Dispersions of polariton and radiative decay rate in a quantum wire grating

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Abstract

In order to study the polariton dispersions and their radiative decays in a semiconductor quantum wire grating, we have calculated the electromagnetic modes generated by the grating when the light incident plane is parallel to the wires. By using Green’s function techniques and solving Maxwell’s equations with a non-local susceptibility, exciton-polarizations induced in quantum wires are then calculated. Dispersion curves show not only exciton-polariton resonances but also the dispersion of the grating’s electromagnetic modes. For a given wire dimension, the polariton can decay radiatively even for higher grating electromagnetic modes. Our model can be also applied for a three-dimensional semiconductor photonic crystal having confined excitons.

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1. Introduction

Recently, the semiconductor photonic crystals (SPCs) are the subject of detailed investigations [1–3]. These particular materials have the ability to affect by the same way the electromagnetic waves and electron motions. Allowed and forbidden electronic and photonic energy bands are then obtained. The spontaneous emission which is the radiative recombination of electron–hole pairs is determined by the electronic properties of the material and the density of electromagnetic modes of the field [4]. The elaboration of photonic crystals based on semiconductors has proved to be more efficient than semiconductor diodes laser, since in these devices, light is transmitted only in few and specific directions. Moreover, a semiconductor-photo-detector deposited between two photonic crystals can inhibit spontaneous emission [2] if the electronic band gap of the semiconductor material is equal to the photonic one. The study of the optical nonlinearities of the SPC has revealed a number of interesting results [5], in particular the nonlinear absorption which can be used to achieve ultrafast-optical control in SPC. Exciton-polarizations induced in SPC can resonate with the electromagnetic modes of the SPC to form mixed states called polaritons. The coupling between these modes strongly enhances the polariton effects in these materials. In fact many coupled electromagnetic modes interact with exciton-dipoles and then increase the nonlinearity of the exciton-polarizabilities. The polariton dispersion, which is extensively studied in semiconductor quantum wells [6,7], considers only one electromagnetic mode interacting with an exciton-dipole, and the calculation of the exciton-polarizability is simple to perform. In this case, and at the vicinity of resonance, the polariton dispersion behaves like exciton and photon dispersions. But in SPC, we have more than one electromagnetic mode and the determination of exciton-polarizabilities needs to solve the coupled Maxwell’s equations in the reciprocal space.

In this work, we consider one-dimensional SPC constituted by GaAs quantum wires (QWs) embedded inside a GaAlAs semiconductor grating. This system offers the
possibility to confine both the exciton motion and the electromagnetic modes. Formalism based on solving Maxwell’s equations for a spatial depending dielectric permittivity and the Green function theory has been developed to describe the coupling of grating electromagnetic waves with the confined one-dimensional excitons. This model was carried out to elaborate the polariton dispersion equations in one-dimensional SPC and can be extended to two- and even to three-dimensional SPCs. In addition, we have tried to analyze through the polariton dispersions and radiative decay rate spectra, how the grating electromagnetic modes interact with confined excitons. In Section 2, we present our model and give general formulas for the dispersion of polaritons in a rectangular QW grating. The illustrated results are discussed in Section 3, where we focus especially on the behavior of the photonic modes for different grating and QW dimensions, and how the higher guided modes can be excited and resonated with excitonic polarizations. Finally, Section 4 is devoted for the conclusion.

2. The model

Let us consider a QW grating of GaAs/GaAlAs. The GaAs (QW) are localized at the middle of the grating. The GaAlAs on both sides of the QWs are considered as a barrier. We suppose that the dielectric permittivity \( \varepsilon_{0} \) in the grooves of GaAs/GaAlAs is uniform. \( L_{x} \) is the lateral dimension of the rectangular wires, \( d \) is the in-plane period and \( L_{z} \) is the width of the GaAs (QW) along the \( z \)-axis and \( h \) is the vertical thickness of the grating (Fig. 1). The polar and azimuthal angles of incidence \( \theta \) and \( \phi \) specify the incoming light incidence with a frequency \( \omega \) and a wave vector \( \mathbf{K} = (k_{x}, k_{y}, k_{z}) \):

\[
k_{x} = \frac{\omega}{c} \sin \theta \cos \phi, \quad k_{y} = \frac{\omega}{c} \sin \theta \sin \phi, \quad k_{z} = \frac{\omega}{c} \cos \theta.
\]

In this work, we are interested in the case where the azimuthal angle \( \phi \) is equal to \( \pi/2 \), namely, the incident plan is parallel to the wires. The electric and the displacement fields \( \mathbf{E}(x, y, z) \) and \( \mathbf{D}(x, y, z) \) in periodically optical materials can be derived from the following Maxwell’s equation:

\[
\nabla \times (\nabla \times \mathbf{E}) = -\frac{\omega^{2}}{c^{2}} \mathbf{D}.
\]

In order to evaluate the electromagnetic eigenmodes generated inside the grating, we suppose the whole structure as a dielectric. Then, the periodicity of the QW grating along the \( Ox \) axis and the translational invariance along \( y \) and \( z \) lead to this solution form:

\[
\mathbf{E}_{0}(x, y, z) = e^{i(k_{x}x + k_{y}y + k_{z}z - \omega t)} \sum_{G} e^{iGx} \mathbf{E}_{0}(k_{x} + G, k_{y}, k_{z}),
\]

where \( G = 2\pi n / d \) is the grating reciprocal wave vector and \( m = 0, \pm 1, \pm 2, \ldots \).

