very interesting not only because of its attractive potential applications but also in and of itself, and that many fundamental problems remain unsolved to date.

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Application of the scattering matrix method for calculating the optical properties of metamaterials

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We consider the application of the scattering matrix formalism for calculating the eigenfrequencies, radiation widths, and field distributions of quasiwaveguide modes in photonic crystal layers (PCLs) of finite thickness.

At present, investigations are being performed of one-dimensional (1D) or two-dimensional (2D) periodic layers of photonic crystals whose vertical geometry can be arbitrarily complex [1–3]. Such PCLs have proved to be very interesting and promising structures; they can be prepared by the modern methods of layer-by-layer lithography; their optical properties are of practical interest in connection with their potential compatibility with microelectronic devices.

We note that PCLs are in fact diffraction gratings. Diffraction gratings play an extremely important role in optics and its applications. Therefore, their history, of course, is considerably older than the term 'photonic crystal.' The first diffraction grating was created and investigated by the American astronomer D Rittenhause in 1786 [4]. (The curious history of the creation of the first diffraction grating is described in [5].) But this discovery remained unnoticed, and in the majority of optics courses and encyclopedias, the creation of the diffraction grating (in 1821) is credited to Fraunhofer [6]. In 1902, Wood [7] experimentally detected narrow-frequency features in the reflection spectra of metallic diffraction gratings, which have been called Wood's anomalies since then. Two types of Wood's anomalies are distinguished. Diffraction anomalies, or Rayleigh anomalies [8], appear upon opening (with increasing frequency of incident light) new diffraction channels; the threshold frequency of opening a channel is characterized by the fact that the arising diffracted beam is parallel to the surface of the lattice (see also [9]). Resonance anomalies are connected with the excitation of resonance modes in the lattice, namely, surface plasmons or quasiwaveguide (Fabry–Perot) modes, depending on the type of structure. The qualitative laws governing the behavior of such resonances were first analyzed, as far as we know, by Fano [10]. Twenty years later, Fano in his famous work [11] analyzed the general laws governing the behavior of a discrete level in the background of the continuum; the arising asymmetric resonances are now called Fano resonances. Wood's resonance anomalies refer to precisely this type of resonance.

In view of the importance of the effect of the resonance optical response of diffraction gratings for many applications, including, for example, lasers with a distributed feedback, optical filters, and polarizers, this issue has been considered in an enormous number of studies. The majority of methods are based on the expansion of the scattered field of the diffraction grating in terms of three-dimensional Fourier harmonics (plane waves), as was first suggested by Rayleigh [8]. With the advent of computers, very powerful methods of calculation of optical spectra of arbitrarily complex diffraction gratings were developed. In this connection, we note the important work by Hessel and Oliner [12] and the development of the scattering matrix formalism in [13, 14]. Very powerful computational methods were developed [15] and [16], but, unfortunately, they are practically unknown to modern researchers working in this field.

A convenient method of constructing a scattering matrix for 1D or 2D PCLs with an arbitrarily complex structure in the direction perpendicular to the layer was developed in [17, 18]. The authors of these works extended the method of constructing the scattering matrix in [19] to electrodynamics for calculating electron tunneling in complex heterostructures. The scattering matrix method allows efficiently removing the numerical instabilities that appear in the method of transfer matrices because of the presence of exponentially decreasing and exponentially increasing linearly independent solutions. This method allows constructing a scattering matrix on the complex frequency plane [20] and developing efficient approximate descriptions of photonic resonances in such structures.

We note that the application of the scattering matrix method for metamaterials involves certain difficulties because of the poor convergence of Fourier series for the metal–dielectric structures. Recently, we succeeded in con-siderably improving the convergence of the method [21], using Li factorization rules [22] and the Granet method of adaptive spatial resolution [23], by supplementing the latter with a special curvilinear transformation of coordinates matched to the shape of the metal–dielectric interface.

The modes in a planar waveguide, as is known, have real eigenenergies Ω, and the corresponding field distributions are localized near the waveguide layer and exponentially attenuate outside the waveguide. But in the case of a periodic modulation of the waveguide, a coupling of modes occurs with the continuum in the vacuum and in the substrate, and the quasiwaveguide modes acquire a finite radiation width. Only the waveguide modes with energies less than all diffraction thresholds remain undamped [24]. The spatial distributions of the electromagnetic fields of quasiwaveguide modes calculated at the natural *complex* frequency exponentially diverge as $z \to \pm\infty$. Although such solutions make no physical sense at first glance, a detailed analysis shows that this is not the case [15, 25]. These solutions increasing as $z \to \pm\infty$ have the physical meaning of eigenoscillations of the field in the waveguide that become damped in time; moreover, the solutions propagating into the vacuum and the substrate are finite because their exponential spatial growth is compensated by the decay of the eigenmode $\exp(-|\operatorname{Im}\Omega|\,t)$ damped in time. The space–time dependence of the solution, which is proportional to $\exp[|\operatorname{Im}\Omega|(z-ct)/c]$, describes the propagation of the front of the solution decaying in time.

