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Quantization of the Electromagnetic Field in Three-Dimensional Photonic Structures on the Basis of the Scattering Matrix Formalism (*S* Quantization)

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Abstract—A technique for quantization of the electromagnetic field in photonic nanostructures with three-dimensional modulation of the dielectric constant is developed on the basis of the scattering matrix formalism (*S* quantization in the three-dimensional case). Quantization is based on equating the eigenvalues of the scattering matrix to unity, which is equivalent to equating each other the sets of Fourier expansions for the fields of the waves incident on the structure and propagating away from the structure. The spatial distribution of electromagnetic fields of the modes in a photonic nanostructure is calculated on the basis of the R and T matrices describing the reflection and transmission of the Fourier components by the structure. To calculate the reflection and transmission coefficients of individual real-space and Fourier-space components, the structure is divided into parallel layers within which the dielectric constant varies as a function of two-dimensional coordinates. Using the Fourier transform, Maxwell's equations are written in the form of a matrix connecting the Fourier components of the electric field at the boundaries of neighboring layers. Based on the calculated reflection and transmission vectors for all polarizations and Fourier components, the scattering matrix for the entire structure is formed and quantization is carried out by equating the eigenvalues of the scattering matrix to unity. The developed method makes it possible to obtain the spatial profiles of eigenmodes without solving a system of nonlinear integro-differential equations and significantly reduces the computational resources required for calculating the probability of spontaneous emission in three-dimensional systems.

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1. INTRODUCTION

Understanding the interaction of radiation with matter [1] is an important problem in modern physics, which attracts much interest due to the possibility of creating optoelectronic devices with adjustable characteristics. It is known that media with an inhomogeneous dielectric constant allow control of the direction and probability of spontaneous emission [2]. In particular, the probability of spontaneous emission can significantly increase for the eigenmode of a resonator [3]. In media in which the dielectric constant varies periodically in space and the Bragg diffraction of light is observed, there forms a photonic band gap where spontaneous emission can be completely suppressed [4, 5]. In recent years, attention has been drawn to studies of nanostructures designed in a special way [6] that possess a number of interesting properties; thus, lasing was obtained in metal/semiconductor resonators with three-dimensional modulation of the dielectric constant [7]. Of interest are systems featuring a complex photonic band structure [8], potentially applicable in the terahertz range.

To describe the interaction of radiation with matter, a procedure for quantization of the electromagnetic field in a homogeneous "quantization box" was developed, which makes it possible to deal with a quasi-continuous frequency spectrum instead of a continuous one. The quantization procedure involves setting the boundary conditions at the boundaries of the quantization box. Traditionally, Born–Karman periodic boundary conditions have been used [1, 9, 10]. To calculate the probability of spontaneous emission in layered structures, a method taking into account changes in the spatial structure of the electromagnetic-field modes was proposed in [11]. However, in the case of an inhomogeneous medium, the analysis of the mode structure of a field on the basis of periodic boundary conditions is not strict and self-consistent:

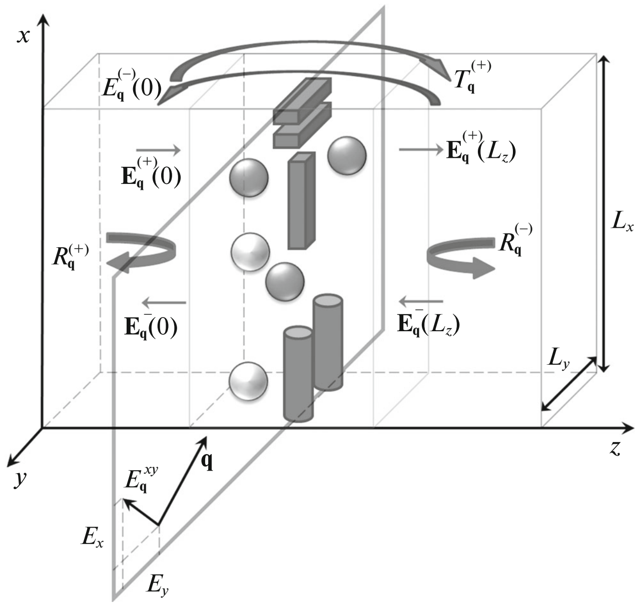

Fig. 1. Layout of the structure placed in a quantization box.