By solving Eq. (2) in the reciprocal space, we can have all the \( k_{z} \) eigenvalue vectors generated inside QW grating (see Appendix A):

\[
\tilde{\mathbf{R}} \mathbf{E}_{0}(x, y, z) = k_{z}^{2} \tilde{Q} \mathbf{E}_{0}(x, y, z).
\]

\( \tilde{\mathbf{R}} \) and \( \tilde{Q} \) are matrices calculated in Appendix A. We define by \( \mathbf{E}_{0}(x, y, z) \), an electric field of \( 2N_{x} \) dimensions made up of the lateral components \( E_{0x}(G, K) \) and \( E_{0y}(G, K) \):

\[
\mathbf{E}_{0}(x, y, z) = \begin{pmatrix} E_{0x} \\ E_{0y} \end{pmatrix}.
\]

The eigenvalues \( k_{z}^{2} \) are the \( z \) components of the wave vectors confined in the grating which can be positive or negative. The positive values are related to propagating and guided modes, whereas the negative ones are referred to evanescent waves or surface modes. Exciton-polarizations should be also considered, if we want to obtain an exact solution of the electric field in the QW grating. Then the displacement field is given by

\[
\mathbf{D}(x, y, z) = \varepsilon_{0} \mathbf{E}(x, y, z) + \mathbf{P}(x, y, z).
\]

The total electric field in QW grating computed in terms of Green’s function formalism [8,9] splits into two contributions:

\[
E_{i}(k_{x}, k_{y}, z) = E_{0}(k_{x}, k_{y}, z) - \frac{\omega^{2}}{c^{2}d} \sum_{pm} N_{pm} \times \frac{S_{0}}{E_{0}(k_{x}, k_{y}) - \hbar \omega - \imath \gamma} \int_{0}^{L_{z}} dz' \times G_{0}(k_{x} + G, k_{y}, z') \times R_{p}(z'),
\]

where \( i, j = x, y \) and \( z \).

\[
I_{1}^{i}(k_{x}, k_{y}) = N_{pm} \sum_{G} Q_{m}(k_{x} + G) \times \int_{0}^{L_{z}} dz' R_{p}(z')E_{i}(k_{x} + G, k_{y}, z')
\]

\( R_{p}(z) \) and \( Q_{m}(k_{x} + G) \) are the wave function and the Fourier transformed wave function of exciton, respectively, along the \( z \)- and \( x \)-axis. The indices \( p \) and \( m \) refer to the

![Fig. 1. Quantum wire grating of GaAlAs/GaAs/GaAlAs; the wires GaAs are embedded in the half height of the grating.](image-url)
number of the exciton subband and \( G_{ij}(k_x + G, k_y, z, z') \) are Green’s functions calculated in Appendix B. We denote by \( S_0 \) a factor which is proportional to the squared matrix element of the momentum operator between the valence and conduction bands and \( N_{pm} \) is the normalization constant of the excitonic wave function [8].

The first term of Eq. (6) is related to the unperturbed electric field when the QW grating is considered as a dielectric material, whereas the second term contains the contribution of polarizations induced by electron–hole pairs confined in QWs. So, we can conclude that the coupling between the electromagnetic modes generated by the grating and the one-dimensional excitons is not simple as was found in quantum wells where only one electromagnetic mode interacts with the exciton. In this case, we expect that the calculated polariton dispersions and their radiative attenuations will display interesting features. In order to understand the coupling between the incident wave and those generated by the grating, we analyze the Maxwell equations in the reciprocal space show that more than one wave can exist in the grating. The wave vectors \( k_n \) for a grating of periodicity \( d = 300 \) nm, vertical thickness \( h = 350 \) nm and dielectric constants \( \varepsilon_0 = 12.3 \) and \( \varepsilon_0 = 1 \), can be real or imaginary. Correspondingly, the modes are purely propagating or evanescent.

\[
\sum_{j_{pmG}} \mathcal{C}_{ij}^{\pm}(k_x, k_y) = N_{pm} \frac{\omega^2}{c^2} S_{pm} Q_{pm}^*(k_x + G) \mathcal{I}_{pm}^{\mp}(k_x, k_y), \tag{8}
\]

with \( S_{pm} = \frac{E_{pm}(k_y) - \hbar \omega - i\gamma}{\hbar \omega} \).

