Chapter 5

Analytical Grounds for Modern Theory of Two-Dimensionally Periodic Gratings

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1. Introduction

Rigorous models of one-dimensionally periodic diffraction gratings made their appearance in the 1970s, when the corresponding theoretical problems had been considered in the context of classical mathematical disciplines such as mathematical physics, computational mathematics, and the theory of differential and integral equations. Periodic structures are currently the objects of undiminishing attention. They are among the most called-for dispersive elements providing efficient polarization, frequency and spatial signal selection. Fresh insights into the physics of wave processes in diffraction gratings are being implemented into radically new devices operating in gigahertz, terahertz, and optical ranges, into new materials with inclusions ranging in size from micro- to nanometers, and into novel circuits for in-situ man-made and natural material measurements.

However, the potentialities of classical two-dimensional models [1-7] are limited. Both theory and applications invite further investigation of three-dimensional, vector models of periodic structures in increasing frequency. In our opinion these models should be based on time-domain (TD) representations and implemented numerically by the mesh methods [8,9]. It follows from the well-known facts: (i) TD-approaches are free from the idealizations inherent in the frequency domain; (ii) they are universal owing to minimal restrictions imposed on geometrical and material parameters of the objects under study; (iii) they allow explicit computational schemes, which do not require inversion of any operators and call for an adequate run time when implementing on present-day computers; (iv) they result in data easy convertible into a standard set of frequency-domain characteristics. To this must be added that in recent years the local and nonlocal exact absorbing conditions (EAC) have been derived and tested [6,7]. They allow one to replace an open initial boundary value problem occurring in the electrodynamic theory of gratings with a closed problem. In addition, the efficient fast Fourier transform accelerated finite-difference schemes with EAC for characterizing different resonant structures have been constructed and implemented [10].

It is evident that the computational scheme solving a grating problem must be stable and convergent, computational error must be predictable, while the numerical results are bound to be unambiguously treated in physical terms. To comply with these requirements, it is important to carry out theoretical analysis at each stage of the modeling (formulation of boundary value and initial boundary value problems, determination of the correctness classes for them, study of qualitative characteristics of singularities of analytical continuation for solutions of model boundary value problems into a domain of complex-valued frequencies, etc.).

In the present work, we present a series of analytical results providing the necessary theoretical background to the numerical solution of initial boundary value problems as applied to two-dimensionally periodic structures. Section 1 is an Introduction. In Section 2 we give general information required to formulate a model problem in electrodynamic theory of gratings. Sections 3 and 4 are devoted to correct and efficient truncation of the computational space in the problems describing spatial-temporal electromagnetic wave transformation in two-dimensionally periodic structures. Some important characteristics and properties of transient and steady-state fields in regular parts of the rectangular Floquet channel are discussed in Sections 5 and 7. In Section 6, the method of transformation operators (the TD-analog of the generalized scattering matrix method) is described; by applying this method the computational resources can be optimized when calculating a multi-layered periodic structure or a structure on a thick substrate. In Section 8, elements of spectral theory for two-dimensionally periodic gratings are given in view of its importance to physical analysis of resonant scattering of pulsed and monochromatic waves by open periodic resonators.

2. Fundamental Equations, Domain of Analysis, Initial and Boundary Conditions

Space-time and space-frequency transformations of electromagnetic waves in diffraction gratings, waveguide units, open resonators, radiators, etc. are described by the solutions of initial boundary value problems and boundary value problems for Maxwell's equations. In this chapter, we consider the problems of electromagnetic theory of gratings resulting from the following system of Maxwell's equations for waves propagating in stationary, locally inhomogeneous, isotropic, and frequency dispersive media [9,11]:

$$\mathrm{rot}\vec{H}(g,t)=\eta_0^{-1}\frac{\partial\left[\vec{E}(g,t)+\chi_\varepsilon(g,t)*\vec{E}(g,t)\right]}{\partial t}+\chi_\sigma(g,t)*\vec{E}(g,t)+\vec{j}(g,t), \tag{1}$$

$$\mathrm{rot}\vec{E}(g,t)=-\eta_0\frac{\partial\left[\vec{H}(g,t)+\chi_\mu(g,t)*\vec{H}(g,t)\right]}{\partial t}, \tag{2}$$

where

$g=\{x, y, z\}$ is the point in a three-dimensional space R^3;

x, y, and z are the Cartesian coordinates;

$\vec{E}(g, t)=\{E_x, E_y, E_z\}$ and $\vec{H}(g, t)=\{H_x, H_y, H_z\}$ are the electric and magnetic field vectors;

$\eta_0=(\mu_0/\varepsilon_0)^{1/2}$ is the intrinsic impedance of free space;

ε_0 and μ_0 are permittivity and permeability of free space;

$\vec{j}(g, t)$ is the extraneous current density vector;

$\chi_\varepsilon(g, t)$, $\chi_\mu(g, t)$, and $\chi_\sigma(g, t)$ are the electric, magnetic, and specific conductivity susceptibilities; $f_1(t) * f_2(t)=\int f_1(t-\tau) f_2(\tau) d\tau$ stands for the convolution operation.

We use the SI system of units. From here on we shall use the term "time" for the parameter t, which is measured in meters, to mean the product of the natural time and the velocity of light in vacuum.

With no frequency dispersion in the domain $G\subset R^3$, for the points $g\in G$ we have

$\chi_\varepsilon(g, t)=\delta(t)[\varepsilon(g)-1]$, $\chi_\mu(g, t)=\delta(t)[\mu(g)-1]$, $\chi_\sigma(g, t)=\delta(t)\sigma(g)$,

where $\delta(t)$ is the Dirac delta-function; $\varepsilon(g)$, $\mu(g)$, and $\sigma(g)$ are the relative permittivity, relative permeability, and specific conductivity of a locally inhomogeneous medium, respectively. Then equations (1) and (2) take the form:

$$\mathrm{rot}\vec{H}(g, t)=\eta_0^{-1}\varepsilon(g)\frac{\partial\vec{E}(g, t)}{\partial t}+\sigma(g)\vec{E}(g, t)+\vec{j}(g, t), \tag{3}$$

$$\mathrm{rot}\vec{E}(g, t)=-\eta_0\mu(g)\frac{\partial\vec{H}(g, t)}{\partial t}. \tag{4}$$

In vacuum, where $\varepsilon(g)=\mu(g)=1$ and $\sigma(g)=0$, they can be rewritten in the form of the following vector problems [6]:

$$\begin{gathered}\left[\Delta-\mathrm{grad\,div}-\frac{\partial^2}{\partial t^2}\right]\vec{E}(g, t)=\vec{F}_E(g, t), \quad \frac{\partial}{\partial t}\vec{H}(g, t)=-\eta_0^{-1} rot\,\vec{E}(g, t), \\ \vec{F}_E(g, t)=\eta_0\frac{\partial}{\partial t}\vec{j}(g, t)\end{gathered} \tag{5}$$

or

$$\begin{gathered}\left[\Delta-\frac{\partial^2}{\partial t^2}\right]\vec{H}(g, t)=\vec{F}_H(g, t), \quad \eta_0^{-1}\frac{\partial}{\partial t}\vec{E}(g, t)=\mathrm{rot}\vec{H}(g, t)-\vec{j}(g, t), \\ \vec{F}_H(g, t)=-\mathrm{rot}\,\vec{j}(g, t)\ .\end{gathered} \tag{6}$$

By Δ we denote the Laplace operator. As shown in [6], the operator grad div$\vec{E}$ can be omitted in (5) from the following reasons. By denoting the volume density of induced and external electric charge through $\rho_1(g, t)$ and $\rho_2(g, t)$, we can write grad div$\vec{E}=\varepsilon_0^{-1}$grad$(\rho_1+\rho_2)$. In homogeneous medium, where ε and σ are positive and non-negative constants, we have $\rho_1(g, t)=\rho_1(g,0)\exp(-t\sigma/\varepsilon)$, and if $\rho_1(g,0)=0$, then $\rho_1(g, t)=0$ for any$t>0$. The remaining term ε_0^{-1}gradρ_2 can be moved to the right-hand side of (5) as a part of the function defining current sources of the electric field.

To formulate the initial boundary value problem for hyperbolic equations (1)-(6) [12], initial conditions at $t=0$ and boundary conditions on the external and internal boundaries of the domain of analysis Q should be added. In 3-D vector or scalar problems, the domain Q is a part of the R^3-space bounded by the surfaces S that are the boundaries of the domains int$S$, filled with a perfect conductor:$Q=R^3\setminus\overline{\text{int}S}$. In the so-called open problems, the domain of analysis may extend to infinity along one or more spatial coordinates.

The system of boundary conditions for initial boundary value problems is formulated in the following way [11]:

- on the perfectly conducting surface S the tangential component of the electric field vector is zero at all times t

$$E_{tg}(g, t)\big|_{g\in S}=0 \quad \text{for} \quad t\geq 0; \tag{7}$$

the normal component of the magnetic field vector on S is equal to zero $(H_{nr}(g, t)\big|_{g\in S}=0)$, and the function $H_{tg}(g, t)\big|_{g\in S}$ defines the so-called surface currents generated on S by the external electromagnetic field;

- on the surfaces$S^{\varepsilon,\mu,\sigma}$, where material properties of the medium have discontinuities, as well as all over the domain$Q$, the tangential components $E_{tg}(g, t)$ and $H_{tg}(g, t)$ of the electric and magnetic field vectors must be continuous;
- in the vicinity of singular points of the boundaries of$Q$, i.e. the points where the tangents and normals are undetermined, the field energy density must be spatially integrable;
- if the domain Q is unbounded and the field $\{\vec{E}(g, t), \vec{H}(g, t)\}$ is generated by the sources having bounded supports in Q then for any finite time interval $(0,T)$ one can construct a closed virtual boundary $M\subset Q$ sufficiently removed from the sources such that

$$\{\vec{E}(g, t), \vec{H}(g, t)\}\big|_{g\in M, t\in(0,T)}=0. \tag{8}$$

The initial state of the system is determined by the initial conditions at$t=0$. The reference states $\vec{E}(g,0)$ and $\vec{H}(g,0)$ in the system (1), (2) or the system (3), (4) are the same as $\vec{E}(g,0)$ and $[\partial\vec{E}(g, t)/\partial t]\big|_{t=0}$ ($\vec{H}(g,0)$and$[\partial\vec{H}(g, t)/\partial t]\big|_{t=0}$) in the differential forms of the second order (in the terms of t), to which (1), (2) or (3), (4) are transformed if the vector $\vec{H}$ (vector $\vec{E}$) is eliminated (see, for example, system (5), (6)). Thus, (5) should be complemented with the initial conditions

$$\vec{E}(g,0)=\vec{\varphi}(g),\ \frac{\partial}{\partial t}\vec{E}(g,\ t)\Big|_{t=0}=\vec{\psi}(g),\ g\in\bar{Q}. \tag{9}$$

The functions $\vec{\varphi}(g)$, $\vec{\psi}(g)$, and $\vec{F}(g,\ t)$ (called the instantaneous and current source functions) usually have limited support in the closure of the domain Q. It is the practice to divide current sources into hard and soft [9]: soft sources do not have material supports and thus they are not able to scatter electromagnetic waves. Instantaneous sources are obtained from the pulsed wave $\vec{U}^i(g,\ t)$ exciting an electrodynamic structure: $\vec{\varphi}(g)=\vec{U}^i(g,0)$ and $\vec{\psi}(g)=[\partial\vec{U}^i(g,\ t)/\partial t]\big|_{t=0}$. The pulsed signal $\vec{U}^i(g,\ t)$ itself should satisfy the corresponding wave equation and the causality principle. It is also important to demand that the pulsed signal has not yet reached the scattering boundaries by the moment $t=0$.

The latter is obviously impossible if infinite structures (for example, gratings) are illuminated by plane pulsed waves that propagate in the direction other than the normal to certain infinite boundary. Such waves are able to run through a part of the scatterer's surface by any moment of time. As a result a mathematically correct modeling of the process becomes impossible: the input data required for the initial boundary value problem to be set are defined, as a matter of fact, by the solution of this problem.

3. Time Domain: Initial Boundary Value Problems

The vector problem describing the transient states of the field nearby the gratings whose geometry is presented in Figure 1 can be written in the form

$$\begin{cases} \mathrm{rot}\vec{H}(g,t)=\eta_0^{-1}\dfrac{\partial\left[\vec{E}(g,t)+\chi_\varepsilon(g,t)*\vec{E}(g,t)\right]}{\partial t}+\chi_\sigma(g,t)*\vec{E}(g,t)+\vec{j}(g,t), \\ \mathrm{rot}\vec{E}(g,t)=-\eta_0\dfrac{\partial\left[\vec{H}(g,t)+\chi_\mu(g,t)*\vec{H}(g,t)\right]}{\partial t}, \quad g=\{x,y,z\}\in\mathbf{Q}, \quad t>0 \\ \vec{E}(g,0)=\vec{\varphi}_E(g), \quad \vec{H}(g,0)=\vec{\varphi}_H(g), \quad g\in\bar{\mathbf{Q}} \\ E_{tg}(g,t)\big|_{g\in\mathbf{S}}=0, \quad H_{nr}(g,t)\big|_{g\in\mathbf{S}}=0, \quad t\geq 0 \end{cases} \tag{10}$$

Here, $\bar{Q}$ is the closure of Q, $\chi_{\varepsilon,\mu,\sigma}(g,\ t)$ are piecewise continuous functions and the surfaces S are assumed to be sufficiently smooth. From this point on it will be also assumed that the continuity conditions for tangential components of the field vectors are satisfied, if required. The domain of analysis $Q=R^3\setminus\overline{\mathrm{int}S}$ occupies a great deal of the R^3-space. The problem formulated for that domain can be resolved analytically or numerically only in two following cases.

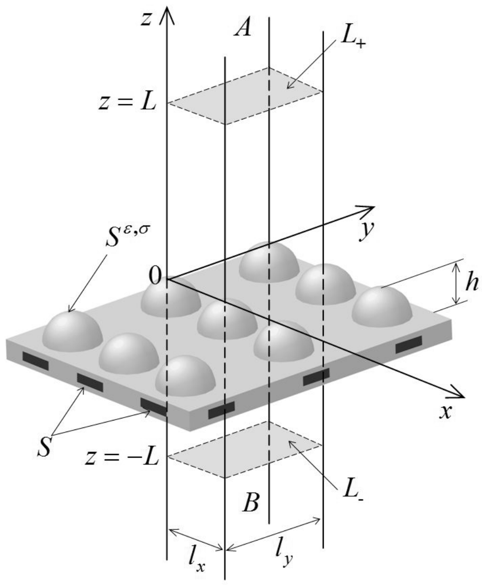

Figure 1. Geometry of a two-dimensionally periodic grating.

- The problem (10) degenerates into a conventional Cauchy problem ($\overline{\mathrm{int}S} = \varnothing$, the medium is homogeneous and nondispersive, while the supports of the functions $\vec{F}(g, t)$, $\vec{\varphi}(g)$, and $\vec{\psi}(g)$ are bounded). With some inessential restrictions for the source functions, the classical and generalized solution of the Cauchy problem does exist; it is unique and is described by the well-known Poisson formula [12].
- The functions $\vec{F}(g, t)$, $\vec{\varphi}(g)$, and $\vec{\psi}(g)$ have the same displacement symmetry as the periodic structure. In this case, the domain of analysis can be reduced to $Q^N = \{g \in Q : 0 < x < l_x; 0 < y < l_y\}$, by adding to problem (10) periodicity conditions [7] on lateral surfaces of the rectangular Floquet channel $R = \{g \in R^3 : 0 < x < l_x; 0 < y < l_y\}$.

