = 0$ for the value $k = \bar{k}$) as well as the existence of the sequences $\{x_N\}_N$ and $\{\bar{k}_N\}_N$ converging to all the exact values x and $\bar{k}$ only if the matrix-function $A(k)$ has the number of specific properties for such mathematical objects [8, 9].

We show with a simple example that the corresponding conditions cannot be performed using the standard approach to the solution of spectral problems for the 2-D photonic crystals. This means that the standard computational schemes are not correct enough and should be regularized. One of the possible methods of analytical regularization previously used in the theory of the non-self-adjoint operators [9] is discussed in Section 4.

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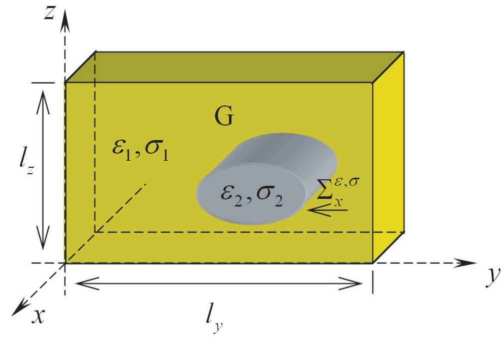

Figure 1. The cross section of one cells of the 2-D photonic crystal by two parallel planes $x = \text{const}$.

2. PROBLEM STATEMENT

A dielectric structure which is infinite and homogeneous in x direction but periodic in y and z ones [1, 2] is usually named 2-D photonic crystal (see, for example, Fig. 1: ℓ_y and ℓ_z are the lengths of the periods of the structure in axes y and z; $\Sigma^{\varepsilon,\sigma} = \Sigma_x^{\varepsilon,\sigma} \times (|x| \leq \infty)$ is a sufficiently smooth surface, where the material parameters of the wave propagation medium are discontinuous). The electromagnetic waves generated in the structure by the quasi-periodic current sources

$$\begin{aligned} F(g,k) &= \sum_{m,n=-\infty}^{\infty} f_{m,n}(k)\,\mu_{m,n}(g); \qquad g = \{y,z\} \in \mathrm{R}, \\ \mu_{m,n}(g) &= (\ell_y \ell_z)^{-1/2} \exp\left[i\left(\alpha_m y + \beta_n z\right)\right], \\ &\alpha_m = 2\pi\left(\Phi_y + m\right)/\ell_y \quad \text{and} \quad \beta_n = 2\pi\left(\Phi_z + n\right)/\ell_z \end{aligned} \tag{1}$$

and propagating harmonics in perpendicular directions to x are given by problem (see [5, 7])

$$\begin{cases} \left[\dfrac{\partial^2}{\partial y^2} + \dfrac{\partial^2}{\partial z^2} + k^2 \tilde{\varepsilon}(g)\right] U(g,k,\Phi_y,\Phi_z) = F(g,k); \quad g \in \mathrm{G} = \{g:\ 0 < y < \ell_y,\ 0 < z < \ell_z\} \\ \vec{E}_{tg}(q,k), \quad q = \{x,y,z\} \quad \text{and} \quad \vec{H}_{tg}(q,k) \quad \text{are continuous when crossing} \quad \Sigma^{\varepsilon,\sigma}, \\ U\left\{\dfrac{\partial U}{\partial y}\right\}(\ell_y,z,k,\Phi_y,\Phi_z) = \mathrm{e}^{2\pi i \Phi_y} U\left\{\dfrac{\partial U}{\partial y}\right\}(0,z,k,\Phi_y,\Phi_z), \\ \tilde{U}\left\{\dfrac{\partial \tilde{U}}{\partial z}\right\}(\ell_z,z,k,\Phi_y,\Phi_z) = \mathrm{e}^{2\pi i \Phi_z} \tilde{U}\left\{\dfrac{\partial \tilde{U}}{\partial z}\right\}(y,0,k,\Phi_y,\Phi_z). \end{cases} \tag{2}$$