The dispersion equations can be determined by substituting the solution of Eq. (7) back into Eqs. (8) and (6). We obtain

\[
\sum_{j_{pmG}} \mathcal{C}_{ij}^{\pm}(\omega, G') \delta_{ij} \delta_{pm} \delta_{pq} \mathcal{G}_{ij} \mathcal{E}_{pm}(\omega, k_y) \\
+ \frac{\omega^2}{c^2} S_{0} N_{pm} Q_{pm}^*(k_x + G) Q_{pm}(k_x + G') \mathcal{A}_{ij}^{\pm}(k_x + G', k_y, z') \times \int_0^{L_z} dz' R_p(z') E_{ij}(k_x + G', k_y, z'). \tag{9}
\]

where

\[
\mathcal{E}_{pm}(\omega, k_y) = E_{pm} + \frac{\hbar^2 k_y^2}{2M} - \hbar \omega - i\gamma, \tag{10}
\]

\[
\mathcal{A}_{ij}^{\pm}(k_x + G, k_y) = \int_0^{L_x} dz \int_0^{L_z} dz' R_p(z) R_p(z') G_{ij}(k_x + G, k_y, z, z'). \tag{11}
\]

\( E_{pm} \) is the total exciton energy, \( M \) is the in-plane electron–hole mass and \( \gamma \) is its damping. The polariton resonances are calculated by diagonalizing and minimizing the following equation:

\[
\sum_{j_{pmG}} \mathcal{C}_{ij}^{\pm}(\omega, G') \delta_{ij} \delta_{pm} \delta_{pq} \mathcal{G}_{ij} \mathcal{E}_{pm}(\omega, k_y) \\
+ \frac{\omega^2}{c^2} S_{0} N_{pm} Q_{pm}^*(k_x + G) Q_{pm}(k_x + G') \mathcal{A}_{ij}^{\pm}(k_x + G', k_y, z') = 0. \tag{12}
\]

![Fig. 2. The real part of the eigenvalues \( k_n \) as a function of the energy for a dielectric grating dimensions \( d = 300 \) nm, \( h = 350 \) nm and for incident angles \( \theta = \pi/3 \) and \( \phi = \pi/2 \): (a) \( L_x = 225 \) nm and (b) \( L_x = 100 \) nm.](image-url)
as a function of the incident energy $\hbar \omega$ for the incidence angles $\theta = \frac{\pi}{4}$ and $\phi = \frac{\pi}{2}$. We remark that the curves are coupled and are, respectively, attributed to the $S$ and $P$ light polarizations. By comparing these figures, we find that the energy gap between the eigenmodes for grating lateral dimension $L_x = 225$ nm is larger than that related to $L_x = 100$ nm. To explain this effect, we can consider the grating as a layer having a dielectric permittivity $\varepsilon = \varepsilon_0 + \frac{\omega_p^2}{\omega^2} (\varepsilon_0 - \varepsilon_b)$. So, the system behaves as a wave guide which the number of the $k_n$ guided waves depends essentially not only on the values of $\varepsilon_0$ and $\varepsilon_b$ but also on the grating dimensions. We notice that these curves reveal a cut off energies from which the evanescent eigenvalues $k_n$ become traveling. In addition, we remark that the non diagonal terms $M_{12}(G, G')$, $N_{12}(G, G')$ and $N_{21}(G, G')$ of Eq. (4) are nonnegligible, and have a large contribution for the coupling between electric field components. As a result, the number of guided and propagating wave vectors in the grating has clearly increased [see Figs. 2(a) and (b)]. Furthermore, we can see that the $k_n$ modes are linear on the low-energy side of these figures, while the high-energy side is characterized by a nonlinear behavior. This nonlinearity arises from the increase of grating modes and their mutual coupling. Figs. 2(a) and (b) show also for given energies, degenerated modes resulting from some crossing optical modes.

For grating dimensions $d = 300$ nm, $L_x = 100$ nm, $h = 350$ nm and a width of the QW $L_z = 8$ nm, we report on Fig. 3(a) the light hole exciton-polariton dispersion as a function of $q_y/k_0$, where $k_0 = \sqrt{\varepsilon_0 \omega / \hbar}$ is the wave vector of the light in the GaAs layers. The dispersions shown in this figure are evaluated for only the eigenmode $n = 1$ and only one reciprocal grating wave vector $G = 0$. In addition, the exciton state considered here is the ground state where $m = 1$ and $p = 1$. In Fig. 3(a) the $T$ mode refers to the $S$ light polarization, whereas $L$ and $Z$ modes correspond to the $P$ light polarization. Initially, we remark that a $ZT$ splitting of 0.6 meV occurs at $q_y = 0$ which is due to the strong anisotropy of the exciton-light hole oscillator strength. Far from $0.5k_0$, this $ZT$ splitting has slightly decreased. These curves, which are the combination of the photon and the exciton dispersions in the QW grating, show many resonances resulting from the light redistribution in the grating, or in other terms, specific electromagnetic modes are generated and will be coupled to the exciton-dipoles. In fact these resonances correspond to the...