The domain of analysis can also be reduced to Q^N in a more general case. The objects of analysis are in this case not quite physical (complex-valued sources and waves). However, by simple mathematical transformations, all the results can be presented in the customary, physically correct form. There are several reasons (to one of them we have referred at the end of Section 3) why the modeling of physically realizable processes in the electromagnetic theory of gratings should start with the initial boundary value problems for the images $f^N(g, t, \Phi_x, \Phi_y)$ of the functions $f(g, t)$ describing the actual sources:

$$
\begin{aligned}
f(g, t) &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \tilde{f}(z, t, \Phi_x, \Phi_y)\exp\left(2\pi i \Phi_x \frac{x}{l_x}\right)\exp\left(2\pi i \Phi_y \frac{y}{l_y}\right) d\Phi_x d\Phi_y \\
&= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f^N(g, t, \Phi_x, \Phi_y) d\Phi_x d\Phi_y
\end{aligned} \tag{11}
$$

From (11) it follows that

$$f^N\left\{\frac{\partial f^N}{\partial x}\right\}(x+l_x,\, y,\, z,\, t,\, \Phi_x,\, \Phi_y) = \mathrm{e}^{2\pi i\Phi_x} f^N\left\{\frac{\partial f^N}{\partial x}\right\}(x,\, y,\, z,\, t,\, \Phi_x,\, \Phi_y),$$

$$f^N\left\{\frac{\partial f^N}{\partial y}\right\}(x,\, y+l_y,\, z,\, t,\, \Phi_x,\, \Phi_y) = \mathrm{e}^{2\pi i\Phi_y} f^N\left\{\frac{\partial f^N}{\partial y}\right\}(x,\, y,\, z,\, t,\, \Phi_x,\, \Phi_y)$$

or, in other symbols,

$$D[f^N](x+l_x,\, y) = \mathrm{e}^{2\pi i\Phi_x} D[f^N](x,\, y), D[f^N](x,\, y+l_y) = \mathrm{e}^{2\pi i\Phi_y} D[f^N](x,\, y).$$

The use of the foregoing conditions truncates the domain of analysis to the domain Q^N, which is a part of the Floquet channel R, and allows us to rewrite problem (10) in the form

$$\vec{E}(g,\, t) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \vec{E}^N(g,\, t,\, \Phi_x,\, \Phi_y)\, d\Phi_x d\Phi_y,\ \vec{H}(g,\, t) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \vec{H}^N(g,\, t,\, \Phi_x,\, \Phi_y)\, d\Phi_x d\Phi_y \tag{12}$$

and

$$\begin{cases} \mathrm{rot}\vec{H}^N(g,t) = \eta_0^{-1}\dfrac{\partial\left[\vec{E}^N(g,t) + \chi_\varepsilon(g,t) * \vec{E}^N(g,t)\right]}{\partial t} + \chi_\sigma(g,t) * \vec{E}^N(g,t) + \vec{j}^N(g,t), \\ \mathrm{rot}\vec{E}^N(g,t) = -\eta_0\dfrac{\partial\left[\vec{H}^N(g,t) + \chi_\mu(g,t) * \vec{H}^N(g,t)\right]}{\partial t}, \quad g \in Q^N, \quad t > 0 \\ \vec{E}^N(g,0) = \vec{\varphi}_E^N(g), \quad \vec{H}^N(g,0) = \vec{\varphi}_H^N(g), \quad g \in \bar{Q}^N \\ D\left[\vec{E}^N\left(\vec{H}^N\right)\right](l_x,y) = \mathrm{e}^{2\pi i\Phi_x} D\left[\vec{E}^N\left(\vec{H}^N\right)\right](0,y), \quad 0 \le y \le l_y \\ D\left[\vec{E}^N\left(\vec{H}^N\right)\right](x,l_y) = \mathrm{e}^{2\pi i\Phi_y} D\left[\vec{E}^N\left(\vec{H}^N\right)\right](x,0), \quad 0 \le x \le l_x \\ E_{tg}^N(g,t)\big|_{g\in \mathbf{S}} = 0, \quad H_{nr}^N(g,t)\big|_{g\in \mathbf{S}} = 0, \quad t \ge 0\,. \end{cases} \tag{13}$$

It is known [6-8] that initial boundary value problems for the above discussed equations can be formulated such that they are uniquely solvable in the Sobolev space $W_2^1(Q^T)$, where $Q^T = Q \times (0,T)$ and $0 \le t \le T$. On this basis we suppose in the subsequent discussion that the problem (13) for all $t \in [0,T]$ has also a generalized solution from the space $W_2^1(Q^{N,T})$ and that the uniqueness theorem is true in this space. Here symbol $\times$ stands for the operation of direct product of two sets, $(0,T)$ and $[0,T]$ are open and closed intervals, $W_m^n(G)$ is the set of all elements $\vec{f}(g)$ from the space $L_m(G)$ whose generalized derivatives up to the order n inclusive also belong to $L_m(G)$. $L_m(G)$ is the space of the functions $\vec{f}(g) = \{f_x,\, f_y,\, f_z\}$ (for $g \in G$) such that the functions $|f_{\dots}(g)|^m$ are integrable on the domain G.

4. Exact Absorbing Conditions for the Rectangular Floquet Channel

In this section, we present analytical results relative to the truncation of the computational space in open 3-D initial boundary value problems of the electromagnetic theory of gratings. In Section 3, by passing on to some special transforms of the functions describing physically realizable sources, the problem for infinite gratings have been reduced to that formulated in the rectangular Floquet channel R or, in other words, in the rectangular waveguide with quasi-periodic boundary conditions. Now we perform further reduction of the domain Q^N to the region $Q_L^N = \{g \in Q^N : |z| < L\}$ (all the sources and inhomogeneities of the Floquet channel R are supposedly located in this domain). For this purpose the exact absorbing conditions [6,7,10,13,14] for the artificial boundaries $L_{\pm}$ $(z = \pm L)$ of the domain Q_L^N will be constructed such that their inclusion into (13) does not change the correctness class of the problem and its solution $\vec{E}^N(g, t), \vec{H}^N(g, t)$.

From here on we omit the superscripts N in (13). By applying the technique similar to that described in [13,14], represent the solution $\vec{E}(g, t)$ of (13) in the closure of the domains $A = \{g \in R : z > L\}$ and $B = \{g \in R : z < -L\}$ in the following form:

$$\vec{E}(g, t) = \sum_{n,m=-\infty}^{\infty} \vec{u}_{nm}^{\pm}(z, t)\mu_{nm}(x, y),\ \{x, y\} \in \bar{R}_z,\ t \geq 0, \tag{14}$$

where the superscript '+ ' corresponds to $z \geq L$ and '− ' to $z \leq -L$ and the following notation is used:

$R_z = (0 < x < l_x) \times (0 < y < l_y)$;

$\{\mu_{nm}(x, y)\}$ $(n, m = 0, \pm 1, \pm 2, ...)$ is the complete in $L_2(R_z)$ orthonormal system of the functions $\mu_{nm}(x, y) = (l_x l_y)^{-1/2} \exp(i\alpha_n x)\exp(i\beta_m y)$;

$\alpha_n = 2\pi(\Phi_x + n)/l_x$, $\beta_m = 2\pi(\Phi_y + m)/l_y$, and $\lambda_{nm}^2 = \alpha_n^2 + \beta_m^2$.

The space-time amplitudes $\vec{u}_{nm}^{\pm}(z, t)$ satisfy the equations

$$\begin{cases} \left[-\dfrac{\partial^2}{\partial t^2} + \dfrac{\partial^2}{\partial z^2} - \lambda_{nm}^2\right]\vec{u}_{nm}^{\pm}(z, t) = 0,\ t > 0 \\ \vec{u}_{nm}^{\pm}(z, 0) = 0, \quad \dfrac{\partial}{\partial t}\vec{u}_{nm}^{\pm}(z, t)\Big|_{t=0} = 0 \end{cases}, \quad \begin{Bmatrix} z \geq L \\ z \leq -L \end{Bmatrix}. \tag{15}$$

Equations (14) and (15) are obtained by separating variables in the homogeneous boundary value problems for the equation $[\Delta - \partial^2/\partial t^2]\vec{E}(g, t) = \vec{0}$ (see formula (5)) and taking into account that in the domains A and B we have grad div $\vec{E}(g, t) = 0$ and $\vec{F}_E(g, t) = 0$. It is also assumed that the field generated by the current and instantaneous sources located in Q_L has not yet reached the boundaries $L_{\pm}$ by the moment of time $t = 0$.

The solutions $\vec{u}^{\pm}_{nm}(z, t)$ of the vector problems (15), as well as in the case of scalar problems [13,14], can be written as

$$\vec{u}^{\pm}_{nm}(\pm L, t) = \mp \int_0^t J_0[\lambda_{nm}(t-\tau)]\vec{u}^{\pm}_{nm}{}'(\pm L, \tau)d\tau, \ t \ge 0 \quad . \tag{16}$$

The above formula represents nonlocal EAC for the space-time amplitudes of the field $\vec{E}(g, t)$ in the cross-sections $z = \pm L$ of the Floquet channel R. The exact nonlocal and local absorbing conditions for the field $\vec{E}(g, t)$ on the artificial boundaries $L_{\pm}$ follow immediately from (16) and (14):

$$\begin{gathered}\vec{E}(x, y, \pm L, t) \\ = \mp \sum_{n,m=-\infty}^{\infty} \left\{ \int_0^t J_0[\lambda_{nm}(t-\tau)] \left[\int_0^{l_x}\int_0^{l_y} \frac{\partial \vec{E}(\tilde{x}, \tilde{y}, z, \tau)}{\partial z}\bigg|_{z=\pm L} \mu^*_{nm}(\tilde{x}, \tilde{y})d\tilde{x}d\tilde{y} \right] d\tau \right\} \mu_{nm}(x, y), \\ \{x, y\} \in \bar{R}_z, \quad t \ge 0 \end{gathered} \tag{17}$$

and

$$\vec{E}(x,y,\pm L,t) = \frac{2}{\pi}\int_0^{\pi/2} \frac{\partial \vec{W}_E(x,y,t,\varphi)}{\partial t} d\varphi, \quad \{x,y\} \in \bar{R}_z, \quad t \ge 0$$

$$\begin{cases} \left[\dfrac{\partial^2}{\partial t^2} - \sin^2\varphi \left(\dfrac{\partial^2}{\partial x^2} + \dfrac{\partial^2}{\partial y^2} \right) \right] \vec{W}_E(x,y,t,\varphi) = \mp \dfrac{\partial \vec{E}(g,t)}{\partial z}\bigg|_{z=\pm L}, \quad \{x,y\} \in R_z, \quad t > 0 \\ \vec{W}_E(x,y,t,\varphi)\big|_{t=0} = \dfrac{\partial \vec{W}_E(x,y,t,\varphi)}{\partial t}\bigg|_{t=0} = 0, \quad \{x,y\} \in \bar{R}_z \\ D\left[\vec{W}_E\right](l_x,y) = e^{2\pi i \Phi_x} D\left[\vec{W}_E\right](0,y), \quad 0 \le y \le l_y \\ D\left[\vec{W}_E\right](x,l_y) = e^{2\pi i \Phi_y} D\left[\vec{W}_E\right](x,0), \quad 0 \le x \le l_x, \quad t \ge 0 \quad . \end{cases} \tag{18}$$

Here, $\vec{u}^{\pm}_{nm}{}'(\pm L, \tau) = \partial \vec{u}^{\pm}_{nm}(z, \tau)/\partial z\,|_{z=\pm L}$, $J_0(t)$ is the zero-order Bessel function, the superscript '$*$' stands for the complex conjugation operation, $\vec{W}_E(x, y, t, \varphi)$ is some auxiliary function, where the numerical parameter φ lies in the range $0 \le \varphi \le \pi/2$.

It is obvious that the magnetic field vector $\vec{H}(g, t)$ of the pulsed waves $\vec{U}(g, t) = \{\vec{E}(g, t), \vec{H}(g, t)\}$ outgoing towards the domains A and B satisfies similar boundary conditions on $L_{\pm}$. The boundary conditions for $\vec{E}(g, t)$ and $\vec{H}(g, t)$ (nonlocal or local) taken together reduce the computational space for the problem (13) to the domain Q_L (a part of the Floquet channel R) that contains all the sources and obstacles.

Now suppose that in addition to the sources $\vec{j}(g, t)$, $\vec{\varphi}_E(g)$, and $\vec{\varphi}_H(g)$, there exist sources $\vec{j}^A(g, t)$, $\vec{\varphi}_E^A(g)$, and $\vec{\varphi}_H^A(g)$ located in A and generating some pulsed wave $\vec{U}^i(g, t)=\{\vec{E}^i(g, t), \vec{H}^i(g, t)\}$ being incident on the boundary L_+ at times $t>0$. The field $\vec{U}^i(g, t)$ is assumed to be nonzero only in the domain A. Since the boundary conditions (17), (18) remain valid for any pulsed wave outgoing through $L_\pm$ towards $z=\pm\infty$ [13,14], then the total field $\{\vec{E}(g, t), \vec{H}(g, t)\}$ is the solution of the initial boundary value problem (13) in the domain Q_L with the boundary conditions (17) or (18) on L_- and the following conditions on the artificial boundary L_+:

$$\begin{gathered}\vec{E}^s(x, y, L, t)\\ =-\sum_{n,m=-\infty}^{\infty}\left\{\int_0^t J_0[\lambda_{nm}(t-\tau)]\left[\int_0^{l_x}\int_0^{l_y}\frac{\partial\vec{E}^s(\tilde{x}, \tilde{y}, z, \tau)}{\partial z}\bigg|_{z=L}\mu_{nm}^*(\tilde{x}, \tilde{y})d\tilde{x}d\tilde{y}\right]d\tau\right\}\mu_{nm}(x, y),\\ \{x, y\}\in\bar{R}_z,\quad t\geq 0\end{gathered}\tag{19}$$

or

$$\begin{gathered}\vec{E}^s(x,y,L,t)=\frac{2}{\pi}\int_0^{\pi/2}\frac{\partial\vec{W}_E(x,y,t,\varphi)}{\partial t}d\varphi,\quad \{x,y\}\in\bar{R}_z,\quad t\geq 0\\ \begin{cases}\left[\dfrac{\partial^2}{\partial t^2}-\sin^2\varphi\left(\dfrac{\partial^2}{\partial x^2}+\dfrac{\partial^2}{\partial y^2}\right)\right]\vec{W}_E(x,y,t,\varphi)=-\dfrac{\partial\vec{E}^s(g,t)}{\partial z}\bigg|_{z=L}, & \{x,y\}\in R_z,\quad t>0\\ \vec{W}_E(x,y,t,\varphi)\big|_{t=0}=\dfrac{\partial\vec{W}_E(x,y,t,\varphi)}{\partial t}\bigg|_{t=0}=0, & \{x,y\}\in\bar{R}_z\\ D\left[\vec{W}_E\right](l_x,y)=e^{2\pi i\Phi_x}D\left[\vec{W}_E\right](0,y), & 0\leq y\leq l_y\\ D\left[\vec{W}_E\right](x,l_y)=e^{2\pi i\Phi_y}D\left[\vec{W}_E\right](x,0), & 0\leq x\leq l_x,\quad t\geq 0\ .\end{cases}\end{gathered}\tag{20}$$

Here $\vec{U}^s(g, t)=\{\vec{E}^s(g, t), \vec{H}^s(g, t)\}=\vec{U}(g, t)-\vec{U}^i(g, t)$ $(g\in A, t>0)$ is the pulsed wave outgoing towards $z=+\infty$. It is generated by the incident wave $\vec{U}^i(g, t)$ ('reflection' from the virtual boundary L_+) and the sources $\vec{j}(g, t)$, $\vec{\varphi}_E(g)$, and $\vec{\varphi}_H(g)$.

5. Some Important Characteristics of Transient Fields in the Rectangular Floquet Channel

For numerical implementation of the computational schemes involving boundary conditions like (19) or (20), the function $\vec{U}^i(g, t)$ for $t\in[0,T]$ and its normal derivative with respect to the boundary L_+ are to be known. To obtain the required data for the wave $\vec{U}^i(g, t)$ generated by a given set of sources $\vec{j}^A(g, t)$, $\vec{\varphi}_E^A(g)$, and $\vec{\varphi}_H^A(g)$, the following initial boundary value problem for a regular hollow Floquet channel R are to be solved:

$$\begin{cases} \left[-\frac{\partial^2}{\partial t^2}+\Delta\right]\begin{Bmatrix}\vec{E}^i\\ \vec{H}^i\end{Bmatrix}=\begin{Bmatrix}\eta_0\partial\vec{j}^{\mathbf{A}}/\partial t+\varepsilon_0^{-1}\operatorname{grad}\rho_2^{\mathbf{A}}\\ -\operatorname{rot}\vec{j}^{\mathbf{A}}\end{Bmatrix}=\begin{Bmatrix}\vec{F}_E^{\mathbf{A}}\\ \vec{F}_H^{\mathbf{A}}\end{Bmatrix}, \quad g=\{x,y,z\}\in R, \quad t>0 \\ \begin{Bmatrix}\vec{E}^i(g,0)\\ \vec{H}^i(g,0)\end{Bmatrix}=\begin{Bmatrix}\vec{\varphi}_E^{\mathbf{A}}\\ \vec{\varphi}_H^{\mathbf{A}}\end{Bmatrix}, \quad \begin{Bmatrix}\partial\vec{E}^i(g,t)/\partial t\big|_{t=0}=\eta_0\operatorname{rot}\vec{H}^i(g,0)\\ \partial\vec{H}^i(g,t)/\partial t\big|_{t=0}=-\eta_0^{-1}\operatorname{rot}\vec{E}^i(g,0)\end{Bmatrix}=\begin{Bmatrix}\vec{\psi}_E^{\mathbf{A}}\\ \vec{\psi}_H^{\mathbf{A}}\end{Bmatrix}, \quad g\in\bar{R} \\ D\left[\vec{E}^i\left(\vec{H}^i\right)\right](l_x,y)=e^{2\pi i\Phi_x}D\left[\vec{E}^i\left(\vec{H}^i\right)\right](0,y), \quad 0\le y\le l_y \\ D\left[\vec{E}^i\left(\vec{H}^i\right)\right](x,l_y)=e^{2\pi i\Phi_y}D\left[\vec{E}^i\left(\vec{H}^i\right)\right](x,0), \quad 0\le x\le l_x, \quad t\ge 0 \ . \end{cases} \tag{21}$$

The function $\rho_2^A(g,\ t)$ here determines the volume density of foreign electric charge.

