Progress In Electromagnetics Research, PIER 59, 113–149, 2006

C-METHOD: SEVERAL ASPECTS OF SPECTRAL THEORY OF GRATINGS

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Abstract—The goal of the present paper is two folded. The first, the methodological one, is the complementation of well established in diffraction theory of gratings C method with certain elements of spectral theory and the development of interactive numerical algorithm that made feed back conjunction between diffraction and spectral problems. As a natural result the second goal appeared: the appearing of such tool for numerical experiments resulted in profound qualitative and quantitative study of rather peculiar phenomena in resonant scattering from periodic surface. Special attention has been paid to the investigation of electromagnetic waves diffraction from periodic boundaries of material with single and double negative parameters.

1. INTRODUCTION

There is no need nowadays to discuss the importance of diffraction gratings (DG) study in modern applied optics and MW engineering [1–22]. They have found their well-established place as a key dispersive element in numerous devices. The utilization of DG within a rather large range of parameters (wavelength, material properties the DG are made with and put on, shape and depth of grooves) put certain

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requirements on the accuracy and reliability of the mathematical modeling of electromagnetic wave scattering by DG. There are no doubt that the solution of simulated electromagnetic boundary value problem (BVP) and corresponding numerical algorithms including their code implementation must be: robust, fitting the requirements concerning efficiency and accuracy within a rather wide parameter range (including resonant scattering), for the real time simulation and analyses to be possible

Presently, a huge number of approaches and methods exist in the area of wave diffraction by periodic wavy surfaces, including periodic boundary between two or several media. It should be outlined that most of them are certain modifications of corresponding general methods used for the problems of wave diffraction by local inhomogeneities. Just this possibility of "local" methods application to infinite boundary surfaces of multilayered structure is the principal advantage of "embedding" such surface (namely, its essential part) into relevant periodic structure.

Existing methods and approaches for wave diffraction by local or periodic inhomogeneity can be separated conditionally in the following way (having no possibility to make detailed survey of such huge amount of information, we restricted ourselves on basic publications of the fields):

1. Approaches, using Green's formulae technique, volume, surface and boundary integral equations of the first and the second kind (see [1–3], for example), including methods of analytical regularization [4].
2. Method of partial domains, including semi-inversion procedures [5–7].
3. Methods of perturbation theory (small inhomogeneities, small inclinations of boundary surface, etc.) — see, for example, [8].
4. "Differential" methods — see, for example, [1, 9] and references cited here.
5. Methods of boundary "straightening", which are rather efficient specialization of "differential" methods, mentioned above, — see [10–16] and references cited here.
6. Incomplete Galerkin method — see [17] and, for example, [18].
7. Methods based on field representations by means of Rayleigh harmonics (theory of series, involving non-orthogonal function, in general) — see [1, 19, 20].
8. Asymptotic methods — see [21, 22].

In present DG theory C method [10–16] holds rather special place: it is efficient and accurate in rather wide area of its applicability, clear in implementation, and it performs numerical modeling of diffraction processes by arbitrary profiled DG, coated or not coated with dielectrics.

Here we shall discuss several mathematical issues concerning the C method that earlier skipped attention of its authors [10–16]: the continuation of diffraction problems into the complex plane of frequency parameters and a comparative investigation of diffraction and spectral problems.

There is a wide set of different possibilities to formulate the spectral problems. Among them there are ones for eigen frequencies and eigen waves of corresponding diffraction boundary value problem. From mathematical point of view, all of them have equal rights for existence. But, as it often happens in theoretical physics, the "correctness" of one or other models can be justified by its mathematical consequences only, i.e., by mathematical results following from the formulation, by possibility of their reasonable physical interpretation and their utility level for modeling of corresponding physical processes, as well as for profound understanding of the processes inner nature. Just this makes up the principal reason that made us to chose (among many possibilities) such posing of spectral problem, which is, from one side, strictly connected with excitation problem and, from the other side, is based on the idea of analytical continuation of operator of this excitation problem in relevant complex valued frequency domain.

It is clear that any correctly formulated diffraction problem (for real valued frequencies) should have the solution, which is unique. From the other side, there are well known resonant phenomena, which become apparent, when frequency of excitation field is varying. It is natural to think these phenomena as a result of an existence of some eigen oscillation of the obstacle. As such eigen oscillation can not exist for real frequencies, relevant question arises: do they exist in a domain of complex valued frequencies? Moreover: are they allowed and are they able to exist? What mathematical object can be treated as such eigen oscillation? It is necessary to outline that within the scope of one of the possible and even traditional way of spectral problems posing (when eigen function supposed to be square integrable in the space R^2 or R^3) the answers are negative: eigen oscillations are forbidden for complex valued frequencies.

That is why we have chosen the formulation of spectral problem in which eigen oscillations are allowed to exist and they are in strong connection with solutions of diffraction problem for real valued frequencies. This strong connection is based on the idea of analytical continuation of diffraction boundary value problem operator from real frequencies into the relevant domain (Riemannian surface) of complex-valued frequencies. More exactly, it was necessary to construct the relevant posing of diffraction problem considered for complex valued frequencies.

The procedure of analytical continuation of resolvent of corresponding operator in complex valued domain of spectral parameter, which is frequency in our case, is well known in functional analysis (and in the theory of boundary value problems). The presence of poles of this continuation means the absence of uniqueness and existence of non-trivial solution of corresponding homogeneous functional equation for such values of spectral parameter, the residuals of resolvent in these poles are strictly connected with eigen vectors of "direct" initial operator and so on. It can be shown (see [4, 7]) that the approach of analytical continuation of "direct" operator of boundary value problem, which we are using here, is essentially equivalent to analytical continuation of the operator resolvent above mentioned.

Thus, the principal step in our way of construction of spectral theory is the formulation of diffraction boundary value problem in relevant domain (infinite-sheeted Riemannian surface) of complex valued frequencies.

We would like to point out once again that the formulation of the problem chosen here has predetermined the mathematical consequences and the utility for understanding of physical essence of "real" diffraction problem — with real valued frequencies.

2. THE DIFFRACTION PROBLEM FORMULATION FOR REAL-VALUED FREQUENCY

In this section, we consider the standard posing of diffraction problem for real-valued wave number $k = 2\pi/\lambda$, where λ is a wavelength of incident field in vacuum, doing this in the way similar to [16]. After that, in the next section, we discuss the necessary changes of the posing for complex-valued k.

We consider the structure of two dielectric media, which both together fill whole three-dimensional space R^3 — see Fig. 1. The structure is homogenous along the OX axis as well as the boundary surface S between two media. The smooth and one-connected contour L is a generator of surface in plane ZOY (i.e., L is boundary line between two media for $x = 0$). Contour L is given by 2π-periodic function $z = ha(y)$; $0 \leq a(y) \leq 1$, its maximum deviation from the axis OY is equal to $h < \infty$. The upper and the low media have dielectric constant parameters ε_1, μ_1, and ε_2, μ_2, respectively.

It is necessary to note that the case of arbitrary period $d \neq 2\pi$

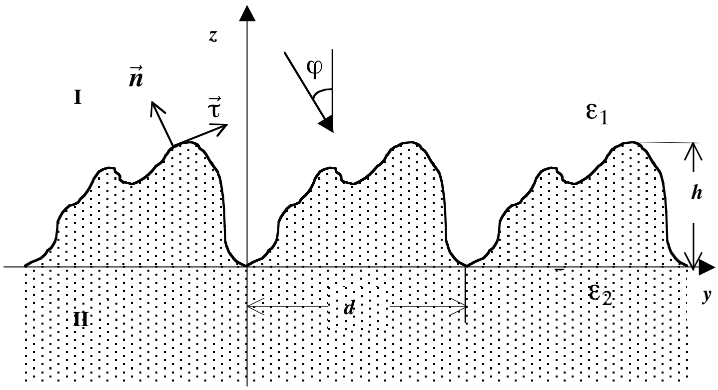


Figure 1. Presentation of the problem.

of function $z = ha(y)$ can be easily reduced to the case considered by means of introducing of new space variables $\hat{x} = (2\pi/d)x$, $\hat{y} = (2\pi/d)y$, $\hat{z} = (2\pi/d)z$. Correspondingly, instead of a wave number $k = 2\pi/\lambda$, one may use a parameter $\kappa = d/\lambda$ in all formulae and statements below without loss of their correctness. Actually, such substitution of κ instead of k is the only difference for $d \neq 2\pi$.

The incident time harmonic field (E^i, H^i) is given in the upper media and is supposed to be E-polarized: vector E^i is parallel to OX axis (the case of H-polarized incident field can be investigated in a very similar way). The time factor is chosen as $e^{-i\omega t}$, and it is omitted everywhere below.

It is evident and can be shown easily that scattered field (E^s, H^s) is E-polarized too. Because all electromagnetic fields considered satisfying time-harmonic Maxwell's equations:

$$rot\, E = ik\mu H; \qquad rot\, H = -ik\varepsilon E, \tag{1}$$

any E-polarized field (E, H) can be expressed (as well known and immediately follows from (1)) by means of one scalar generic function $U = U(y, z)$, which satisfies two-dimensional Helmholtz equation:

$$(\Delta + k^2\varepsilon\mu)U(y, z) = 0, \tag{2}$$

and

$$\begin{aligned} E_x &= U(y, z); \qquad E_y = 0; \qquad E_z = 0; \\ H_x &= 0; \qquad H_y = \frac{1}{ik\mu}\frac{\partial U}{\partial z}; \quad H_z = -\frac{1}{ik\mu}\frac{\partial U}{\partial y}. \end{aligned} \tag{3}$$

Here ε and μ are constant material parameters of corresponding dielectric media and subscripts x, y, and z denote corresponding vector component in Cartesian coordinate system. We suppose additionally that incident field is 2π-quasi-periodic one of the kind (see Eq. (3))

$$U(y + 2\pi, z) = e^{i2\pi\Phi} U(y, z), \tag{4}$$

where Φ is some real-valued parameter of quasi-periodicity:

$$|\Phi| \leq 1/2. \tag{5}$$

The simplest example of such quasi-periodic field is plane wave with an amplitude A and directional parameters α and γ:

$$U^{pw}(y, z) = Ae^{i(\alpha y + \gamma z)}; \tag{6}$$

$$\alpha^2 + \gamma^2 = k^2 \varepsilon\mu \tag{7}$$

with real-valued parameter α. Here a parameter Φ is equal to that positive or negative fractional part of value $\alpha/2\pi$, which has the smallest modulus (and that is why satisfies condition (15)). As well, formula (6) includes both homogenous (γ is real) and inhomogeneous (γ is complex) plane waves.

