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Quantization of Electromagnetic Field and Analysis of Purcell Effect Based on Formalism of Scattering Matrix[1]

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Abstract—We have developed a rigorous self-consistent approach for the quantization of electromagnetic field in inhomogeneous structures. The approach is based on utilization of the scattering matrix of the system. Instead of the use of standard periodic Born-Karman boundary conditions, we use the quantization condition implying equating eigenvalues of the scattering matrix (S-matrix) of the system to unity (S-quantization). In the trivial case of uniform medium boundary condition for S-quantization is nothing but periodic boundary condition. S-quantization allows calculating modification of the spontaneous emission rate for arbitrary inhomogeneous structure and direction of the emitted radiation. S-quantization solves the long-standing problem coupled to normalization of the quasi-stationary electromagnetic modes. Examples of application of S-quantization for the calculation of spontaneous emission rate for the cases of Bragg reflector and microcavity are demonstrated.

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INTRODUCTION

Solution of a wave equation for electromagnetic field in infinite uniform media with refractive index n

$$\nabla \times \nabla \times \mathbf{E} = n^2 \left(\frac{\omega}{c}\right)^2 \mathbf{E} \tag{1}$$

gives continuous spectrum of eigenfrequencies of the mode ω. In order to provide quantum-mechanical desription of interaction of radiation and matter, field should be quantized: continuous spectrum of electromagnetic (EM) modes should be replaced by discrete one [1–3]. For this purpose EM field is considered in "quantization box" of "large" size (see Fig. 1a) and boundary conditions (BC) are to be set on the facets of the box. The natural choice is to set periodic (Born-Karman) BC

$$\begin{cases} E|_{x=0} = E|_{x=L_x} \\ \left.\dfrac{\partial E}{\partial x}\right|_{x=0} = \left.\dfrac{\partial E}{\partial x}\right|_{x=L_x} \end{cases},$$

$$\begin{cases} E|_{y=0} = E|_{y=L_y} \\ \left.\dfrac{\partial E}{\partial y}\right|_{y=0} = \left.\dfrac{\partial E}{\partial y}\right|_{y=L_y} \end{cases}, \tag{2}$$

$$\begin{cases} E|_{z=0} = E|_{z=L_z} \\ \left.\dfrac{\partial E}{\partial z}\right|_{z=0} = \left.\dfrac{\partial E}{\partial z}\right|_{z=z} \end{cases},$$

Wave equation (1) with BC (2) can be considered as eigenvalue and eigenfunction problem and the solution of the problem is given by a discrete set wavevectors $\mathbf{k} = (k_x, k_y, k_z)$ obeying

$$k_{x,y,z} = \pm 2\pi n N_{x,y,z} / L_{x,y,z}, \tag{3}$$

where $N_{x,y,z}$ are integers; corresponding eigenfunctions have the form of propagating planewaves

$$E = E_0 \exp(i(k_x x + k_y y + k_z z)). \tag{4}$$

We should note, that the same set of eigenvalues of the wave vector is provided by equating eigenvalues of the transfer matrix $\hat{M}$ along each direction x, y, and z through quantization box to unity, since the matrix along any particular direction (for example direction z) in the uniform media has a form

$$\hat{M}_z = \begin{pmatrix} \exp(ik_z z) & 0 \\ 0 & \exp(-ik_z z) \end{pmatrix}, \tag{5}$$

and its eigenvalues are equal to $\exp(\pm ik_z z)$.

[1] The article was translated by the authors.

