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Optical Fano resonances in photonic crystal slabs near diffraction threshold anomalies

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Optical Fano resonances due to resonant eigenmodes in a layered periodically-modulated structure (photonic crystal slab) are investigated theoretically. The special attention is focused on the behavior of the resonances near a diffraction threshold. A new formulation of the resonant mode approximation for the optical scattering matrix near the diffraction threshold anomalies is proposed.

Layered periodic structures or photonic crystal slabs (PCS) [1] attract a great interest in modern nanooptics. A very convenient formalism for the numerical investigation of periodic structures is the Fourier modal method, also known as the rigorous coupled wave analysis [2], especially in the form of the optical scattering matrix (S-matrix) approach [3–5]. It is based on a decomposition of the solutions of the Maxwell's equations into a set of the Bloch waves. S-matrix connects the hypervectors of complex amplitudes of Bloch harmonics corresponding to the incoming and outgoing waves, $|I\rangle$ and $|O\rangle$,

$$S|I\rangle = |O\rangle. \tag{1}$$

The S-matrix method has been greatly improved in recent years with several techniques, such as factorization rules [6] and adaptive spatial resolution [7] (see, e.g., [8]). Due to this progress it is now possible to consider periodic structures with a complicated unit cell consisted of arbitrary materials including metals and anisotropic crystals. However, the needed computational time can still be very long. Therefore, physically clear approximations giving a qualitative, and, if possible, quantitative prediction of the system's properties are crucially important. In this paper we suggest a generalization of the resonant mode approximation (RMA) [9–11], which allows one to describe correctly the optical properties of PCS with the Fano-type resonances [12] near the Wood-Rayleigh diffraction threshold anomalies [13] (see an early analysis in [14]). The approximation is free of fitting parameters: all needed quantities are calculated from the eigenproblem for the linearized inverse S-matrix.

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Within the scattering matrix formalism, a resonant mode corresponds to the pole of the S-matrix or zero of the inverse S-matrix,

$$S^{-1}\left(\Omega_r, \mathbf{k}_\parallel\right)|O_r\rangle = 0. \tag{2}$$

Here Ω_r is a complex eigenfrequency of the mode and $|O_r\rangle$ is the corresponding output eigenvector. Equation (2) defines the dependencies of Ω_r and $|O_r\rangle$ on the in-plane component of the incoming light wavevector $\mathbf{k}_\parallel = (k_x, k_y)$, thus allowing to find the dispersion law of the resonant mode and its optical properties.

Far from the diffraction thresholds, if N different poles are located near the frequency range of interest, S-matrix can be represented [9–11] as a sum of slowly varying background and resonant parts S_b and S_r,

$$S = S_b + S_r = S_b + \sum_{r=1}^{N} \frac{A_r}{\omega - \Omega_r}. \tag{3}$$

Here matrices A_r depend on the corresponding input and output resonant vectors, $|I_r\rangle$ and $|O_r\rangle$,

$$A_r = |O_r\rangle\langle I_r|. \tag{4}$$

The details of this resonant mode approximation can be found in [10, 11, 15]. It allows one to evaluate the S-matrix near the resonances without fitting parameters. However, RMA in form of Eqs. (3), (4) fails near the diffraction thresholds where the folded dispersion curves cross the folded light cones

$$\Omega_t = \frac{c}{\sqrt{\varepsilon}}\left|\mathbf{k}_\parallel + \mathbf{G}\right|, \tag{5}$$

where $\mathbf{G}$ is the two-dimensional reciprocal lattice of the PCS and ε is the dielectric constant of the media to which the corresponding diffraction order is opened at this threshold photon frequency Ω_t.

On the other side, as shown in [16], S-matrix in the vicinity of the threshold can be represented as

$$S = S_0 + B\kappa, \tag{6}$$

where the parameter

$$\kappa = \frac{\sqrt{\varepsilon}}{c}\sqrt{\omega^2 - \Omega_t^2} \tag{7}$$

is a z-component of the wavevector of the new diffracted wave. This parameter is real above the threshold ($\omega > \Omega_t$) where the diffracted wave is propagating, and pure imaginary below the threshold.

However, if resonances approach the diffraction threshold, Eq. (6) becomes applicable only in a very narrow frequency range around the threshold. In order to propose a better approximation for this case, let us note first of all that Ω_t is the branching point of the S-matrix, thus, the analytical continuations of the inverse scattering matrix $S^{-1}(\omega)$ into $\mathrm{Im}\,\omega < 0$ part of the complex frequency plane, needed to describe the resonances, are different depending on whether the continuation is done from the segment $\omega > \Omega_t$ or $\omega < \Omega_t$ of the real frequency axis.