![Fig. 3. Polariton dispersions in a QW grating with $L_x = 100$ nm, $d = 300$ nm, $h = 350$ nm, $L_z = 8$ nm and $\theta = \pi/3$ and $\phi = \pi/2$: (a) for the first travelling eigenmode $k_n$ ($n = 1$) and $G = 0$ (b) for $n = 1$ and all the grating reciprocal wave vectors $G$ (c) for all evanescent eigenmodes $k_n$ with all $G$ wavevectors. (d) For all travelling eigenmodes $k_n$ with all $G$ wavevectors.](image)
singularities of the photonic density of states in the grating
\[ \rho(k_y, \omega) = \sum_{\mathbf{n}} \delta(\omega - \omega_0) \hat{G} \rho_0 \delta(k_n^2 + G^2 + k_y^2). \]
The exciton resonances modes in the grating are clearly distinguished in the curves of the radiative decay rates. These resonances are called polariton modes which are the mixed state of excitonic and photonic modes. We also note that the resonances in the dispersion curve are regular, periodic and spaced by \( \frac{2\pi}{L_z} \). These dispersions display a strong resonance peak at \( q_y \) near 0.5k_0 value due to the large coupling of the electromagnetic mode (\( G = 0, k_n \)) with the exciton. In quantum wells [11–13], where barriers and wells have similar dielectric permittivity, this resonance is usually localized at \( q_y = 0 \), but in QW grating, due to the inhomogeneous value of the dielectric constant, the resonance is found at \( q_y \neq 0 \). On either sides of \( q_y = 0.5k_0 \), other secondary resonances appear and are closely related to the overlap of the principal photonic mode \( n = 1, G = 0 \) with the higher ones \( n = 1, G \neq 0 \).

The case of an eigenmode \( n = 1 \) and all the \( G \) reciprocal grating wave vectors is illustrated in Fig. 3(b). We find that the resonances have clearly increased and are more sharper which can be explained by the coupling between the higher grating photonic modes \( n = 1, G \neq 0 \). Alternatively, we report in Fig. 3(c) the dispersion spectrum, where only evanescent eigenmodes \( k_n \) and all \( G \) reciprocal grating wave vectors are taken into account. The regular peaks found in the spectra are related to the singularities of the first term of \( G_{zz}(z, z') \) in Eq. (B.18), whereas the second and the third terms in \( G_{zz}(z, z') \) equation are small. The surface or evanescent eigenmodes \( k_n \) considered here have no effect on the spectra.

Curves attributed to the only traveling waves \( k_n \) with all \( G \) wave vectors [see Fig. 3(d)] display different features from that depicted in Fig. 3(c). In fact, we obtain secondary resonances around the main ones which are related to the contribution of the guided modes \( k_n \). Here, we shall mention that an exciton with \( k_y \) wavevector interacts with photons having the same \( k_y \) wavevector with all possible values of \( G \) and \( k_n \). The last two cases, where we studied separately the effect of evanescent and traveling modes generated by the QW grating on the dispersions, are a mean to understand how these modes interact with the one-dimensional exciton.

In quantum wells, when we consider the exciton in its ground state, the \( Z \) polariton dispersion displays only one resonance which is obviously the mixed state polariton and in this case, the probability of the exciton to decay radiatively is enhanced. But in QW grating, the results show that the polariton resonances in dispersion spectra are not all associated with an enhancement of the radiative decay. In fact, we can obtain polariton resonance without an amplification in the radiative decay, then, in the calculations, the polariton dispersions should be evaluated with the radiative decays to identify the radiative polaritons from those nonradiative. In Fig. 4, we report the polariton radiative decay rates \( \Gamma \) which are the imaginary part of the polariton eigenenergies obtained from Eq. (12).

We deduce that an amplification of the spontaneous emission has occurred only at the vicinity of \( q_y = 0.5k_0 \) for the \( Z \) light polarization. Eventually, this radiative process is obtained if the exciton resonates with one of the traveling electromagnetic eigenmodes \( (k_n, G) \), while we notice that the evanescent ones do not affect the polariton radiative decay rates.

When we reduce the QW grating dimensions and precisely the wire width \( L_z \), the confining energy of the exciton increases. In this case higher electromagnetic modes with \( G \neq 0 \) can be excited and interact with excitonic polarizations. At this range of energy, the overlap between the exciton and photon wave functions at \( G \neq 0 \) is not to be neglected with respect to the \( G = 0 \) ones and they will contribute to the amplification of the radiative decays. As shown by Figs. 5(a) and (b), the resonate polariton states can be obtained even with electromagnetic modes \( G \neq 0 \) and the probability of the exciton to decay radiatively is enhanced for \( G \neq 0 \).

4. Conclusion

In the QW grating, the change in the light incident plane modifies considerably the dispersion of electromagnetic eigenmodes generated inside this periodical structure. This change can affect the number of the guided and surface modes \( k_n \). Nonlinear dispersion has been noticed in the spectra which results from the strong coupling between the different electric field components. Electromagnetic fields in the QW grating induced exciton-polarizations and will interact with grating photonic modes to give mixed states called polaritons. By using Green’s function formalism,
polariton dispersions and their radiative decay rates have been calculated. Furthermore, many resonance peaks have been obtained in these curves, which are attributed to the polariton resonances, resulting from the interaction of grating photonic modes with exciton-dipoles. The calculated polariton dispersions in QW grating are in fact the combination of the dispersion of the grating photonic modes with the exciton ones and they show that only travelling eigenmodes $k_n$ resonate with the one-dimensional exciton, whereas the evanescent modes have no effect on the radiative decay rates. Unlike the quantum well case, an amplification of the spontaneous emission is obtained at $q_y \neq k_0$ which can be explained by the inhomogeneous characteristic of the dielectric permittivity. By decreasing the wire width $L_z$, polariton resonances can also occur at higher grating photonic modes $G \neq 0$, in this case exciton-polarizabilities with $G \neq 0$ are nonnegligible and will interact with the generated eigenmodes of the grating to induce polariton radiative decays at given frequencies. Our model which is based on solving Maxwell’s equations can be also extended to the three-dimensional SPCs.