We denote generic functions of the kind (2), (3) for an incident, scattering and a total field respectively as U^i, U^s and U^t, where U^t is defined as follows:

$$U^t(y, z) = \begin{cases} U^i(y, z) + U^s(y, z), & z > a(y); \\ U^s(y, z), & z < a(y) \end{cases} \tag{8}$$

The standard boundary (transform) condition on the boundary surface between two media is requirement of continuity of the tangential components of the total electromagnetic field. By means of the formulae (3), these conditions can be re-written in the following standard form [1]:

$$U^{t(+)}(p) = U^{t(-)}(p), \quad \frac{\partial U^{t(+)}(p)}{\partial n_p} = \gamma \frac{\partial U^{t(-)}(p)}{\partial n_p} \quad p \in L, \tag{9}$$

where

$$\gamma = \begin{cases} \mu_1/\mu_2 & E\text{-polarization} \\ \varepsilon_1/\varepsilon_2 & H\text{-polarization} \end{cases}.$$

Subscripts $(+)$ and $(-)$ denote (uniform on the contour L) limits of functions $U^t(p)$ and $\partial U^t(p)/\partial n_p$ of arguments $p + sn_p$ and $p - sn_p$ respectively, when $s \to +0$. Here n_p is the unit normal to the contour

L in a point $p \in L$ (which direction is arbitrary chosen for the contour L and fixed after that).

The essential part of the problem formulation is a radiation condition formulation. Several comments worth to be done about the "philosophy" and the history of the question before the radiation condition formulating.

We would like to remind the reader that a radiation condition from mathematical point of view is a kind of such "closure" of the boundary value problem posing, which guarantees the uniqueness of the solution to the diffraction boundary value problem. At the same time, the radiation condition should be chosen in such a form that this unique solution has reasonable physical sense. Standard choice of the radiation condition is that one, which corresponds to the presence of outgoing waves only, without waves coming from the infinity. Last statements above look like something trivial and well known. Nevertheless, it looks like the meaning of the words "outgoing waves" should be explained in more thoroughly.

One of the most fundamental physical principal is the energy conservation law. Thus, "outgoing waves", in this context, means that energy of scattered field must always go to the infinity (and never comes from the infinity). That is, the energy must go to infinity not only in the case, when it means that the wave itself should go to infinity, but even if the wave itself must be coming from infinity, if necessary. The point is that nowadays there is enormous flash of interest to so called Veselago materials [24] with both negative $\varepsilon < 0$ and $\mu < 0$ (left-handed or double negative media in another terminology). Thus, their product is positive $\varepsilon\mu > 0$, and such "principal" question arises as what is physical value of $\sqrt{\varepsilon\mu}$? Is this $\sqrt{|\varepsilon\mu|}$ or $-\sqrt{|\varepsilon\mu|}$?

The answer for this question is known from textbooks at least last 45 years or more. For example, L. A. Vainshtein explains in his textbook [23] the theory of complex Maxwell equations (when electromagnetic fields and material parameters are complex-valued vectors and scalars correspondingly). He shows that because of the energy conservation law, the material parameters ε and μ of passive media must be situated in the first or second quadrant of complex plane only:

$$\varepsilon = |\varepsilon|e^{i\delta}, \quad 0 \le \delta \le \pi, \quad \mu = |\mu|e^{i\Delta}, \quad 0 \le \Delta \le \pi; \tag{10}$$

i.e., $\mathrm{Im}\varepsilon \ge 0$, $\mathrm{Im}\mu \ge 0$. At that, all arithmetic operations with ε and μ should be made according to standard rules for complex numbers, and square root branch in all formulae of electromagnetic theory should be taken as one of the kind $\sqrt{1} = 1$. In particular,

$$\varepsilon\mu = |\varepsilon\mu|e^{i\rho}, \qquad \rho = \delta + \Delta \in [0, 2\pi], \tag{11}$$

$$n = \sqrt{\varepsilon\mu} = |\varepsilon\mu|^{1/2} e^{i\rho/2}, \quad \rho/2 \in [0, \pi]; \quad \zeta = \sqrt{\mu/\varepsilon} = |\mu/\varepsilon|^{1/2} e^{i(\Delta-\delta)/2}; \tag{12}$$

$$K = kn = k\sqrt{\varepsilon\mu}, \quad k = 2\pi/\lambda = \omega/c, \quad \operatorname{Re} k \geq 0, \quad \operatorname{Im} k = 0 \tag{13}$$

Thus, an index of refraction $n = \sqrt{\varepsilon\mu}$ is a complex number, it can be real valued, and its real part can be positive (if $0 \leq \delta + \Delta \leq \pi$) or negative (if $\pi \leq \delta + \Delta \leq 2\pi$), its imaginary part is always non-negative; real part of wave resistance (wave impedance) $\zeta = \sqrt{\mu/\varepsilon}$ is always non-negative, and so on. Values κ and λ are a wave number and a wavelength of monochromatic wave of angular frequency ω in vacuum respectively, and K is (complex valued in general) wave number in media with material parameters ε and μ. Here k is real valued, and, consequently, $K = kn$ is complex valued with the same above-mentioned properties as index of refraction n.

In section devoted to plane waves in [23], L. A. Vainshtein considers as the simplest example of monochromatic plane wave such wave of amplitude A propagating along OZ axis in some media, namely

$$E_x = Ae^{iKz-i\omega t}, \quad H_y(1/\zeta)Ae^{iKz-i\omega t}, \quad E_y = E_z = H_x = H_z = 0. \tag{14}$$

According to standard formulae $E(t) = \operatorname{Re}\{E(\omega)e^{-i\omega t}\}$ and $H(t) = \operatorname{Re}\{H(\omega)e^{-i\omega t}\}$ for real electromagnetic field, this wave is propagating with its phase velocity

$$u = \omega/\operatorname{Re}(K) = c/\operatorname{Re}(n), \tag{15}$$

i.e., it propagates in a positive (if $\operatorname{Re}(K) > 0$, $\operatorname{Re}(n) > 0$) or a negative (if $\operatorname{Re}(K) < 0$, $\operatorname{Re}(n) < 0$) direction of axis OZ. In the same time, Umov-Pointing vector S of this wave has the only component S_z of the kind

$$S_z = \frac{c}{8\pi}\left(E_z H_y^* - E_y^* H_x\right) = \frac{c}{8\pi} E_x H_y^* = \frac{c}{8\pi\zeta^*}|A|^2 e^{-(\operatorname{Im} K)z}; \tag{16}$$

$$\operatorname{Re} S_z = \cos\frac{\delta - \Delta}{2}\frac{c}{8\pi|\zeta|}|A|^2 e^{-2(\operatorname{Im} K)z}. \tag{17}$$

Thus, the vector ReS is always directed in positive direction of OZ axis, i.e., the wave considered always propagates the energy in positive direction of OZ axis, even in the case $\operatorname{Re}(K) < 0$, $\operatorname{Re}(n) < 0$, when the wave itself is propagating (its phase velocity is oriented) in negative direction of OZ axis.

There is a kind of idee fixe in minds that harmonic wave propagates in direction of its phase velocity. The only reason for this is just tradition. The example considered shows that much more correct from physical point of view is idea that the wave propagates in direction of its energy propagation. For traditional materials (with $\mathrm{Re}\,\varepsilon > 0$, $\mathrm{Re}\,\mu > 0$) the difference between these two directions, if exists, is out of principal importance. But in general, as we have seen, the directions can be even opposite.

From these formulae the simplest recipe for correct radiation condition formulation in arbitrary passive media follows: use always the same radiation condition as one for vacuum, but change parameter κ by parameter $K = \kappa n = \kappa\sqrt{\varepsilon\mu}$ of the media; the calculation of K must be done according to formulae above described.

Veselago materials [33] are within the scope of this recipe. That is why, it is not a surprise that authors of paper [34, 35] came into the same conclusion about correct formulation of radiation condition.

It is noteworthy that in the case of Veselago materials energy of scattered waves goes to the infinity if and only if the waves themselves are incoming from infinity, all parameters ε, μ, n and K of Veselago medium are real, but negative; value ζ is real and positive. The same treatment of signs of n and ζ can be found in the paper of Veselago [33].

The canonic choice of radiation condition for the structure considered is the requirement that outside certain vicinity of contour L the scattered field must be presented in the form of the uniformly converging series of the outgoing and decaying plane waves, namely

$$U^s(y,z) = \begin{cases} \displaystyle\sum_{n=-\infty}^{\infty} R_n e^{i\Phi_n y + \Gamma_{n1}(z-A_0)}, & z > A_0; \\ \displaystyle\sum_{n=-\infty}^{\infty} T_n e^{i\Phi_n y - \Gamma_{n2} z}, & z < 0, \end{cases} \tag{18}$$

where

$$\Phi_n = \Phi + n, \quad \Gamma_{nj} = \sqrt{K_j^2 - \Phi_n^2},\ K_j = k^2\varepsilon_j\mu_j,\ A_0 = \frac{2\pi h}{d},\ k = d/\lambda. \tag{19}$$

The branch of $\Gamma_{nj} = \sqrt{K_j^2 - \Phi_n^2}$ in formula (19) is chosen according to formulae (10)–(13).

The physical meaning of radiation condition (18), (19) is the restriction of scattering field by outgoing and decaying waves only i.e., elimination of plane waves that bring (produce!) energy from infinity to some vicinity of the contour L. Thus, we need not introduce any new radiation condition and can use the canonic one with proper understanding of its complex valued parameters according to formulas (10)–(13).

If the contour L is piecewise smooth only and, for example, some point $p_0 \in L$ is an edge point of L, then boundary condition (9) can not be applied in point p_0 (even because normal vector in p_0 is not defined). Without going into too deep mathematical details (connected with the theory of generalized functions and Sobolev's spaces) for more general mathematical posing of the diffraction problem, one may use instead of (9) the condition of field energy finiteness in any bounded domain of the space R^2:

$$\int_V \left\{ |U^s(p)|^2 + |grad\, U^s(p)| \right\} dv < \infty. \tag{20}$$

For the case, when p_0 is an edge point of contour L, the well known edge condition [1, 25] follows from (20).

Thus, the diffraction problem considered can be formulated as the necessity to find out the scattered field $U^s(y, z)$, which satisfies:

1. Helmholtz equation (2) in both media — for (ε, μ) equal to (ε_1, μ_1) and (ε_2, μ_2);
2. Quasi-periodicity condition (4) with given parameter Φ;
3. Boundary conditions (9);
4. Radiation condition (18);
5. Condition (20) of energy finiteness (which is necessary only if contour L is not smooth).