the presence of inhomogeneities can cause significant changes in the mode structure calculated on the basis of periodic boundary conditions, which can lead to inaccurate results in the study of finite-size systems [12]. Numerical algorithms for calculating the probability of spontaneous emission on the basis of Green's functions [13] or expansion of the field by eigenmodes or quasi-guided states [14] require significant computational resources when implemented for large three-dimensional systems and can encounter problems concerning the convergence of the results.

A strict and self-consistent procedure for the quantization of an electromagnetic field and calculation of the probability of spontaneous emission in inhomogeneous media can be implemented on the basis of the S-quantization formalism [15], in which the quantization condition is the equivalence of the amplitudes of waves incident on the structure and those of outgoing waves.

Here, we develop the S-quantization formalism for media with three-dimensional modulation of the dielectric constant.

2. QUANTIZATION OF AN ELECTROMAGNETIC FIELD

Let us consider an arbitrary structure with three-dimensional inhomogeneities. It is necessary to choose a system of coordinates within this medium. Since most structures currently fabricated have a preferred axis (the growth axis), we choose it as the z axis. Typically, the thickness of the structure along this axis (denoted here as L_z) is much smaller than the transverse dimensions of the structure in the xy plane. We assume that the characteristic transverse dimensions of the structure in this plane are $L_x \times L_y$ (see figure 1). This makes it possible to expand any variable pertaining to the field-quantization problem into a Fourier series in two dimensions. For example, an electric field can be represented as

$$\mathbf{E}(x, y, z) = \sum_{\mathbf{q}} \mathbf{E}(z)_{\mathbf{q}} \exp(i\mathbf{q}\boldsymbol{\rho}). \tag{1}$$

Here, the components of the two-dimensional vector $\mathbf{q} = (q_x, q_y)$ take on values of $2\pi M_{x,y}/L_{x,y}$, where $M_{x,y}$ are integers, and vector $\boldsymbol{\rho}$ lies in the xy plane. Evidently, this transformation does not generally allow an arbitrary angle of incidence of a wave on the structure. However, one can choose rather large transverse dimensions of the structure, so that the transverse wave vector will be close to one of the vectors $\mathbf{q}$, provided that the number of terms in the expansion is large enough. In particular, for waves of the optical range it is sufficient that the transverse dimensions of the structure exceed 100 μm.

Furthermore, due to the linearity of Maxwell's equations, any wave incident on the structure can be presented as the sum of two polarizations with either the E_x or E_y component vanishing. We note that these polarizations have nothing to do with the TE or TM polarizations, since there is no plane of incidence as such.

As will be shown in the next section, the x and y components of the electric and magnetic fields uniquely determine the solution of Maxwell's equations, and, thus, to solve the quantization problem it is sufficient to determine the vector of Fourier coefficients for the x and y components of an electric field. It is assumed below in this section that, wherever the index q occurs in matrix notation, it runs twice the entire set of values in Fourier space, once for each of the coordinate components of the electric field.