Here, $U(g,k) = E_x(g,k)$ in the case of E-polarization (TE-waves: $\partial/\partial x \equiv 0$, $H_x = E_y = E_z = 0$, $ikH_y = \eta_0^{-1}\partial U/\partial z$, $-ikH_z = \eta_0^{-1}\partial U/\partial y$) and $U(g,k) = H_x(g,k)$ in the case of H-polarization (TM-waves: $\partial/\partial x \equiv 0$, $E_x = H_y = H_z = 0$, $-ik\varepsilon\eta_0 E_y + \sigma E_y + j_y = \partial U/\partial z$, $-ik\varepsilon\eta_0^{-1} E_z + \sigma E_z + j_z = -\partial U/\partial y$); $\vec{E}_{tg}$, $\vec{H}_{tg}$, E_x, H_x, etc. are the components of the intensity vectors of the electric ($\vec{E}(g,k)$) and the magnetic ($\vec{H}(g,k)$) field; $k = 2\pi/\lambda$ is the wave number; λ is the electromagnetic wavelength in free space; $\tilde{\varepsilon}(g) = \varepsilon(g) + i\sigma(g)\eta_0/k$ is a piecewise continuous (in E-polarization case) or a piecewise constant (in H-polarization case) function of coordinates; functions $\sigma(g) \geq 0$ and $\varepsilon(g) \geq 1$ are the specific conductivity and relative permittivity of the dielectric elements; $\eta_0 = (\mu_0/\varepsilon_0)^{1/2}$ is the impedance of free space; ε_0 and μ_0 are the electric and magnetic vacuum constants; R is the plane $y0z$; $\operatorname{Im}\Phi_y = \operatorname{Im}\Phi_z = 0$ è $|\Phi_y| \leq 0.5$, $|\Phi_z| \leq 0.5$. The time-dependence of the processes under consideration is determined by multiplier $\exp(-ikt)$. All physical parameters are measured in the SI system. But time t is measured in meters: it is the product of the natural time and the velocity of light in vacuum.

The orthonormal system of the functions $\{\mu_{m,n}(g)\}_{m,n=-\infty}^{\infty}$ is complete in $L_2(G)$ [10]. This makes it possible to represent the solution $U(g,k,\Phi_y,\Phi_z) \in L_2(G)$ of problem (2) by infinite series

$$U\left(g,k,\Phi_y,\Phi_z\right) = \sum_{m,n=-\infty}^{\infty} u_{m,n}\left(k\right)\mu_{m,n}\left(g\right). \tag{3}$$

Function (3) satisfies the quasi-periodicity conditions (the last two rows of problem (2)). The unknown complex amplitudes $u_{m,n}(k)$ should be chosen in such a way as to satisfy the differential equation of the problem and the boundary conditions (on $\Sigma^{\varepsilon,\sigma}$) imposed on the tangential components of the field that are uniquely determined by the function $U(g,k,\Phi_y,\Phi_z)$.

Spectral problems of the 2-D photonic crystals theory can be obtained from Eq. (2) assuming $F(g,k) \equiv 0$. When the real values Φ_y and Φ_z are fixed, one arrives at the problem of the complex eigenfrequencies $\bar{k}(\Phi_y,\Phi_z)$ and the corresponding free oscillations of the field inside the crystal $\bar{U}(g,\bar{k},\Phi_y,\Phi_z)$. When the value of real k is fixed, we have the problem of the complex propagation constants $\bar{\Phi}_y$ and $\bar{\Phi}_z$ of the eigenwaves in the crystal $\bar{U}(g,k,\bar{\Phi}_y,\bar{\Phi}_z)$. In practice, as a rule, one usually addresses the first of these problems when calculating the isofrequencies of periodic structure for the chosen bandwidth in coordinates related with the wave vectors of eigenwaves or dispersion dependencies calculation for the finite number of such waves (usually along the boundary segments of the nonconducting part of the Brillouin zone). This problem in the E-polarization case is considered below.