3. DIFFRACTION PROBLEM FOR COMPLEX-VALUED FREQUENCY

In this section we discuss the necessary changes in the problem formulation for complex κ.

For better understanding the situation, one can consider canonic 2π-quasi-periodic Green function G_{gr} of free space R^2 (where $\varepsilon = 1$ and $\mu = 1$):

$$G_{gr}(y, z, k, \Phi) = -\frac{i}{4\pi} \sum_{n=-\infty}^{\infty} e^{i2\pi n\Phi} H_0^{(1)}(kD_n(y, z)) \tag{21}$$

$$D_n(y, z) = \{z^2 + (y + 2\pi n)^2\}^{1/2}, \tag{22}$$

where $H_0^{(1)}\xi$ is zero-order Hankel function of the first kind.

We would like to remind the reader that $-\frac{i}{4}H_0^{(1)}(kD_0(y, z))$ is Green function (field of point source) of free space R^2. Thus, function

(21) describes field composed as the superposition of a corresponding 2π-periodic system of unit point sources with $e^{i2\pi n\Phi}$ factors, and it is evident that (21) is 2π-quasi-periodic function of the kind (4).

As well known (see proof, for example, in [4, 7]), Green function (21) can be rewritten by means of Poisson summation formula [4, 7] as follows

$$G_{gr}(y, z, k, \Phi) = -\frac{i}{4} \sum_{n=-\infty}^{\infty} e^{i[\Phi_n y + \Gamma_n |z|]} \Gamma_n^{-1}, \tag{23}$$

$$\Phi_n = n + \Phi; \qquad \Gamma_n = (k^2 - \Phi_n^2)^{1/2}. \tag{24}$$

For real-valued k the branches of square roots of Γ_n are of the kind

$$\operatorname{Im}\Gamma_n \geq 0, \qquad \operatorname{Re}\Gamma \geq 0, \qquad n = 0, \pm 1, \pm 2, \ldots. \tag{25}$$

It can be proved (see, for example [1, 4, 7]) that function (21), considered as one of argument k, can be analytically continued (by means of the same formula (21)) from real axis $\operatorname{Im} k = 0$ into Riemannian surface R_0 with complex plane cuts, which are starting in points $k_n^2 = \Phi_n^2$ and going to infinity $\operatorname{Im} k \to \infty$ like, for example, curves described in [7] (see Fig. 2):

$$(\operatorname{Re} k)^2 = (\operatorname{Im} k)^2 - \Phi_n^2 = 0, \quad n = 0, \pm 1, \pm 2, \ldots, \operatorname{Im} k \leq 0. \tag{26}$$

The function thus obtained is an analytic function for any $\kappa \neq \kappa_n$ in any sheet of Riemannian surface. The only singular points of this function are κ_n, $n = 0, \pm 1, \pm 2$, and for local variable $\tau = \tau(\kappa)$ (in vicinity $\kappa = \kappa_n$ or $\kappa = -\kappa_n$) of the kind $\tau^2 = \kappa^2 - \kappa_n^2$ the function has the only simple pole in $\tau = 0$ (i.e., the set of the function singularities is the set of the same branch points of functions Γ_n^{-1}, $n = 0, \pm 1, \pm 2, \ldots$).

The first sheet (which sometimes is referred as the zeroth or "physical" one) of Riemannian surface R_0 is defined by condition (25) and cuts (26). The consequent sheets differ from the first one by opposite choice of signs of Γ_n for a few corresponding indices n.

It is necessary to underline that function $G_{gr}(y, z, k, \Phi)$ gives the solution to the "diffraction problem" for the system of quasi-periodic point sources in the absence of an obstacle. The function evidently satisfies radiation condition (18) in the trivial case $\varepsilon_1 = \varepsilon_2 = \varepsilon$ and $\mu_1 = \mu_2 = \mu$. However, even for such the simplest case the procedure of analytical continuation gives rather complicated Riemannian surface, as above described.

The question arises: what new quality should one expect in the presence of an obstacle and, especially, for the boundary surface, which separates two different media, when both media are extending to infinity (in the way half-space like)? It is clear that two Green functions

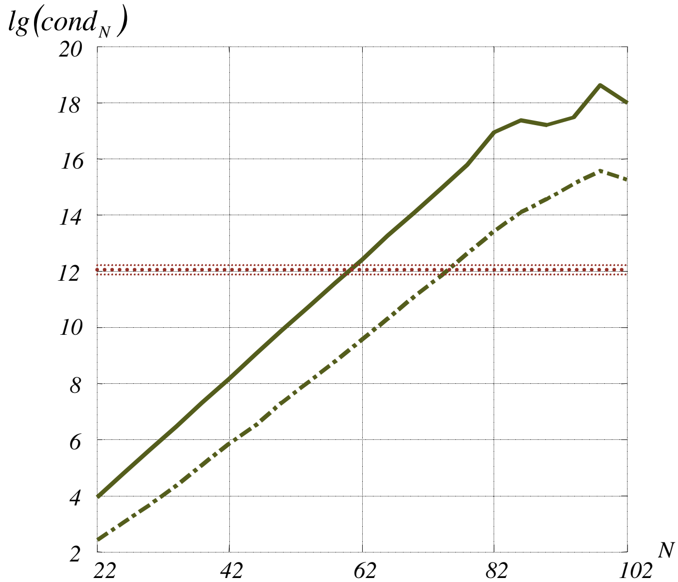


Figure 2. The boundary of the shape $a(y) = 0.5(1 + \cos y)$, $\varepsilon_2 = 4.1$; $\kappa = 0.6$; $h = \pi$; $\varphi = 0$. Solid line corresponds to numerical solution to the equation of the fist kind (30), dashed lines — to numerical solution of regularized system of the second kind (31).

are naturally involved now, namely, $G_{gr}^{(j)} = G_{gr}^{(j)}(y, z, k\sqrt{\varepsilon_j \mu_j}, \Phi)$, $j = 1, 2$, which satisfy radiation conditions (18) in the upper and the low half-spaces respectively.

Due to this the Riemannian surface R of analytical continuation of boundary value problem operator in respect to κ be somehow "doubled" Riemannian surface R_0 of free space. More exactly, it is necessary to consider two sets $j = 1, 2$ of branch points (of functions Γ_{nj} — see (19))

$$K_{jn}^2 = \Phi_n^2, \qquad n = 0, \pm 1, \pm 2, \ldots, \ j = 1, 2, \tag{27}$$

where

$$K_j = \kappa\sqrt{\varepsilon_j \mu_i}. \tag{28}$$

and κ in (26) is replaced by $K_j = \kappa\sqrt{\varepsilon_j \mu_i}$; index of refraction $n = \sqrt{\varepsilon\mu}$ is a complex number calculated according to formula (12). See Riemannian surface and cuts depicted in Fig. 3.

That is why, it is natural to generalize the formulation of diffraction problem (considered in the previous section for real-valued

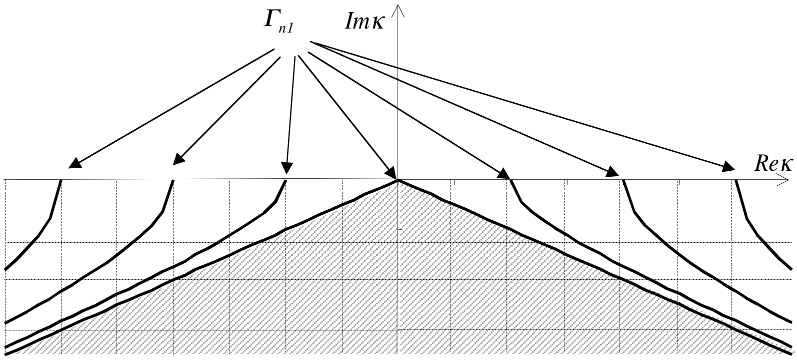


Figure 3. Riemannian surface with cuts defined by equation (23).

κ) for the case of complex-valued κ in the following way. At first, we suppose that wave number κ belongs to Riemannian surface R. At second, radiation condition (18) for each given $\kappa \in R$ has the same form, but the signs of square roots of Γ_n in formula (19) must be taken according to the sheet, which κ is belonging to. At third, all the other conditions are exactly the same as ones for real-valued κ.

Thus, the only formal difference in the diffraction problems posing for complex- and real-valued k is that now we consider k belonging to relevant Riemannian surface, instead of the previous case $\mathrm{Im}\,\kappa = 0$.

We would like to emphasize the significant difference between the diffraction problem considered in comparison with diffraction problem for finite obstacles, where well known Sommerfeld radiation condition traditionally applied. The procedure of analytical continuation into the domain of complex-valued κ requires changing of Sommerfeld condition by Reichardt radiation condition (see details in [4, 7, 26]). However, for the infinite periodic structure under consideration the radiation condition in form (18) are valid (see below) for both real- and complex-valued κ as above described. The reason of such difference is that Sommerfeld condition is one of a kind of asymptotic requirement, but Reichardt conditions as well as condition (18) are the exact series representations in a vicinity of the infinite point.

As we have had already mentioned in Introduction, the usefulness of one or another formulation of diffraction problem for complex-valued κ is based on the mathematical consequences from such posing, namely, on qualitative properties of the solution and on its connection with the solutions for real valued κ. The detailed explanation of such qualitative mathematical consequences requires a lot of space, and we shall not dwell on it here. We restrict ourselves here by brief explanation of the several facts that to justify the formulation, which we have been chosen above.

Taking into account radiation condition (18) and using standard Green formulae technique, one can represent scattered field $U^s(q),\ q = (y_q, z_q) \in R^2 \backslash L$ as an integral over one period of the boundary contour L with integrand formed by the linear combination of the functions

$$G_{gr}^{(j)}\left(y_q - y_p, z_q - z_p, k\sqrt{\varepsilon_j \mu_j}, \Phi\right) \frac{\partial U^s(p)^s}{\partial n_p},$$
$$\frac{\partial G_{gr}^{(j)}\left(y_q - y_p, z_q - z_p, k\sqrt{\varepsilon_j \mu_j}, \Phi\right)}{\partial n_p} U^s(p),\ p = (y_p, z_p) \in L,\ j = 1, 2. \tag{29}$$

Here, as usually, the values of $U^s(p)$ and normal derivative $\partial U^s(p)/\partial n_p$ should be treated as limiting values of these functions on the contour L and limits are taken along the normal n_p from the side, where the medium with corresponding value of index j is situated (i.e., medium with such ε_j, μ_j)). Substitution of this representation into the boundary conditions (9) gives the system of two integral-differential equations of the first kind [1]. Analytical Regularization Method reduces this system to functional equation of the second kind in the way similar to one described in [4, 29, 32]. After that the technique similar to one described in [1, 4, 7] gives the result that a resolvent of a diffraction boundary value problem operator treated as a function of $\kappa \in R$ is a finite-meromorphic operator-function in surface R, and the function may have poles of finite multiplicity only, and upper half-plane of first sheet of R has no singularity at all; this resolvent coincides with analytical continuation of such resolvent for real-valued κ.