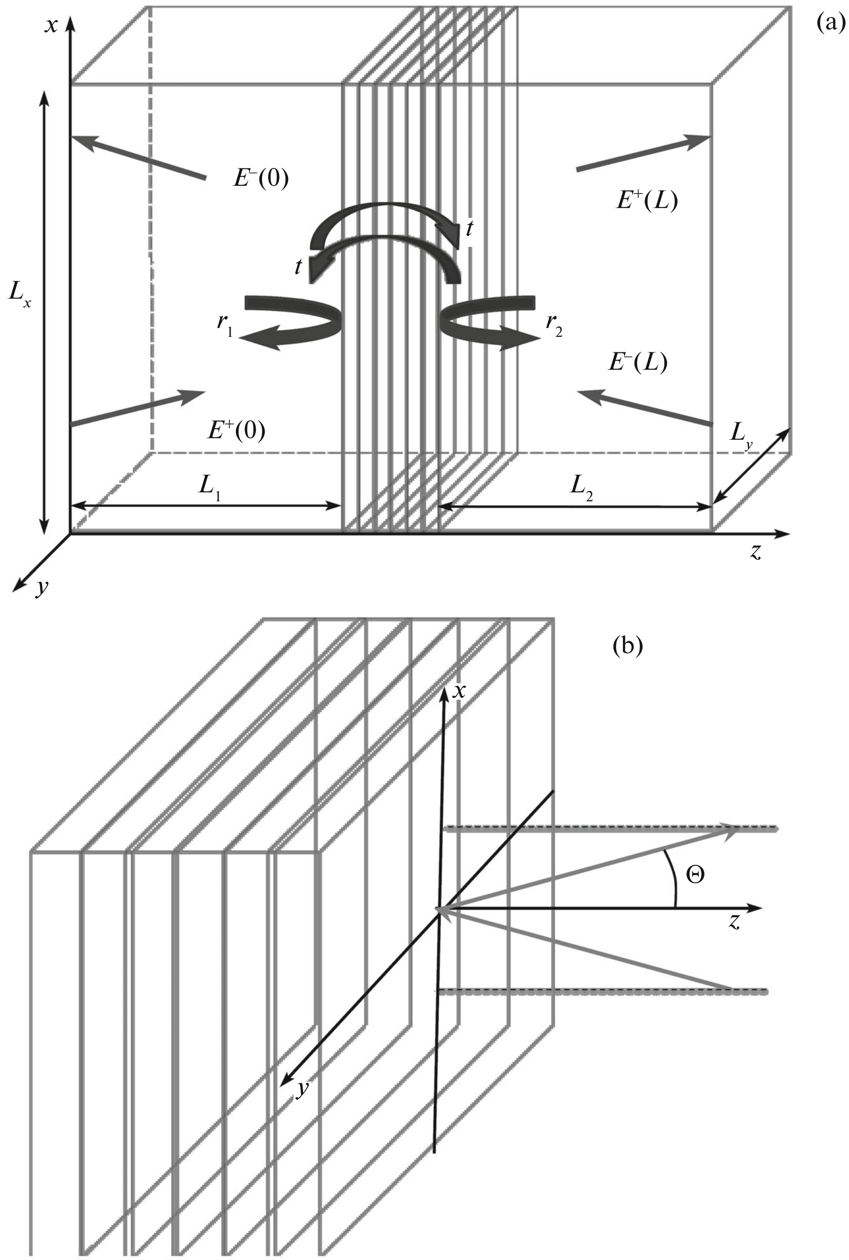

Fig. 1. (a) Layered structure in the quantization box. (b) Plane of incidence xOz, polar angle θ is reckoned from z-axis, azimuthal angle φ is reckoned from x- axis.

An analysis provided above leads to an expression for the density of states in K-space

$$\rho_k = \frac{dN}{dk_x dk_y dk_z} = \frac{n^3 V}{(2\pi)^3}, \tag{6a}$$

where $V = L_x L_y L_z$ is the volume of quantization box. Then, an expression for the density of states in respect energy reads

$$\rho = \frac{dN}{d(\hbar\omega)} = \frac{dN}{dK}\frac{dK}{d(\hbar\omega)} = \frac{n^3\omega^2}{\pi^2 c^3}\frac{V}{\hbar}. \tag{6b}$$

Each EM mode can be considered as quantum oscillator with an energy $\hbar\omega/2$, and this energy should be associated with an integral of the density of EM energy of the mode over quantization box [4]

$$\frac{1}{4\pi}\int_V n^2 E^2 d^3\mathbf{r} = \hbar\omega/2. \tag{7}$$

In the case of uniform media and periodic BC, the eigenmode of EM field is nothing but a plane wave with spatially uniform amplitude, and the amplitude of electric field for the quantized EM mode can be obtained,

$$E_0 = \frac{1}{n}\sqrt{2\pi\hbar\omega/V}, \quad (8)$$

which allows to obtain a probability of spontaneous emission W for the quantum transition characterized by dipole moment $\mathbf{d} = e\mathbf{r} = e\mathbf{r}(\cos\varphi_d\sin\theta_d, \sin\varphi_d\sin\theta_d, \cos\theta_d))$ using Fermi golden rule:

$$W = \frac{2\pi}{\hbar}|\langle f|\mathbf{Ed}|i\rangle|^2\rho, \quad (9)$$

where $\langle f|Ed|i\rangle$ is the matrix element for the transition between states $|i\rangle$ and $\langle f|$. Equations (6) and (8) allow to obtain Fermi golden rule in the form which does depend on a virtual quantization box [5]:

$$W = \alpha|\langle f|\boldsymbol{\epsilon}\mathbf{r}|i\rangle|^2\frac{4n\omega^3}{c^2}, \quad (10)$$

where we introduce dimensionless function $\boldsymbol{\epsilon}$ describing spatial distribution of the electric field of the mode satisfying relation $\mathbf{E} = nE_0\boldsymbol{\epsilon}$, where $\alpha = e^2/(\hbar c) \approx 1/137$ is the fine structure constant and $\boldsymbol{\epsilon}$ is a normalized vector describing an electric field of the EM mode. Note that function $\boldsymbol{\epsilon}$ satisfies normalization condition

$$\frac{1}{V}\int_V n^2\boldsymbol{\epsilon}^2 d^3\mathbf{r} = 1. \quad (11)$$

Half-century ago Purcell have shown experimentally [6], that probability of spontaneous emission can be increased substantially, if emitter is placed into a cavity. Purcell has proposed that density of states is no longer described by equation (6), but should be replaced by the quantity corresponding to a single oscillator in frequency range corresponding to the mode of the cavity, i.e.

$$\rho = Q/\omega_0, \quad (12a)$$

where Q is a quality factor of the cavity and ω_0 is the resonant frequency, and volume of the quantization box had to be replaced by actual (or effective) volume of the cavity V_c defined as

$$V_c = \frac{\int n^2E^2d^3\mathbf{r}}{(n^2E^2)_{\max}}, \quad (12b)$$

where term in the denominator describes maximal value of the density of electromagnetic energy for the cavity mode. As a result it was concluded that the probability of spontaneous emission is increased by the factor f (named Purcell factor)

$$f = \frac{3}{4\pi^2}\frac{Q\lambda^3}{V_c}, \quad (13)$$

where $\lambda = 2\pi c/\omega$. The equation (13) is correct when the decay of the cavity mode exceeds radiative decay of the emitter.