Appendix A

In order to find the grating electromagnetic modes $k_n$ along the Oz axis, we should calculate the eigenvalues of the Fourier transformed Maxwell’s equations:

$$\sum_G K_{zz}^{(2)}(G, G')E_{0z}(G', K)$$

$$= k_x^2 E_{0z}(G, K) - (k_x + G)k_y E_{0y}(G, K)$$

$$- k_z(k_x + G)E_{0z}(G, K),$$

$$\sum_G K_{zz}^{(2)}(G, G')E_{0y}(G', K)$$

$$= -(k_x + G)k_y E_{0z}(G, K)$$

$$+ k_y^2 E_{0y}(G, K) - k_z k_y E_{0z}(G, K),$$

$$\sum_G K_{zz}^{(2)}(G, G')E_{0z}(G', K)$$

$$= -k_z[(k_x + G)E_{0z}(G, K) + k_y E_{0y}(G, K)],$$

$$\text{where } K = (k_x, k_y, k_z) \text{ and } K^{(2)}_{zz}(G, G'), K^{(2)}_{zz}(G, G'), K^{(2)}_{zz}(G, G') \text{ are the matrix elements of } K_{zz}, K_{zy} \text{ and } K_{zz}.$$  

$$K^{(2)}_{zz}(G, G') = \frac{\alpha^2}{c^2} k_{G, G'} - k_z^2 \delta_{G, G'},$$

$$K^{(2)}_{zy}(G, G') = \frac{\alpha^2}{c^2} k_{G, G'} - (k_x + G')^2 \delta_{G, G'},$$

$$K^{(2)}_{zz}(G, G') = \frac{\alpha^2}{c^2} k_{G, G'} - [(k_x + G')^2 + k_y^2] \delta_{G, G'}.$$  

(A.2)

In reciprocal space, the modulated dielectric function $\varepsilon(x, y, z)$ takes the following form:

$$\varepsilon_{G, G'} = \varepsilon_0 + \frac{2}{d} (\varepsilon_b - \varepsilon_0) \frac{\sin((G - G') \frac{L_z}{2})}{(G - G')}.$$  

(A.3)

Multiplying the third equation of Eq. (A.1) by the inverse matrix $K^{(2)}_{zz}^{-1}$, we obtain

$$E_{0z}(G, K) = -k_z \sum_G K^{(2)}_{zz}^{-1}(G, G')$$

$$\times [(k_x + G')E_{0z}(G', K) + k_y E_{0y}(G', K)].$$  

(A.4)
Eq. (A.1) is reduced by substituting Eq. (A.4) into Eq. (A.1):

\[
\sum_{G'} K^{(2)}_{\chi z}(G,G') E_{0x}(G', K) + M_{12}(G, G') E_{0y}(G', K) = k_x^2 \sum_{G'} N_{11}(G, G') E_{0x}(G', K) + k_y^2 \sum_{G'} N_{12}(G, G') E_{0y}(G', K),
\]

\[
\sum_{G'} M_{21}(G, G') E_{0x}(G', K) + K^{(2)}_{\chi z}(G, G') E_{0y}(G', K) = k_x^2 \sum_{G'} N_{21}(G, G') E_{0x}(G', K) + k_y^2 \sum_{G'} N_{22}(G, G') E_{0y}(G', K).
\]

(A.5)

Eq. (A.5) can be written in a simple form as

\[
\vec{R} E_{0xy} = k_x^2 \vec{Q} E_{0xy},
\]

(A.6)

where \( \vec{R} = (\vec{k}_x, \vec{k}_y, \overrightarrow{M_{12}}, \overrightarrow{M_{21}}) \) and \( \vec{Q} = (\overrightarrow{N_{11}}, \overrightarrow{N_{12}}, \overrightarrow{N_{21}}, \overrightarrow{N_{22}}) \) matrices of dimensions \( 2N_G \times 2N_G \). \( N_G \) is the number of the \( G \) reciprocal grating wave vectors.

Multiplying Eq. (A.6) by the inverse unitary matrix \( U_R^{-1} \) of \( \vec{R} \) then we obtain

\[
\vec{\eta} E'_{0xy} = k_x^2 \vec{Q} E'_{0xy},
\]

(A.7)

where \( \vec{\eta} = \overrightarrow{U_R} \vec{R} \overrightarrow{U_R} \) and \( \vec{Q} = \overrightarrow{U_R} \overrightarrow{Q} \overrightarrow{U_R} \).