The situation simplifies greatly if S-matrix is considered as a function of κ instead of ω. Then the branching point at Ω_t is removed, and S-matrix as a two-sheet function of ω is mapped into a single-sheet function of κ. The "physical" segments of the real frequency axis above the threshold $\omega > \Omega_t$ and below the threshold $\omega < \Omega_t$ then correspond to the rays on the complex κ plane $\mathcal{A} = (\mathrm{Re}\,\kappa > 0, \mathrm{Im}\,\kappa = 0)$ and $\mathcal{B} = (\mathrm{Re}\,\kappa = 0, \mathrm{Im}\,\kappa > 0)$, respectively (see the straight thick lines in Fig. 1). The analytical continuation of $S(\kappa)$ into complex κ plane cannot have poles in the quadrant $\mathrm{Re}\,\kappa > 0$, $\mathrm{Im}\,\kappa > 0$, because $S(\omega)$ is analytical when $\mathrm{Im}\,\omega > 0$. Thus, all the poles of $S(\kappa, \mathbf{k}_\parallel)$ are below $\mathcal{A}$ and/or to the left of $\mathcal{B}$; the physically important resonances have to be close to these physical rays $\mathcal{A}$ and/or $\mathcal{B}$.

In what follows we consider the simplest case when there are only two poles κ_1 and κ_2 in the vicinity of the physical rays $\mathcal{A}$ and $\mathcal{B}$, respectively. Instead of Eq. (3) we can now write the Breit-Wigner type expression for the S-matrix as a function of κ as

$$S = S_b + S_r = S_b + \sum_{r=1,2} |O_r\rangle \frac{1}{\kappa - \kappa_r} \langle I_r|. \tag{8}$$

We will now demonstrate that Eq. (8) is really a very convenient approximation for S-matrix in the vicinity of the diffraction threshold, on example of a one dimensionally periodic PCS.

Let us consider, for simplicity, the near-threshold behavior of so called quasiguided modes [5]. Such resonances exist in periodically modulated planar dielectric waveguides; they originate from guided modes of the homogenized planar waveguide but acquire a finite lifetime due to multiple scattering on the periodic inhomogeneities of the modulated structure.

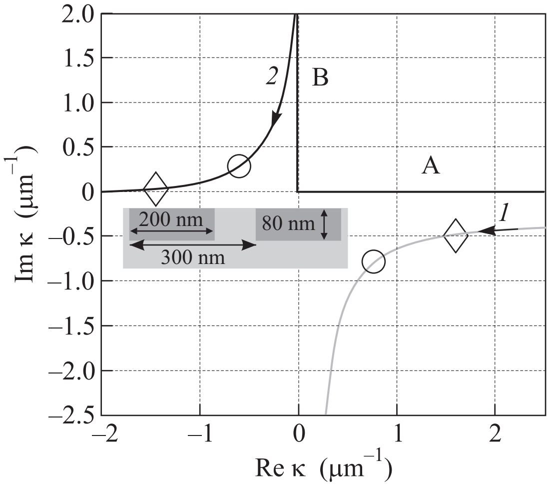

Fig. 1. The calculated trajectories of the poles $\kappa_{1,2}$ (curves 1,2, respectively) of $S(\kappa)$-matrix of the model structure on the complex κ plane. The in-plane momentum k_x is changed (see arrows) from 0 to 0.3 μm^{-1} in case of curve 2 and in the opposite direction in case of curve 1. The circles and rectangles denote the positions of poles at $k_x = 0.17\,\mu\mathrm{m}^{-1}$ and $k_x = 0.2\,\mu\mathrm{m}^{-1}$, respectively. Thick straight rays $\mathcal{A}$ and $\mathcal{B}$ correspond to the real frequency ranges above and below the threshold frequency Ω_t. The crossection of the model structure is shown in the insert

The model grating-type PCS (see the scheme in Fig. 1 inset) consists of the ZnO rectangular wires ($\varepsilon_w = 6.25$) embedded into quartz ($\varepsilon = 2.25$) substrate. The period of the structure is $d = 300$ nm, the height and the width of the wires are 80 nm and 200 nm, respectively. For the sake of simplicity we restrict ourselves to the case of inclined and perpendicular to the wires ($k_y = 0$) incidence from air of the incoming TM-polarized light wave (magnetic field parallel to the wires). We focus our attention on the first diffraction channel opening to the substrate. The corresponding folded light cone is given by

$$\Omega_t = \frac{c}{\sqrt{\varepsilon}}\left(\frac{2\pi}{d} - k_x\right). \tag{9}$$

The calculated trajectories of the poles $\kappa_{1,2}(k_x)$ when k_x is changed between 0 and 0.3 μm^{-1} are shown in Fig. 1. The calculation was done via the eigenproblem for the linearized inverse S-matrix near its zeroes as described in [10] (with the only difference that instead of the frequency plane, the linearization is done on the complex κ plane). It is clear that near the threshold ($\kappa = 0$) both κ_1 and κ_2 become important in Eq. (8), because they both are located at comparable distances from the physical rays $\mathcal{A}$ and $\mathcal{B}$. However, far from the threshold only one pole remains important: κ_1 above the threshold and κ_2 below the threshold.