Note that the argument used by Purcell (replacement of the density of states defined by Eq. (6) with inverse spectral width of the cavity mode) is not the solution of a rigorously formulated mathematical problem (eigenstate problem for EM field with specific BC) but a flash of intuition.

An Eq. (13) does not allow to calculate the probability of spontaneous emission to the mode with specific directions and polarization (for example directionality of the emission from photonic crystals). Also, the use of Eq. (13) is problematic in the case of open optical systems, when the integral in Eq. (12) does not converge.

Quantization of electromagnetic field can be also done using outgoing wave BC [7], which results in a set of quasi-stationary states with complex energies. These states are analogues of the eigen-modes of Fabry–Perot cavity, and are also known in literature as quasi-stationary states [8], decaying states [9], resonant states (RS) [10], leaky modes [11], quasi-guided modes [12], quasi-normal modes [13, 14].

However, outgoing wave BC are not universal: they do not provide solutions for uniform media and within photonic band gaps of periodic structures. Numerical recipes based on application of Brillouin-Wigner (BW) perturbation theory [15, 16] to the set of quasi-stationary states can in principle treat the problem of renormalization of effective mode volume, but the formalism describing these numerical methods is rather cumbersome, and substantial computational efforts are required to achieve convergence of the results. The attempts to develop the procedure for the quantization of electromagnetic fields in inhomogeneous media based on canonical quantization of Lagrangian and Hamiltonian of the electromagnetic field [17, 18] can be formally considered as solution of the problem, but such attempts are characterized by extreme awkwardness of the developed formalism, which is impractical to use, in particular for the calculation of probability of spontaneous emission in arbitrary structures.

This paper is aimed at development of the procedure of quantization of electromagnetic field that would allow rigorous self-consistent description of the mode structure in the quantization box with inhomogeneity, and providing a way for the calculation of probability of spontaneous emission (Purcell effect) from multilayered structure for modes characterized by arbitrary direction of propagation and polarization.

THE FORMALISM

As was noted above periodic BC can be set by equating eigenvalues of transfer matrix through uniform quantization box to unity, providing a set of eigenvalues in the form of wavevectors. When inhomogeneity is inserted into quantum box, then wavevectors are not good quantum numbers anymore. On other hand, adequate description of inhomogeneous structure can be given by scattering matrix, which couples the waves incident on the structure (incoming waves) and outgoing waves.

We propose the procedure of quantization of electromagnetic field, based on *equating to unity eigenvalues of scattering matrix of the system*, or by equating incoming amplitudes and outgoing amplitudes.

Now we will define quantization procedure in details. Let us consider quantization box with layered structure within, as shown in Fig. 1a. The normal to the interfaces of the layers is parallel to the Oz axis, and the distances from the left and the right facet of the quantization box to layered structures are L_1 and L_2, as shown in Fig. 1a. In the case of such layered structure, it is convenient to consider mode of electromagnetic field with specific angular frequency ω in the form

$$E_{K_x,K_y}(x,y,z) = E(z)\exp(iK_x x)\exp(iK_y y), \quad (14a)$$

where the lateral components of the wavevector K_x and K_y relate to direction of propagation of the waves in empty parts of quantization box via relations

$$K_x = \frac{\omega}{c}\sin\theta\cos\varphi, \quad (14b)$$

and

$$K_y = \frac{\omega}{c}\sin\theta\sin\varphi. \quad (14c)$$

In the case of TE polarization electric field of the wave has the component E_y only, while for TM polarization there are components E_x and E_z.

In each layer of the structure, spatial dependence of electric field along z-axis is defined as superposition of the waves propagating in opposite directions along z-axis, and in the subsequent discussion we denote the wave with positive K_z with upper index "+," for negative K_z we will use upper index "–."

We denote amplitudes of the waves incident on the left and right facets of the quantization box as $E^+(0)$ and $E^-(L)$, and amplitudes of the waves outgoing from right and left boundaries as $E^+(L)$ and $E^-(0)$.

Amplitudes of the wave on left and right facets of the quantization box are coupled by relation

$$\begin{pmatrix} \lambda_2^* E^+_{K_x,K_y}(L) \\ \lambda_1^* E^-_{K_x,K_y}(0) \end{pmatrix} = \begin{pmatrix} t & r_1 \\ r_2 & t \end{pmatrix} \begin{pmatrix} \lambda_1 E^+_{K_x,K_y}(0) \\ \lambda_2 E^-_{K_x,K_y}(L) \end{pmatrix}, \quad (15)$$

where r_1 and r_2 are the amplitude reflection coefficients of layered structure for the waves incident from the left and right sides respectively, t is the amplitude transmission coefficient of layered structure, and the phases gained by waves propagating from the facets of quantization boxes to layered structures are given by $\lambda_{1,2} = \exp(iK_z L_{1,2})$. It follows from (9) that amplitudes of incoming waves $[E^+_{K_x,K_y}(0), E^-_{K_x,K_y}(L)]$ are coupled with amplitudes of outgoing waves $[E^+_{K_x,K_y}(L), E^-_{K_x,K_y}(0)]$ by scattering matrix $\hat{S}$

$$\begin{pmatrix} E^+_{K_x,K_y}(L) \\ E^-_{K_x,K_y}(0) \end{pmatrix} = \hat{S} \begin{pmatrix} E^+_{K_x,K_y}(0) \\ E^-_{K_x,K_y}(L) \end{pmatrix}, \quad (16)$$

and $\hat{S}$ reads

$$\hat{S} = \begin{pmatrix} \lambda t & \lambda_2^2 r_2 \\ \lambda_1^2 r_1 & \lambda t \end{pmatrix}, \quad (17)$$

where $\lambda = \lambda_1\lambda_2$.