Thus, the diffraction problem formulation that is chosen for the complex-valued κ really gives “natural” analytical continuation of diffraction problem for real-valued κ.

Unfortunately, the Riemannian surface constructed in such way has rather complicated structure in the presence of several dielectric media (several periodic layers). Even in the case of two media considered herein the set of the cuts and branch points is rather complicated, especially if one takes into account that the change of ε_2 and μ_2, namely, the changes δ and Δ in formulae (10) leads to the rotation of the branch points as well as to the rotation of the contours of the corresponding cuts and, consequently, to crossing of such curves generated by the first (upper) and the second (lower) media. Thus, it is necessary to change the cuts curves, and it is not easy to make this in a uniform way (especially for a considerable number of the media).

From formal mathematical point of view the positions and shapes of cuts are out of any importance (if the cuts have the same starting and ending points), because all Riemannian surfaces thus obtained are equivalent. But the complexity or the simplicity of the system of these cuts is very important from practical and, in particular, numerical points of view. The simpler the better, especially when complexity is higher than the limits of our ability to understand, and it seems to us that for cuts structure of a few media we are very near to these limits.

That is why we call the formulation of diffraction problem in complex domain, which is above described, as the "global" one with the only one frequency parameter for all media. The alternative posing is the "local" one, when for each media its own spectral parameter is chosen and all others parameters of the others media are "frozen", i.e., are fixed in "physical domain" of their definition.

More precisely, the idea is the following. Let us take certain real valued κ and calculate all $K_j = \kappa\sqrt{\varepsilon_j\mu_j}$, $j = 1, 2, 3, \ldots, N$ for each media, where N is number of layers (here we have considered above diffraction problem for $N = 2$). Now one can fix all K_j with exception of K_{j_0} for some index j_0. After that it is possible to consider diffraction problem for complex valued , when all the others parameters K_j, $j \neq j_0$ are fixed as above described. It is clear that natural domain of analytical continuation in respect to parameter K_{j_0} is the same Riemannian surface as that one for the canonic Green functions (23) and (24), where parameter is changed for parameter K_{j_0}.

For each $j = 1, 2, 3, \ldots, N$ we denote as R^j such Riemannian surfaces of variable K_j as the parameter of analytical continuation, when the others parameters K_s, $s \neq j$ are fixed. Such analytical continuations in the complex domain of one parameter K_j we shall call as the local formulations of the diffraction problem, i.e., one in respect to each media separately.

The local formulation has a few evident advantages in comparison with the global one. The first of them is the simplicity: corresponding Riemannian surface has much more simple structure. The second advantage is that it is possible to investigate influence of the corresponding media, including resonance properties of each layer, independently that may essentially simplify the understanding of inner nature of diffraction processes.

4. SPECTRAL PROBLEM

In this section we formulate the spectral problem for complex κ. The formulation is strictly connected with corresponding diffraction problem considered in the previous section.

As well known (and can be easy proved), the diffraction problem for real valued κ (see Section 2) always has the solution and the solution is unique, if $\Gamma_{nj} \neq 0$ for all n and j — see (19). In particular, radiation condition (18) guarantees the solution uniqueness for real-valued κ. But such uniqueness (as well as existence) of a solution can not be guaranteed for arbitrary $\kappa \in R$ and even more: it does not take place for some values $\kappa^m \in R$. This fact can be shown analytically for the simplest obstacles. It means, of course, that the operator of diffraction boundary value problem is not invertible for $\kappa = \kappa^m$ and a set Ω of such κ^m can be treated as a part of spectrum of the operator.

Thus, the following spectral problem naturally arises: it is necessary to find such values $\kappa^m \in R$, for which homogeneous (i.e., $U^i(y,z) \equiv 0$) boundary value problem has non-trivial solution $u^m(y,z) = U^s(y,z)$. Such values κ^m correspondent to their functions $u^m(y,z)$ and can be called as eigen wave numbers and eigen waves (or modes, or oscillations) respectively. Evidently, value κ^m can not belong to real axis of first sheet of R.

Due to the qualitative properties of the resolvent of the boundary value operator (see the previous section) the set Ω of eigen wave numbers includes all possible spectral points of boundary value problem operator (i.e., the continuous spectrum is absent!). Moreover, it can be proved that the set Ω coincides with set of poles of above mentioned resolvent, and cardinality of Ω cannot be more than countable, and Ω is the set of isolated points without any accumulation point in any bounded part of Riemannian surface R.

In accordance with the terminology of the previous section, we call the spectral problem described as global spectral problem (one parameter k for all media). It is clear that the local spectral problems in respect to each complex valued parameter K_j, $j = 1, 2, 3, \ldots, N$ can be posed in very similar and evident way as homogeneous problem for corresponding diffraction problem in Riemannian surface $K_j \in R^j$. The qualitative properties of each local spectral problem are the same as ones described above for the global spectral problem.

These qualitative properties mean that solution of spectral problems is able to give important information about diffraction problem operator and, consequently, about resonant properties of the obstacle, is able to give new physical understanding of complicated physical phenomena of wave scattering by periodic boundary between two media. This statement is illustrated with the numerical examples in the Section 6 of this paper.

5. ALGORITHMS, NUMERICAL TECHNIQUES AND IMPLEMENTATION

Following the scheme of C method [10–16] we arrive to the operator equation of the first kind

$$Fx = B \tag{30}$$

in respect to unknowns x with operator F and right-hand side vector B that have the following block structures:

$$F = \left\| \begin{array}{cc} F_1 & -F_2 \\ G_1 & -\gamma G_2 \end{array} \right\|, \qquad x = \left\| \begin{array}{c} R \\ T \end{array} \right\|, \quad B = \left\| \begin{array}{c} B_1 \\ B_2 \end{array} \right\|.$$

Here we remind the expression of the matrix operators

$$F^p = \|F^p_{mn}\|^{\infty}_{m=1,\ n=-\infty}, \qquad G^p = \|G^p_{mn}\|^{\infty}_{m=1,\ n=-\infty}; \quad p = 1, 2$$

$$F^1_{mn} = L_{m-n}(\rho_{n1} A_0); \qquad F^2_{mn} = \overline{L}_{m-n}(\rho_{n2} A_0)$$

$$\begin{aligned}
L_n(\gamma) &= \frac{1}{2\pi}\int_0^{2\pi} \exp\{i\gamma a(y) - iny\}dy; \\
\overline{L}_n(\gamma) &= \frac{1}{2\pi}\int_0^{2\pi} \exp\{i\gamma(1 - a(y)) - iny\}dy; \\
G^1_{mn} &= \rho_{n1} F^1_{mn} - \Phi_n A_0 \sum_{s=-\infty}^{+\infty} a_{m-s} F^1_{ms}(m - s); \\
G^2_{mn} &= -\rho_{n2} F^2_{mn} + \Phi_n A_0 \sum_{s=-\infty}^{+\infty} a_{m-s} F^2_{ms}(m - s); \\
a_n &= \frac{1}{2\pi}\int_0^{2\pi} a(y)\exp\{-iny\}dy;
\end{aligned}$$

$$\begin{aligned}
B_1 &= (B_{n1})^{\infty}_{n=-\infty}; \qquad B_{n1} = -L_n(-\kappa_1 \cos(\varphi) A_0); \\
B_2 &= (B_{n2})^{\infty}_{n=-\infty}; \quad B_{n2} = \begin{cases} -\kappa_1 \cos(\varphi) B_{01}; & n = 0 \\ (ntg(\varphi) - \kappa_1 \cos(\varphi)) B_{n1}; & n \neq 0; \end{cases}.
\end{aligned}$$

ρ_{mp}, $p = 1, 2$, are the solutions to the spectral problem of C-method [16], φ is the angle between the wave vector of incident wave and OZ axis.

Analysis of the matrix entries of (30) made clear that operator equation (30) is an equation of the first kind. Formally it follows from the asymptotical estimation for entries of operators F^1 and F^2. It can be proved that for $|n|$, $|m| \to \infty$ the following asymptotic estimations are valid

$$F^1_{mn} \sim \sum_{k=1}^{P_1} \frac{e^{-i(m-n)y^1_k} e^{-\frac{(m-n)^2}{2A_0(|n|+1)\ddot{a}(y^1_k)}}}{\sqrt{2\pi A_0(|n|+1)\ddot{a}(y^1_k)}};$$

$$F^2_{mn} \sim \sum_{k=1}^{P_2} \frac{e^{-i(m-n)y^2_k} e^{-\frac{(m-n)^2}{2A_0(|n|+1)\ddot{a}(y^2_k)}}}{\sqrt{2\pi A_0(|n|+1)\ddot{a}(y^2_k)}}.$$

They are obtained under assumption that function $z = A_0 a(y)$ (that is describing the periodic boundary between two media) has finite sets of points $Y^1 = \{y^1_k\}^{P_1}_{k=1}$, $Y^2 = \{y^2_k\}^{P_2}_{k=1}$ for which the following relations hold

$$\begin{aligned} a(y^1_k) &= 0; \quad \dot{a}(y^1_k) = 0; \quad \ddot{a}(y^1_k) > 0; \\ a(y^2_k) &= 1; \quad \dot{a}(y^2_k) = 0; \quad \ddot{a}(y^2_k) < 0. \end{aligned}$$

For matrix elements of operators G^1 and G^2 we obtain the following asymptotic behavior:

$$G^1_{mn} \sim m\frac{|n|}{n}F^1_{mn}; \quad G^2_{mn} \sim -im\frac{|n|}{n}F^2_{mn}.$$

Such behavior of entries of operator F from (30) allows us to state that the condition numbers of corresponding truncated systems of algebraic equations

$$F_N x_N = B_N$$

tends to the infinity rather quickly ($cond(F_N) \to \infty$), when truncation number $N \to \infty$. We remind here that the condition number of the system (30) is defined as $cond(F) = \|F\| \cdot \|F\|^{-1}$ and plays the crucial role in the connection of the errors including round off errors of input data (entries of matrix F and right hand side part B) and the solution accumulated error δx:

$$\frac{\|\delta x\|}{\|x\|} \approx cond(F)\left(\frac{\|\delta F\|}{\|F\|} + \frac{\|\delta B\|}{\|B\|}\right).$$

We calculated the matrix F_N norm $\|F_N\| = \sum_{m=1}^{N}\sum_{n=1}^{N}|f_{mn}|^2$ as Frobenius's one.