3. ALGORITHMIZATION OF PROBLEMS AND THEIR ANALYSIS

Let us construct the canonical Green function of the 2-D photonic crystal — the solution of problem (2) for $F(g,k) = \delta(g,p)$, $p = \{y_p, z_p\} \in G$ ($\delta(g,p)$ is the Dirac delta function) and $\tilde{\varepsilon}(g) \equiv 1$. Function (3) is the solution of problem (2) only if

$$\left(k^2 - \alpha_m^2 - \beta_n^2\right) u_{m,n} = f_{m,n}; \quad -\infty \leq m,n \leq \infty. \tag{4}$$

From Eqs. (3), (2) and (1) we derive

$$\begin{aligned} U\left(k,g,\Phi_y,\Phi_z\right) &= \sum_{m,n=-\infty}^{\infty} \frac{f_{m,n}}{k^2-\alpha_m^2-\beta_n^2}\mu_{m,n}\left(g\right) = \sum_{m,n=-\infty}^{\infty} \frac{\mu_{m,n}\left(g\right)}{k^2-\alpha_m^2-\beta_n^2}\int_G F\left(p,k\right)\mu_{m,n}^*\left(p\right)dp \\ &= \int_G \left[\sum_{m,n=-\infty}^{\infty} \frac{\mu_{m,n}\left(g\right)\mu_{m,n}^*\left(p\right)}{k^2-\alpha_m^2-\beta_n^2}\right] F\left(p,k\right)dp = \int_G G_0\left(g,p,k,\Phi_y,\Phi_z\right)F\left(p,k\right)dp \end{aligned}$$

(symbol '$*$' stands for the complex conjugation). A simple analysis [11, 12] shows that the function

$$G_0\left(g,p,k,\Phi_y,\Phi_z\right) = \sum_{n,m=-\infty}^{\infty} \frac{\mu_{m,n}\left(g\right)\mu_{m,n}^*\left(p\right)}{k^2-\alpha_m^2-\beta_n^2}; \quad p = \{y_p, z_p\} \in G \tag{5}$$

has all the properties of the sought Green function for the real k and preserves these properties in the analytic extension to the complex values of the frequency parameter. The natural boundaries of such a continuation determine the complex plane C as the variation range of the complex eigenfrequencies of the 2-D photonic crystals.

Let us consider problem (2), when function $F(g,k)$ is restricted in G, and $\tilde{\varepsilon}(g)$ is continuous in G and has the continuous partial derivatives of y and z. We assume that $F(g,k)$ as the function of parameter k does not have any singularities in C. It is not difficult to show, as follows from [12], that function $U(g,k,\Phi_y,\Phi_z)$ holomorphic in some region $C_0 \in C$ is defined by the equation

$$U\left(g,k,\Phi_y,\Phi_z\right) = \int_G G_0\left(g,p,k,\Phi_y,\Phi_z\right)\left[\left(1-\tilde{\varepsilon}\left(p\right)\right)k^2 U\left(p,k,\Phi_y,\Phi_z\right) + F\left(p,k\right)\right]dp; \quad g \in G, \tag{6}$$

and extends from the region $C_0 \in C$ to the whole plane C as the meromorphic function of variable k. In the part of C, where the function $U(g,k)$ remains holomorphic, it is the solution of problem (2).

In fact, the solution $U(g,k,\Phi_y,\Phi_z)$ of Eq. (6) (in case it exists and is unique) is the solution of problem (2), as it follows from the properties of the canonical Green function (5). Furthermore, all the eigenfrequencies of the crystal are located on the real axis when $\sigma(g)\equiv 0$, but all the eigenfrequencies $\bar{k}$ of the crystal are in the lower half-plane C in case the specific conductivity $\sigma(g)$ is nontrivial, as it is evident from the complex power theorem in the integral form formulated for the nontrivial solution of homogeneous (spectral) problem (2). It means that there are points k, where the solution of problem (2) exists, and it is unique for any values $\sigma(g)$ on the plane C. The compactness of the finitely meromorphic operator-function