Eigenvalues of $\hat{S}$ matrix reads

$$\beta^{(1,2)} = \lambda(t \pm \sqrt{r_1 r_2}), \quad (18)$$

and related eigenvectors are

$$B^{(1,2)} = [1, \pm(\lambda_1/\lambda_2)\sqrt{r_1/r_2}]. \quad (19)$$

Periodic BC imply equating the field on the opposite sides of the quantization box, which is equivalent to the equating eigenvalues of scattering matrix to unity. Here we provide quantization of the field using different BC: we equate "incoming" and "outgoing" fields, what means equating the eigenvalues of the scattering matrix $\hat{S}$ to unity:

$$\beta^{(1,2)} = 1. \quad (20)$$

Solution of eq. (20) in respect to frequency thus gives the spectrum of eigenfrequencies. Using the set of quantum numbers, one can obtain the eignenvectors $B^{(1)}$ and $B^{(2)}$, and calculate the field profile of the mode using the transfer matrix method. The components of the eignevectors $B^{(1,2)}$ are the complex amplitudes of the fields incident on the edges of the box, and the field of the mode is the superposition of the fields, excited by waves incident on the structure from opposite directions, and corresponding spatial profiles of the electric field described by the functions $\tilde{\epsilon}^{(1,2)}$.

Similar to the case of periodic BC, we can consider the mode obtained using S-quantization as elementary quantum oscillator and normalize it using equation (11). The field of the mode should be normalized according to eq. (7). We denote BC (20) as S-conditions, and the procedure of quantization described above as S-quantization.

In the case of uniform media, BC given by Eq. (20) is nothing but periodic BC. At the same time, the modes defined by eigenvectors $B^{(1)}$ and $B^{(2)}$ with field distribution described by functions $\epsilon^{(1)}$ and $\epsilon^{(2)}$ respectively, will not be plane waves, propagating in opposite directions, but will be standing waves of equal amplitude, shifted by the quarter of wavelength.

In non-absorbing media eigenfrequencies defined by Eq. (20) are real, which reflects equity of incoming and outgoing fluxes. Eq. (18) can be rewritten in the form

$$\beta^{(1,2)} = \exp(iK_z L + \alpha), \tag{21}$$

where α is a phase, defined by reflection and transmission coefficients of layered structure and is depending on frequency of the light. When size of quantization box is large enough in respect to layered structure, $K_z L$ varies much faster then α with increasing frequency, and one-dimentional density of states in K-space reads $\frac{dN}{dK_z} = L/(2\pi)$, as in the case of uniform media, and 3D density of states is given by Eq. (6).

In non-uniform media, spatial envelope function of electric field of the mode is not constant, and probability of spontaneous emission is defined by the magnitude of an electric field of the mode at the position of emitting dipole. For each eigenvalue $\beta^{(1,2)}$ the spatial profile of the field of EM mode is a superposition of the fields excited by the two waves incident from left and right sides of the structure with the frequencies defined by Eq. (20), and the amplitudes of these two waves are coupled by Eq. (19). As usual, each mode should be considered as elementary quantum oscillator, and normalized using Eq. (7).

Let us consider the situation when the K-vector of light in empty quantization box is within the light cone, i.e. $K_x < \omega/c$. The formalism corresponding to waveguide modes will be given elsewhere [19]. In this case light can leak from the structure into the quantization box. If the size of quantization box goes to infinity, then the contribution of the layered structure to value of integral (7) will be negligible, and the integral (7) will be equal to the contribution given by the wave in empty parts of quantization box. Thus, the amplitude of electric field of EM mode, normalized using Eq. (7) incident on empty quantization box, and incident on quantization box with layered structure, will be equal.

Since density of states provided by S-quantization is the same density of states as setting periodic BC, for the specific EM mode probability of spontaneous emission given by Eq. (10) for the dipole in layered structure will be defined by modification of the amplitude of electric field vector $\tilde{\boldsymbol{\epsilon}}$ in layered structure.

The physical results should not depend on the size of quantization box. The size of quantization box can be chosen to provide equity of the solution of Eq. (20) to any predefined frequency, and λ_1 can always be chosen equal to λ_2. When the size of quantization box is approaching infinity, the spectrum of eigen-frequencies defined by Eq. (20) become quasi-continuous. Thus, the modification of spatial profile of the field within layered structure defined by functions $\tilde{\boldsymbol{\epsilon}}^{(1,2)}$ does not depend on the size of the left and right empty parts of quantization box, and is defined only by reflection coefficients r_1 and r_2 and transmission coefficient t of the layered structures see Eq. (19).

An approach based on modification of spatial profile of the modes in microcavities has been used by De Martini [20], though the use of periodic BC limits an applicability of results obtained in this work. An approach used in [20] corresponds to the use of only "symmetric" eigenvector $B^{(1)}$, while the mode corresponding to "antisymmetric" eigenvector $B^{(2)}$ is missed in [20, 21]. However, if an emitter is placed at the center of a symmetric structure (as has been done in [20]) absence of $B^{(2)}$ does not affect the validity of the results, since the value of the mode field corresponding to $B^{(2)}$ is zero in center of the symmetric structure. If the dipole is placed into arbitrary place in the structure without specific symmetry, the modes corresponding to both $B^{(1)}$ and $B^{(2)}$ should be taken into account.