In Fig. 2 we present the results of the numerical study of condition number $cond_N = cond(F_N(N))$ for grating with boundary function $a(y) = A_0(1+\cos y)/2$, $\kappa = d/\lambda = 0.6$, $\varphi = 0$, $A_0 = \frac{2\pi h}{d} = \pi$, solid line. As it has been shown in [37], the number m_r of correct binary figures in approximate solution x_N (rounded off to m_e binary figures, in other words, m_e is the binary length of mantissa) does not exceed the value

$$m_r = m_e - \log_2 cond_N.$$

The computer has fixed mantissa length m_e. So, the value m_r may become negative, when the condition number $cond_N$ is big enough. In such a case there is no one a correct digit in the approximate numerical solution x_N. Besides the order of the value of residual $\|\delta_N\| = F_N x_N - B_N$ will be $\|\delta_N\| \sim N 2^{-m_e}\|x_N\|$, i.e., the residual is very small even if the solution has not any correct figures. The accurate solution of the system (30) rounded off up to m_e binary digits, gives the same order of the error — see [37]. This shows the potential impossibility of straightforward application of truncation method for numerical solution of (30) with large numbers of truncation N, and means that the application of regularizing procedure may be useful.

In order to obtain more stable numerical algorithm we applied two-side regularization (left and right hand side regularization similar to [4, 29]). For this purpose we consider the contour L, given by formula $z = ha(y)$, $0 \le a(y) \le 1$ with additional restriction that function $a(y)$ has the finite numbers P_1 and P_2 of maximums $\{y_k^1\}_{k=1}^{P_1}$ and minimums $\{y_k^2\}_{k=1}^{P_2}$ only, and $\ddot{a}(y) \ne 0$ for $j = 1, 2$ and all possible k, where $\ddot{a}(y)$ is second derivative of function $a(y)$. Relaying on the asymptotic estimation for the entries of F, we introduce matrix-operator $T_1 = \|\delta_{mn}\sqrt{|n|+1}\|_{m,n=-\infty}^{\infty}$, $T_2 = \|\delta_{mn}\tau_n\|_{m,n=-\infty}^{\infty}$, $\tau_0 = 1$, $\tau_n = i/n$, $n \ne 0$, and now one can make right hand side $x_1 = T_1 y_1$, $x_2 = T_1 y_2$ and left-hand side regularization. The below-presented formulae explain the idea clearly:

$$\begin{pmatrix} I & 0 \\ 0 & T_2 \end{pmatrix}\begin{pmatrix} F_1 & -F_2 \\ G_1 & -\gamma G_2 \end{pmatrix}\begin{pmatrix} T_1 & 0 \\ 0 & T_1 \end{pmatrix} \Rightarrow$$

$$\begin{cases} F_1 T_1 y_1 - F_2 T_1 y_2 = B_1; \\ T_2 G_1 T_1 y_1 - \gamma T_2 G_2 T_1 y_2 = T_2 B_2; \end{cases} \Rightarrow$$

$$\begin{cases} c_1 y_1 - c_2 y_2 + A^{11} y_1 - A^{12} y_2 = B_1; \\ -c_1 y_1 + c_2 \gamma y_2 + A^{21} y_1 - A^{22} y_2 = T_2 B_2, \end{cases}$$

where c_1, c_2 are constants, defined by the boundary shape (under mentioned above restrictions on function $a(y)$):

$$c_1 = \sum_{k=1}^{P_1} \frac{1}{\sqrt{2\pi A_0 \ddot{a}(y_k^1)}}, \qquad c_2 = \sum_{k=1}^{P_2} \frac{1}{\sqrt{2\pi A_0 \ddot{a}(y_k^2)}},$$

where $\ddot{a}(y)$ is the derivative of second order of function $a(y)$.

The analytical inversion of

$$\begin{cases} c_1 y_1 - c_2 y_2 \\ -c_1 y_1 + c_2 y_2 \end{cases}$$

gives the operator equation of the second kind

$$y + Hy = d. \tag{31}$$

In Fig. 2 we presented with dashed line the condition number of truncated system (31) for the same gratings at the same frequency. We can see that application of regularizing procedure gave us the decreasing of condition number of the system that we have to solve numerically by more than 100 times and increased the acceptable value of number of truncation, and, as a result, extended the range of parameters h (depth of grooves up to 2π) and κ (frequency parameter up to 2).

Let us now consider homogeneous problem

$$y + Hy = 0. \tag{32}$$

This operator H depends on spectral parameter κ analytically. The condition of existence of nontrivial solution to (32) is the equality to zero of the determinant of (32) that arrives to

$$\det[I + H(\kappa)] = 0.$$

Numerical algorithm has been developed for the spectral problem numerical solution is strongly based on the experience that had been acquired during the study of eigen frequencies in fields of DG and open waveguide resonators [7, 30–32].

From the point of view of numerical methods, the key feature of the algorithm is the numerical search of the complex valued frequencies in multi sheeted Riemannian surface and the calculation of electromagnetic field density distribution corresponding to the certain eigen frequency.

Thus, the first problem is the calculation of the complex valued roots of function $f(z) = \det[I + H(z)]$, which is determinant of the system (32), and z is corresponding complex valued variables (namely,

z is κ or K_j) belonging to the relevant Riemannian surface. The routine for these roots searching had been constructed as adaptive set of several methods. Linear and quadratic interpolations of direct $f = f(z)$ and inverse $z = z(f)$ functions are among them (we used Traub's interpolation scheme that has a few numerical advantages over more popular Muller's one — see [38]). Using already calculated approximations of the root, the computer routine chooses the best interpolation method for each next step of more accurate approach construction. It is necessary to take into account that, at first, the root can be situated in the different from initial guess sheet of Riemannian surface. At second, during the root search current approximation to the root may be placed in another sheet than the previous one, even if exact value of root is situated in the same sheet. Thus, the routine while operating must automatically switch the search into relevant Riemannian sheet. The routine constructed analyses the possibility of such switching and makes proper choice of such a sheet, which minimizes the difference between two successive approximations. As numerical experiments have already shown, the strategy explained is rather fast and robust and it gives required precision of the root value.

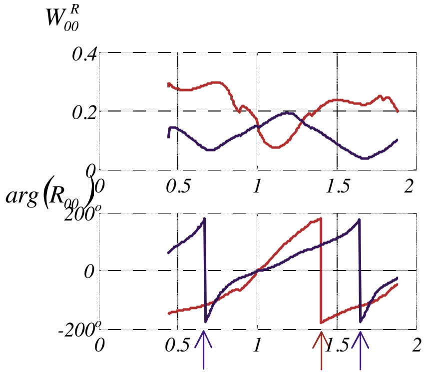
The numerical reconstruction of the electromagnetic field density distribution in the boundary domain is an important and always required characteristic of eigen regimes. In order to get it we have to find out numerically corresponding eigen vector x. Namely, if some characteristic value z_c of matrix-operator $I + H(z)$ is found (i.e., $f(z_c) = 0$), system (32) for $z = z_c$ is a degenerated one, and it is necessary to find eigen vector corresponding to zero eigen value of operator $I + H(z_c)$. This problem has been solved by means of well known algorithm of inverse iteration — see [36–38] (which, of course, was applied to the reduced matrix that is the finite approximation to the infinite matrix-operator $I + H(z_c)$).

In such way, we constructed efficient and powerful tool for numerical study of spectral properties of periodic boundary between two media within rather wide range of parameters. That is to be illustrated in the following section.

6. NUMERICAL RESULTS DESCRIPTION, DISCUSSION AND INTERPRETATION

6.1. Connection between Spikes in Diffraction Characteristics and Eigen Regimes

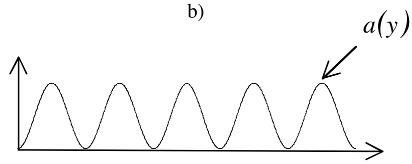
In present paper we have considered rather wide range of theoretical aspects of spectral theory of gratings. Each of them, due to existence of numerical algorithm that is efficient and reliable tool for computational



a)

E/H	κ_n	κ'_n	κ''_n
E	1.403	1.4379	-0.2067
H	0.674	0.7117	-0.1123
	1.648	1.75987	-0.3021

b)



c)

Figure 4. Correlation between diffraction characteristics and excitation in the POR regimes, close to natural ones. Red curves correspond to E-polarization, the blue ones to the H-polarization. The boundary is described by the curve $a(y) = \sin^2(y/2)$, $h = \pi$, $\varepsilon_2 = 5$; $\mu_2 = 1$.

experiments, may be illustrated with numerous interesting examples, and numerical results can provide a good background for profound electromagnetic analysis. But keeping our study within the frames of a paper we shall just outline the major, from out point of view, qualitative properties of the studies spectra of dielectric grating with arbitrary profile of grooves.

In our investigation of diffraction properties of gratings we followed the approach [7, 30, 31], considering the periodic boundary (DG) as periodic open resonator (POR).

The assumption that resonant transmission/reflection from the periodic boundary treated as POR is related to the excitation of regimes close to eigen ones in the region of the boundary ($0 < z < a(y)$) has been inspired by the following facts: when parameters of the problem are close to ones providing the spikes in diffraction characteristics a decrease in the value of the determinant of the system of equations of corresponding BVP and an increase in the field intensity near the boundary do emerge.

To prove this statement we have studied the frequency responses of the electromagnetic field scattered from the DG of the shape $a(y) = \sin^2(y/2)$, depicted in Fig. 4c. The structure under consideration — a periodic boundary between dielectrics with limited depth does not support pronounced (with high quality $\boldsymbol{Q}$ factor) resonances. That is why, in order to follow the connection between so called low $\boldsymbol{Q}$ resonances with excitation of natural oscillation, we have to study the behavior of the phase of reflected zero order efficiency $\arg R_{00}(\kappa)$. It is known that in the vicinity of resonant frequency the phase has to be changed by the value approximately equal to π, so it may serve a good pointer to the close existents of eigen regime.