The S-quantization procedure is based on constructing a scattering matrix, which relates the amplitudes of the waves incident on the structure to those of waves emitted by the structure. Thus,

$$\begin{pmatrix} E_{\mathbf{q}}^{(+)} & (L_z) \\ E_{\mathbf{q}}^{(-)} & (0) \end{pmatrix} = \hat{S} \times \begin{pmatrix} E_{\mathbf{q}}^{(+)} & (0) \\ E_{\mathbf{q}}^{(-)} & (L_z) \end{pmatrix}, \tag{2}$$

$$\hat{S} = \begin{pmatrix} \hat{T}^{(+)} & \hat{R}^{(-)} \\ \hat{R}^{(+)} & \hat{T}^{(-)} \end{pmatrix}. \tag{3}$$

Here, we introduce the following designations: the superscript denotes the positive or negative direction of wave propagation along the z axis, while the matrices $\hat{T}$ and $\hat{R}$ describe the transmission and reflection of the Fourier components through the structure. For example, if there is only a wave propagating in the positive direction of the z axis, we can write

$$E_{\mathbf{q}}^{(+)}(L_z) = \hat{T}_{\mathbf{q},\mathbf{q}'}^{(+)} E_{\mathbf{q}'}^{(+)}(0). \tag{4}$$

The calculation of the reflection and transmission matrices is described in the next section.

The procedure of S quantization implies that we equate the eigenvalues of the scattering matrix to unity:

$$\|\hat{S} - \lambda(\omega)\hat{I}\| = 0, \quad (5)$$

$$\lambda(\omega) = 1. \quad (6)$$

In this way, we obtain the eigenmodes of the electromagnetic field in the structure. For each eigenvalue, we can determine the associated eigenvector, which yields the initial values of the field at the boundaries. Subsequently, using the transfer matrix method discussed in the next section, we can reconstruct the distribution of the field in the given mode at any point in the structure. Then, using the field distribution, we can calculate such values as the probability of dipole spontaneous emission and, as a consequence, the Purcell factor [12, 15].

3. CALCULATING THE REFLECTION AND TRANSMISSION COEFFICIENTS

The reflection and transmission matrices $\hat{R}^{(\pm)}$ and $\hat{T}^{(\pm)}$, entering Eq. (3), can be determined by a number of different techniques [16], usually using the finite-difference method. The disadvantage of these approaches is primarily their computational complexity, especially when working in real space. When calculations are done in reciprocal space, there may also occur divergences for some types of materials. In one-dimensional structures, it is reasonable to use the transfer matrix method [17], which is well suited for calculating the reflection and transmission coefficients and was already used in the S-quantization method for lower dimensions [12, 15, 18]. In this paper, we propose a generalized transfer matrix technique for the case of three-dimensional structures that meet the requirements listed in the previous section. In this section, we retain the convention on the index $\mathbf{q}$ in matrix notation, but now it runs the set of values in reciprocal space four times, as it counts the x and y components of the electric and magnetic fields.

The method is based on dividing the structure into N layers parallel to the xy plane. Let the thickness of the l_{th} layer be d_l. We assume that the dielectric constant ε inside each layer depends only on x and y

$$\varepsilon = f(x, y), \quad (7)$$

and expand it into a Fourier series similar to the field in Eq. (1):

$$\varepsilon(x, y) = \sum_{\mathbf{q}} \varepsilon_{\mathbf{q}} \exp(i\mathbf{q}\boldsymbol{\rho}). \quad (8)$$

We note that the Fourier coefficients tend to zero as the absolute value of q increases, and it is this fact that makes it possible to replace an infinite set of Fourier components of a field with a finite one. Then, the expansion for electric displacement can be found by the convolution theorem:

$$\mathbf{D}_{\mathbf{q}}(z) = \sum_{\mathbf{q}'} \varepsilon_{\mathbf{q}-\mathbf{q}'} \mathbf{E}_{\mathbf{q}'}(z). \quad (9)$$