For a development of the formalism it is convenient to relate components of vector $\tilde{\boldsymbol{\epsilon}}^{(1,2)}$ describing electric field in layered structure to the components of vector $\boldsymbol{\epsilon}^{(1,2)}$ for uniform medium, via coefficients X, Y, and Z as specified below. For TE mode

$$\tilde{\boldsymbol{\epsilon}}^{(1,2)} = (0 \;\; \tilde{\epsilon}_y^{(1,2)} \;\; 0) = (0 \;\; Y^{(1,2)}\epsilon_y^{(1,2)} \;\; 0), \tag{22}$$

while for TM mode

$$\tilde{\boldsymbol{\epsilon}}^{(1,2)} = (\tilde{\epsilon}_x^{(1,2)} \;\; 0 \;\; \tilde{\epsilon}_z^{(1,2)}) = (X^{(1,2)}\epsilon_x^{(1,2)} \;\; 0 \;\; Z^{(1,2)}\epsilon_z^{(1,2)}). \tag{23}$$

It is also convenient to define *directional Purcell factor* for a specific mode characterized by direction of propagation defined by the polar angle θ of wave in free space as a ratio of probability of spontaneous emission for this mode to probability of spontaneous emission in the free space, when dipole is parallel to the field of the mode:

$$F_\theta^{(TE)} = \frac{|\langle f|\tilde{\boldsymbol{\epsilon}}\mathbf{r}|i\rangle|^2}{|\langle f|\epsilon r|i\rangle|^2}. \tag{24}$$

Such definition of directional Purcell factor will be convenient for the subsequent analysis of the Purcell effect in the case of waveguide modes.

Similarly, the dot product in Eq. (24) for TE modes reads

$$\tilde{\boldsymbol{\epsilon}}^{(1,2)}\mathbf{r} = \tilde{\epsilon}_y^{(1,2)} r_y = Y^{(1,2)}\epsilon_y^{(1,2)} r_y, \tag{25}$$

and for TM mode

$$\tilde{\boldsymbol{\epsilon}}^{(1,2)}\mathbf{r} = \tilde{\epsilon}_x^{(1,2)} r_x + \tilde{\epsilon}_z^{(1,2)} r_z = X^{(1,2)}\epsilon_x^{(1,2)} r_x + Z^{(1,2)}\epsilon_z^{(1,2)} r_z. \tag{26}$$

Therefore, the Purcell factor for specific TE mode characterized by emission angle θ is

$$F_\theta^{(TE)} = \sum_{i=1,2} |Y^{(i)}|^2 (r_y/r)^2 = \sum_{i=1,2} |Y^{(i)}|^2 \sin^2\varphi_d \sin^2\theta_d, \tag{27}$$

while for TM mode

$$F_\theta^{(TM)} = \sum_{i=1,2}\left|X^{(i)}\frac{\epsilon_x^{(i)}}{|\epsilon^{(i)}|}\frac{r_x}{r} + Z^{(i)}\frac{\epsilon_z^{(i)}}{|\epsilon^{(i)}|}\frac{r_z}{r}\right|^2$$
$$= \sum_{i=1,2}|X^{(i)}\cos\theta\cos\varphi_d\sin\theta_d + Z^{(i)}\sin\theta\cos\theta_d|^2. \tag{28}$$

In the case of TE polarization, for the dipole oriented along y-axis, directional Purcell factor is nothing but

$$F_\theta^{(TE)} = \sum_{i=1,2}|Y^{(i)}|^2. \tag{29a}$$

For the dipole, oriented along axis Ox the Purcell factor for TM modes reads

$$F_\theta^{(TM)} = \sum_{i=1,2}|X^{(i)}|^2\cos^2\theta, \tag{29b}$$

and for the orientation of dipole along Oz axis

$$F_\theta^{(TM)} = \sum_{i=1,2}|Z^{(i)}|^2\sin^2\theta. \tag{29c}$$

Thus the quantities X, Y, and Z define the probability of spontaneous emission in layered structure within the light cone.

The Purcell factor in its usual sense, describing the total probability emission of emission rate into the free space is given by integration of directional Purcell factor $F_\theta^{(TM)}$ over the whole solid angle 4π. Note that such integration should imply averaging over all possible orientation of a dipole, where necessary.

RESULTS AND DISCUSSION

The equations for eigenvalues (18) and eigenvectors (19) of scattering matrix become extremely simple in the case of symmetric structure. When $\lambda_1 = \lambda_2$ and $r_1 = r_2 = r$, eigenvalues reads $\lambda(t \pm r)$ while corresponding $B^{(1,2)} = [1, \pm 1]$. In this case the mode $\tilde{\epsilon}^{(1)}$ corresponding to eigen-vector $B^{(1)}$ becomes purely symmetric, while the mode $\tilde{\epsilon}^{(2)}$ becomes anti-symmetric. For subsequent analytical transformations of the formalism, it is interesting to note that for symmetric structure amplitude reflection and transmission coefficients r and t are coupled by a relation $|t \pm r| = 1$ [22]. For uniform space, variations of $\tilde{\epsilon}^{(1)}$ and $\tilde{\epsilon}^{(2)}$ is described by standing waves shifted by quarter-wave.