By setting \( \vec{\eta} = \overrightarrow{I_x} \vec{I}_x \) and \( \vec{I}_x = | \vec{\eta} |^{-1} \vec{I}_x \) is a diagonal matrix where its elements are the signs of the \( \eta \) eigenvalues of \( \overrightarrow{R} \), Eq. (A.7) can be transformed into

\[
\frac{E''_{0xy}}{k_x^2} = \overrightarrow{S} E'_{0xy}.
\]

(A.8)

We multiply Eq. (A.8) by \( | \eta |^{-1/2} \vec{I}_x \) and we try to express it in a simple form:

\[
\frac{E''_{0xy}}{k_x^2} = \overrightarrow{S} E'_{0xy},
\]

(A.9)

where \( \overrightarrow{S} = | \eta |^{-1/2} \vec{I}_x \vec{Q} | \vec{\eta} |^{-1/2} \) and \( E'_{0xy} = | \eta |^{-1/2} E_{0xy} \).

Afterwards, the \( k_n \) eigenvalues would be replaced by \( k_n \), where \( n \) represents the eigenvalue index. The matrix elements of \( K^{(2)}_{\chi z}, K^{(2)}_{\chi y}, M_{12}, M_{21}, N_{11}, N_{12}, N_{21}, N_{22} \) are as follows:

\[
K^{(2)}_{\chi z}(G, G') = \frac{\alpha^2}{c^2} \delta_{G, G'} - k_y^2 \delta_{G, G'},
\]

\[
M_{12}(G, G') = M_{21}(G, G') = (k_x + G') k_y \delta_{G, G'},
\]

\[
N_{11}(G, G') = \delta_{G, G'} + (k_x + G) K^{(2)}_{\chi z}^{-1}(G, G') (k_x + G'),
\]

\[
N_{12}(G, G') = (k_x + G) K^{(2)}_{\chi z}^{-1}(G, G'),
\]

\[
N_{21}(G, G') = (k_x + G') k_y K^{(2)}_{\chi z}^{-1}(G, G'),
\]

\[
N_{22}(G, G') = \delta_{G, G'} + k_y^2 K^{(2)}_{\chi z}^{-1}(G, G').
\]

Appendix B

In this appendix we calculate Green’s functions expressed in the total electric field (Eq. (6)). We take \( G_{ij} = G_{ij}(x, y, z) \) where their components \( G_{ij}(x, G) \) and \( k_x, k_y, k_z \) verify the following differential equations:

\[
\frac{\partial^2 G_{xx}}{\partial z^2} - i k_x \frac{\partial G_{xx}}{\partial z} + k_y G_{xy} + \frac{\partial^2}{\partial z^2} G_{xx} = (z - z') V_+, \\
\frac{\partial^2 G_{yx}}{\partial z^2} + i k_x G_{xy} + k_y \frac{\partial G_{xy}}{\partial z} + \frac{\partial^2}{\partial z^2} G_{xx} = 0.
\]

(1.1)

We denote by \( K \) a diagonal matrix whose elements are \( K_{ij}(G, G') = (k_x + G) \delta_{ij, G'} \) and \( V_+ \) is a vector of \( N_G \) dimensions with its components are equal to 1. Eq. (1.1) can be reduced to give the system of equations:

\[
\frac{\partial^2 G_{xx}}{\partial z^2} + R \left( \frac{\partial G_{xx}}{\partial z} \right) = \delta(z - z') V_{10},
\]

(1.2)

where \( V_{10} = (V, 0, \ldots) \) a vector of \( 2N_G \) dimensions. In addition, Green’s functions \( G_{xy}, G_{yy} \) and \( G_{xy} \) verify Eq. (B.3):

\[
\frac{\partial^2 G_{xy}}{\partial z^2} - i k_x \frac{\partial G_{xy}}{\partial z} + k_y G_{xy} + \frac{\partial^2}{\partial z^2} G_{xy} = 0,
\]

(1.3)

\[
\frac{\partial^2 G_{yx}}{\partial z^2} + i k_x G_{xy} + k_y \frac{\partial G_{xy}}{\partial z} + \frac{\partial^2}{\partial z^2} G_{xy} = 0.
\]

(1.3)

By reducing it

\[
\frac{\partial^2 G_{xy}}{\partial z^2} + R \left( \frac{\partial G_{xy}}{\partial z} \right) = \delta(z - z') V_{01},
\]