First we determine the longitudinal components E_z^i and H_z^i of the field $\{\vec{E}^i,\ \vec{H}^i\}$ at all points $g$of the domain R for all times$t>0$. Let us consider the scalar initial boundary value problems following from (21):

$$\begin{cases} \left[-\frac{\partial^2}{\partial t^2}+\Delta\right]\begin{Bmatrix}E_z^i\\ H_z^i\end{Bmatrix}=\begin{Bmatrix}F_{z,E}^{\mathbf{A}}\\ F_{z,H}^{\mathbf{A}}\end{Bmatrix}, \quad g\in R, \quad t>0 \\ \begin{Bmatrix}E_z^i(g,0)\\ H_z^i(g,0)\end{Bmatrix}=\begin{Bmatrix}\varphi_{z,E}^{\mathbf{A}}\\ \varphi_{z,H}^{\mathbf{A}}\end{Bmatrix}, \quad \begin{Bmatrix}\partial E_z^i(g,t)/\partial t\big|_{t=0}\\ \partial H_z^i(g,t)/\partial t\big|_{t=0}\end{Bmatrix}=\begin{Bmatrix}\psi_{z,E}^{\mathbf{A}}\\ \psi_{z,H}^{\mathbf{A}}\end{Bmatrix}, \quad g\in\bar{R} \\ D\left[E_z^i\left(H_z^i\right)\right](l_x,y)=e^{2\pi i\Phi_x}D\left[E_z^i\left(H_z^i\right)\right](0,y), \quad 0\le y\le l_y \\ D\left[E_z^i\left(H_z^i\right)\right](x,l_y)=e^{2\pi i\Phi_y}D\left[E_z^i\left(H_z^i\right)\right](x,0), \quad 0\le x\le l_x, \quad t\ge 0 \ . \end{cases} \tag{22}$$

By separating of the transverse variables x and y in (22) represent the solution of the problem as

$$\begin{Bmatrix}E_z^i(g,\ t)\\ H_z^i(g,\ t)\end{Bmatrix}=\sum_{n,m=-\infty}^{\infty}\begin{Bmatrix}v_{nm(z,E)}(z,\ t)\\ v_{nm(z,H)}(z,\ t)\end{Bmatrix}\mu_{nm}(x,\ y) \tag{23}$$

To determine the scalar functions $v_{nm(z,E)}(z,\ t)$ and$v_{nm(z,H)}(z,\ t)$, we have to invert the following Cauchy problems for the one-dimensional Klein-Gordon equations:

$$\begin{cases} \left[-\frac{\partial^2}{\partial t^2}+\frac{\partial^2}{\partial z^2}-\lambda_{nm}\right]\begin{Bmatrix}v_{nm(z,E)}(z,t)\\ v_{nm(z,H)}(z,t)\end{Bmatrix}=\begin{Bmatrix}F_{nm(z,E)}^A\\ F_{nm(z,H)}^A\end{Bmatrix}, \quad t>0, \quad -\infty<z<\infty \\ \begin{Bmatrix}v_{nm(z,E)}(z,0)\\ v_{nm(z,H)}(z,0)\end{Bmatrix}=\begin{Bmatrix}\varphi_{nm(z,E)}^A\\ \varphi_{nm(z,H)}^A\end{Bmatrix}, \quad \frac{\partial}{\partial t}\begin{Bmatrix}v_{nm(z,E)}(z,t)\\ v_{nm(z,H)}(z,t)\end{Bmatrix}\Bigg|_{t=0}=\begin{Bmatrix}\psi_{nm(z,E)}^A\\ \psi_{nm(z,E)}^A\end{Bmatrix}, \\ \qquad -\infty<z<\infty, \qquad n,m=0,\pm1,\pm2,\ldots \ . \end{cases} \tag{24}$$

Here $F^{A}_{nm(z,E)}$, $\varphi^{A}_{nm(z,E)}$, $\psi^{A}_{nm(z,E)}$ and $F^{A}_{nm(z,H)}$, $\varphi^{A}_{nm(z,H)}$, $\psi^{A}_{nm(z,H)}$ are the amplitudes of the Fourier transforms of the functions $F^{A}_{z,E}$, $\varphi^{A}_{z,E}$, $\psi^{A}_{z,E}$ and $F^{A}_{z,H}$, $\varphi^{A}_{z,H}$, $\psi^{A}_{z,H}$ in the basic set $\{\mu_{nm}(x, y)\}$.

Let us continue analytically the functions $v_{nm(z,E)}(z, t)$, $v_{nm(z,H)}(z, t)$ and $F^{A}_{nm(z,E)}$, $F^{A}_{nm(z,H)}$ by zero on the semi-axis $t0$ and pass on to the generalized formulation of the Cauchy problem (24) [12]:

$$\begin{aligned}
&B(\lambda_{nm})\begin{bmatrix} v_{nm(z,E)}(z, t) \\ v_{nm(z,H)}(z, t)\end{bmatrix} \equiv \left[-\frac{\partial^2}{\partial t^2}+\frac{\partial^2}{\partial z^2}-\lambda^2_{nm}\right]\begin{Bmatrix} v_{nm(z,E)}(z, t) \\ v_{nm(z,H)}(z, t)\end{Bmatrix} \\
&= \begin{Bmatrix} F^{A}_{nm(z,E)} \\ F^{A}_{nm(z,H)}\end{Bmatrix} - \delta^{(1)}(t)\begin{Bmatrix} \varphi^{A}_{nm(z,E)} \\ \varphi^{A}_{nm(z,H)}\end{Bmatrix} - \delta(t)\begin{Bmatrix} \psi^{A}_{nm(z,E)} \\ \psi^{A}_{nm(z,H)}\end{Bmatrix} = \begin{Bmatrix} f_{nm(z,E)} \\ f_{nm(z,H)}\end{Bmatrix}, \\
&-\infty<z<\infty, \quad -\infty<t<\infty, \quad n, m=1, \pm 2, \pm 3, \ldots ,
\end{aligned} \tag{25}$$

where $\delta(t)$ and $\delta^{(m)}(t)$ are the Dirac delta-function and its derivative of the order m. Taking into account the properties of the fundamental solution $G(z, t, \lambda)=-(1/2)\chi(t-|z|)J_0\left(\lambda\sqrt{t^2-z^2}\right)$ of the operator $B(\lambda)$ [6,13,14] ($\chi(t)$ is the Heaviside step function), the solutions $v_{nm(z,E)}(z, t)$ and $v_{nm(z,H)}(z, t)$ of equations (25) can be written as

$$\begin{aligned}
&\begin{Bmatrix} v_{nm(z,E)}(z, t) \\ v_{nm(z,H)}(z, t)\end{Bmatrix} = G(z, t, \lambda_{nm}) * \begin{Bmatrix} f_{nm(z,E)} \\ f_{nm(z,H)}\end{Bmatrix} = \\
&-\frac{1}{2}\int_{-\infty}^{t-|z-\omega|}\int_{-\infty}^{\infty} J_0\left(\lambda_{nm}\sqrt{(t-\tau)^2-(z-\omega)^2}\right)\left(\begin{Bmatrix} F^{A}_{nm(z,E)} \\ F^{A}_{nm(z,H)}\end{Bmatrix} - \delta^{(1)}(t)\begin{Bmatrix} \varphi^{A}_{nm(z,E)} \\ \varphi^{A}_{nm(z,H)}\end{Bmatrix} - \delta(t)\begin{Bmatrix} \psi^{A}_{nm(z,E)} \\ \psi^{A}_{nm(z,H)}\end{Bmatrix}\right) d\omega d\tau, \\
&\qquad -\infty<z<\infty, \quad t\geq 0, \quad n, m=1, \pm 2, \pm 3, \ldots .
\end{aligned} \tag{26}$$

Relations (23) and (26) completely determine the longitudinal components of the field $\{\vec{E}^i, \vec{H}^i\}$.

Outside the bounded domain enclosing all the sources, in the domain $G\subset R$, where the waves generated by these sources propagate freely, the following relations [6,14] are valid:

$$\begin{cases}
\vec{E}^i = \left(\dfrac{\partial^2 U^E}{\partial x\partial z} - \dfrac{\partial^2 U^H}{\partial y\partial t}\right)\vec{x} + \left(\dfrac{\partial^2 U^E}{\partial y\partial z} + \dfrac{\partial^2 U^H}{\partial x\partial t}\right)\vec{y} + \left(\dfrac{\partial^2 U^E}{\partial z^2} - \dfrac{\partial^2 U^E}{\partial t^2}\right)\vec{z} \\
\eta_0\vec{H}^i = \left(\dfrac{\partial^2 U^E}{\partial y\partial t} + \dfrac{\partial^2 U^H}{\partial x\partial z}\right)\vec{x} + \left(-\dfrac{\partial^2 U^E}{\partial x\partial t} + \dfrac{\partial^2 U^H}{\partial y\partial z}\right)\vec{y} + \left(\dfrac{\partial^2 U^H}{\partial z^2} - \dfrac{\partial^2 U^H}{\partial t^2}\right)\vec{z}
\end{cases} \tag{27}$$

in which

$$U^{E,H}(g,\ t) = \sum_{n,m=-\infty}^{\infty} u_{nm}^{E,H}(z,\ t)\mu_{nm}(x,\ y) \tag{28}$$

are the scalar Borgnis functions such that $[\Delta - \partial^2/\partial t^2][\partial U^{E,H}(g,\ t)/\partial t] = 0$. Equations (23), (26)-(28) determine the field $\{\vec{E}^i,\ \vec{H}^i\}$ at all points g of the domain G for all times $t > 0$. Really, since at the time point $t = 0$ the domain G is undisturbed, then we have $[\Delta - \partial^2/\partial t^2]U^{E,H} = 0$ $(g \in G, t > 0)$. Hence, in view of (27), (28), it follows:

$$E_z = \frac{\partial^2 U^E}{\partial z^2} - \frac{\partial^2 U^E}{\partial t^2} = -\left(\frac{\partial^2 U^E}{\partial x^2} + \frac{\partial^2 U^E}{\partial y^2}\right) = \sum_{n,m=-\infty}^{\infty} \lambda_{nm}^2 u_{nm}^E \mu_{nm},$$

$$\eta_0 H_z = \frac{\partial^2 U^H}{\partial z^2} - \frac{\partial^2 U^H}{\partial t^2} = -\left(\frac{\partial^2 U^H}{\partial x^2} + \frac{\partial^2 U^H}{\partial y^2}\right) = \sum_{n,m=-\infty}^{\infty} \lambda_{nm}^2 u_{nm}^H \mu_{nm}$$

and (see representation (23))

$$u_{nm}^E(z,\ t) = (\lambda_{nm})^{-2} v_{nm(z,E)}(z,\ t),\ u_n^H(z,\ t) = \eta_0(\lambda_{nm})^{-2} v_{nm(z,H)}(z,\ t). \tag{29}$$

Hence the functions $U^{E,H}(g,\ t)$ as well as the transverse components of the field $\{\vec{E}^i,\ \vec{H}^i\}$ are determined.

The foregoing suggests the following important conclusion: the fields generated in the reflection zone (the domain A) and transmission zone (the domain B) of a periodic structure are uniquely determined by their longitudinal (directed along z-axis) components and can be represented in the following form (see also formulas (14) and (23)). For the incident wave we have

$$\left\{\begin{matrix} E_z^i(g,\ t) \\ H_z^i(g,\ t) \end{matrix}\right\} = \sum_{n,m=-\infty}^{\infty} \left\{\begin{matrix} v_{nm(z,E)}(z,\ t) \\ v_{nm(z,H)}(z,\ t) \end{matrix}\right\} \mu_{nm}(x,\ y),\ g \in \bar{A},\ t \geq 0, \tag{30}$$

for the reflected wave $\vec{U}^s(g,\ t)$(which coincides with the total field $\vec{U}(g,\ t)$ if $\vec{U}^i(g,\ t) \equiv 0$) we have

$$\left\{\begin{matrix} E_z^s(g,\ t)\text{or}E_z(g,\ t) \\ H_z^s(g,\ t)\text{or}H_z(g,\ t) \end{matrix}\right\} = \sum_{n,m=-\infty}^{\infty} \left\{\begin{matrix} \overset{+}{u}_{nm(z,E)}(z,\ t) \\ \overset{+}{u}_{nm(z,H)}(z,\ t) \end{matrix}\right\} \mu_{nm}(x,\ y),\ g \in \bar{A},\ t \geq 0 \tag{31}$$

and for the transmitted wave (coinciding in the domain B with the total field $\vec{U}(g,\ t)$) we can write

$$\begin{Bmatrix} E_z(g,t) \\ H_z(g,t) \end{Bmatrix} = \sum_{n,m=-\infty}^{\infty} \begin{Bmatrix} u^-_{nm(z,E)}(z,t) \\ u^-_{nm(z,H)}(z,t) \end{Bmatrix} \mu_{nm}(x,y),\ g\in\bar{B},\ t\geq 0. \tag{32}$$

In applied problems, the most widespread are situations where a periodic structure is excited by one of the partial components of TE-wave (with $E_z^i(g,t)=0$) or TM-wave (with $H_z^i(g,t)=0$) [7]. Consider, for example, a partial wave of order pq. Then we have

$$\vec{U}^i(g,t)=\vec{U}^i_{pq(H)}(g,t): H_z^i(g,t)=v_{pq(z,H)}(z,t)\mu_{pq}(x,y)$$

or

$$\vec{U}^i(g,t)=\vec{U}^i_{pq(E)}(g,t): E_z^i(g,t)=v_{pq(z,E)}(z,t)\mu_{pq}(x,y).$$

The excitation of this kind is implemented in our models in the following way. The time function $v_{pq(z,H)}(L,t)$ or $v_{pq(z,E)}(L,t)$ is defined on the boundary L_+. This function determines the width of the pulse $\vec{U}^i(g,t)$, namely, the frequency range $[K_1, K_2]$ such that for all frequencies k from this range ($k=2\pi/\lambda$, λ is the wavelength in free space) the value

$$\gamma=\frac{|\tilde{v}_{pq(z,H\,\mathrm{or}\,E)}(L,k)|}{\max\limits_{k\in[K_1;K_2]}|\tilde{v}_{pq(z,H\,\mathrm{or}\,E)}(L,k)|}$$

where $\tilde{v}_{pq(z,H\,\mathrm{or}\,E)}(L,k)$ is the spectral amplitude of the pulse $v_{pq(z,H\,\mathrm{or}\,E)}(L,t)$, exceeds some given value $\gamma=\gamma_0$. All spectral characteristics $\tilde{f}(k)$ are obtainable from the temporal characteristics $f(t)$ by applying the Laplace transform

$$\tilde{f}(k)=\int_0^{\infty} f(t)e^{ikt}dt \leftrightarrow f(t)=\frac{1}{2\pi}\int_{i\alpha-\infty}^{i\alpha+\infty}\tilde{f}(k)e^{-ikt}dk,\ 0\leq\alpha\leq\mathrm{Im}k. \tag{33}$$

For numerical implementation of the boundary conditions (19) and (20) and for calculating space-time amplitudes of the transverse components of the wave $\vec{U}^i(g,t)$ in the cross-section $z=L$ of the Floquet channel (formulas (27) and (29)), the function $(v_{pq(z,H\,\mathrm{or}\,E)})'(L,t)$ are to be determined. To do this, we apply the following relation [7,14]:

$$\vec{v}_{pq(H\,\mathrm{or}\,E)}(L,t)=\int_0^t J_0[\lambda_{pq}(t-\tau)](\vec{v}_{pq(H\,\mathrm{or}\,E)})'(L,t)d\tau,\ t\geq 0. \tag{34}$$

which is valid for all the amplitudes of the pulsed wave $\vec{U}^i(g,t)$ outgoing towards $z=-\infty$ and does not violate the causality principle.