Figure 2 shows the profiles of electric field for the modes $\tilde{\epsilon}^{(1)}$ and $\tilde{\epsilon}^{(2)}$ characterized by $\theta = 0$ (normal incidence) for the Bragg reflector placed into the quantization box for the frequencies below stop band, at the center of stop band, and on the edge of the stopband. The Bragg reflector was constructed from 16 pairs of quarter-wave layers with the refractive indices 1.45 and 2.2 (corresponding to silica and titania); the structure is surrounded by vacuum. Thus the thicknesses satisfy the condition

$$n_1d_1 = n_2d_2 = \pi c/2\omega_{BR}. \tag{30}$$

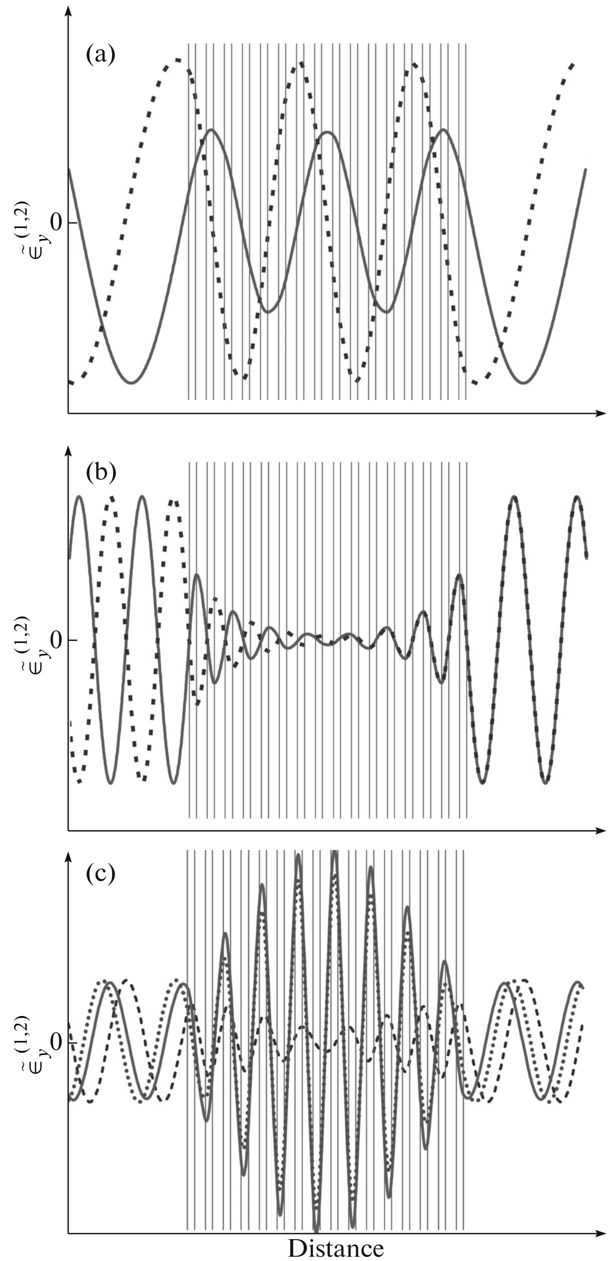

Fig. 2. The profiles of the electric field for the modes $\tilde{\epsilon}^{(1)}$ and $\tilde{\epsilon}^{(2)}$ (solid and dashed curves) the modes obtained by using BC (20) for the Bragg reflector placed in a "box of quantization," for the frequency of eigenmodes (a) the lower allowed band, (b) in the center of PBG, and (c) on the edge of the PBG. The dotted line in the Fig. 2c shows the profile of the field obtained using outgoing wave boundary conditions.