Maxwell's equations for the field inside the layer are

$$\nabla \times \mathbf{E} = -\frac{i\omega}{c}\mathbf{H}, \quad \nabla \times \mathbf{H} = \frac{i\omega}{c}\mathbf{D}, \quad (10)$$

and

$$\nabla \cdot \mathbf{E} = \nabla \cdot \mathbf{H} = 0 \quad (11)$$

by transforming the curl of both sides of Eq. (10) and substituting Eqs. (9) and (11), we obtain a system of homogeneous second-order differential equations for the Fourier components:

$$\Delta \mathbf{E}_{\mathbf{q}}(z) + \frac{\omega^2}{c^2} \sum_{\mathbf{q}'} \varepsilon_{\mathbf{q}-\mathbf{q}'} \mathbf{E}_{\mathbf{q}'}(z) = 0, \quad (12)$$

$$\Delta \mathbf{H}_{\mathbf{q}}(z) + \frac{\omega^2}{c^2} \sum_{\mathbf{q}'} \varepsilon_{\mathbf{q}-\mathbf{q}'} \mathbf{H}_{\mathbf{q}'}(z) = 0. \quad (13)$$

The Laplace operator is written in the chosen Fourier representation as

$$\Delta = \left(-q_x^2, -q_y^2, \frac{d^2}{dz^2}\right). \quad (14)$$

Using it in Eqs. (12) and (13), we obtain a system of equations for the electric and magnetic field components:

$$E''_{x,\mathbf{q}} = q^2 E_{x,\mathbf{q}} - \frac{\omega^2}{c^2} \sum_{\mathbf{q}'} \varepsilon_{\mathbf{q}-\mathbf{q}'} E_{x,\mathbf{q}'}, \quad (15)$$

$$E''_{y,\mathbf{q}} = q^2 E_{y,\mathbf{q}} - \frac{\omega^2}{c^2} \sum_{\mathbf{q}'} \varepsilon_{\mathbf{q}-\mathbf{q}'} E_{y,\mathbf{q}'}, \quad (16)$$

$$H''_{x,\mathbf{q}} = q^2 H_{x,\mathbf{q}} - \frac{\omega^2}{c^2} \sum_{\mathbf{q}'} \varepsilon_{\mathbf{q}-\mathbf{q}'} H_{x,\mathbf{q}'}, \quad (17)$$

$$H''_{y,\mathbf{q}} = q^2 H_{y,\mathbf{q}} - \frac{\omega^2}{c^2} \sum_{\mathbf{q}'} \varepsilon_{\mathbf{q}-\mathbf{q}'} H_{y,\mathbf{q}'}. \quad (18)$$

We note that the equations for the y components are unnecessary (see below). This system is solved in the conventional way by introducing the first derivatives with respect to z as auxiliary functions. Then, the vector of unknown variables is written as

$$\mathbf{x}(z) = (E_{x,\mathbf{q}}, E_{y,\mathbf{q}}, H_{x,\mathbf{q}}, H_{y,\mathbf{q}}, E'_{x,\mathbf{q}}, E'_{y,\mathbf{q}}, H'_{x,\mathbf{q}}, H'_{y,\mathbf{q}}), \quad (19)$$

and the system of equations as

$$\mathbf{x}'(z) = \mathbf{A}\mathbf{x}(z), \quad (20)$$

$$\mathbf{A} = \begin{pmatrix} 0 & \delta_{\mathbf{q},\mathbf{q}'} \\ q^2\delta_{\mathbf{q},\mathbf{q}'} - \frac{\omega^2}{c^2}\varepsilon_{\mathbf{q}-\mathbf{q}'} & 0 \end{pmatrix}. \quad (21)$$

The coordinates of the layer boundaries are $z_1 = \sum_{j=1}^{l-1} d_j$ and $z_2 = \sum_{j=1}^{l} d_j = z_1 + d_l$. Then, the solution to Eq. (20) can be written as

$$\mathbf{x}(z_2 - 0) = e^{d_l \mathbf{A}} \mathbf{x}(z_1 + 0). \quad (22)$$

We also have to determine the rule for the transfer of the vector of unknowns across the boundaries. Using Eq. (10), we obtain

$$E'_{x,\mathbf{q}} = iq_x E_{z,\mathbf{q}} - i\frac{\omega}{c} H_{y,\mathbf{q}}, \quad (23)$$