$$A\left(k\right)\left[U\right]=k^{2}\int\limits_{\mathrm{G}} G_{0}\left(g,p,k,\Phi_{y},\Phi_{z}\right)\left[1-\tilde{\varepsilon}\left(p\right)\right]U\left(p,k,\Phi_{y},\Phi_{z}\right)dp;\quad \mathrm{L}_{2}\left(\mathrm{G}\right)\rightarrow \mathrm{L}_{2}\left(\mathrm{G}\right),\quad k\in \mathrm{C} \tag{7}$$

permits one to take the advantage of the meromorphic Fredholm theorem [12–15] in order to justify the conclusion formulated in the previous paragraph.

This conclusion can be generalized to the case of the functions $\tilde{\varepsilon}(g)$ discontinuous along the curve consisting of the finite number of the differentiable arcs [11]: the function $U(g,k,\Phi_y,\Phi_z)$ and its first partial derivatives remain continuous along this curve, and, consequently, the continuity condition for the tangential components of the electromagnetic field on the surface $\Sigma^{\varepsilon,\sigma}$ holds.

Formally, by simplifying the situation, we assume that the poles $\bar{k}$ of the function $U(g,k,\Phi_y,\Phi_z)$ are simple. This assumption does not restrict us fundamentally. In addition, we can justify it rigorously of all real values $\bar{k}$ [12]. The poles $\bar{k}$ form the spectrum $\Omega_{\underline{k}}$ of the eigenfrequencies of the photonic crystal, which is nothing more than a countable set of points $\bar{k}\in$ C that are not accumulated anywhere in the finite part of plane C, and residues $\operatorname*{Res}_{k=\bar{k}} U(g,k,\Phi_y,\Phi_z)=\sum_{j=1}^{J} B_j\bar{U}_j(g,\bar{k},\Phi_y,\Phi_z)$ determine linearly independent free oscillations $\bar{U}_j(g,\bar{k},\Phi_y,\Phi_z)$ of the field corresponding to these frequencies. The last mentioned statement follows from Keldysh theorem on the representation of the principal part of the resolvent $[E-A(k)]^{-1}$ of the operator equation (6) [7,13]. Here, E is the unit operator, and $A(k)[U]$ is operator-function [7] with the values from space $\Re_\infty$ of the completely continuous (compact) operators [9]. The number J of the free oscillations corresponding to each eigenfrequency $\bar{k}$ is finite. The coefficients B_j are determined by the function $F(g,k)$ as well as by the choice of the canonical system $\bar{U}_j(g,\bar{k},\Phi_y,\Phi_z)$ of the eigen elements of the operator-function $E-A(k)$ [7,13].

We determine all the eigenfrequencies $\bar{k}$ and the fields $\bar{U}_j(g,\bar{k},\Phi_y,\Phi_z)$ of the free oscillations which are connected to these frequencies by solving the operator equation $[E-A(k)][U]=0$ equivalent to homogeneous (spectral) problem (2). The plane waves method allows one to pass to the matrix form $[\tilde{E}-\tilde{A}(k)][\tilde{U}]=0$ of this equation, namely, to perform the following changes

$$[E-A\left(k\right)]\left[U\right]=0\ \Rightarrow\ \sum_{s=1}^{\infty}\left[\delta_r^s-a_{r,s}\left(k\right)\right]u_s=0;\quad r=1,2,3,\ldots,$$

$$E\quad\Rightarrow\quad \tilde{E}=\{\delta_r^s\}_{r,s=1}^{\infty},\quad A\left(k\right)\Rightarrow\tilde{A}\left(k\right)=\{a_{r,s}\left(k\right)\}_{r,s=1}^{\infty},\quad U\quad\Rightarrow\quad\tilde{U}=\{u_s\}_{s=1}^{\infty}\in\ell_2.$$

Here, δ_r^s is the Kronecker delta; $a_{r,s}(k)=(A\mu_s,\mu_r)$; $u_s=(U,\mu_s)$; $(\cdot,\cdot)$ is the scalar product in $\mathrm{L}_2(\mathrm{G})$; $\ell_2=\{a=\{a_s\}:\sum_s|a_s|^2<\infty\}$ is the space of infinite sequences; $\mu_s=\mu_{m(s),n(s)}$, and it makes no difference whether one of the possible rules of recalculation of the index s or r by the values n or m is realized here.