6. Transformation Operator Method

6.1. Evolutionary basis of a signal and transformation operators

Let us place an arbitrary periodic structure of finite thickness between two homogeneous dielectric half-spaces $z_1 = z - L > 0$ (with$\varepsilon = \varepsilon_1$) and $z_2 = -z - L > 0$ (with$\varepsilon = \varepsilon_2$). Let also a local coordinate system $g_j = \{x_j, y_j, z_j\}$ be associated with each of these half-spaces (Figure 2). Assume that the distant sources located in the domain A of the upper half-space generate a primary wave $\vec{U}_1^i(g, t) = \{\vec{E}_1^i(g, t), \vec{H}_1^i(g, t)\}$ being incident on the artificial boundary L_+ (on the plane$z_1 = 0$) as viewed from$z_1 = \infty$.

Denote by $\vec{U}_j^s(g, t) = \{\vec{E}_j^s(g, t), \vec{H}_j^s(g, t)\}$ the fields resulting from scattering of the primary wave $\vec{U}_1^i(g, t)$ in the domains A (where the total field is $\vec{U}(g, t) = \{\vec{E}(g, t), \vec{H}(g, t)\} = \vec{U}_1^s(g, t) + \vec{U}_1^i(g, t)$) and B (where$\vec{U}(g, t) = \vec{U}_2^s(g, t)$). In Section 5, we have shown that the fields under consideration are uniquely determined by their longitudinal components, which can be given, for example, as:

$$\begin{Bmatrix} E_z^i(g, t) \\ H_z^i(g, t) \end{Bmatrix} = \sum_{n,m=-\infty}^{\infty} \begin{Bmatrix} v_{nm(1,E)}(z_1, t) \\ v_{nm(1,H)}(z_1, t) \end{Bmatrix} \mu_{nm}(x, y),\ z_1 \geq 0,\ t \geq 0 \tag{35}$$

$$\begin{Bmatrix} E_z^s(g, t) \\ H_z^s(g, t) \end{Bmatrix} = \sum_{n,m=-\infty}^{\infty} \begin{Bmatrix} u_{nm(j,E)}(z_j, t) \\ u_{nm(j,H)}(z_j, t) \end{Bmatrix} \mu_{nm}(x, y),\ z_j \geq 0,\ t \geq 0,\ j = 1,2 \tag{36}$$

(see also formulas (30)-(32)). Here, as before, $\{\mu_{nm}(x, y)\}_{n,m=-\infty}^{\infty}$is the complete (in$L_2(R_z)$) orthonormal system of transverse eigenfunctions of the Floquet channel R (see Section 4), while the space-time amplitudes $u_{nm(j,E)}(z_j, t)$ and $u_{nm(j,H)}(z_j, t)$ are determined by the solutions of the following problems (see also problem (15)) for the one-dimensional Klein-Gordon equations:

$$\begin{cases} \left[-\varepsilon_j \dfrac{\partial^2}{\partial t^2} + \dfrac{\partial^2}{\partial z_j^2} - \lambda_{nm}^2 \right] u_{nm(j,E\text{ or }H)}(z_j, t) = 0, \quad t > 0 \\ u_{nm(j,E\text{ or }H)}(z_j, 0) = 0, \quad \dfrac{\partial}{\partial t} u_{nm(j,E\text{ or }H)}(z_j, t)\Big|_{t=0} = 0 \end{cases}, \qquad j = 1,2, \qquad n, m = 0, \pm 1, \pm 2, \ldots\ . \tag{37}$$

Compose from the functions$v_{nm(1,E)}(z_1, t)$, $v_{nm(1,H)}(z_1, t)$, $u_{nm(j,E)}(z_j, t)$, $u_{nm(j,H)}(z_j, t)$and the eigenvalues λ_{nm} $(n, m = 0, \pm 1, \pm 2, \ldots)$ the sets$v_{(1)}(z_1, t) = \{v_{p(1)}(z_1, t)\}_{p=-\infty}^{\infty}$, $u_{(j)}(z_j, t) = \{u_{p(j)}(z_j, t)\}_{p=-\infty}^{\infty}$, and $\{\lambda_p\}_{p=-\infty}^{\infty}$ such that their members are defined according to the rules depicted in Figure 3. The sets $v_{(1)}(z_1, t)$ and $u_{(j)}(z_j, t)$ are said to be evolutionary bases of signals $\vec{U}_1^i(g, t)$ and$\vec{U}_j^s(g, t)$. They describe completely and unambiguously transformation of the corresponding nonsine waves in the regular Floquet channels A and Bfilled with dielectric.

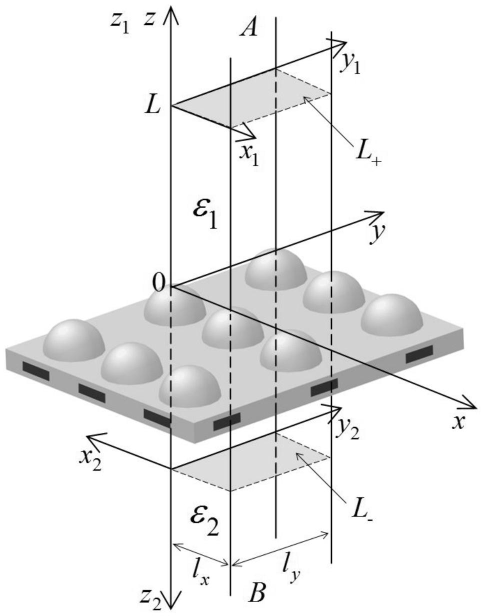

Figure 2. A two-dimensionally periodic grating between two dielectric half-spaces as element of a multi-layered structure.

Let us introduce by the relations

$$u_{p(j)}{}'(0,t) \equiv \frac{\partial}{\partial z_j} u_{p(j)}(z_j,\, t)\Big|_{z_j=0} = \int_0^t \sum_{q=-\infty}^{\infty} \left[S_{pq}^{AA}(t-\tau)\delta_j^1 + S_{pq}^{BA}(t-\tau)\delta_j^2 \right] v_{q(1)}(0,\tau)d\tau, \tag{38}$$

$t \geq 0,\ p = 0, \pm 1, \pm 2, \ldots,\ j = 1,2$

$$u_{(j)}{}'(0,t) = \left\{ u_{p(j)}{}'(0,t) \right\}_p = \left[S^{AA}\delta_j^1 + S^{BA}\delta_j^2 \right] \left[v_{(1)}(0,\tau) \right],\ t \geq 0, j = 1,2 \tag{39}$$

the boundary (on the boundaries $z_j = 0$) transformation operators S^{AA} and S^{BA} of the evolutionary basis $v_{(1)}(z_1,\, t)$ of the wave $\vec{U}_1^i(g,\, t)$ incoming from the domain A. Here δ_m^n stands for the Kronecker delta, the operators' elements S_{nm}^{XY} specify the space-time energy transformation from the domain Y into the domain X and from the mode of order m into the mode of order n.

It is evident that the operators S^{AA} and S^{BA} working in the space of evolutionary bases are intrinsic characteristics of the periodic structure placed between two dielectric half-spaces. They totalize an impact of the structure on elementary excitations composing any incident signal $\vec{U}_1^i(g,\, t)$. Thus for $v_{q(1)}(0,t) = \delta_q^r \delta(t-\eta)$, where r is an integer and $\eta > 0$, we have $u_{p(1)}{}'(0,t) = S_{pr}^{AA}(t-\eta)$ and $u_{p(2)}{}'(0,t) = S_{pr}^{BA}(t-\eta)$. We use this example with an abstract non-physical signal by methodological reasons in order to associate the transformation operators' components $S_{pr}^{AA}(t-\tau)$ and $S_{pr}^{BA}(t-\tau)$ with an 'elementary excitation'.

http://dx.doi.org/10.5772/51007

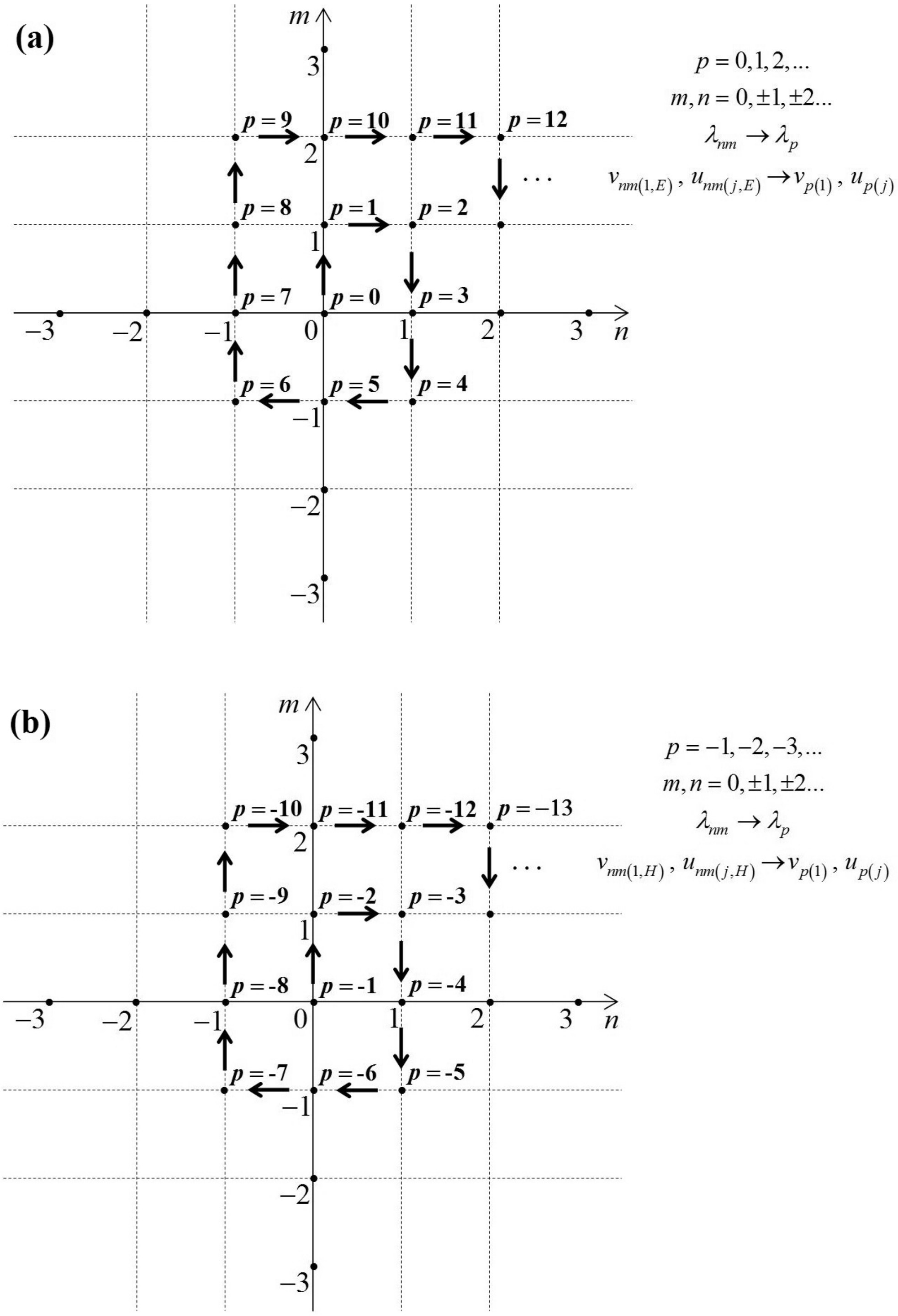

Figure 3. Construction of sets of the values $v_{p(1)}$, $u_{p(j)}$, and λ_p ($p=0,\pm 1,\pm 2,\ldots$) from sets of the values $v_{nm(1,E)}$, $u_{nm(j,E)}$, $v_{nm(1,H)}$, $u_{nm(j,H)}$, and λ_{nm} (m, $n=0,\pm 1,\pm 2,\ldots$): (a) $p=0,1,2,\ldots$; (b) $p=-1,-2,-3,\ldots$.

The operators S^{AA} and S^{BA} determine all the features of transient states on the upper and bottom boundaries of the layer enclosing the periodic structure. Secondary waves outgoing from these boundaries propagate freely in the regular Floquet channels A and B therewith undergoing deformations (see, for example, [6]). The space-time amplitudes $u_{p(j)}(z_j, t)$ of the partial components of these waves (the elements of the evolutionary bases of the signals $\vec{U}_j^s(g, t)$) vary differently for different values of p and j. These variations on any finite sections of the Floquet channels A и B are described by the diagonal transporting operators $Z_{0\to z_1}^A$ and $Z_{0\to z_2}^B$ acting according the rule:

$$u_{(j)}(z_j, t)=\{u_{p(j)}(z_j, t)\}=\left[Z_{0\to z_1}^A\delta_j^1+Z_{0\to z_2}^B\delta_j^2\right][u_{(j)}{}'(0,\tau)],\ j=1,2. \tag{40}$$

The structure of the operators given by (40) can be detailed by the formula

$$\begin{gathered}u_{p(j)}(z_j, t)=-\frac{1}{\varepsilon_j}\int_0 J_0\left[\lambda_p\sqrt{\frac{(t-\tau)^2}{\varepsilon_j}-z_j^2}\right]\chi\left(\frac{t-\tau}{\sqrt{\varepsilon_j}}-z_j\right)u_{p(j)}{}'(0,\tau)d\tau,\\ t\geq 0,\ z_j\geq 0,\ p=0,\pm 1,\pm 2,...,\ j=1,2,\end{gathered} \tag{41}$$

which reflects general properties of solutions of homogeneous problems (37), i.e. the solutions that satisfy zero initial conditions and are free from the components propagating in the direction of decreasing z_j. The derivation technique for (41) is discussed at length in [6,13,14].

6.2. Equations of the operator method in the problems for multilayer periodic structures

The operators S^{AA} and S^{BA} completely define properties of the periodic structure excited from the channel A. By analogy with (38) we can determine transformation operators S^{BB} and S^{AB} for evolutionary basis $v_{(2)}(z_2, t)=\{v_{p(2)}(z_2, t)\}_{p=-\infty}^{\infty}$ of the wave $\vec{U}_2^i(g, t)=\left\{\vec{E}_2^i(g, t), \vec{H}_2^i(g, t)\right\}$ incident onto the boundary $z_2=0$ from the channel B:

$$\begin{gathered}u_{p(j)}{}'(0,t)=\int_0^t\sum_{m=-\infty}^{\infty}[S_{pq}^{AB}(t-\tau)\delta_j^1+S_{pq}^{BB}(t-\tau)\delta_j^2]v_{q(2)}(0,\tau)d\tau,\\ t\geq 0,\ p=0,\pm 1,\pm 2,...,\ j=1,2.\end{gathered} \tag{42}$$

Let us construct the algorithm for calculating scattering characteristics of a multilayer structure consisting of two-dimensionally periodic gratings, for which the operators S^{AA}, S^{BA}, S_{pq}^{AB}, and S_{pq}^{BB} are known. Consider a double-layer structure, whose geometry is given in Figure 4. Two semi-transparent periodic gratings I and II are separated by a dielectric layer of finite thickness M (here $\varepsilon=\varepsilon_2(\mathrm{I})=\varepsilon_1(\mathrm{II})$) and placed between the upper and the bottom dielectric half-spaces with the permittivity $\varepsilon_1(\mathrm{I})$ and $\varepsilon_2(\mathrm{II})$, respectively. Let also a pulsed wave like (35) be incident onto the boundary $z_1(\mathrm{I})=0$ from the Floquet channel A.

Retaining previously accepted notation (the evident changes are conditioned by the presence of two different gratings I and II), represent the solution of the corresponding initial boundary value problem in the regular domains A, B, and C in a symbolic form

$$U(A)=\sum_{p=-\infty}^{\infty}\left[v_{p(1)}(z_1(\mathrm{I}),\ t)+u_{p(1)}(z_1(\mathrm{I}),\ t)\right]\mu_p(x,\ y),$$

$$U(B)=\sum_{p=-\infty}^{\infty}\left[u_{p(2)}(z_2(\mathrm{I}),\ t)+u_{p(1)}(z_1(\mathrm{II}),\ t)\right]\mu_p(x,\ y),$$

$$U(C)=\sum_{p=-\infty}^{\infty}u_{p(2)}(z_2(\mathrm{II}),\ t)\mu_p(x,\ y).$$

The first terms in the square brackets correspond to the waves propagating towards the domain C, while the second ones correspond to the waves propagating towards the domain A (Figure 4). The set $\{\mu_p(x,\ y)\}_{p=-\infty}^{\infty}$ is formed from the functions $\mu_{nm}(x,\ y)$, $(n,\ m=0,\pm 1,\pm 2,...)$, while the set $\{\lambda_p\}_{p=-\infty}^{\infty}$ is composed from the values λ_{nm}, $(n,\ m=0,\pm 1,\pm 2,...)$ (Figure 3).