$$E'_{x,\mathbf{q}} = iq_y E_{z,\mathbf{q}} + i\frac{\omega}{c} H_{x,\mathbf{q}}, \quad (24)$$

$$H'_{y,\mathbf{q}} = iq_x H_{z,\mathbf{q}} + i\frac{\omega}{c} \sum_{\mathbf{q}'} \varepsilon_{\mathbf{q}-\mathbf{q}'} E_{y,\mathbf{q}'}, \quad (25)$$

$$H'_{y,\mathbf{q}} = iq_y H_{z,\mathbf{q}} - i\frac{\omega}{c} \sum_{\mathbf{q}'} \varepsilon_{\mathbf{q}-\mathbf{q}'} E_{x,\mathbf{q}'}, \quad (26)$$

$$\frac{\omega}{c} \sum_{\mathbf{q}'} \varepsilon_{\mathbf{q}-\mathbf{q}'} E_{z,\mathbf{q}'} = q_x H_{y,\mathbf{q}} - q_y H_{x,\mathbf{q}}, \quad (27)$$

$$\frac{\omega}{c} H_{z,\mathbf{q}} = q_y E_{x,\mathbf{q}} - q_x E_{y,\mathbf{q}}. \quad (28)$$

Evidently, we can get rid of the y components of the field altogether by expressing them via other components, and then express the derivatives via these components. Since the tangential components of the field are conserved at the boundaries between different media, the $E_{x,\,\mathbf{q}}$, $E_{y,\,\mathbf{q}}$, $H_{x,\,\mathbf{q}}$, and $H_{y,\,\mathbf{q}}$ Fourier components are also conserved, so that the transfer rule for the x vector can be written as

$$\mathbf{x}(z_1 + 0) = \mathbf{B}\mathbf{x}(z_1 - 0), \quad (29)$$

$$\mathbf{B} = \begin{pmatrix} \delta_{\mathbf{q},\mathbf{q}'} & 0 \\ \mathbf{C} & 0 \end{pmatrix}. \quad (30)$$

Now, let us introduce the transfer matrix for the l_{th} layer

$$\hat{V}_l = e^{d_l \mathbf{A}_l} \mathbf{B}_l, \quad (31)$$

and the transfer matrix for the entire structure

$$\hat{V} = \prod_{l=1}^{N} \hat{V}_l. \quad (32)$$

Using this matrix, we can calculate the transmission and reflection of an arbitrary wave incident at any boundary of the structure. Since one needs to know the reflection and transmission coefficients for individual coordinate and Fourier components in order to obtain the scattering matrix, let us demonstrate how these components can be determined. The wave vector of a given component is

$$\mathbf{k}_\mathbf{q} = (q_x, q_y, \sqrt{\omega^2/c^2 - q^2}), \quad (33)$$

$$\mathbf{n}_\mathbf{q} = \mathbf{k}_\mathbf{q}/k_\mathbf{q}. \quad (34)$$

Then, e.g., for the case of x polarization we have

$$\mathbf{E}_\mathbf{q} = \mathbf{e}_y \times \mathbf{n}_\mathbf{q}, \quad (35)$$

$$\mathbf{H}_\mathbf{q} = (\mathbf{e}_y \times \mathbf{n}_\mathbf{q}) \times \mathbf{n}_\mathbf{q}. \quad (36)$$

These relations are sufficient to compose the $\mathbf{x}$ vectors corresponding to the incident, reflected, and transmitted waves, because the z dependence in free space is given by a simple exponential factor.