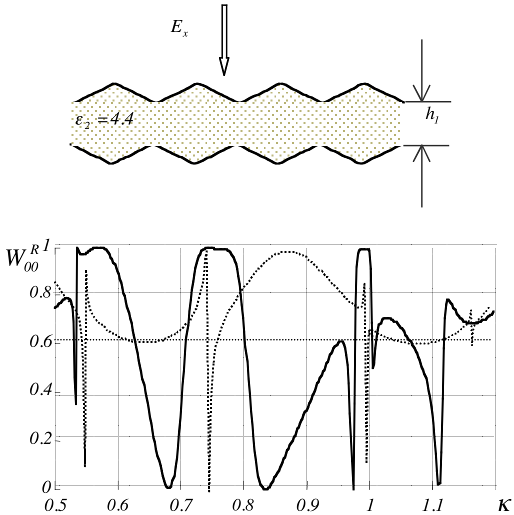
In Fig. 4a the reflected energy $W_{00}^R(\kappa)$ and the phase $\arg(R_{00}(\kappa))$ of the 0-th harmonic for E and H polarized wave when real frequency parameter $\kappa = d/\lambda$ varying are presented. The amplitude of the scattered waves have calculated from the solution to diffraction problem (for real frequencies) (31); and the nearest eigen complex frequencies $\kappa_n' + i\kappa_n''$ have been found as the solution to the spectral problem (32). In the table (Fig. 4b) the values of κ_n corresponding to the spikes in the curves $\arg(R_{00}(\kappa))$ and nearest complex eigen frequencies $\kappa_n' + i\kappa_n''$ are presented. The correspondence of the resonances in the frequency characteristic of $\arg R_{00}(\kappa)$ and excitation in the structure the oscillations close to natural ones is clearly seen.

The field pattern formed by grating in resonant regime is rather interesting and useful characteristic, giving more profound understanding of the resonant phenomena. By studying the various field patterns, calculated at different eigen frequencies, we can analyze the peculiarities of spectral properties of grating. In order to obtain qualitative characteristics of eigen field, we have calculated the patterns of the distribution $|E_x(y,z)|$ for E-polarized wave or $|H_x(y,z)|$, for H polarized plane wave, corresponding to their eigen frequencies. In the calculation we used the routine for numerical determination of eigen vectors corresponding to their eigen frequency.

We would like to attract the attention to the fact that in the case of H polarization the first resonances appears at much smaller frequency parameter, that is for more long waves. This resonance exists due to the possibility of excitation of TEM wave that is propagating along the grooves and, under certain parameters, is able to provide the resonances. Naturally, this resonance disappears at certain value of that corresponds to the minimal depth of grooves that can provide resonance conditions for TEM wave.

Much more pronounced resonances may be seen in the diffraction by the dielectric layer, limited with periodic boundary, see for example Fig. 5. Fig. 5a presents the curve $W_{00}^R(\kappa)$ and in Fig. 5b the table, demonstrating the correspondence of resonances in real frequencies and relevant complex eigen frequencies.

It is clearly seen here that the eigen complex frequencies of oscillations in DG or POR, which are close to the natural ones, are in strict correlation with the resonances in diffraction characteristics



h_1	κ_n	κ'_n	κ''_n
0.1π	0.549	0.5485	-0.0004i
	0.749	0.7455	-0.00000i
	0.999	0.9971	-0.00001i
	1.171	1.1691	-0.00066i
0.5π	0.528	0.5255	-0.0000i
	0.680	0.6600	-0.00001i
	0.728	0.7085	-0.0484i
	0.822	0.8067	-0.03045i
	0.972	0.975	-0.005i
	0.981	0.987	-0.00000i
	1.03	1.0058	-0.0048i
	1.15	1.1144	-0.005i

Figure 5. The diffraction and spectral characteristics for the dielectric layer with $\varepsilon_2 = 4.4$, $\mu_2 = 1$, limited with the boundaries $a(y) = 0.5 - 4\pi^{-2}(\cos(y) + \cos(3y)/9 + \cos(5y)/25)$ and $1 - a(y)$ of thickness h_1 normally excited with E polarized plane wave. Solid line corresponds to $h_1 = 0.5\pi$, dashed line corresponds to the layer with $h_1 = 0.1\pi$.

of this structure. In particular (and it is to be demonstrated in our future article devoted to the multilayered periodic structures study) the operation on the frequency that is close to the eigen one of certain POR can provide the regimes of total reflection or transmission of electromagnetic waves scattered by this resonator.

6.2. General Regularities in POR Spectrum Behavior

Having performed rather extensive study of the eigen complex frequencies of POR with material and geometrical parameters varying, we can make several comments on the regularities of spectrum behavior.

First of all, we have to point out that the spectral properties of POR for two different polarizations manifest the principal difference. Further on, following the analogy with waveguide open resonators [30, 31], we shall call eigen oscillations, corresponding to E-polarization as TM eigen modes, and that ones, corresponding to H-polarization as TE modes. It is not possible to carry out the classification of the natural oscillation in the way it has been done for waveguide open resonators [30, 31], open resonators [4] or for DG with so-called coordinate shape grooves [7]. So here we shall for the present time make numeration for the eigen modes starting with the smallest real part of eigen frequency.

The parameter region where certain type of eigen oscillations is allowed, is strictly bounded by the domain of eigen frequencies existence and corresponding cuts in the Riemannian surface, see Fig. 2. Eigen complex frequencies, in the first (physical) sheet of Riemannian surface continuously depend on the parameters of the problem (geometrical, constitutive). The values of real and imaginary parts of eigen frequencies of TM modes weekly change with the ε_2 or μ_2 varying. Real and imaginary part of κ decrease with ε_2 increasing that is the $\boldsymbol{Q}$ factor of natural oscillation is increasing. The eigen fields density is, naturally more concentrated inside the second material.

For TM modes similar situation appears for real part of complex frequency κ' with the depth of grooves h is increasing. Imaginary part of complex eigen frequency is also decreasing, but with certain oscillations, the mean value of $\boldsymbol{Q}$ factor is definitely growing. The field of eigen oscillation for DG with deep grooves is concentrated in the grooves.

Situation similar to the one described above may be observed for small values of ε_2/μ_2 and for not deep grooves for modes.

But, when the grooves of DG become of considerable size and $\varepsilon_2 >\cong 3$, the "regular" behavior of eigen frequencies with parameter change does not exist any more, and we have the spectral curves behavior of rather complicated type, having resemblance with Vienne graphs that are well-known from the circuit theory.

6.3. Certain Irregularities in POR Spectrum Behavior

Rather special behavior of spectral curves for TE modes is illustrated by Fig. 6. The curves, that correspond to real ($\mathrm{Re}(\kappa)$) and imaginary parts ($\mathrm{Im}(\kappa)$) of eigen frequencies (Fig. 6a) come very close and even cross each other when depth of grooves h increases. It more easy to grasp this phenomena presenting calculated values of eigen frequencies in parametric form as function $\kappa(h)$ in the fist sheet of the plane R, see Fig. 6b. Note, the crossing of curves $\kappa_2(h)$ and $\kappa_3(h)$ occurs at the point $(1.6681, -0.3591)$ for different values of parameters $h_i,\ i = 2, 3$.

One can see clearly the resemblance with diagrams for eigen frequencies of close resonators and naturally the question about degeneration and coupling of oscillation arises.

We have to remind here that similar situation had been already revealed and discussed for open resonators [29], gratings [7] and open waveguide resonators [30, 31]. Relying on the results, [7, 30, 31, 39]

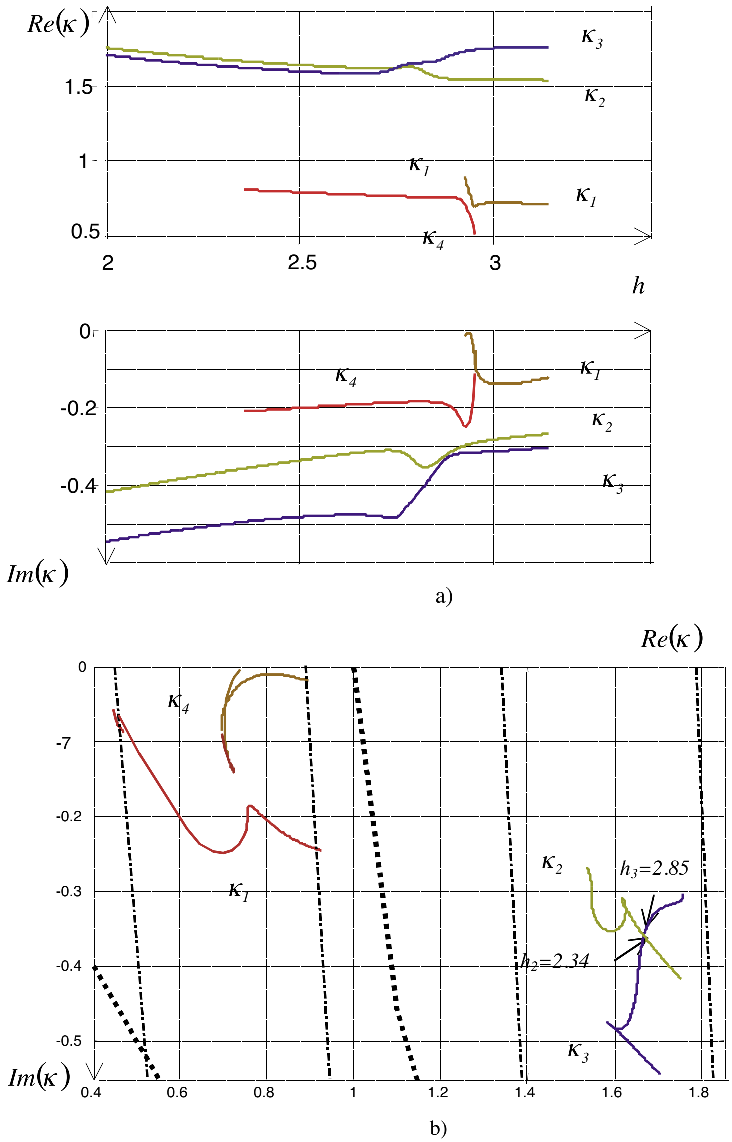


Figure 6. The spectral curves for TE modes, boundary $a(y) = \sin^2(y/2)$, $\varepsilon_2 = 5$, $\mu_2 = 1$. In Fig. a) the spectral curves $\kappa_i(h)$, $i = 1, \dots, 4$ are presented. In Fig. b) spectral curves $\kappa_i(h)$, $i = 1, \dots, 4$ are depictured in the plane $\boldsymbol{R}$. The dashed lines correspond to the cuts Eq. (23).

we can treat the spectrum characteristics, presented in Fig. 6, as the mode coupling phenomena. The "coupling" phenomena we treat here as the mutual influence of eigen modes, resulting in the eigen frequencies and $\boldsymbol{Q}$ factor variation and accompanied with appearance in resonator "inter-mode" complicated field structures, corresponding to eigen frequencies.