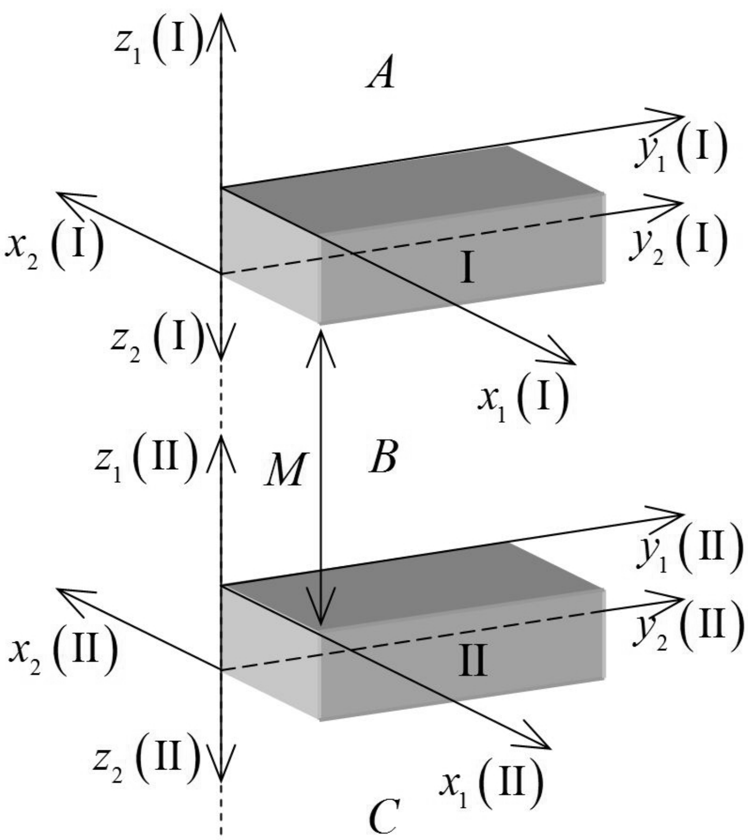

Figure 4. Schematic drawing of a double-layered structure.

By denoting

$$u_{(j)}'(\mathrm{I}) \equiv \frac{\partial}{\partial z_j(\mathrm{I})} u_{(j)}(z_j(\mathrm{I}),\, t)\Big|_{z_j(\mathrm{I})=0}, \qquad u_{(j)}(\mathrm{I}) = \{u_{p(j)}(z_j(\mathrm{I}),\, t)\}\big|_{z_j(\mathrm{I})=0},$$

according to formulas (38)-(42), we construct the following system of operator equations:

$$\begin{cases} u_{(1)}'(\mathrm{I}) = S^{AA}(\mathrm{I})\left[v_{(1)}(\mathrm{I})\right] + S^{AB}(\mathrm{I})Z^{B}_{z_1(\mathrm{II})=0\to M}\left[u_{(1)}'(\mathrm{II})\right] \\ u_{(2)}'(\mathrm{I}) = S^{BA}(\mathrm{I})\left[v_{(1)}(\mathrm{I})\right] + S^{BB}(\mathrm{I})Z^{B}_{z_1(\mathrm{II})=0\to M}\left[u_{(1)}'(\mathrm{II})\right] \\ u_{(1)}'(\mathrm{II}) = S^{BB}(\mathrm{II})Z^{B}_{z_2(\mathrm{I})=0\to M}\left[u_{(2)}'(\mathrm{I})\right] \\ u_{(2)}'(\mathrm{II}) = S^{CB}(\mathrm{II})Z^{B}_{z_2(\mathrm{I})=0\to M}\left[u_{(2)}'(\mathrm{I})\right] \;. \end{cases} \tag{43}$$

Equations (43) clearly represent step-by-step response of the complex structure on the excitation by the signal $\vec{U}_1^{i}(g,\, t)$ with the evolutionary basis $v_{(1)}(z_1(\mathrm{I}),\, t) = \{v_{p(1)}(z_1(\mathrm{I}),\, t)\}_{p=-\infty}^{\infty}$ (or simply$v_{(1)}(\mathrm{I})$). Thus, for example, the first equation can be interpreted as follows. A signal $u_{(1)}(\mathrm{I})$ (the secondary field in$A$) is a sum of two signals, where the first signal is a result of the reflection of the incident signal $v_{(1)}(\mathrm{I})$ by the gratingI, while another one is determined by the signal $u_{(1)}(\mathrm{II})$being deformed during propagation in the channel $B$and interaction with the gratingI.

By method of elimination the system (43) is reduced to the operator equation of the second kind

$$u_{(2)}'(\mathrm{I}) = S^{BA}(\mathrm{I})[v_{(1)}(\mathrm{I})] + S^{BB}(\mathrm{I})Z^{B}_{z_1(\mathrm{II})=0\to M}\, S^{BB}(\mathrm{II})Z^{B}_{z_2(\mathrm{I})=0\to M}[u_{(2)}'(\mathrm{I})] \tag{44}$$

and some formulas for calculating the electromagnetic field components in all regions of the two-layered structure. The observation time t for the unknown function $u_{(2)}'(\mathrm{I})$ from the left-hand side of equation (44) strictly greater of any moment of time τ for the function $u_{(2)}'(\mathrm{I})$ in the right-hand side of the equation (owing to finiteness of wave velocity). Therefore equation (44) can be inverted explicitly in the framework of standard algorithm of step-by-step progression through time layers. Upon realization of this scheme and calculation of the boundary operators by (38), (42), the two-layered structure can be used as 'elementary' unit of more complex structures.

Turning back to (38)-(42), we see that the operators entering these equations act differently that their analogues in the frequency domain, where the boundary operators relate a pair 'field $\rightarrow$ field'. Reasoning from the structure of the transport operators $Z^{A}_{0\to z_1}$ and $Z^{B}_{0\to z_2}$ (formulas (40) and (41)), we relate a pair 'field $\rightarrow$ directional derivative with respect to the propagation direction' to increase numerical efficiency of the corresponding computational algorithms.

7. Some Important Properties of Steady-State Fields in the Rectangular Floquet Channel

7.1. Excitation by a TM-wave

Let a grating (Figure 1) be excited form the domain A by a pulsed TM-wave $\vec{U}^i(g, t)=\vec{U}^i_{pq(E)}(g, t): E_z^i(g, t)=v_{pq(z,E)}(z, t)\mu_{pq}(x, y)$ and the region Q_L is free from the sources $\vec{j}(g, t)$, $\vec{\varphi}_E(g)$, and $\vec{\varphi}_H(g)$. The field generated in the domains A and B is determined completely by their longitudinal components. They can be represented in the form of (31), (32). Define steady-state fields $\{\vec{\tilde{E}}(g, k), \vec{\tilde{H}}(g, k)\}$ (see formula (33) with $\mathrm{Im}k=0$) corresponding to the pulsed fields $\{\vec{E}^i, \vec{H}^i\}$, $\{\vec{E}^s, \vec{H}^s\}$ in A and the pulsed field $\{\vec{E}, \vec{H}\}$ in B, by their z-components:

$$\begin{Bmatrix}\tilde{E}_z^i(g, k)\\ \tilde{H}_z^i(g, k)\end{Bmatrix}=\begin{Bmatrix}\tilde{v}_{pq(z,E)}(k)\\ 0\end{Bmatrix}e^{-i\Gamma_{pq}(z-L)}\mu_{pq}(x, y),\ g\in\bar{A} \tag{45}$$

$$\begin{Bmatrix}\tilde{E}_z^s(g, k)\\ \tilde{H}_z^s(g, k)\end{Bmatrix}=\sum_{n,m=-\infty}^{\infty}\begin{Bmatrix}\tilde{u}^+_{nm(z,E)}(k)\\ \tilde{u}^+_{nm(z,H)}(k)\end{Bmatrix}e^{i\Gamma_{nm}(z-L)}\mu_{nm}(x, y),\ g\in\bar{A} \tag{46}$$

$$\begin{Bmatrix}\tilde{E}_z(g, k)\\ \tilde{H}_z(g, k)\end{Bmatrix}=\sum_{n,m=-\infty}^{\infty}\begin{Bmatrix}\tilde{u}^-_{nm(z,E)}(k)\\ \tilde{u}^-_{nm(z,H)}(k)\end{Bmatrix}e^{-i\Gamma_{nm}(z+L)}\mu_{nm}(x, y),\ g\in\bar{B} \tag{47}$$

where the following notation is used: $\tilde{v}_{pq(z,E)}(k)\leftrightarrow v_{pq(z,E)}(L, t)$, $\tilde{u}^{\pm}_{nm(z,E\,\mathrm{or}\,H)}(k)\leftrightarrow u^{\pm}_{nm(z,E\,\mathrm{or}\,H)}(\pm L, t)$, $\Gamma_{nm}=\left(k^2-\lambda^2_{nm}\right)^{1/2}$, $\mathrm{Re}\Gamma_{nm}\mathrm{Re}k\geq 0$, $\mathrm{Im}\Gamma_{nm}\geq 0$[7].

The amplitudes $\tilde{u}^{\pm}_{nm(z,E\,\mathrm{or}\,H)}(k)$ form the system of the so-called scattering coefficients of the grating, namely, the reflection coefficients

$$R^{nm(H)}_{pq(E)}=\frac{\tilde{u}^+_{nm(z,H)}(k)}{\tilde{v}_{pq(z,E)}(k)},\quad R^{nm(E)}_{pq(E)}=\frac{\tilde{u}^+_{nm(z,E)}(k)}{\tilde{v}_{pq(z,E)}(k)},\quad n, m=0, \pm 1, \pm 2, ... \tag{48}$$

specifying efficiency of transformation of pq-th harmonic of a monochromatic TM-wave into of order nm-th harmonics of the scattered field $\{\vec{\tilde{E}}^s, \vec{\tilde{H}}^s\}$ in the reflection zone, and the transmission coefficients

$$T^{nm(H)}_{pq(E)}=\frac{\tilde{u}^-_{nm(z,H)}(k)}{\tilde{v}_{pq(z,E)}(k)},\quad T^{nm(E)}_{pq(E)}=\frac{\tilde{u}^-_{nm(z,E)}(k)}{\tilde{v}_{pq(z,E)}(k)},\quad n, m=0, \pm 1, \pm 2, ... \tag{49}$$

determining the efficiency of excitation of the transmitted harmonics in the domain B.

These coefficients are related by the energy balance equations

$$\sum_{n,m=-\infty}^{\infty}\frac{1}{\lambda_{nm}^2}\left[\left(\left|R_{pq(E)}^{nm(E)}\right|^2+\left|T_{pq(E)}^{nm(E)}\right|^2\right)\pm\eta_0^2\left(\left|R_{pq(E)}^{nm(H)}\right|^2+\left|T_{pq(E)}^{nm(H)}\right|^2\right)\right]\begin{Bmatrix}\mathrm{Re}\Gamma_{nm}\\ \mathrm{Im}\Gamma_{nm}\end{Bmatrix}$$
$$=\frac{1}{\lambda_{pq}^2}\begin{Bmatrix}\mathrm{Re}\Gamma_{pq}+2\mathrm{Im}\Gamma_{pq}\mathrm{Im}R_{pq(E)}^{pq(E)}\\ \mathrm{Im}\Gamma_{pq}-2\mathrm{Re}\Gamma_{pq}\mathrm{Im}R_{pq(E)}^{pq(E)}\end{Bmatrix}\mp\frac{1}{\varepsilon_0}\begin{Bmatrix}W_1\\ W_2\end{Bmatrix},\ p,\ q=0,\pm1,\pm2,\ldots, \tag{50}$$

$$W_1=\frac{\varepsilon_0\eta_0}{k}\int_{Q_L}\sigma(g,\ k)\left|\vec{\tilde{E}}(g,\ k)\right|^2dg,$$
$$W_2=\int_{Q_L}\left[\mu_0\mu(g,\ k)\left|\vec{\tilde{H}}(g,\ k)\right|^2-\varepsilon_0\varepsilon(g,\ k)\left|\vec{\tilde{E}}(g,\ k)\right|^2\right]dg \tag{51}$$

They follow from the complex power theorem (Poynting theorem) in the integral form [11]

$$\oint_{S_L}\left(\left[\vec{\tilde{E}}\times\vec{\tilde{H}}^*\right]\cdot\vec{ds}\right)=\int_{Q_L}\mathrm{div}\left[\vec{\tilde{E}}\times\vec{\tilde{H}}^*\right]dg=ik\eta_0\int_{Q_L}\mu\left|\vec{\tilde{H}}\right|^2dg-\frac{ik}{\eta_0}\int_{Q_L}\varepsilon\left|\vec{\tilde{E}}\right|^2dg-\int_{Q_L}\sigma\left|\vec{\tilde{E}}\right|^2dg \tag{52}$$

where $\varepsilon(g,\ k)-1=\tilde{\chi}_\varepsilon(g,\ k)\leftrightarrow\chi_\varepsilon(g,\ t)$, $\mu(g,\ k)-1=\tilde{\chi}_\mu(g,\ k)\leftrightarrow\chi_\mu(g,\ t)$, $\sigma(g,\ k)=\tilde{\chi}_\sigma(g,\ k)\leftrightarrow\chi_\sigma(g,\ t)$, $\vec{ds}$ is the vector element of the surface S_L bounding the domain Q_L. Equations (50)-(52) have been derived starting from the following boundary value problem for a diffraction grating illuminated by a plane TM-wave $\vec{\tilde{U}}_{pq(E)}^i(g,\ k):\tilde{E}_z^i(g,\ k)=\exp[-i\Gamma_{pq}(z-L\ )]\mu_{pq}(x,\ y)$:

$$\begin{cases}\eta_0\mathrm{rot}\vec{\tilde{H}}(g,k)=-ik\bar{\varepsilon}(g,k)\vec{\tilde{E}}(g,k),\\ \mathrm{rot}\vec{\tilde{E}}(g,k)=ik\eta_0\mu(g,k)\vec{\tilde{H}}(g,k),\quad g\in Q_L\\ D\left[\vec{\tilde{E}}\left(\vec{\tilde{H}}\right)\right](l_x,y)=e^{2\pi i\Phi_x}D\left[\vec{\tilde{E}}\left(\vec{\tilde{H}}\right)\right](0,y),\quad 0\le y\le l_y,\quad |z|<L\\ D\left[\vec{\tilde{E}}\left(\vec{\tilde{H}}\right)\right](x,l_y)=e^{2\pi i\Phi_y}D\left[\vec{\tilde{E}}\left(\vec{\tilde{H}}\right)\right](x,0),\quad 0\le x\le l_x,\quad |z|<L\\ \tilde{E}_{tg}(g,k)\Big|_{g\in S}=0,\quad \tilde{H}_{nr}(g,k)\Big|_{g\in S}=0\end{cases} \tag{53}$$

$$\begin{Bmatrix}\tilde{E}_z(g,\ k)\\ \tilde{H}_z(g,\ k)\end{Bmatrix}=\begin{Bmatrix}1\\ 0\end{Bmatrix}e^{-i\Gamma_{pq}(z-L\ )}\mu_{pq}(x,\ y)+\sum_{n,m=-\infty}^{\infty}\begin{Bmatrix}R_{pq(E)}^{nm(E)}(k)\\ R_{pq(E)}^{nm(H)}(k)\end{Bmatrix}e^{i\Gamma_{nm}(z-L\ )}\mu_{nm}(x,\ y),\ g\in\bar{A},$$
$$\begin{Bmatrix}\tilde{E}_z(g,\ k)\\ \tilde{H}_z(g,\ k)\end{Bmatrix}=\sum_{n,m=-\infty}^{\infty}\begin{Bmatrix}T_{pq(E)}^{nm(E)}(k)\\ T_{pq(E)}^{nm(H)}(k)\end{Bmatrix}e^{-i\Gamma_{nm}(z+L\ )}\mu_{nm}(x,\ y),\ g\in\bar{B}. \tag{54}$$

When deriving (50), (51) we have also used the equations relating z-components of the eigenmode of the Floquet channel

$$\vec{\widetilde{U}}(g,\,k):\ \widetilde{E}_z(g,\,k)=A\mathrm{e}^{\pm i\Gamma z}\mu(x,\,y)\quad\text{and}\quad \widetilde{H}_z(g,\,k)=B\mathrm{e}^{\pm i\Gamma z}\mu(x,\,y) \tag{55}$$

(subscripts nm are omitted) with its longitudinal components:

$$\begin{aligned}&\widetilde{E}_x=-\frac{\beta k\eta_0}{\lambda^2}\widetilde{H}_z\mp\frac{\alpha\Gamma}{\lambda^2}\widetilde{E}_z,\ \widetilde{E}_y=\frac{\alpha k\eta_0}{\lambda^2}\widetilde{H}_z\mp\frac{\beta\Gamma}{\lambda^2}\widetilde{E}_z,\\&\widetilde{H}_x=\mp\frac{\alpha\Gamma}{\lambda^2}\widetilde{H}_z+\frac{\beta k}{\eta_0\lambda^2}\widetilde{E}_z,\ \widetilde{H}_y=\mp\frac{\beta\Gamma}{\lambda^2}\widetilde{H}_z-\frac{\alpha k}{\eta_0\lambda^2}\widetilde{E}_z.\end{aligned} \tag{56}$$

Here, $\bar{\varepsilon}(g,\,k)=\varepsilon(g,\,k)+i\eta_0\sigma(g,\,k)/k$, $\mu(x,\,y)=(l_x l_y)^{-1/2}\exp(i\alpha x)\exp(i\beta y)$, $\Gamma=\sqrt{k^2-\lambda^2}$, $\lambda^2=\alpha^2+\beta^2$.