The poles of the S-matrix as a function of frequency are then

$$\Omega_{1,2} = \sqrt{\Omega_t^2 + \frac{c^2\kappa_{1,2}^2}{\varepsilon}}. \qquad (10)$$

Figure 2 shows the real and imaginary parts of $\Omega_{1,2}$, corresponding to $\kappa_{1,2}$ in Fig. 1, as functions of k_x. It

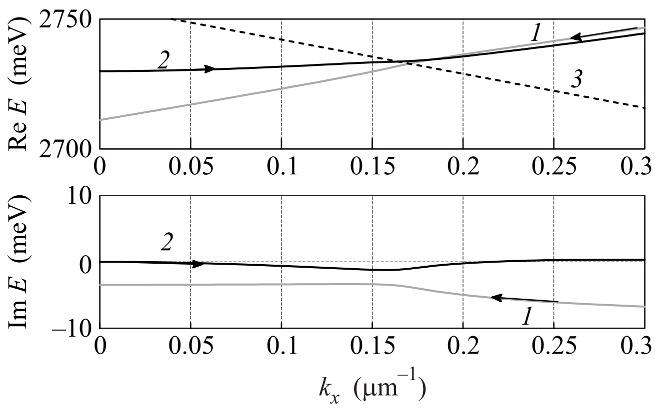

Fig. 2. The real and imaginary parts (upper and lowers panel, respectively) of the eigenenergies $\hbar\Omega_{1,2}$ (curves 1,2) as functions of k_x. Arrows correspond to the arrows in Fig. 1. Dashed straight line 3 in the upper panel is the folded light cone Eq. (9)

can be understood from Eq.(10) and Figs. 1,2 that Ω_1 and Ω_2 are the poles of the analytical continuation of S-matrix as a function of energy above and below the threshold, respectively. Note that the imaginary part of the pole frequency can even become positive if it is located far from the physical segment of the real frequency axis, i.e., far into the unphysical sheet of the S-matrix as a function of frequency.

For checking the approximation Eq. (8) it is representative to consider the cases of $k_x = 0.17\ \mu\mathrm{m}^{-1}$ and $0.2\ \mu\mathrm{m}^{-1}$. The results of calculations within the S-matrix method [5] (with 15 plane waves) in comparison with the modified resonant mode approximation Eq. (8) are shown in Fig. 3. As already noted above, the eigenvalues $\kappa_{1,2}$, input and output eigenvectors $|I_{1,2}\rangle$ and $|O_{1,2}\rangle$ in Eq. (8) are calculated via the eigenproblem for the linearized inverse S-matrix. This still leaves some freedom in defining the background matrix S_b. In both cases shown in Fig. 3 S_b was found from the condition that the exact S-matrix is equal to the approximate one on the threshold $\kappa = 0$. It can be seen that both the Fano-type anomaly and the kink-type Wood-Rayleigh

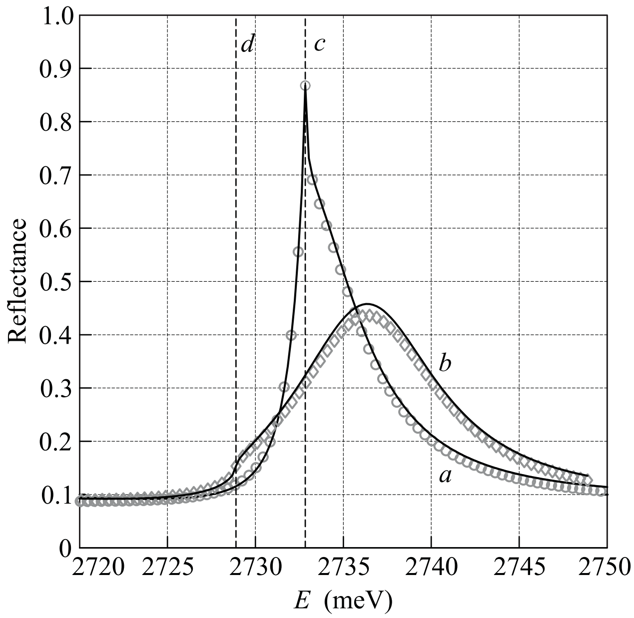

Fig. 3. The calculated reflectance spectra for $k_x = 0.17\ \mu\mathrm{m}^{-1}$ – a and $0.2\ \mu\mathrm{m}^{-1}$ – b. 15 spatial harmonics were taken. The vertical lines c and d denote the corresponding threshold frequencies. The solid lines are calculated via full S-matrix method, circles and diamonds show the resonant mode approximation Eq. (8)

peculiarity are correctly described by Eq. (8). Note that in case of $k_x = 0.17\ \mu\mathrm{m}^{-1}$ the asymmetric Fano-type resonance disappears, but the Wood-Rayleigh kink becomes resonantly enhanced.

To conclude, we have shown that the resonant mode approximation for the S-matrix of a photonic structure remains applicable near thresholds of new diffraction channels if one considers its wavevector parameter κ as the argument of the S-matrix instead of the photon frequency ω. We have demonstrated that this approximation describes very well the peculiarities of the optical spectra of a dielectric photonic crystal slab with a quasiguided mode near a diffraction threshold. We believe that this approach is more general and is applicable to all resonant modes in PCS, including, e.g., plasmonic resonances in metal-dielectric structures. The suggested formula generalizes the resonant mode approximation to the vicinity of diffraction thresholds and allows to describe both the Fano resonances and the Wood-Rayleigh anomalies in the optical spectra.

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