Let us write the components of the vector $\mathbf{x}$ corresponding to the Fourier component $\mathbf{q}$, the positive direction of propagation, and the x polarization of the wave (the index $\mathbf{q}$ is omitted in these expressions):

$$E_x = \sqrt{1 - \frac{q^2}{\omega^2/c^2}}, \quad E_y = 0, \quad (37)$$

$$H_x = \frac{q_x q_y}{\omega^2/c^2}, \quad H_y = \frac{q_y^2}{\omega^2/c^2} - 1, \quad (38)$$

$$E'_x = i\frac{\omega}{c}\left(1 - \frac{q^2}{\omega^2/c^2}\right), \quad E'_y = 0, \quad (39)$$

$$H'_x = i\frac{q_x q_y}{\omega/c}\sqrt{1 - \frac{q^2}{\omega^2/c^2}}, \quad H'_y = i\left(\frac{q_y^2}{\omega^2/c^2} - 1\right)\sqrt{\omega^2/c^2 - q^2}. \quad (40)$$

We designate this vector as $\mathbf{1}_\mathbf{q}^{(+)}$. We note that the signs of the components E_x and E_y and the derivatives H'_x and H'_y are reversed upon reversal of the propagation direction (the direction of decreasing z). Thus, to write the vector of unknowns $\mathbf{R}_\mathbf{q}^{(+)}$, corresponding to the column of the reflection matrix in Eq. (3), we need to multiply the components corresponding to the magnetic field and the derivative of the electric field from Eqs. (38) and (39) by $R_{\mathbf{q},\,x}$ and the components of the electric field and the derivative of the magnetic field from Eqs. (37) and (40) by $(-R_{\mathbf{q},\,x})$. The vector $\tilde{T}_\mathbf{q}^{(+)}$ describing the transmitted wave is obtained by simply multiplying Eqs. (37)–(40) by $T_{\mathbf{q},\,x}$, because its propagation direction is the same as that of the incident wave.

To find the reflection and transmission matrices, let us formally write expressions for the transmission and reflection of a single Fourier component through the structure:

$$\mathbf{1}_\mathbf{q}^{(+)} + \tilde{\mathbf{R}}_\mathbf{q}^{(+)} = \hat{V}\tilde{\mathbf{T}}_\mathbf{q}^{(+)}, \quad (41)$$

$$\tilde{\mathbf{T}}_\mathbf{q}^{(-)} = \hat{V}(\mathbf{1}_\mathbf{q}^{(-)} + \tilde{\mathbf{R}}_\mathbf{q}^{(-)}). \quad (42)$$

Since the original vectors $\mathbf{R}_\mathbf{q}^{(\pm)}$ and $\mathbf{T}_\mathbf{q}^{(\pm)}$ in Eq. (3) have dimensions two times smaller than the new vectors $\tilde{\mathbf{R}}_\mathbf{q}^{(\pm)}$ and $\tilde{\mathbf{T}}_\mathbf{q}^{(\pm)}$, the system of Eqs. (41) and (42) is sufficient to determine them uniquely. After finding the reflection and transmission vectors for all polarizations and Fourier components, we can construct the scattering matrix and proceed to the procedure of S quantization.

4. CONCLUSIONS

We have developed a procedure for quantization of the electromagnetic field in photonic nanostructures with three-dimensional modulation of the dielectric constant. The quantization of three-dimensional structures was carried out in a quantization box with boundary conditions based on equating the amplitudes of traveling waves at opposite sides of the box (S boundary conditions), which corresponds to equating the eigenvectors of the scattering matrix (S matrix) to unity. Expressions for the complete S matrix in the three-dimensional case written in terms of the reflection and transmission matrices of the inhomogeneous structure under consideration are obtained. A method for determining the reflection and transmission matrices of arbitrary structures with three-dimensional modulation of the dielectric constant is presented. The method is based on reducing to a problem depending on two Cartesian coordinates, dividing the structure into parallel layers, and calculating individual coordinate and Fourier components. The proposed procedure for quantization of the electromagnetic field in the three-dimensional case allows the implementation of a direct and self-consistent method for calculating the spontaneous emission for an emitter placed inside three-dimensional photonic nanostructures that avoids convergence problems in solving integro-differential equations and significantly reduces the required computational resources.

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