According to the Lorentz lemma [11], the fields $\{\vec{\widetilde{E}}^{(1)},\,\vec{\widetilde{H}}^{(1)}\}$ and $\{\vec{\widetilde{E}}^{(2)},\,\vec{\widetilde{H}}^{(2)}\}$ resulting from the interaction of a grating with two plane TM-waves

$\vec{\widetilde{U}}^{i(1)}_{pq(E)}(g,\,k):\widetilde{E}^{i(1)}_z(g,\,k)=\exp[-i\Gamma_{pq}(\Phi_x,\,\Phi_y)(z-L\,)]\mu_{pq}(x,\,y,\,\Phi_x,\,\Phi_y)$ and

$\vec{\widetilde{U}}^{i(2)}_{-r,-s(E)}(g,\,k):\widetilde{E}^{i(2)}_z(g,\,k)=\exp[-i\Gamma_{-r,-s}(-\Phi_x,\,-\Phi_y)(z-L\,)]\mu_{-r,-s}(x,\,y,\,-\Phi_x,\,-\Phi_y)$,

satisfy the following equation

$$\oint_{S_L}\left(\left([\vec{\widetilde{E}}^{(1)}\times\vec{\widetilde{H}}^{(2)}]-[\vec{\widetilde{E}}^{(2)}\times\vec{\widetilde{H}}^{(1)}]\right)\cdot\vec{ds}\right)=0. \tag{57}$$

From (57), using (54) and (56), we obtain

$$\begin{gathered}\frac{R^{rs(E)}_{pq(E)}(\Phi_x,\,\Phi_y)\lambda^2_{p,q}(\Phi_x,\,\Phi_y)}{\Gamma_{pq}(\Phi_x,\,\Phi_y)}=\frac{R^{-p,-q(E)}_{-r,-s(E)}(-\Phi_x,\,-\Phi_y)\lambda^2_{-r,-s}(-\Phi_x,\,-\Phi_y)}{\Gamma_{-r,-s}(-\Phi_x,\,-\Phi_y)},\\ p,\,q,\,r,\,s=0,\pm 1,\pm 2,\ldots\end{gathered} \tag{58}$$

– the reciprocity relations, which are of considerable importance in the physical analysis of wave scattering by periodic structures as well as when testing numerical algorithms for boundary problems (53), (54).

Assume now that the first wave $\vec{\widetilde{U}}^{i(1)}_{pq(E)}(g,\,k)$: $:\widetilde{E}^{i(1)}_z(g,\,k)=\exp[-i\Gamma_{pq}(\Phi_x,\,\Phi_y)(z-L\,)]\mu_{pq}(x,\,y,\,\Phi_x,\,\Phi_y)=\vec{\widetilde{U}}^{i(1)}_{pq(E)}(g,\,k,\,A)$ be incident on the grating from the domain A, as in the case considered above, while another wave $\vec{\widetilde{U}}^{i(2)}_{-r,-s(E)}(g,\,k):\widetilde{E}^{i(2)}_z(g,\,k,\,B)=\exp[i\Gamma_{-r,-s}(-\Phi_x,\,-\Phi_y)(z+L\,)]\mu_{-r,-s}(x,\,y,\,-\Phi_x,\,-\Phi_y)$ is incident from B. Both of these waves satisfy equation (57), whence we have

$$\frac{T_{pq(E)}^{rs(E)}(\Phi_x,\ \Phi_y,\ A)\lambda_{p,q}^2(\Phi_x,\ \Phi_y)}{\Gamma_{pq}(\Phi_x,\ \Phi_y)}=\frac{T_{-r,-s(E)}^{-p,-q(E)}(-\Phi_x,\ -\Phi_y,\ B)\lambda_{-r,-s}^2(-\Phi_x,\ -\Phi_y)}{\Gamma_{-r,-s}(-\Phi_x,\ -\Phi_y)},\qquad p,\ q,\ r,\ s=0,\pm 1,\pm 2,... \tag{59}$$

7.2. Excitation by a *TE*-wave

Let a grating be excited form the domain A by a pulsed TE-wave $\vec{U}^i(g,\ t)=\vec{U}^i_{pq(H)}(g,\ t):H_z^i(g,\ t)=v_{pq(z,H)}(z,\ t)\mu_{pq}(x,\ y)$ and the region Q_L is free from the sources $\vec{j}(g,\ t)$, $\vec{\varphi}_E(g)$, and $\vec{\varphi}_H(g)$. The field generated in the domains A and B is determined completely by their longitudinal components. They can be represented in the form of (31), (32). Define steady-state fields $\{\vec{\tilde{E}}(g,\ k),\ \vec{\tilde{H}}(g,\ k)\}$ corresponding to the pulsed fields $\{\vec{E}^i,\ \vec{H}^i\}$, $\{\vec{E}^s,\ \vec{H}^s\}$ in A and the pulsed field $\{\vec{E},\ \vec{H}\}$ in B, by their z-components as was done for the TM-case (see equations (45)-(47)). Introduce the scattering coefficients $R_{pq(H)}^{nm(E)}$, $R_{pq(H)}^{nm(H)}$, $T_{pq(H)}^{nm(E)}$, and $T_{pq(H)}^{nm(H)}$ by the relations like (48). These coefficients can be determined from the problems

$$\begin{cases}\eta_0\mathrm{rot}\vec{\tilde{H}}(g,k)=-ik\bar{\varepsilon}(g,k)\vec{\tilde{E}}(g,k),\\ \mathrm{rot}\vec{\tilde{E}}(g,k)=ik\eta_0\mu(g,k)\vec{\tilde{H}}(g,k), \qquad g\in Q_L\\ D\left[\vec{\tilde{E}}\left(\vec{\tilde{H}}\right)\right](l_x,y)=\mathrm{e}^{2\pi i\Phi_x}D\left[\vec{\tilde{E}}\left(\vec{\tilde{H}}\right)\right](0,y), \qquad 0\le y\le l_y, \qquad |z|<L\\ D\left[\vec{\tilde{E}}\left(\vec{\tilde{H}}\right)\right](x,l_y)=\mathrm{e}^{2\pi i\Phi_y}D\left[\vec{\tilde{E}}\left(\vec{\tilde{H}}\right)\right](x,0), \qquad 0\le x\le l_x, \qquad |z|<L\\ \tilde{E}_{tg}(g,k)\big|_{g\in\mathbf{S}}=0, \qquad \tilde{H}_{nr}(g,k)\big|_{g\in\mathbf{S}}=0,\end{cases} \tag{60}$$

$$\begin{gathered}\begin{Bmatrix}\tilde{E}_z(g,\ k)\\ \tilde{H}_z(g,\ k)\end{Bmatrix}=\begin{Bmatrix}0\\ 1\end{Bmatrix}\mathrm{e}^{-i\Gamma_{pq}(z-L)}\mu_{pq}(x,\ y)+\sum_{n,m=-\infty}^{\infty}\begin{Bmatrix}R_{pq(H)}^{nm(E)}(k)\\ R_{pq(H)}^{nm(H)}(k)\end{Bmatrix}\mathrm{e}^{i\Gamma_{nm}(z-L)}\mu_{nm}(x,\ y),\ g\in\bar{A},\\ \begin{Bmatrix}\tilde{E}_z(g,\ k)\\ \tilde{H}_z(g,\ k)\end{Bmatrix}=\sum_{n,m=-\infty}^{\infty}\begin{Bmatrix}T_{pq(H)}^{nm(E)}(k)\\ T_{pq(H)}^{nm(H)}(k)\end{Bmatrix}\mathrm{e}^{-i\Gamma_{nm}(z+L)}\mu_{nm}(x,\ y),\ g\in\bar{B}\end{gathered} \tag{61}$$

and satisfy the following relations, which are corollaries from the Poynting theorem and the Lorentz lemma:

$$\begin{gathered}\sum_{n,m=-\infty}^{\infty}\frac{1}{\lambda_{nm}^2}\left[\left(\left|R_{pq(H)}^{nm(H)}\right|^2+\left|T_{pq(H)}^{nm(H)}\right|^2\right)\pm\frac{1}{\eta_0^2}\left(\left|R_{pq(H)}^{nm(E)}\right|^2+\left|T_{pq(H)}^{nm(E)}\right|^2\right)\right]\begin{Bmatrix}\mathrm{Re}\Gamma_{nm}\\ \mathrm{Im}\Gamma_{nm}\end{Bmatrix}=\\ =\frac{1}{\lambda_{pq}^2}\begin{Bmatrix}\mathrm{Re}\Gamma_{pq}+2\mathrm{Im}\Gamma_{pq}\mathrm{Im}R_{pq(H)}^{pq(H)}\\ \mathrm{Im}\Gamma_{pq}-2\mathrm{Re}\Gamma_{pq}\mathrm{Im}R_{pq(H)}^{pq(H)}\end{Bmatrix}-\frac{1}{\mu_0}\begin{Bmatrix}W_1\\ W_2\end{Bmatrix},\ p,\ q=0,\pm 1,\pm 2,\ldots\end{gathered} \tag{62}$$

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and

$$\frac{R_{pq(H)}^{rs(H)}(\Phi_x,\ \Phi_y)\lambda_{p,q}^2(\Phi_x,\ \Phi_y)}{\Gamma_{pq}(\Phi_x,\ \Phi_y)} = \frac{R_{-r,-s(H)}^{-p,-q(H)}(-\Phi_x,\ -\Phi_y)\lambda_{-r,-s}^2(-\Phi_x,\ -\Phi_y)}{\Gamma_{-r,-s}(-\Phi_x,\ -\Phi_y)}, \quad p,\ q,\ r,\ s=0,\pm 1,\pm 2,... \tag{63}$$

$$\frac{T_{pq(H)}^{rs(H)}(\Phi_x,\ \Phi_y,\ A)\lambda_{p,q}^2(\Phi_x,\ \Phi_y)}{\Gamma_{pq}(\Phi_x,\ \Phi_y)} = \frac{T_{-r,-s(H)}^{-p,-q(H)}(-\Phi_x,\ -\Phi_y,\ B)\lambda_{-r,-s}^2(-\Phi_x,\ -\Phi_y)}{\Gamma_{-r,-s}(-\Phi_x,\ -\Phi_y)}, \quad p,\ q,\ r,\ s=0,\pm 1,\pm 2,... \tag{64}$$

7.3. General properties of the grating's secondary field

Let now k be a real positive frequency parameter, and let an arbitrary semi-transparent grating (Figure 1) be excited from the domain A by a homogeneous TM- or TE-wave

$$\vec{\tilde{U}}_{pq(E\text{ or }H)}^{i}(g,\ k):\left\{\tilde{E}_z^i(g,\ k)\quad\text{or}\quad\tilde{H}_z^i(g,\ k)\right\}=e^{-i\Gamma_{pq}(z-L\ )}\mu_{pq}(x,\ y),\qquad p,\ q:\operatorname{Im}\Gamma_{pq}=0\ . \tag{65}$$

The terms of infinite series in (54) and (61) are z-components of nm-th harmonics of the scattered field for the domains A and B. The complex amplitudes $R_{pq(E\text{or}H)}^{nm(E\text{or}H)}$ and $T_{pq(E\text{or}H)}^{nm(E\text{or}H)}$ are the functions of $k,\ \Phi_x,\ \Phi_y$, as well as of the geometry and material parameters of the grating. Every harmonic for which $\operatorname{Im}\Gamma_{nm}=0$ and $\operatorname{Re}\Gamma_{nm}>0$ is a homogeneous plane wave propagating away from the grating along the vector $\vec{k}_{nm}:k_x=\alpha_n,\ k_y=\beta_m,\ k_z=\Gamma_{nm}$(in A; Figure 5) or $k_z=-\Gamma_{nm}$ (in B). The frequencies k such that $\Gamma_{nm}(k)=0$ $(k=k_{nm}^{\pm}=\pm|\lambda_{nm}|)$ are known as threshold frequency or sliding points [1-6]. At those points, a spatial harmonic of order nm with $\operatorname{Im}\Gamma_{nm}>0$ are transformed into a propagating homogeneous pane wave.

It is obvious that the propagation directions $\vec{k}_{nm}$ of homogeneous harmonics of the secondary field depends on their order nm, on the values of k and on the directing vector of the incident wave $\vec{k}_{pq}^{i}:k_x^i=\alpha_p,\ k_y^i=\beta_q, k_z^i=-\Gamma_{pq}$. According to (50) and (62), we can write the following formulas for the values, which determine the 'energy content' of harmonics, or in other words, the relative part of the energy directed by the structure into the relevant spatial radiation channel:

$$\begin{aligned}(WR)_{pq}^{nm}&=\left(\left|R_{pq(E)}^{nm(E)}\right|^2+\eta_0^2\left|R_{pq(E)}^{nm(H)}\right|^2\right)\frac{\operatorname{Re}\Gamma_{nm}}{\lambda_{nm}^2}\frac{\lambda_{pq}^2}{\Gamma_{pq}}=(WR)_{pq(E)}^{nm(E)}+(WR)_{pq(E)}^{nm(H)},\\(WT)_{pq}^{np}&=\left(\left|T_{pq(E)}^{nm(E)}\right|^2+\eta_0^2\left|T_{pq(E)}^{nm(H)}\right|^2\right)\frac{\operatorname{Re}\Gamma_{nm}}{\lambda_{nm}^2}\frac{\lambda_{pq}^2}{\Gamma_{pq}}=(WT)_{pq(E)}^{np(E)}+(WT)_{pq(E)}^{np(H)}\end{aligned} \tag{66}$$

(for TM-case) and

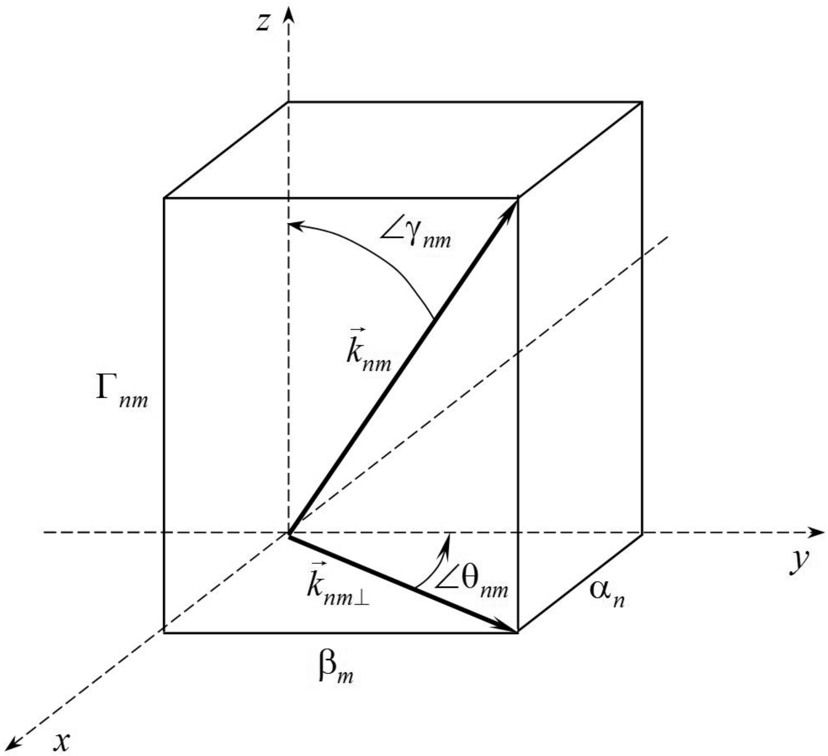

Figure 5. On determination of propagation directions for spatial harmonics of the field formed by a two-dimensionally periodic structure.

$$\begin{aligned}(WR)_{pq}^{nm}&=\left(\left|R_{pq(H)}^{nm(H)}\right|^2+\frac{1}{\eta_0^2}\left|R_{pq(H)}^{nm(E)}\right|^2\right)\frac{\mathrm{Re}\Gamma_{nm}}{\lambda_{nm}^2}\frac{\lambda_{pq}^2}{\Gamma_{pq}}=(WR)_{pq(H)}^{nm(H)}+(WR)_{pq(H)}^{nm(E)},\\(WT)_{pq}^{np}&=\left(\left|T_{pq(H)}^{nm(H)}\right|^2+\frac{1}{\eta_0^2}\left|T_{pq(H)}^{nm(E)}\right|^2\right)\frac{\mathrm{Re}\Gamma_{nm}}{\lambda_{nm}^2}\frac{\lambda_{pq}^2}{\Gamma_{pq}}=(WT)_{pq(H)}^{nm(H)}+(WT)_{pq(H)}^{nm(E)}\end{aligned}\tag{67}$$

(for TE-case). The channel corresponding to the nm-th harmonic will be named 'open' if $\mathrm{Im}\Gamma_{nm}=0$. The regime with a single open channel ($nm=pq$) will be called the single-mode regime.