The algorithm of solving the spectral problem is usually designed using the inversion of the reduced system of the linear algebraic equations to order N

$$\sum_{s=1}^{\infty}\left[\delta_r^s-a_{r,s}\left(k\right)\right]u_s=0;\quad r=1,2,3,\ldots, \tag{8}$$

and as the approximate value $\bar{k}$ one choose the solution $k=\bar{k}_N$ of the following scalar equation

$$\Delta_N\left(k\right)=\det\left\{\delta_r^s-a_{r,s}\left(k\right)\right\}_{r,s=1}^{N}=0 \tag{9}$$

when the value N is sufficiently large.

Let us consider the reliable enough basis for justifying the steps described above. First, we note the results of [8] that permit one to do the following conclusions. If (i) $\tilde{A}(k) = \{a_{r,s}(k)\}_{r,s=1}^{\infty}$ is holomorphic in some region $C_0 \in C$ matrix-function with the values from $\Re_\infty$; (ii) the sequence of the reduced matrices $\tilde{E}_N - \tilde{A}_N(k) = \{\delta_r^s - a_{r,s}(k)\}_{r,s=1}^{N}$, when $N \to \infty$ converges properly [8] to infinite matrix $\tilde{E} - \tilde{A}(k) = \{\delta_r^s - a_{r,s}(k)\}_{r,s=1}^{\infty}$ for all $k \in C_0$; and (iii) if $\bar{k} \in C_0$, then there is a sequence $\{\bar{k}_N\}_N$, $\bar{k}_N \in C_0$, that $\bar{k}_N \to \bar{k}$ when $N \to \infty$. On the other hand, if the conditions (i), (ii) are fulfilled and in (iii) the sequence $\{\bar{k}_N\}_N$, $\bar{k}_N \in C_0$ converges to a point $k = \bar{k} \in C_0$ when $N \to \infty$, then this point is $\bar{k} \in \Omega_k$.

If the operator-function $A(k) : L_2(G) \to L_2(G)$ generates the kernel matrix-function $\tilde{A}(k)$ ($A(k) \in \Re_1$) or Koch matrix $\tilde{E} - \tilde{A}(k)$ [9] in the domain $C_0 \in C$, where it is holomorphic, then there exists holomorphic function-determinant $\Delta(k) = \det[E - A(k)]$ in C_0, which has the following properties [9, 14, 15] that allow one to justify the usage of Eq. (9) for the derivation of the approximate solutions of spectral problem (8). The order J of the eigenvalue $\bar{k}$ of the operator-function coincides with the multiplicity of zero of the scalar function $\Delta(k)$, when $k = \bar{k}$. Function $\Delta_N(k) = \det\{\delta_r^s - a_{r,s}(k)\}_{r,s=1}^{N}$ when $N \to \infty$ converges uniformly to $\Delta(k)$ for all $k \in C_0$. For all $k \in C_0$

$$\left|\Delta(k) - \Delta_N(k)\right| \le \left\|A(k) - \tilde{A}_N(k)\right\|_{\Re_1} \exp\left(\left\|A(k)\right\|_{\Re_1} + \left\|\tilde{A}_N(k)\right\|_{\Re_1} + 1\right). \tag{10}$$