In the theory of diffraction gratings, a traditional procedure is to construct the scattering matrix as a function of the complex propagation constant [13, 14] rather than the complex frequency [15]. The supporters of this approach believe that because the scattering matrix leads to 'nonphysical' solutions in the complex frequency plane, exponentially increasing in space, this method is mathematically inconsistent. Such increasing solutions have been known since the work of Thomson [26], who calculated the emission of an ideally conducting sphere. (For some reason, it has not been noticed that in constructing a scattering matrix as a function of the complex propagation constant, such exponentially increasing solutions also inevitably appear.) This apparent mathematical inconsistency, is removed by passing to non-stationary scattering, for example, to a decay; the exponential increase with moving away from the system is cut off by the exponentially decreasing time-dependent coefficient; as a result, the decay front moves with a limited amplitude. We also note that an essential advantage of constructing the scattering matrix in the complex frequency plane is the possibility of using causality relations.

The linear system eigenmodes are the nontrivial solutions of the equation

$$\mathbf{B}_{\text{out}} = S(\omega, \mathbf{k})\,\mathbf{B}_{\text{in}}, \tag{1}$$

which correspond to the zero vector of the amplitudes of the incoming waves $\mathbf{B}_{\text{in}}$. To find the eigenfrequencies of the system, it is necessary to find the scattering matrix on the complex plane. The causality principle ensures the absence of singularities in the scattering matrix on the upper half-plane of complex frequencies ω; but the S matrix can have poles at $\omega = \Omega - \mathrm{i}\gamma$, $\gamma \geqslant 0$, including those on the real axis. Such poles correspond to the decay of the mode in time at a rate proportional to $\propto \exp(-\mathrm{i}\Omega t - \gamma t)$ as $t \to \infty$, and γ determines their inverse lifetime. For $0 < \gamma \ll \Omega$, these modes are associated with sharp changes in the transmission spectra of

the photonic crystal structure and with a strong resonance increase in the field near it.

For each fixed value of the wave vector in the $\mathbf{k}$ plane, S matrix (1) as a function of ω on the complex plane can be obtained by an analytic continuation from the real ω axis on which it is defined uniquely [20]. We note that the analytic continuation of the S matrix from the real ω axis to the lower half-plane depends on the choice of the axis interval limited by the points of opening of diffraction channels from which this continuation is performed. We consider this problem in more detail.

A two-dimensional diffraction grating couples the incident electromagnetic wave with a frequency ω and a wave vector $\mathbf{k} = (k_x, k_y, k_z)$,

$$k_x = \frac{\omega}{c} \sin \vartheta \cos \varphi, \; k_y = \frac{\omega}{c} \sin \vartheta \sin \varphi, \; k_z = \frac{\omega}{c} \cos \vartheta, \; (2)$$

to all Bragg harmonics with the same frequency ω and the wave vectors

$$\mathbf{k}_{\mathbf{G},a}^{\pm} = (k_{x,\mathbf{G}}, k_{y,\mathbf{G}} \pm k_{z,\mathbf{G},a}), \tag{3}$$

where

$$k_{x,\mathbf{G}} = k_x + G_x, \; k_{y,\mathbf{G}} = k_y + G_y, \tag{4}$$

$$k_{z,\mathbf{G},a} = \sqrt{\frac{\omega^2 \varepsilon_a}{c^2} - (k_x + G_x)^2 - (k_y + G_y)^2}, \tag{5}$$

($a = $ v for the vacuum ($\varepsilon_v = 1$) and $a = $ s for a substrate), and

$$\mathbf{G} = \frac{2\pi}{d} (g_x, g_y, 0), \quad g_{x,y} = 0, \pm 1, \pm 2, \ldots \tag{6}$$

are the vectors of the reciprocal 2D lattice. In what follows, the following rule for choosing the square root sign is used: $\mathrm{Re}\sqrt{A} \geqslant 0$ for all complex A, and $\mathrm{Im}\sqrt{B} > 0$ for $\mathrm{Im}\, B = 0$ and $\mathrm{Re}\, B < 0$.