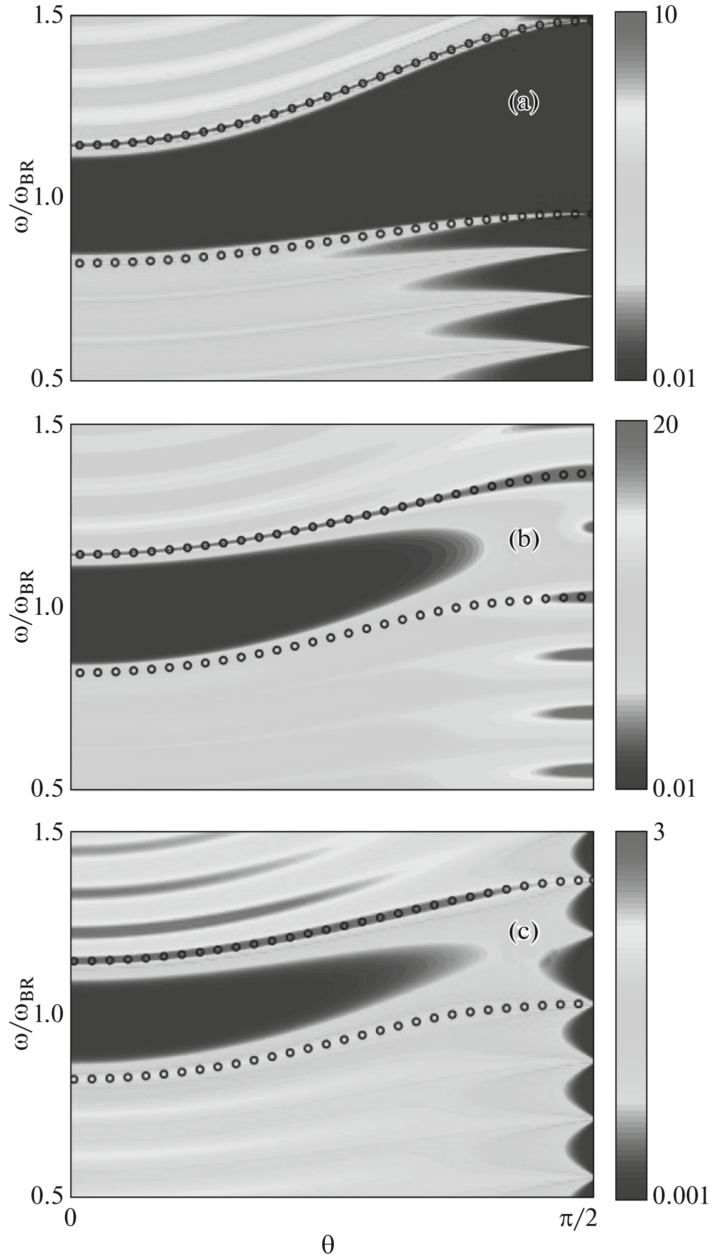

Fig. 3. Dependencies of the quantities Y (a); X (b); and Z (c) on the emission angle θ and frequency ω for the Bragg reflector; emitter is positioned at the centre of the structure. The circles mark the dispersion of the mode obtained using outgoing wave boundary conditions.

In the photonic band structure of Bragg reflector the band gap is centered at frequency ω_{BR}, and the width of the band gap is defined by the contrast of the refractive indices n_1 and n_2. It was predicted [23, 24], that in infinite photonic crystal probability of spontaneous emission is reduced to zero for the frequencies corresponding to bandgap, but for the structures of the finite size it is obviously not the case.

For the modes within the first allowed band, the fields are standing waves outside the structure and standing Bloch waves within the structure.

For the mode, corresponding to the ω_{BR}, shown in Fig. 2b, the spatial structure of the mode is dramatically changed: the modes exponentially decay towards the center of the structure, and then, growth toward the opposite edge. In the surrounding media the modes are standing waves of constant amplitude, but unlike the case of uniform media the modes $\tilde{\boldsymbol{\epsilon}}^{(1)}$ and $\tilde{\boldsymbol{\epsilon}}^{(2)}$ are either coincides or shifted by half wavelength in respect to each other. Such peculiar spatial profile indicate that there are areas *outside* the structure, where emission is either suppressed or enhanced. Within the structure, the field (and probability of emission) is falling into the depth of the structure, but the decrease is not monotonic, an envelope of the field also oscillates. Thus, the proposed procedure of S-quantization describes qualitatively suppression of spontaneous emission inside photonic crystals.

For the mode, corresponding to the edge of the bandgap, (see Fig. 2c), envelop of the field, corresponding to $\tilde{\boldsymbol{\epsilon}}^{(1)}$ is reducing when approaching center of the structure, while for $\tilde{\boldsymbol{\epsilon}}^{(2)}$ the field in the structure is increased. For comparison, the profile of the mode obtained using outgoing wave BC with complex frequency (1.16–0.0025i) eV, is also shown. It can be seen that this mode is very similar to the mode, decribed by the function $\tilde{\boldsymbol{\epsilon}}^{(1)}$. This is a manifestation of eigenmodes of the photonic crystals called edge states which are used in distributed feedback lasers [25] and are responsible for appearance of Bragg polaritons states [26].

Figure 3 shows the dependencies of the quantities

$$Y = (Y^{(1)})^2 + (Y^{(2)})^2 \tag{31a}$$

(Fig. 3a),

$$X = (X^{(1)})^2 + (X^{(2)})^2 \tag{31b}$$

(Fig. 3b), and

$$Z = (Z^{(1)})^2 + (Z^{(2)})^2 \tag{31c}$$

(Fig. 3c), defining Purcell effect for the Bragg reflector described above for the dipole, placed into the center of the structure. For all cases, a pronounced band reduced emission probability, mimicking a photonic band gap of the Bragg reflector is clearly seen. For TE polarization, the bandgap is increased with increasing emission angle, while for TM polarization, the quantities X and Z mark a reduction of the width of photonic band gap with increasing Θ.

There is also line of enhanced efficiency of emission, near the upper boundary of the band gap. This line corresponds to gap edge state, shown in Fig. 2c. Note, that there is no feature in the emission pattern, corresponding to edge state in the lower boundary of the bandgap, since upper and lower band edge states have different parity.

Figure 4 shows the profiles of the electric field for the modes $\tilde{\boldsymbol{\epsilon}}^{(1)}$ and $\tilde{\boldsymbol{\epsilon}}^{(2)}$ obtained by using BC (20) for the microcavity placed in a "box of quantization," for the frequency corresponding to an eigenmode of a microcavity. The microcavity structure is formed by two Bragg reflectors as described above that confine a layer with optical thickness corresponding to one wavelength for the frequency ω_{BR}. It can be seen, that an envelope of the field corresponding to $\tilde{\boldsymbol{\epsilon}}^{(1)}$ exponentially increases from edges towards center of the structure repeating the profile corresponding to eigenmode with complex frequency $(1.0 - 0.0002i)\omega_{BR}$, obtained using outgoing wave BC, while $\tilde{\boldsymbol{\epsilon}}^{(2)}$ quickly vanishes within a depth of the structure. Dependence of the quantities Y, X and Z on angle θ and the frequency of the emitted light is shown in Fig. 5. Within the bandgap probability of emission is suppressed, but for eigenmode of the microcavity, whose frequency is defined by outgoing wave BC [26] probability of emission is substantially increased. Thus S-quantization depicts simultaneously the features of corresponding to band gap (suppression of the emission probability) and localized eigenstates (increase of the emission probability).