From Eq. (10) and relation

$$\left|\bar{k}_N - \bar{k}\right|^J = J! \left|\Delta\left(\bar{k}_N\right)\left[\frac{d^J}{dk^J}\Delta(k)\bigg|_{k=\bar{k}}\right]^{-1}\right| + O\left[\left(\bar{k}_N - \bar{k}\right)^{J+1}\right];$$
$$\frac{d^j}{dk^i}\Delta(k)\bigg|_{k=\bar{k}} = 0 \quad \text{for} \quad j = 0, 1, \ldots, J-1,$$

obtained by the expansion of the function $\Delta(k)$ into the Taylor series in the vicinity of the point $k = \bar{k}$, it follows the estimation of the real convergence rate when $\bar{k}_N \to \bar{k}$ for the sufficiently large N:

$$\left|\bar{k}_N - \bar{k}\right|^J \le const \left\|A\left(\bar{k}_N\right) - \tilde{A}_N\left(\bar{k}_N\right)\right\|_{\Re_1} = const \sum_{r=N+1}^{\infty} \left|a_{r,r}\left(\bar{k}_N\right)\right|. \tag{11}$$

Now we analyse the results from the mentioned above which are reliable enough while solving the spectral problem $[E - A(k)][U] = 0$. The operator $A(k)$, $k \in C_0$ is a completely continuous operator, but requirement (ii) of the proper convergance of the reduced matrices $\tilde{E}_N - \tilde{A}_N(k)$ to an infinite matrix $\tilde{E} - \tilde{A}(k)$ whose strict checking seems to us quite problematic and substantially complicates the application of the results in [8] that, in general, satisfy our demands.

Matrix $\tilde{A}(k)$ generated by the operator-function $A(k) : L_2(G) \to L_2(G)$, $k \in C_0$ is not the kernel. The necessary and sufficient condition (the series $\sum_{r=1}^{\infty} a_{r,r}(k)$ is convergent) related with the finiteness of the operator $A(k)$ is not fulfilled. The matrix $\tilde{A}(k)$ cannot be referred to Koch matrices ($\sum_{r=1}^{\infty}|a_{r,r}(k)| < \infty$ and $\sum_{r,s=1}^{\infty}|a_{r,s}(k)|^2 < \infty$ [9] are the sufficient conditions). To such a conclusion we arrive by presenting the operator $A(k)$ in the form $A(k) = B(k)C(k)$, where

$$B(k)[U] = k^2 \int_G G_0(g, p, k, \Phi_y, \Phi_z)\, U(p, k, \Phi_y, \Phi_z)\, dp$$

and

$$C(k)[U] = \int_G \delta(g, p)\left[1 - \tilde{\varepsilon}(p)\right] U(p, k, \Phi_y, \Phi_z)\, dp,$$

or in matrix form

$$\begin{aligned} &\tilde{B}(k) = \{b_{r,s}(k)\}_{r,s=1}^{\infty}; \quad b_{r,s}(k) = \frac{k^2\delta_r^s}{k^2 - \alpha_{m(s)}^2 - \beta_{n(s)}^2} \quad \text{and} \\ &\tilde{C}(k) = \{c_{r,s}(k)\}_{r,s=1}^{\infty}; \quad c_{r,s}(k) = \varepsilon_{r-s}, \quad \varepsilon_r = \int_G \left[1 - \tilde{\varepsilon}(g)\right]\mu_r^*(g)\, dg. \end{aligned} \tag{12}$$

From Eq. (12), one obtains $a_{r,s}(k) = k^2\varepsilon_{r-s}(k^2 - \alpha^2_{m(r)} - \beta^2_{n(r)})$, and as the series $\sum_{m,n}(m^2 + n^2)$ is divergent [11], the series $\sum_{r=1}^{\infty} a_{r,r}(k)$, $\sum_{r=1}^{\infty} |a_{r,r}(k)|$ is divergent as well.