For a transparent nonabsorbing substrate, $\mathrm{Im}\,\varepsilon_s = 0$. Under this condition, Bragg harmonics (3), depending on the frequency of the incident light ω (real number), are either propagating ($\mathrm{Im}\,(k_{z,\mathbf{G}}) = 0$) or exponential ($\mathrm{Re}\,(k_{z,\mathbf{G}}) = 0$). Below, the harmonics that exponentially increase (exponentially decay) when moving away from the PCL are called exponential (increasing or decaying). They should not be confused with the damped solutions for a two-dimensional photonic crystal inside the forbidden band. If $k_{z,\mathbf{G},a}^2 > 0$, $a = $ v, s, then the corresponding harmonics are the non-damped propagating solutions both in the vacuum and in the substrate. If $k_{z,\mathbf{G},v}^2 < 0$ and $k_{z,\mathbf{G},s}^2 > 0$, the harmonics are exponential in the vacuum and propagating in the substrate. Finally, if $k_{z,\mathbf{G},a}^2 < 0$, then the corresponding harmonics are exponential on both sides of the PCL.

Thus, the $k_{\mathbf{G},v}^+$ and $k_{\mathbf{G},s}^-$ harmonics on the real ω axis, depending on whether the diffraction channel that corresponds to the reciprocal lattice vector $\mathbf{G}$ is open or is not open, are the solutions that either propagate toward the PCL or exponentially increase when moving away from it. They form a set of 'incoming' waves.

On the complex ω plane, the standard definition of the complex root in (5) for the 'propagating' harmonics, i.e., for $\mathrm{Re}\, k_{z,\mathbf{G},a}^2 > 0$, has a cut below the negative real semiaxis (i.e., at $\mathrm{Re}\, k_{z,\mathbf{G},a}^2 < 0$) and implies an analytic continuation of $k_{z,\mathbf{G},a}$ into the lower half-plane when $k_{z,\mathbf{G},a}^2$ intersects the *positive* real semiaxis, i.e., for open diffraction channels.

However, this cut prevents the analytic continuation of $k_{z,\mathbf{G},a}$ into the lower half-plane for closed diffraction channels. For these, it is therefore necessary to choose a cut in the definition of the square root differently, for example, to draw the cut under the *positive* real axis, as this is always done in the resonance theory.

Because the question of whether $k_{z,\mathbf{G},a}^2$ intersects the positive or negative real semiaxis as ω is shifted into the lower complex half-plane is equivalent to the question of whether the $\mathbf{G}$ diffraction channel is open or not at a given energy, the choice of the position of the square root cut is limited to the segment of the real axis of energies located between the adjacent diffraction thresholds.

The distribution of the amplitudes of the outgoing waves can be found by solving the homogeneous linear set of equations

$$RX = 0, \tag{7}$$

where $R \equiv S^{-1}$. As is well known, a homogeneous set of equations has a nontrivial solution only if its determinant is equal to zero. Therefore, dispersion curves are typically found by solving scalar equations equivalent to the vanishing condition for the determinant of the inverse scattering matrix as a function of ω and $\mathbf{k}$. But in numerical calculations, it is much more convenient to use the method of linearization of the inverse scattering matrix (a variant of the multidimensional Newton algorithm), which is as follows.

Instead of solving a dispersion equation nonlinear in frequency,

$$\det R(\omega, \mathbf{k}) = 0, \tag{8}$$

which gives the spectra of eigenmodes $\omega(k)$ for linear system (7), it is necessary to calculate the inverse scattering matrix and its derivative with respect to energy at a certain point ω_0 (for example, at the point where a certain state is obtained in the approximation of the empty lattice)

$$R_0 = R(\omega_0), \; R_0' = \left.\frac{\partial R}{\partial \omega}\right|_{\omega = \omega_0}. \tag{9}$$

We then obtain

$$R(\omega) \approx R_0 + (\omega - \omega_0) R_0'. \tag{10}$$

Instead of solving system (7), we can, as the first iteration, find nontrivial solutions for the linear approximation of the inverse S matrix in (10):

$$\left(R_0 + (\omega - \omega_0) R_0'\right) X = 0. \tag{11}$$

It can be seen that the last equation is equivalent to the *linear* problem for eigenvalues