Here we remind that behavior of eigen frequencies, similar to presented in Fig. 6, is coursed by the existence (in this parameter range) of degeneracy points (DP) or/and Morse critical points (MCP) of operator-function

$$f = \det(I - H(k, h, \varepsilon_i, \mu_i)), \tag{33}$$

that is analytically continued into the domain of complex values of $h = h' + ih''$.

The study of singular point of $f(\kappa, h)$ in two-dimensional complex space C^2 would allow us to investigate purposefully the regions of POR's parameters where the spectrum curves come closer, and even cross, each other. Those two types of singular points are rather natural [7, 31, 39] for such situation.

In order to determine the coordinates of DP (κ_d, h_d) we have to find out the solution of the system

$$\begin{cases} f(\kappa, h) = 0; & k = k' + i\kappa'' \\ f'_\kappa(\kappa, h) = 0; & h = h' + ih'' \end{cases}. \tag{34}$$

The eigen modes coupling phenomenon is well known in different resonator devices. It displays as an abrupt change in $\boldsymbol{Q}$ factor and as the transformation of internal resonator field structure when the geometrical parameters are varying slightly. It has been shown [7, 31, 39] that the availability of isolated MCP of the boundary value problem operator function causes mode coupling. In order to find the coordinates of MCP, it is necessary to solve the system

$$\begin{cases} f'_\kappa(\kappa, h) = 0; \\ f'_h(\kappa, h) = 0; \end{cases}$$
$$f''_{\kappa\kappa}(\kappa, h) f''_{hh}(\kappa, h) - (f''_{\kappa h}(\kappa, h))^2 \neq 0. \tag{35}$$

The calculation of MCP provides us with the opportunity to approximate the corresponding spectral curves in the (κ_m, h_m) vicinity by a rather simple quadratic form.

$$\begin{aligned} &f''_{\kappa\kappa}(\kappa, h) \cdot (\kappa - \kappa_m)^2 + 2 f''_{\kappa h}(\kappa, h)(\kappa - \kappa_m)(h - h_m) \\ &+ f''_{hh}(\kappa, h)(h - h_m)^2 + 2\delta + O_3 = 0; \\ &\delta = f(\kappa_m, h_m) \neq 0. \end{aligned} \tag{36}$$

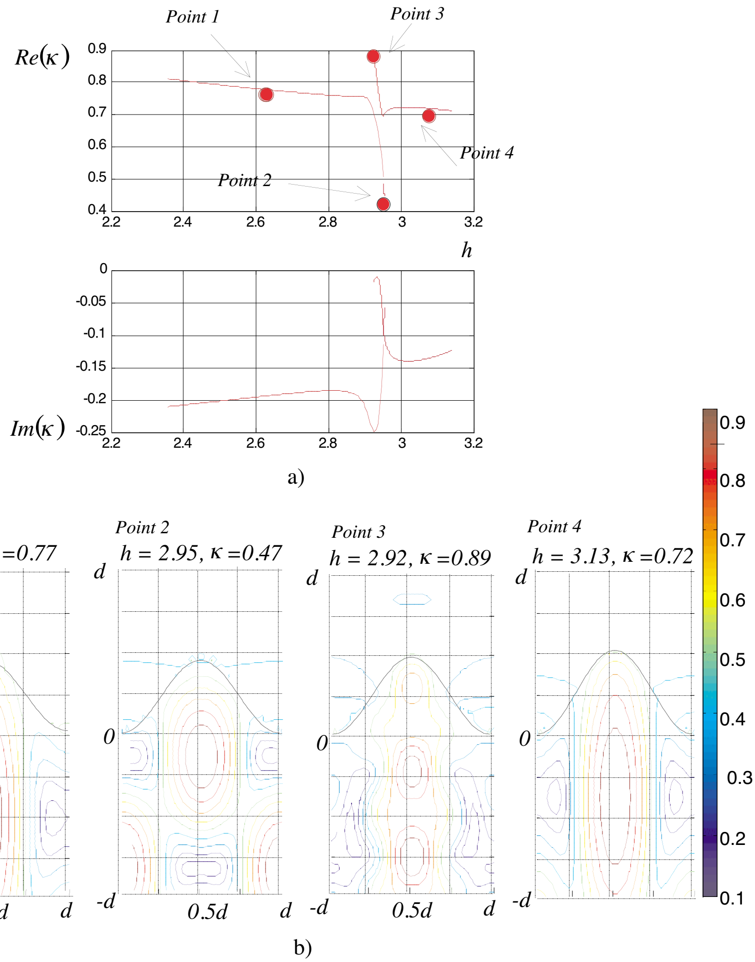


Figure 7. The mode coupling phenomena. $a(y) = \sin^2(y/2)$, $\varepsilon_2 = 5$, $\mu_2 = 1$, H polarization. The behavior of eigen modes in the vicinity of MCP: eigen frequencies ($\kappa(h)$, Fig. a) and eigen fields ($|H_x(y,z)| = const$, computed within one period, Fig. b) calculated consequently in the points, indicated at the curves.

Where $O_3 = O((\kappa-\kappa_m)^3 + (h-h_m)^3)$ denotes cubic small terms, and $f''_{\kappa\kappa}$, $f''_{\kappa h}$, f''_{hh}; are calculated in the point (κ_m, h_m).

In Fig. 7 the detailed piece of variation of eigen values within the interval of parameters, where mode coupling occurs is presented. We can see one of the forms of possible behavior (for details see [31, 39]) of spectral curves: real parts of eigen values take a shape of Vienne graphs, imaginary parts cross each other, the structure of eigen field pattern changes gradually while following along one of the eigen values curves, see *point 1* and *point 2*; *point 3* and *point 4*; in the same time at eigen frequencies chosen at *point 1* and at *point 4*, that belong to the different eigen value curves the field patterns are practically identical; the patterns calculated at eigen values taken from *point 2* and *point 3* reflect the 'transition' (or 'hybrid') character of the eigen field structure.

The study of mode coupling for arbitrary profile periodic boundary between two dielectric media is rather complicated and is actually a new task that has to be fulfilled in the nearest future.

6.4. Spectral Properties of the Grating with Materials $\varepsilon < 0$ or/and $\mu < 0$

Different situation in physics arrives to the study of the materials with negative constitutive parameters [24, 25, 34, 35, 40–42].

The described above solution to the spectral and, naturally, diffraction problem and corresponding to them complementary algorithms, can simulate the electromagnetic field interaction in materials, characterizing by $\varepsilon < 0$ or/and $\mu < 0$, and we are able to provide the "feedback" study: spectral diffraction characteristics.

In order to prove the efficiency and perspective advantages of such a study we shall discuss here one result of the simulation that seems to be rather distinctive for the materials with $\varepsilon < 0$ or/and $\mu < 0$.

In Fig. 8 there are two characteristic cases of TM/TE waves diffraction by periodic boundary between the two media, when one of them (the second) has negative permeability $\mathrm{Re}(\mu_2) < 0$ and $\varepsilon_2 = 2.25$. The Fig. 8a illustrates the resonance that appears for normal excitation of the boundary, when $\mathrm{Im}(\mu_2) = 0$. In this case the resonance may be seen in the curve of $\arg(R_{00})$ for TM waves only, as we have total reflection of the incident wave, and $|R_{00}| = 1$.

By introducing the losses in the second medium we can make the resonance to be manifested for the amplitude of reflection filed also, see Fig. 8b. While oblique excitation, even with rather small angles, say $\varphi = 5$, see Fig. 8c, the resonance splits into two ones, moving from initial position in frequency into two different directions. The amplitudes of evanescent harmonics in scattering field are suffering pronounced resonant spikes also.

Naturally, similar situation emerges for TM polarized wave diffraction by periodic medium with parameters $\mathrm{Re}(\mu_2) < 0,\ \mathrm{Re}(\varepsilon_2) > 0$.

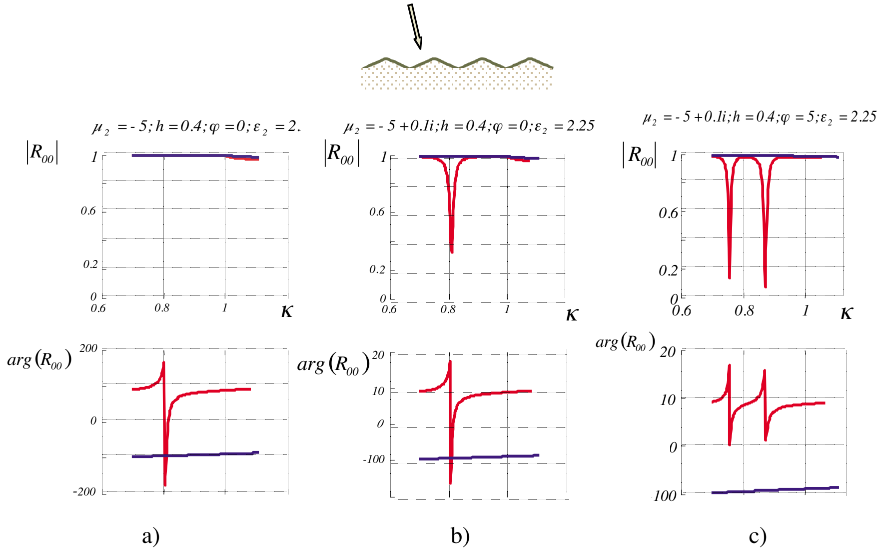


Figure 8. The amplitude $|R_{00}|$ and phase $\arg R_{00}$ of reflected propagating harmonic: red curves correspond to TM modes, blue — to TE modes. The corresponding eigen frequency $\kappa = 0.813 - i0$, $\Phi = 0$.

In contrast to the resonance appearing for TE modes, that has been discussed above, this resonance does not disappear with depth of grooves h decreasing, even for $h \approx 0.001$, see Fig. 9, where the evolution of resonances with h decrease (Fig. 9a) and various ε_2 (Fig. 9b) is presented. It is worthwhile to point out that the $\boldsymbol{Q}$ factor of this resonance increases when h decreases. That allows us to conclude, that resonances of the type are characteristic for periodic boundaries and are connected with excitation of polaritons.

All these resonances have corresponding complex eigen frequencies with $\kappa'' \approx 10^{-8}$, that means within the algorithm accuracy these resonances have real eigen frequencies.