Since $\left|\vec{k}_{pq}^{i}\right|=\left|\vec{k}_{nm}\right|=k$, the nm-th harmonic of the secondary field in the reflection zone propagates in opposition to the incident wave only if $\alpha_n=-\alpha_p$ and $\beta_m=-\beta_q$ or, in other notation, if

$$n=-2\Phi_x-p \quad \text{and} \quad m=-2\Phi_y-q \tag{68}$$

Generation of the nonspecularly reflected mode of this kind is termed the auto-collimation.

The amplitudes $R_{pq(E\,\mathrm{or}H)}^{nm(E\,\mathrm{or}H)}$ or $T_{pq(E\,\mathrm{or}H)}^{nm(E\,\mathrm{or}H)}$ are not all of significance for the physical analysis. In the far-field zone, the secondary field is formed only by the propagating harmonics of the orders nm such that $\mathrm{Re}\Gamma_{nm} \ge 0$. However, the radiation field in the immediate proximity of the grating requires a consideration of the contribution of damped harmonics $(nm:\mathrm{Im}\Gamma_{nm} > 0)$. Moreover, in some situations (resonance mode) this contribution is the dominating one [6].

7.4. The simplest corollaries of the reciprocity relations and the energy conservation law

Let us formulate several corollaries of the relations (50), (58), (59), and (62)-(64) basing on the results presented in [3] and [7] for one-dimensionally periodic gratings and assuming that $\varepsilon(g,\,k) \ge 0$, $\mu(g,\,k) \ge 0$, and $\sigma(g,\,k) \ge 0$.

- The upper lines in (50) and (62) represent the energy conservation law for propagating waves. If $\mathrm{Im}\Gamma_{pq} = 0$, the energy of the scattered field is clearly related with the energy of the incident wave. The energy of the wave $\vec{\tilde{U}}^{\,i}_{pq(E\,\mathrm{or}H)}(g,\,k)$ is partially absorbed by the grating (only if $W_1 \ne 0$), and the remaining part is distributed between spatial TM- and TE-harmonics propagating in the domains A and B (the wave is reradiating into the directions $z = \pm\infty$). If a plane inhomogeneous wave be incident on a grating $(\mathrm{Im}\Gamma_{pq} > 0)$, the total energy is defined by the imaginary part of reflection coefficient $R_{pq(E\,\mathrm{or}H)}^{pq(E\,\mathrm{or}H)}$, which in this case is nonnegative.
- The relations in the bottom lines in (50), (62) limit the values of $\sum_{n,m=-\infty}^{\infty} | R_{pq(E)}^{nm(E)} |^2 \lambda_{nm}^{-2} \mathrm{Im}\Gamma_{nm}$, $\sum_{n,m=-\infty}^{\infty} | T_{pq(E)}^{nm(E)} |^2 \lambda_{nm}^{-2} \mathrm{Im}\Gamma_{nm}$, etc. and determine thereby the class of infinite sequences

$$l_2 = \left\{ a = \{a_{nm}\}_{nm=-\infty}^{\infty} : \sum_{nm=-\infty}^{\infty} \frac{| a_{nm} |^2}{\sqrt{n^2 + m^2}} \infty \right\} \tag{69}$$

or energetic space, to which amplitudes of the scattered harmonics $R_{pq(E)}^{nm(E)}$, $T_{pq(E)}^{nm(E)}$, etc. belong.

- It follows from (58), (59), (63), and (64) that for all semi-transparent and reflecting gratings we can write

$$\begin{aligned} &(WR)_{00(E\,\mathrm{or}H)}^{00(E\,\mathrm{or}H)}(\Phi_x,\,\Phi_y) = (WR)_{00(E\,\mathrm{or}H)}^{00(E\,\mathrm{or}H)}(-\Phi_x,\,-\Phi_y), \\ &(WT)_{00(E\,\mathrm{or}H)}^{00(E\,\mathrm{or}H)}(\Phi_x,\,\Phi_y,\,A) = (WT)_{00(E\,\mathrm{or}H)}^{00(E\,\mathrm{or}H)}(-\Phi_x,\,-\Phi_y,\,B). \end{aligned} \tag{70}$$

The first equation in (70) proves that the efficiency of transformation of the TM- or TE-wave into the specular reflected wave of the same polarization remains unchanged if the grating is rotated in the plane $x0y$ about z-axis through$180°$. The efficiency of transformation into the principal transmitted wave of the same polarizations does not also vary with the grating rotation about the axis lying in the plane $x0y$ and being normal to the vector $\vec{k}_{00}$ (Figure 5).

- When $r=s=p=q=0$ we derive from (58), (59), (63), and (64) that

$$\begin{aligned} R_{00(E\,\mathrm{or}H)}^{00(E\,\mathrm{or}H)}(\Phi_x, \Phi_y) = R_{00(E\,\mathrm{or}H)}^{00(E\,\mathrm{or}H)}(-\Phi_x, -\Phi_y), \\ T_{00(E\,\mathrm{or}H)}^{00(E\,\mathrm{or}H)}(\Phi_x, \Phi_y, A) = T_{00(E\,\mathrm{or}H)}^{00(E\,\mathrm{or}H)}(-\Phi_x, -\Phi_y, B). \end{aligned} \tag{71}$$

That means that even if a semi-transparent or reflecting grating is non symmetric with respect to the any planes, the reflection and transmission coefficients entering (71) do not depend on the proper changes in the angles of incidence of the primary wave.

- Relations (50), (58) allow the following regularities to be formulated for ideal ($\sigma(g, k)\equiv 0$) asymmetrical reflecting gratings. Let the parameters$k$, Φ_x, and Φ_y be such that $\mathrm{Re}\Gamma_{00}(\Phi_x, \Phi_y)>0$ and $\mathrm{Re}\Gamma_{nm}(\Phi_x, \Phi_y)=0$ for$n$, $m\neq 0$. If the incident wave is an inhomogeneous plane wave$\vec{U}^{\,i}_{\pm p,\pm q(E)}(g, k, \pm\Phi_x, \pm\Phi_y)$, then

$$\begin{aligned} \left(\left| R_{\pm p,\pm q(E)}^{00(E)}(\pm\Phi_x, \pm\Phi_y)\right|^2 + \eta_0^2 \left| R_{\pm p,\pm q(E)}^{00(H)}(\pm\Phi_x, \pm\Phi_y)\right|^2\right) \frac{\mathrm{Re}\Gamma_{00}(\pm\Phi_x, \pm\Phi_y)}{\lambda_{00}^2(\pm\Phi_x, \pm\Phi_y)} = \\ = 2\mathrm{Im}R_{\pm p,\pm q(E)}^{\pm p,\pm q(E)}(\pm\Phi_x, \pm\Phi_y) \frac{\mathrm{Im}\Gamma_{\pm p,\pm q}(\pm\Phi_x, \pm\Phi_y)}{\lambda_{\pm p,\pm q}^2(\pm\Phi_x, \pm\Phi_y)}. \end{aligned} \tag{72}$$

Since$R_{pq(E)}^{pq(E)}(\Phi_x, \Phi_y) = R_{-p,-q(E)}^{-p,-q(E)}(-\Phi_x, -\Phi_y)$, we derive from (72)

$$\begin{aligned} \left| R_{p,q(E)}^{00(E)}(\Phi_x, \Phi_y)\right|^2 + \eta_0^2 \left| R_{p,q(E)}^{00(H)}(\Phi_x, \Phi_y)\right|^2 = \\ = \left| R_{-p,-q(E)}^{00(E)}(-\Phi_x, -\Phi_y)\right|^2 + \eta_0^2 \left| R_{-p,-q(E)}^{00(H)}(-\Phi_x, -\Phi_y)\right|^2. \end{aligned} \tag{73}$$

It is easy to realize a physical meaning of the equation (73) and of similar relation for TE-case, which may be of interest for diffraction electronics. If a grating is excited by a damped harmonic, the efficiency of transformation into the unique propagating harmonic of spatial spectrum is unaffected by the structure rotation in the plane $x0y$ about z-axis through$180°$. The above-stated corollaries have considerable utility in testing numerical results and making easier their physical interpretation. The use of these corollaries may considerably reduce amount of calculations.

8. Elements of Spectral Theory for Two-Dimensionally Periodic Gratings

The spectral theory of gratings studies singularities of analytical continuation of solutions of boundary value problems formulated in the frequency domain (see, for example, problems (53), (54) and (60), (61)) into the domain of complex-valued (nonphysical) values of real parameters (like frequency, propagation constants, etc.) and the role of these singularities in resonant and anomalous modes in monochromatic and pulsed wave scattering. The fundamental results of this theory for one-dimensionally periodic gratings are presented in [4,6,7]. We present some elements of the spectral theory for two-dimensionally periodic structures, which follow immediately form the results obtained in the previous sections. The frequency k acts as a spectral parameter; a two-dimensionally periodic grating is considered as an open periodic resonator.

8.1. Canonical Green function

Let a solution $\widetilde{G}_0(g,\ p,\ k)$ of the scalar problem

$$\begin{cases} [\Delta_g + k^2][\widetilde{G}_0(g,\ p,\ k)] = \delta(g-p),\ g=\{x_g,\ y_g,\ z_g\}\in R,\ p=\{x_p,\ y_p,\ z_p\}\in Q_L \\ D[\widetilde{G}_0](l_x,\ y_g) = \mathrm{e}^{2\pi i \Phi_x} D[\widetilde{G}_0](0, y_g),\ 0\le y_g \le l_y,\ |z_g| \le L \\ D[\widetilde{G}_0](x_g,\ l_y) = \mathrm{e}^{2\pi i \Phi_y} D[\widetilde{G}_0](x_g, 0),\ 0\le x_g \le l_x,\ |z_g| \le L \\ \widetilde{G}_0(g,\ p,\ k) = \sum\limits_{n,m=-\infty}^{\infty} \begin{Bmatrix} A_{nm}(p,\ k) \\ B_{nm}(p,\ k) \end{Bmatrix} \mathrm{e}^{\pm i\Gamma_{nm}(z_g \mp L\ )} \mu_{nm}(x_g,\ y_g),\ g\in \begin{Bmatrix} \overline{A} \\ \overline{B} \end{Bmatrix} \end{cases} \tag{74}$$

is named the canonical Green function for 2-D periodic gratings. In the case of the elementary periodic structure with the absence of any material scatterers, the problems of this kind but with arbitrary right-hand parts of the Helmholtz equation are formulated for the monochromatic waves generated by quasi-periodic current sources located in the region $|z| < L$.

Let us construct $\widetilde{G}_0(g,\ p,\ k)$ as a superposition of free-space Green functions:

$$\widetilde{G}_0(g,\ p,\ k) = -\frac{1}{4\pi}\sum_{n,m=-\infty}^{\infty} \frac{\exp[ik\,|g-p_{nm}|]}{|g-p_{nm}|} \mathrm{e}^{2\pi i n\Phi_x} \mathrm{e}^{2\pi i m\Phi_y},\ p_{nm} = \{x_p + nl_x,\ y_p + ml_y,\ z_p\}. \tag{75}$$

By using in (75) the Poisson summation formula [15] and the tabulated integrals [16]

$$\int_{-\infty}^{\infty} \frac{\exp\left(ip\sqrt{x^2+a^2}\right)}{\sqrt{x^2+a^2}} \mathrm{e}^{ibx} dx = \pi i H_0^{(1)}\left(a\sqrt{|p^2-b^2|}\right) \text{ and } \int_{-\infty}^{\infty} H_0^{(1)}\left(p\sqrt{x^2+a^2}\right) e^{ibx} dx = 2\frac{\exp\left(ia\sqrt{p^2-b^2}\right)}{\sqrt{p^2-b^2}},$$

where $H_0^{(1)}(x)$ is the Hankel function of the first kind, we obtain

$$\widetilde{G}_0(g,\ p,\ k) = -\frac{i}{2l_x l_y} \sum_{n,m=-\infty}^{\infty} \mathrm{e}^{i\left[\alpha_n(x_g - x_p) + \beta_m(y_g - y_p)\right]} \frac{\exp[i\ |\ z_g - z_p\ |\ \Gamma_{nm}]}{\Gamma_{nm}} \tag{76}$$

The surface K of analytic continuation of the canonical Green function (76) into the domain of complex-valued k is an infinite-sheeted Riemann surface consisting of the complex planes $k \in C$ with cuts along the lines$(\mathrm{Re}k)^2 - (\mathrm{Im}k)^2 - \lambda_{nm}^2 = 0,\ n,\ m = 0, \pm 1, \pm 2, \ldots,\ \mathrm{Im}k \le 0$(Figure 6). The first (physical) sheet C_k of the surface K is uniquely determined by the radiation conditions for $\widetilde{G}_0(g,\ p,\ k)$ in the domains A and$B$, i.e. by the choice of $\mathrm{Re}\Gamma_{nm}\mathrm{Re}k \ge 0$ and $\mathrm{Im}\Gamma_{nm} \ge 0$ on the axis$\mathrm{Im}k = 0$. On this sheet, in the domain$0 \le \arg k < \pi$, we have$\mathrm{Im}\Gamma_{nm} > 0$, while $\mathrm{Re}\Gamma_{nm} \ge 0$ for $0 \arg k \le \pi/2$ and $\mathrm{Re}\Gamma_{nm} \le 0$ for$\pi/2 \le \arg k \pi$. In the domain $3\pi/2 \le \arg k < 2\pi$ for finite number of functions $\Gamma_{nm}(k)$ (with n and m such that$(\mathrm{Re}k)^2 - (\mathrm{Im}k)^2 - \lambda_{nm}^2 > 0$), the inequalities $\mathrm{Im}\Gamma_{nm} < 0$ and $\mathrm{Re}\Gamma_{nm} > 0$ hold; for the rest of these functions we have $\mathrm{Im}\Gamma_{nm} > 0$ and$\mathrm{Re}\Gamma_{nm} \le 0$. In the domain$\pi < \arg k \le 3\pi/2$, the situation is similar only the signs of $\mathrm{Re}\Gamma_{nm}$ are opposite. On the subsequent sheets (each of them with its own pair$\{k; \Gamma_{nm}(k)\}$), the signs (root branches) of $\Gamma_{nm}(k)$ are opposite to those they have on the first sheet for a finite number of n and$m$. The cuts (solid lines in Fig. 6) originate from the real algebraic branch points$k_{nm}^{\pm} = \pm\ |\ \lambda_{nm}\ |$.

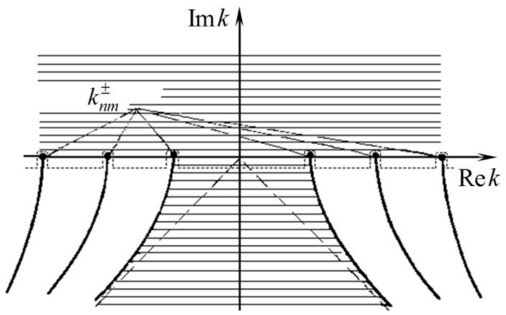

Figure 6. Natural domain of variation of the spectral parameter$k$: the first sheet of the surface$K$.