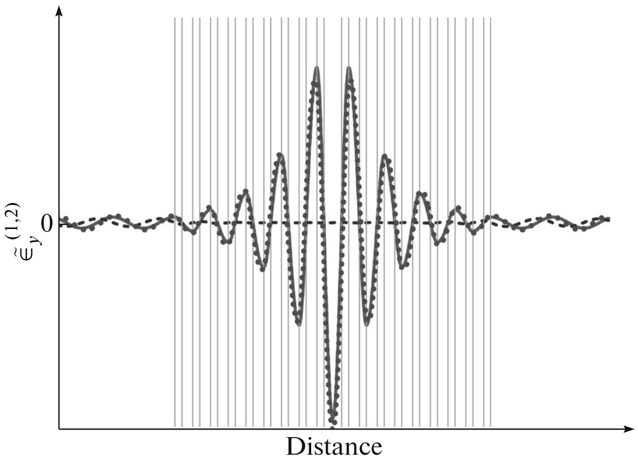

Fig. 4. The profiles of the electric field for the modes $\tilde{\boldsymbol{\epsilon}}^{(1)}$ and $\tilde{\boldsymbol{\epsilon}}^{(2)}$ (solid and dashed curves) obtained by using BC (20) for the microcavity placed in a "box of quantization," for the frequency corresponding to an eigenmode of a microcavity. Green dotted line shows the profile of the field of microcavity eigenmode obtained using outgoing wave boundary conditions.

CONCLUSION

We have developed a rigorous self-consistent procedure of quantization of electromagnetic field for non-uniform media, when arbitrary layered structure is present in the quantization box (S-quantization). Instead of using periodic (Born- von Karman) boundary conditions, implying an equating the wave amplitude and its derivative on opposite facets of quantization box, our model requires equity of incoming and outgoing amplitudes, and quantizes electromagnetic field by equating eigennumber of scattering matrix of the system to unity (S-boundary conditions). In the case of uniform media, S-conditions become equivalent to Born- von Karman boundary conditions. The procedure of the calculation of direction-dependent modification of spontaneous emission rate (Purcell effect) for arbitrary layered structure based on S-quan-

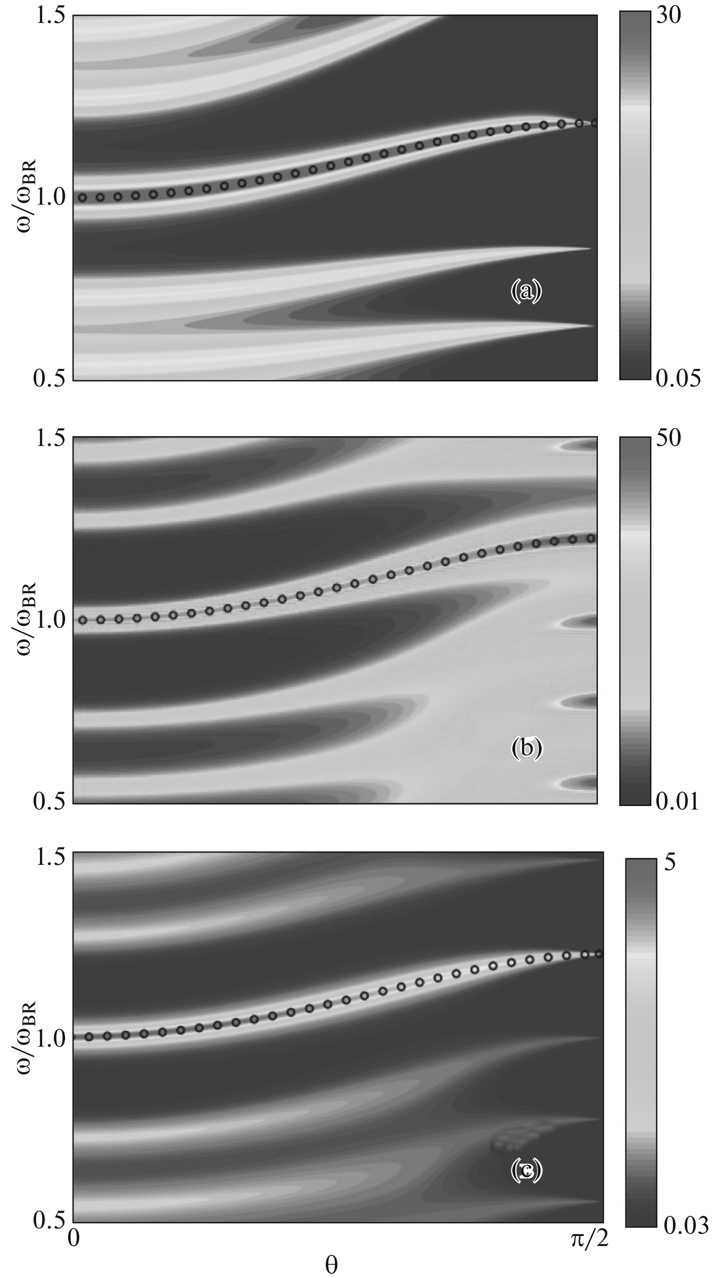

Fig. 5. Dependencies of the quantities Y (a); X (b); and Z (c) on the emission angle θ and frequency ω for the microcavity. The circles mark the dispersion of microcavity eigenmode obtained using outgoing wave boundary conditions.

tization has been developed. The procedure is rigorous and allows to avoid difficulties, coupled to normalization of quasi-stationary mode and originating from divergence of the integral, describing a mode volume in open system. The procedure is applied to calculation of directional dependence of spontaneous emission rate for Bragg reflectors and microcavities.

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