$$-(R_0')^{-1} R_0 X = (\omega - \omega_0) X. \tag{12}$$

The computational effort for solving this linear problem is typically less than that required for calculating the inverse scattering matrix R. As a result, the $4N_g$ eigenvalues δ_j are found, which give approximate values for the solutions of Eqn (7): $\Omega_j = \omega_0 + \delta_j$. The closer to the point of linear expansion ω_0, i.e., the less the value of δ_j, the more precise these approximation become.
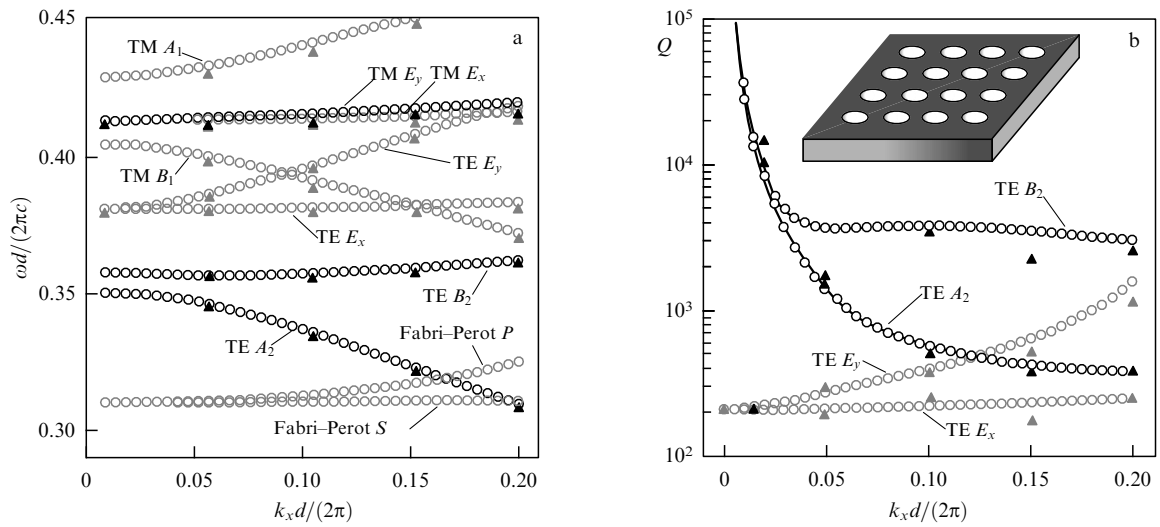
Figure. (a) Energies and (b) quality factors of quasiwaveguide modes of a photonic crystal layer schematically shown in the inset in Fig. 1b. The circles show the results of calculations by the scattering matrix method described in this paper; triangles correspond to the results of calculations by the finite-difference time-domain (FDTD) method [28].

The choice of the linear expansion point for the next iteration depends on which mode is sought and, correspondingly, which of the approximate solutions we should shift to. Typically, three iterations are found to be already sufficient for finding the nearest eigenvalue with a relative accuracy better than 10^{-5}.

The advantages of this method are obvious; instead of the repeated cumbersome calculation of the S matrix and the search for zeroes of the nonlinear scalar function of energy $\det R(\omega, \mathbf{k})$, which contains no information about the structure of the mode, we can implement the search by taking the structure of approximate modes into account, which allows a virtually complete automatization of data processing.

Furthermore, the 'remote' eigenvalues Ω_j and the corresponding vectors X_j allow judging on the qualitative structure of the spectrum and symmetry of resonance states, because the procedure described preserves all the symmetry properties of the S matrix.

If X is an eigenvector and and Δ is the eigenvalue of the matrix $-(R'_0)^{-1}R_0$, then by definition we have

$$-(R'_0)^{-1}R_0X = X\Delta. \tag{13}$$

It follows from (13) that

$$R_0 = -R'_0X\Delta X^{-1}. \tag{14}$$

Substituting this expression in (10), we obtain approximations for $R(\omega)$ as

$$R(\omega) \approx R'_0X(\omega - \omega_0 - \Delta)X^{-1}, \tag{15}$$

and for the matrix $S(\omega) = R^{-1}(\omega)$ as

$$S(\omega) \approx X(\omega - \omega_0 - \Delta)^{-1}(R'_0X)^{-1}. \tag{16}$$

If we now choose ω_0 to be the resonance energy of the multiplicity n found above, then the first n values $\Delta_{i,i}$ become zero and relations (16) allows explicitly isolating the resonance singularity in the scattering matrix.

We note in conclusion that in the case where the analytic continuation of the S matrix into the lower half-plane from the chosen interval of the real ω axis has poles whose distance to the diffraction thresholds is more than the distance to the real axis, then in order to analyze the optical properties of the system in this energy range, it suffices to examine only the analytic continuation of the S matrix from the selected interval. For example, this approach was used in [27] for an analysis of the manifestation of cell symmetry in the resonance features in the reflection spectra of PCLs. As an illustration of the capacity of this computational method, Fig. 1 shows the energies and the quality factors of the quasiwaveguide modes of a PCL schematically depicted in the inset in Fig. 1b (see also [29]). On the other hand, near the cutoff frequency of the quasiwaveguide mode, the poles of the scattering matrix closely approach the diffraction thresholds and begin to affect the spectral dependence of the S matrix elements on the adjacent intervals of the real ω axis. Such behavior was first analyzed in [30].

Thus, we have demonstrated a very efficient method of calculating eigenfrequencies, radiation widths, and the distribution of fields of quasiwaveguide modes in photonic-crystal layers of a finite thickness, which is based on the scattering matrix formalism.

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