4. SPECTRAL PROBLEMS REGULARIZATION

Eventually, we have not succeeded in providing the strict justification of the stability and convergence of the computation scheme based on the solution of the infinite system of linear algebraic equations (8) reduced to the order N. But obviously $\sum_{r,s=1}^{\infty} |a_{r,s}(k)|^2 < \infty$ and, consequently, $A(k)$ is the Hilbert-Schmidt operator [9] ($A(k) \in \Re_2 \subset \Re_\infty$). This allows us, following [9], to pass on the problem

$$\sum_{s=1}^{\infty} \left[\delta_r^s - d_{r,s}(k)\right] v_s = 0; \quad r = 1, 2, 3, \ldots, \tag{13}$$

equivalent to problem (8). Here, $\delta_r^s - d_{r,s}(k) = [\delta_r^s - a_{r,s}(k)] \exp[a_{s,s}(k)]$, $v_s = \exp[-a_{s,s}(k)]u_s$ and $d_{r,r}(k) = 1 - [1 - a_{r,r}(k)] \exp(a_{r,r}(k)) = O(a^2_{r,r}(k))$ as follows from the expansion $\exp[a_{r,r}(k)]$ into the series over powers of $a_{r,r}(k)$. The last equality allows one to state that the operator $D(k)$ corresponding to the matrix $\tilde{D}(k) = \{d_{r,s}(k)\}_{r,s=1}^{\infty}$ is the kernel operator and generates the Koch matrix $\tilde{E} - \tilde{D}(k)$.

Now we have the necessary background in order to reduce system in Eq. (13) properly and calculate the approximate values of the eigenfrequencies $\bar{k}$ of the 2-D photonic crystal by solving the characteristic equation $\det\{\delta_r^s - d_{r,s}(k)\}_{r,s=1}^{N} = 0$. It should be emphasized that the repetition of the above procedure, according to inequality in Eq. (11), leads to the sequences $\{\bar{k}_N\}_N$ whose convergence rates to the exact values $\bar{k}$ increases greatly at each step.

Let us complete the analysis with an elementary but rather illustrative example. Let the elements $a_{r,s}(k)$ of the matrix operator $\tilde{A}(k) = \{a_{r,s}(k)\}_{r,s=1}^{\infty}$ for the sufficiently large r and s behave as $O[(r+s)^{-1}]$ in system (8). It means that the operator $\tilde{A}(k) : \ell_2 \to \ell_2$ is the Hilbert-type operator [16]. It is bounded but not totally continuous. There is no reason to expect that by the reduction of system (8) and by solving dispersion equation (9) we obtain the result that is expected. After the regularization of the problem (when moving to problem (13)), we obtain $d_{r,r}(k) = O(a^2_{r,r}(k)) = O(r^{-2})$, and from the estimation as Eq. (11), we get $|\bar{k}_N - \bar{k}|^J \leq const(N+1)^{-1}$. The convergence of the reduction method (the method based on the replacement of an infinite system of linear algebraic equations by a finite one) is provided. By repeating the procedure of the regularization, we derive $|\bar{k}_N - \bar{k}|^J \leq const(N+1)^{-3}$, i.e., the convergence rate of the sought quantities to their exact value increases by two orders.

The accurate and complete enough numerical analysis of the real efficiencies of the algorithms for solving spectral problems for the 2-D photonic crystals (both standard and regularized) can be performed with a number of special techniques developed for such research (see, for example, [17]). In this paper, in view of the natural restrictions on the volume of the published material, we do not have the possibilities to give due consideration to this question. We hope to discuss it in detail in the next paper.

5. CONCLUSION

In this paper, the questions related to the algorithmization and to the numerical solution of the spectral problems of the electromagnetic theory of the 2-D photonic crystals are analysed. The actuality of the research area is obvious — the quality of the important results both for the theory and practice which are obtained on the corresponding background mostly depends on how accurate the dispersion characteristics of the considered structures are calculated. For the indicated problems, the conditions whose fulfilment is necessary for stable and convergent numerical schemes construction are formulated. The potentiality of the analytical regularization is demonstrated, and the techniques to improve the convergence rate of the obtained results are indicated.

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