For the special case, say for H polarized wave, when $\varepsilon_1, \mu_1 > 0$, $\mu_2 > 0$; $\varepsilon_2 < 0$ and $|\varepsilon_2| > |\varepsilon_1|$, under condition $A_0 \ll 1$, (we shall remind that $A_0 = 2\pi h/d$) following approximation for this real valued root can be obtained:

$$\operatorname{Re}\kappa_0 = \sqrt{\frac{\varepsilon_2^2 - \varepsilon_1^2}{\varepsilon_1\varepsilon_2(\varepsilon_2\mu_1 - \varepsilon_1\mu_2)}}(1 + O(A_0)), \quad |\operatorname{Im}\kappa_0| = O(A_0^2).$$

The eigen fields, corresponding to these resonances, are concentrated in the vicinity of the boundary, see Fig. 10, where this type of resonances,

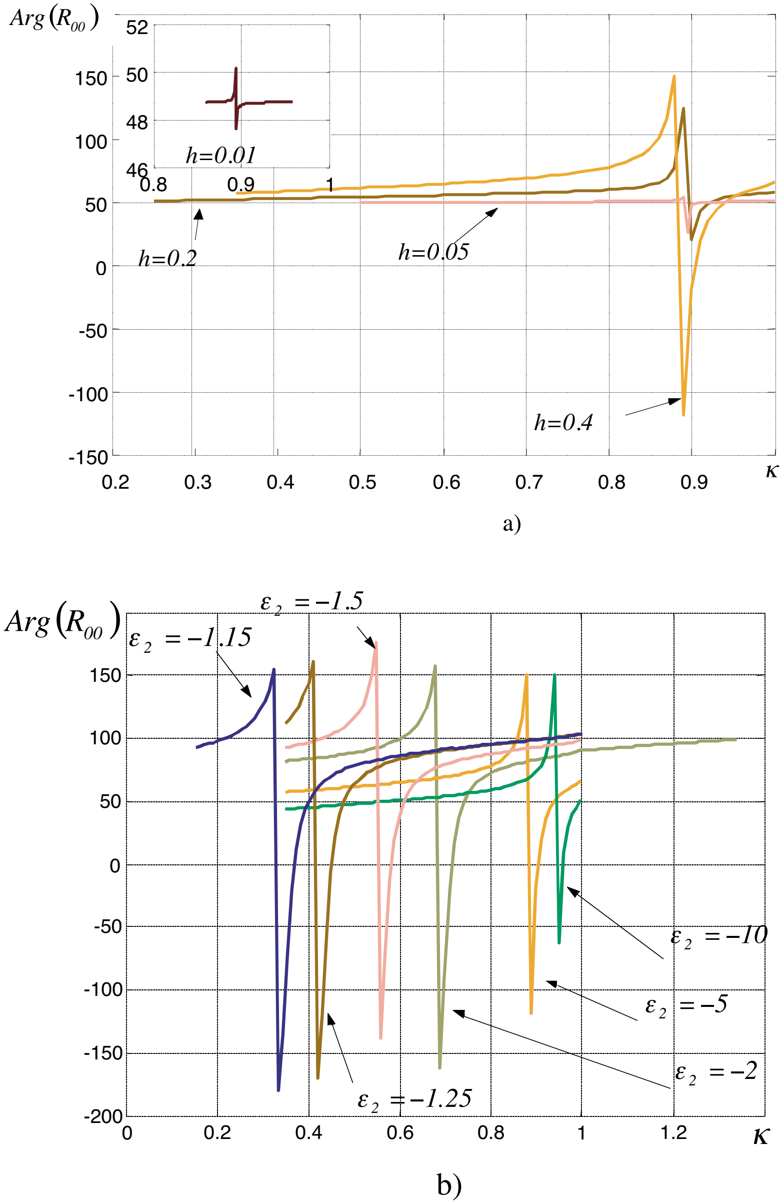


Figure 9. The short wave super high $\boldsymbol{Q}$ resonance of TE mode for different depth of grating profile h (Fig. a) with $\varepsilon_2 = 5$; and constitutive parameter (Fig. b), $h = 0.4$; boundary shape $a(y) = \sin^2(y/2)$. For example for $\varepsilon_2 = -5$; $h = 0.4$ eigen frequency $\kappa = 0.893 - i0.97 \cdot 10^{-13}$.

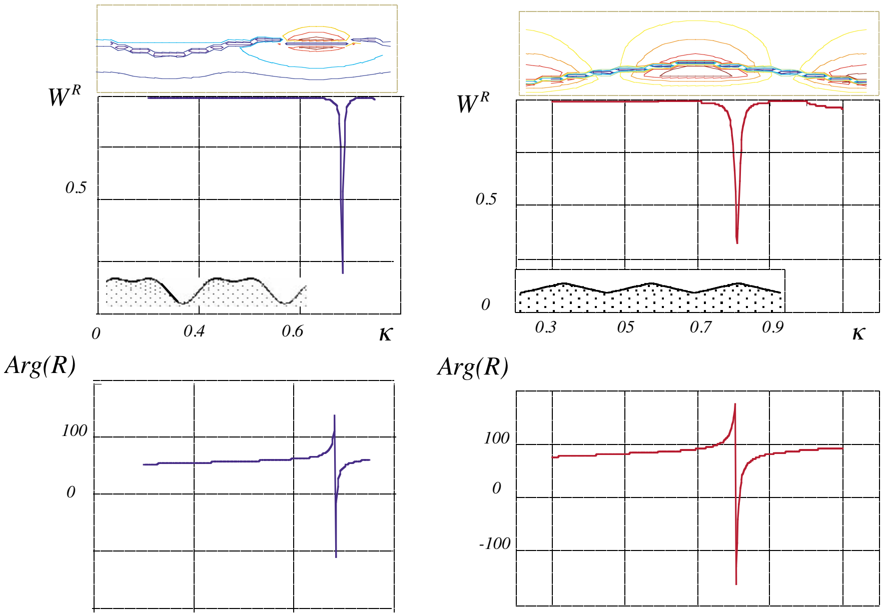


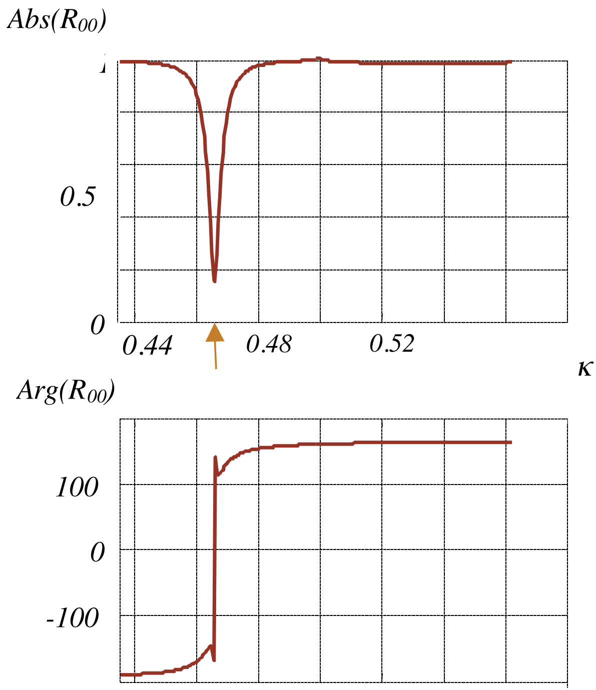
Figure 10. The amplitude and phase of reflected propagating harmonic for two different surfaces: a) TE modes, $\varepsilon_2 = -5+i0.1$; $\mu_2 = 1$, eigen frequency is almost real valued $\kappa = 0.89 + i0$; b) TM modes, $\varepsilon_2 = 2.25$, $\mu_2 = -5 + i0.1$; $\kappa = 0.818 + i0$. The fragments of electromagnetic field density in the vicinity of grating calculated at the frequency of maximal absorption are presented above.

supplied with the eigen filed structures for two different shapes of boundary are presented.

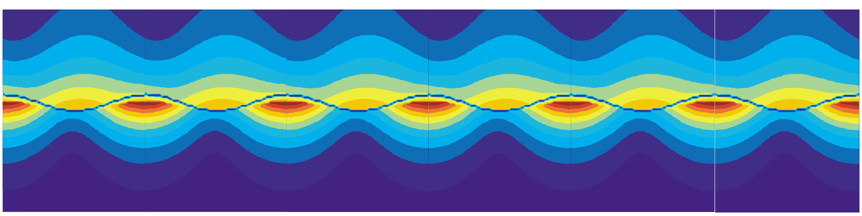
Among numerous results of computational experiments being carried out for double negative materials we have chosen to present here the absorption resonance appearing in diffracted field from periodic surface of lefthanded material when incident plane electromagnetic wave is almost parallel to the axis OY. Fig. 11a) shows the pronounced resonance for rather smooth ($h = 0.1d$) periodic surface of lefthanded (double negative) material illuminated with E polarized planes wave with incidence angle $\varphi = 88$. The real valued resonant frequency may be estimated for surface with $A_0 \ll 1$ from approximate formula

$$\kappa \approx 1/\left(\sin(\varphi) + \sqrt{(\mu_2^2 - 1)\,/\,(\mu_2^2 - \varepsilon_2\mu_2)}\right)$$

and for H polarized plane wave the resonance frequency may be defined



a)



b)

Figure 11. Efficiency (a), eigen field density $|E_x(y,z)| = const$ (b), computed at frequency of maximal absorption (marked with arrow) of the double negative material surface with boundary $a(y) = 0.5(1+\cos(y))$; $h = 0.1d$. TM modes, $\varepsilon_2 = -0.2 - 0.01i$; $\mu_2 = -1.5 + 0.01$; incidence angle $\varphi = 88°$, complex eigen frequency $\kappa = 0.4645 - i0.0012$.

approximately from

$$\kappa \approx 1/\left(\sin(\varphi) + \sqrt{\left(\varepsilon_2^2 - 1\right)/\left(\varepsilon_2^2 - \varepsilon_2\mu_2\right)}\right).$$

When $A_0 \ll 1$ these approximate values of resonant frequencies are in good agreement with calculated ones by rigorous solution (32). The eigen frequency of corresponding natural oscillation that has been found out from the solution to spectral problem Eq. (32) $\kappa = 0.4656 - i0.0012$ is in good correlation with diffraction resonance. Periodic surface eigen field intensity is concentrated near the boundary at the frequency $\kappa = 0.466$, corresponding to maximal electromagnetic energy absorption; the field pattern $|E_x(y,z)| = const$ is presented in the Fig. 11b.

7. CONCLUSION

We have discussed several issues of C method that may prove its high potential for various practical applications. Within the limited frames of this paper we made our choice to provide the essential attention to the mathematical issues of spectral problem and corresponding algorithm descriptions. These items give reliable base for the study of various applied and fundamental questions; among which we can mention the study and apprehension of mode coupling; the properties of Veselago (left handed) materials.

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