(1.4)

where \( V_{01} = (0, V, \ldots) \).
Like Eqs. (B.1) and (B.3), Green’s functions vectors \( \mathbf{G}_{xx} \), \( \mathbf{G}_{xz} \) and \( \mathbf{G}_{zz} \) can be obtained by solving these coupled equations:

\[
\begin{align*}
\frac{\partial^2 \mathbf{G}_{xz}}{\partial z^2} - i \mathbf{K}_x \frac{\partial \mathbf{G}_{xz}}{\partial z} + k_y \mathbf{K}_y \mathbf{G}_{xz} + k_z \mathbf{K}_z \mathbf{G}_{xz} &= 0, \\
\frac{\partial^2 \mathbf{G}_{zz}}{\partial z^2} - i k_y \mathbf{G}_{zz} + k_y \mathbf{G}_{zz} + k_z \mathbf{G}_{zz} &= 0, \\
\frac{\partial^2 \mathbf{G}_{zz}}{\partial z^2} - i k_y \mathbf{G}_{zz} - i k_x \mathbf{G}_{zz} &= \delta(z - z') \mathbf{V}_{+},
\end{align*}
\]

and reducing it

\[
\mathbf{Q} \left( \frac{\partial^2 \mathbf{G}_{xz}}{\partial z^2} \mathbf{G}_{xz} \right) + R \left( \mathbf{G}_{xz} \mathbf{G}_{xz} \right) = \frac{\partial \delta(z - z')}{\partial z} \mathbf{K}_x \mathbf{V}_{+},
\]

where \( \mathbf{K}_q = \left( \begin{array}{cc} \mathbf{K}_{xq} & \mathbf{K}_{yq} \\
\mathbf{K}_{yq} & \mathbf{K}_{zz} \end{array} \right) \) is a matrix of \( 2N_G \times 2N_G \) dimensions and \( \mathbf{V}_{+} = \left( \mathbf{V}_x, \mathbf{V}_z \right) \) is a vector of \( 2N_G \).

Now, let us consider by

\[
\hat{\mathbf{G}}_+ = \begin{pmatrix} \mathbf{G}_{xx} + \mathbf{G}_{xy} \\
\mathbf{G}_{xx} + \mathbf{G}_{yy} \end{pmatrix} \quad \text{and} \quad \hat{\mathbf{G}}_- = \begin{pmatrix} \mathbf{G}_{xx} - \mathbf{G}_{xy} \\
\mathbf{G}_{yx} - \mathbf{G}_{yy} \end{pmatrix},
\]

where \( \hat{\mathbf{G}}_+ \) and \( \hat{\mathbf{G}}_- \) are Green’s functions of \( 2N_G \) dimensions, and solutions of the second-order differential equations obtained from Eqs. (B.2) and (B.4):

\[
\begin{align*}
\mathbf{Q} \frac{\partial^2 \hat{\mathbf{G}}_+}{\partial z^2} + \hat{\eta} \hat{\mathbf{G}}_+ &= \mathbf{V}_{+} \delta(z - z'), \\
\mathbf{Q} \frac{\partial^2 \hat{\mathbf{G}}_-}{\partial z^2} + \hat{\eta} \hat{\mathbf{G}}_- &= \mathbf{V}_{-} \delta(z - z'),
\end{align*}
\]

with \( \mathbf{V}_{+} = \left( \mathbf{V}_x, \mathbf{V}_z \right) \).

Multiplying Eq. (B.7) by the inverse unitary matrix \( \mathbf{U}_R \), we obtain

\[
\begin{align*}
\mathbf{Q} \left( \frac{\partial^2 \hat{\mathbf{G}}_+}{\partial z^2} \right) + \hat{\eta} \hat{\mathbf{G}}_+ &= \mathbf{U}_R \delta(z - z') \mathbf{V}_{+}, \\
\mathbf{Q} \frac{\partial^2 \hat{\mathbf{G}}_-}{\partial z^2} + \hat{\eta} \hat{\mathbf{G}}_- &= \mathbf{U}_R \delta(z - z') \mathbf{V}_{-},
\end{align*}
\]

with \( \mathbf{G}_+ = \left| \eta \right|^{-1} \hat{\mathbf{G}}_+ \), and \( \mathbf{V}_1 = \left| \eta \right|^{-1} \mathbf{U}_R \mathbf{V}_{+} \). Multiplying Eq. (B.10) by the inverse unitary matrix \( \mathbf{U}_S \) of \( \mathbf{S} \) and setting \( \hat{\mathbf{G}}_+(z, z') = \mathbf{U}_S \mathbf{G}_+(z, z') \), we get for each eigenwave vector \( k_n \) the following differential equation:

\[
1 \frac{\partial^2 \hat{\mathbf{G}}_+(n, z, z')}{\partial z'^2} + \hat{\mathbf{G}}_+(n, z, z') = \delta(z - z') \mathbf{w}_1(n),
\]

with \( \mathbf{w}_1(n) = \sum_n \mathbf{U}_S \mathbf{w}_1(n) \).