In the vicinity of some fixed point $K \in K$ the function $\widetilde{G}_0(g,\ p,\ k)$ can be expanded into a Loran series in terms of the local variable [17]

$$\kappa = \begin{cases} k - K; K \notin \{k_{nm}^{\pm}\} \\ \sqrt{k - K}; K \in \{k_{nm}^{\pm}\} \end{cases}.$$

Therefore, this function is meromorphic on the surface$K$. Calculating the residuals $\mathop{\mathrm{Res}}\limits_{k=\bar{k}} \widetilde{G}_0(g,\ p,\ k)$ at the simple poles$\bar{k} \in \{k_{nm}^{\pm}\}$, we obtain nontrivial solutions of homogeneous ($\vec{\widetilde{U}}^i(g,\ k) \equiv 0$) canonical ($\bar{\varepsilon}(g,\ k) \equiv 1,\ \mu(g,\ k) \equiv 1, \overline{\mathrm{int}S} = \varnothing$) problems (53), (54) and (60), (61):

$$\vec{\widetilde{E}}\left(g,\ k_{nm}^{\pm}\right) = \{\widetilde{E}_x,\ \widetilde{E}_y,\ \widetilde{E}_z\};\quad \widetilde{E}_{x,\ y\ \mathrm{or}\ z} = a_{x,\ y\ \mathrm{or}\ z}\exp[i(\alpha_n x + \beta_m y)] \quad \text{and} \quad \vec{\widetilde{H}}\left(g,\ k_{nm}^{\pm}\right) = \left(ik_{nm}^{\pm}\eta_0\right)^{-1}\mathrm{rot}\vec{\widetilde{E}}\left(g,\ k_{nm}^{\pm}\right) \tag{77}$$

where $a_{x,\ y\ \text{or}\ z}$ are the arbitrary constants. These solutions determine free oscillations in the space stratified by the following conditions:

$$D[\vec{\tilde{E}}(\vec{\tilde{H}})](x+l_x,\ y)=\mathrm{e}^{2\pi i\Phi_x}D[\vec{\tilde{E}}(\vec{\tilde{H}})](x,\ y),\ D[\vec{\tilde{E}}(\vec{\tilde{H}})](x,\ y+l_y)=\mathrm{e}^{2\pi i\Phi_y}D[\vec{\tilde{E}}(\vec{\tilde{H}})](x,\ y). \quad (78)$$

8.2. Spectrum qualitative characteristics

Let a set Ω_k of the points $\{\bar{k}_j\}_j\in K$ such that for all $k\in\{\bar{k}_j\}_j$ the homogeneous (spectral) problem

$$\begin{cases} \eta_0\mathrm{rot}\tilde{\vec{H}}(g,k)=-ik\varepsilon(g,k)\tilde{\vec{E}}(g,k), \\ \mathrm{rot}\tilde{\vec{E}}(g,k)=ik\eta_0\mu(g,k)\tilde{\vec{H}}(g,k), \quad g\in Q_L \\ D\left[\tilde{\vec{E}}\left(\tilde{\vec{H}}\right)\right](l_x,y)=\mathrm{e}^{2\pi i\Phi_x}D\left[\tilde{\vec{E}}\left(\tilde{\vec{H}}\right)\right](0,y), \quad 0\le y\le l_y, \quad |z|<L \\ D\left[\tilde{\vec{E}}\left(\tilde{\vec{H}}\right)\right](x,l_y)=\mathrm{e}^{2\pi i\Phi_y}D\left[\tilde{\vec{E}}\left(\tilde{\vec{H}}\right)\right](x,0), \quad 0\le x\le l_x, \quad |z|<L \\ \tilde{E}_{tg}(g,k)\Big|_{g\in\mathbf{S}}=0, \quad \tilde{H}_{nr}(g,k)\Big|_{g\in\mathbf{S}}=0 \quad , \end{cases} \quad (79)$$

$$\begin{aligned} \left\{\begin{matrix}\tilde{E}_z(g,\ k)\\ \tilde{H}_z(g,\ k)\end{matrix}\right\} &= \sum_{n,m=-\infty}^{\infty}\left\{\begin{matrix}A_{nm(E)}(k)\\ A_{nm(H)}(k)\end{matrix}\right\}\mathrm{e}^{i\Gamma_{nm}(z-L)}\mu_{nm}(x,\ y),\ g\in\bar{A} \\ \left\{\begin{matrix}\tilde{E}_z(g,\ k)\\ \tilde{H}_z(g,\ k)\end{matrix}\right\} &= \sum_{n,m=-\infty}^{\infty}\left\{\begin{matrix}B_{nm(E)}(k)\\ B_{nm(H)}(k)\end{matrix}\right\}\mathrm{e}^{-i\Gamma_{nm}(z+L)}\mu_{nm}(x,\ y),\ g\in\bar{B} \end{aligned} \quad (80)$$

has a nontrivial (not necessarily unique) solution $\vec{\tilde{U}}(g,\ \bar{k}_j)=\{\vec{\tilde{E}}(g,\ \bar{k}_j),\ \vec{\tilde{H}}(g,\ \bar{k}_j)\}$be called the point spectrum of the grating. It is obvious that these solutions characterize the so-called free oscillations, whose field pattern, structure of their spatial harmonics and behavior of these harmonics for large $|z|$ and t are determined by the value of $\bar{k}_j=\mathrm{Re}\bar{k}_j+i\mathrm{Im}\bar{k}_j$ and by a position of the point $\bar{k}_j$ (the eigen frequency associated with a free oscillation$\vec{\tilde{U}}(g,\ \bar{k}_j)$) on the surface K [4,6,7]. By continuing analytically the problems (53), (54) and (60), (61) together with their solutions $\vec{\tilde{U}}(g,\ k)=\{\vec{\tilde{E}}(g,\ k),\ \vec{\tilde{H}}(g,\ k)\}$ into the domain K of the complex-valued k, we detect poles of the function $\vec{\tilde{U}}(g,\ k)$at the points$k=\bar{k}_j$. In the vicinity of these poles, the desired solutions can be represented by the Loran series in terms of the local on K variable κ [17]. The analytical findings of this kind may form the basis for detailed study of physical features of resonant wave scattering by one-dimensionally and two-dimensionally periodic structures [4,6,7,18,19].

Derive now the conditions that constrain existence of nontrivial solutions of the problem (79), (80). These conditions can be considered as uniqueness theorems for the problems (53), (54) and (60), (61) formulated for different domains of the surface$K$. Notice that the study of the uniqueness allows one to estimate roughly a domain where elements of the set Ω_k are localized and simplify substantially the subsequent numerical solution of spectral problems owing to reduction of a search zone of the eigen frequencies. The uniqueness theorems serve also as a basis for application of the 'meromorphic' Fredholm theorem [20] when constructing well grounded algorithms for solving diffraction problems as well as when studying qualitative characteristics of gratings' spectra [4,7].

Assume that grating scattering elements are nondispersive ($\varepsilon(g,k)=\varepsilon(g)$, $\mu(g,k)=\mu(g)$, and $\sigma(g,k)=\sigma(g)$). In this case, the analytical continuation of the spectral problem (79), (80) into the domain of complex-valued k are simplified considerably. From the complex power theorem in the integral form formulated for the nontrivial solutions $\vec{U}(g,\bar{k}_j)$ like

$$\begin{aligned}\oint_{S_L}\left([\vec{E}\times\vec{H}^*]\cdot\vec{ds}\right)&=\int_{Q_L}\operatorname{div}[\vec{E}\times\vec{H}^*]dg\\&=ik\eta_0\int_{Q_L}\mu|\vec{H}|^2dg-\frac{ik^*}{\eta_0}\int_{Q_L}\varepsilon|\vec{E}|^2dg-\int_{Q_L}\sigma|\vec{E}|^2dg\end{aligned}\tag{81}$$

the following relations result:

$$\begin{aligned}\sum_{n,m=-\infty}^{\infty}\frac{1}{\lambda_{nm}^2}\begin{Bmatrix}(\mathrm{Re}\Gamma_{nm}\mathrm{Re}k+\mathrm{Im}\Gamma_{nm}\mathrm{Im}k)\\(\mathrm{Im}\Gamma_{nm}\mathrm{Re}k-\mathrm{Re}\Gamma_{nm}\mathrm{Im}k)\end{Bmatrix}&\left[\left(|A_{nm(E)}|^2+|B_{nm(E)}|^2\right)\right.\\\left.\pm\eta_0^2\left(|A_{nm(H)}|^2+|B_{nm(H)}|^2\right)\right]&=\frac{1}{\varepsilon_0}\begin{Bmatrix}-\mathrm{Im}k(V_3+V_2)-V_1\\\mathrm{Re}k(V_3-V_2)\end{Bmatrix}\end{aligned}\tag{82}$$

Notation:$k=\bar{k}_j$, $\vec{E}=\vec{E}(g,\bar{k}_j)$, $\Gamma_{nm}=\Gamma_{nm}(\bar{k}_j)$, $A_{nm(E)}=A_{nm(E)}(\bar{k}_j)$, etc., and

$$V_1=\varepsilon_0\eta_0\int_{Q_L}\sigma|\vec{E}|^2dg,\ V_2=\int_{Q_L}\varepsilon_0\varepsilon|\vec{E}|^2dg, V_3=\int_{Q_L}\mu_0\mu|\vec{H}|^2dg.$$

No free oscillations exist whose amplitudes do not satisfy equations (82). From this general statement, several important consequences follow. Below some of them are formulated for gratings with$\varepsilon(g)>0$, $\mu(g)>0$, and$\sigma(g)\geq 0$.

- There are no free oscillations whose eigen frequencies $\bar{k}_j$ are located on the upper half-plane (Imk0) of the first sheet of the surface$K$. This can be verified by taking into account the upper relation in (82), the function $\Gamma_{nm}(k)$ onC_k, and the inequalities$V_1\geq 0$, $V_2>0$,$V_3>0$.
- If $\sigma(g)\equiv 0$ (the grating is non-absorptive), no free oscillations exist whose eigen frequencies $\bar{k}_j$ are located on the bottom half-plane (Im$k<0$) of the sheet C_k between the cuts corresponding to the least absolute values of$k_{nm}^{\pm}$. In Figure 6, this region of the first sheet of K and the above-mentioned domain are shaded by horizontal lines.

- If $\sigma(g)>0$ on some set of zero-measure points $g \in Q_L$, then there are no elements $\bar{k}_j$ of grating's point spectrum Ω_k that are located on the real axis of the plane C_k.

Investigation of the entire spectrum of a grating, i.e. a set of the points $k \in K$, for which the diffraction problems given by (53), (54) and (60), (61) are not uniquely solvable, is a complicated challenge. Therefore below we do no more than indicate basic stages for obtaining well grounded results. The first stage is associated with regularization of the boundary value problem describing excitation of a metal-dielectric grating by the currents $\tilde{\vec{J}}(g, k) \leftrightarrow \vec{J}(g, t)$ located in the domain Q_L :

$$\begin{cases} \eta_0 \mathrm{rot}\tilde{\vec{H}}(g,k) = -ik\bar{\varepsilon}(g,k)\tilde{\vec{E}}(g,k) + \tilde{\vec{J}}(g,k), \\ \mathrm{rot}\tilde{\vec{E}}(g,k) = ik\eta_0\mu(g,k)\tilde{\vec{H}}(g,k), \quad g \in Q_L \\ D\left[\tilde{\vec{E}}\left(\tilde{\vec{H}}\right)\right](l_x, y) = \mathrm{e}^{2\pi i\Phi_x} D\left[\tilde{\vec{E}}\left(\tilde{\vec{H}}\right)\right](0, y), \quad 0 \le y \le l_y, \quad |z| < L \\ D\left[\tilde{\vec{E}}\left(\tilde{\vec{H}}\right)\right](x, l_y) = \mathrm{e}^{2\pi i\Phi_y} D\left[\tilde{\vec{E}}\left(\tilde{\vec{H}}\right)\right](x, 0), \quad 0 \le x \le l_x, \quad |z| < L \\ \tilde{E}_{tg}(g,k)\Big|_{g\in\mathbf{S}} = 0, \quad \tilde{H}_{nr}(g,k)\Big|_{g\in\mathbf{S}} = 0 \quad , \end{cases} \tag{83}$$

$$\begin{aligned} \begin{Bmatrix} \tilde{E}_z(g, k) \\ \tilde{H}_z(g, k) \end{Bmatrix} &= \sum_{n,m=-\infty}^{\infty} \begin{Bmatrix} A_{nm(E)}(k) \\ A_{nm(H)}(k) \end{Bmatrix} \mathrm{e}^{i\Gamma_{nm}(z-L\ )} \mu_{nm}(x, y), \ g \in \bar{A}, \\ \begin{Bmatrix} \tilde{E}_z(g, k) \\ \tilde{H}_z(g, k) \end{Bmatrix} &= \sum_{n,m=-\infty}^{\infty} \begin{Bmatrix} B_{nm(E)}(k) \\ B_{nm(H)}(k) \end{Bmatrix} \mathrm{e}^{-i\Gamma_{nm}(z+L\ )} \mu_{nm}(x, y), \ g \in \bar{B}. \end{aligned} \tag{84}$$

By regularization is meant (see, for example, [7]) a reduction of the boundary value electrodynamic problem to the equivalent operator equation of the second kind

$$[E + B(\tilde{G}_0, S, \bar{\varepsilon}, \mu, k)]X = Y, \ EX = X \tag{85}$$

with a compact (in some space W of vector fields) finite-meromorphic (in local on K variables κ) operator-function $B(\tilde{G}_0, S, \bar{\varepsilon}, \mu, k)$ [20,21]. If the problem given by (83), (84) is considered separately for metal gratings ($\overline{\mathrm{int}S} \neq \varnothing$ and S are sufficiently smooth surfaces; $\bar{\varepsilon}(g, k) = \mu(g, k) \equiv 1$) and dielectric gratings ($\overline{\mathrm{int}S} = \varnothing$, $\bar{\varepsilon}(g, k) = \varepsilon(g)$ and $\mu(g, k) = \mu(g)$ are sufficiently smooth functions), then its regularization can be performed by applying the potential theory methods [4,7,22].

In the second stage, the following statements should be proved: (i) the resolvent $[E + B(k)]^{-1}$ ($k \in K$) of the problem in (85) is a finite-meromorphic operator-function; (ii) its poles are located at the points $k = \bar{k}_j$ ($j = 1,2,3,...$); (iii) the entire spectrum coincides with its point spectrum Ω_k; (iv) Ω_k is nothing more than a countable set without finite accumulation points. All these statements are corollaries of the 'meromorphic' Fredholm theorem [4,20,21] and the uniqueness theorem proved previously.

By inverting homogeneous operator equation (85), we can construct a numerical solution of the spectral problem given by (79), (80) [4,6], in other words, calculate the complex-valued eigen frequencies $\bar{k}_j$ and associated eigen waves $\vec{\tilde{U}}(g, \bar{k}_j)=\{\vec{\tilde{E}}(g, \bar{k}_j), \vec{\tilde{H}}(g, \bar{k}_j)\}$ or free oscillations of an open two-dimensionnaly periodic resonator. Commonly, this operation is reduced to an approximate solution of the characteristic equation like:

$$\det[C(k)]=0. \tag{86}$$

Here $C(k)$ is some infinite matrix-function; the compactness of the operator $B(k)$ ensures (i) existence of the determinant $\det[C(k)]$ and (ii) the possibility to approximate the solutions $\bar{k}$ of equation (86) by the solutions $\bar{k}(N)$ of the equation $\det[C(k, N)]$ with the matrix $C(k, N)$ reduced to dimension$N\times N$.

Let $\bar{k}$ be a root of characteristic equation (86) that do not coincide with any pole of the operator-function$B(k)$. The multiplicity of this root determines the multiplicity of the eigen value $\bar{k}$ of homogeneous operator equation (85), i.e. the value $M=M(1)+M(2)+\ldots+M(Q)$ [21]. Here, $Q$is the number of linearly-independent eigen functions$\vec{\tilde{U}}^{(q)}(g, \bar{k})$; $q=1,2,\ldots,Q$(the number of free oscillations) corresponding to the eigen value (eigenfrequency)$\bar{k}$, while $M(q)-1$ is the number of the associated functions$\vec{\tilde{U}}_{(m)}^{(q)}(g, \bar{k})$;$m=1,2,\ldots,M(q)-1$. The order of pole of the resolvent $[E+B(k)]^{-1}$ (and of the Green function $\tilde{G}(g, p, k)$ of the problem in (83), (84)) for $k=\bar{k}$is determined by a maximal value of$M(q)$.

9. Conclusion

The analytical results presented in the chapter are of much interest in the development of rigorous theory of two-dimensionally periodic gratings as well as in numerical solution of the associated initial boundary value problems. We derived exact absorbing boundary conditions truncating the unbounded computational space of the initial boundary value problem for two-dimensionally periodic structures to a bounded part of the Floquet channel. Some important features of transient and steady-state fields in rectangular parts of the Floquet channel were discussed. The technique for calculating electrodynamic characteristics of multi-layered structure consisting of two-dimensionally periodic gratings was developed by introducing the transformation operators similar to generalized scattering matrices in the frequency domain. In the last section, the elements of spectral theory for two-dimensionally periodic gratings were discussed.

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