For \( \hat{\mathbf{G}}_+(n, z, z') = k_n \mathbf{w}_1(n) \), Eq. (B.11) can be transformed into a simple expression:

\[
\frac{\partial^2 \hat{\mathbf{G}}(n, z, z')}{\partial z'^2} + k_n^2 \hat{\mathbf{G}}(n, z, z') = \delta(z - z').
\]

The solutions of this differential equation are known [14]:

\[
\hat{\mathbf{G}}(n, z, z') = \frac{1}{2i k_n} \{ \theta(z - z') e^{i k_n(z - z')} + \theta(z' - z) e^{-i k_n(z' - z')} \},
\]

where

\[
\hat{\mathbf{G}}_+(k_x + G, z, z') = \sum_n F_{\mathbf{p}}(G, n) \hat{\mathbf{G}}(n, z, z'),
\]

From Eq. (B.8) we find

\[
\hat{\mathbf{G}}_-(k_x + G, z, z') = \sum_n F_{\mathbf{p}}(G, n) \mathbf{G}_x(n, z, z'),
\]

\[
F_{\mathbf{p}}(G, n) = \sum_{G'} U_R(G, G') |\eta(G')|^{-1/2} U_S(G', n) k_n^2 \mathbf{w}_1(n),
\]

\[
w_2(n) = \sum_{n'} U_S^{-1}(n, n') \mathbf{V}_{2}(n'),
\]

\[
\mathbf{V}_2 = \left| \eta \right|^{-1/2} \mathbf{I}_R \left( \mathbf{I}_R \mathbf{U}_R \mathbf{V}_{+} \right) \left( \mathbf{I}_R \mathbf{U}_R \mathbf{V}_{+} \right)^{-1} \mathbf{I}_R \mathbf{U}_R \mathbf{V}_{+}.
\]

To solve Eq. (B.6), the Green functions \( \mathbf{G}_{xx} \) and \( \mathbf{G}_{zz} \) should be expressed as first derived unknown Green functions \( \mathbf{G}_x \) and \( \mathbf{G}_z \):

\[
\mathbf{G}_{xx} = \frac{\partial \mathbf{G}_x}{\partial z} \quad \text{and} \quad \mathbf{G}_{zz} = \frac{\partial \mathbf{G}_z}{\partial z}.
\]

By replacing them in Eq. (B.6) and integrating it, we obtain

\[
\begin{align*}
\mathbf{Q} \left( \frac{\partial^2 \mathbf{G}_x}{\partial z^2} \right) + R \left( \mathbf{G}_x \mathbf{G}_x \right) &= \mathbf{J}, \\
\mathbf{Q} \left( \frac{\partial^2 \mathbf{G}_z}{\partial z^2} \right) + R \left( \mathbf{G}_z \mathbf{G}_z \right) &= \mathbf{J}.
\end{align*}
\]

Let us consider by \( \mathbf{G}_x = \left( \begin{array}{c} \mathbf{G}_x \\
\mathbf{G}_z \end{array} \right) \) Green’s functions of \( 2N_G \) dimensions and solutions of Eq. (B.17). This kind of equation has been solved for the case of Eqs. (B.7) and (B.8), then we immediately have

\[
\mathbf{G}_x(k_x + G, z, z') = \sum_{G'} U_R(G, G') |\eta(G')|^{-1/2} U_S(G', n) k_n^2 \mathbf{w}_3(n),
\]
\[ w_3(n) = \sum_{n'} U_S^{-1}(n, n') V_3(n'), \]
\[ \mathbf{V}_3 = \begin{bmatrix} \eta \\ -1/2 \\ -1/2 \end{bmatrix}, \quad I_x = U_R K_{y} \mathbf{V}_{1+}. \]  
\[ (B.18) \]

Finally, it is possible now to evaluate exactly Green’s functions:

\[ G_{xx}(k_x + G, z, z') = \frac{1}{2} \sum_{G=0}^{N_y} \sum_{n=1}^{2N_y} \left\{ F_{1p}(G, n) + F_{2p}(G, n) \right\} \tilde{G}(n, z, z'), \quad (B.19a) \]

\[ G_{xy}(k_x + G, z, z') = \frac{1}{2} \sum_{G=0}^{N_y} \sum_{n=1}^{2N_y} \left\{ F_{1p}(G, n) - F_{2p}(G, n) \right\} \tilde{G}(n, z, z'), \quad (B.19b) \]

\[ G_{yx}(k_x + G, z, z') = \frac{1}{2} \sum_{G=N_y+1}^{2N_y} \sum_{n=1}^{2N_y} \left\{ F_{1p}(G, n) + F_{2p}(G, n) \right\} \tilde{G}(n, z, z'), \quad (B.19c) \]

\[ G_{yy}(k_x + G, z, z') = \frac{1}{2} \sum_{G=0}^{N_y} \sum_{n=1}^{2N_y} \left\{ F_{3p}(G, n) \right\} \tilde{G}(n, z, z'), \quad (B.19d) \]

\[ G_{zz}(k_x + G, z, z') = \frac{1}{2} \sum_{G=N_y+1}^{2N_y} \sum_{n=1}^{2N_y} \left\{ F_{3p}(G, n) \right\} \tilde{G}(n, z, z'), \quad (B.19e) \]

\[ G_{xy}(z, z') = i \vec{K}_{zz}^{(2)-1} \left\{ k_y \frac{\partial G_{yx}(z, z')}{\partial z} + k_x \frac{\partial G_{xy}(z, z')}{\partial z} \right\}, \quad (B.19f) \]

\[ G_{yz}(z, z') = K_{zz}^{(2)-1} \left\{ \delta(z - z') \mathbf{V}_+ + i(k_y \frac{\partial G_{yz}(z, z')}{\partial z} \right\}, \quad (B.19g) \]

References