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Spontaneous Emission in Multilayer Semiconductor Structures

Christa Hooijer, Gao-xiang Li, Klaas Allaart, and Daan Lenstra

Abstract—A theoretical analysis of spontaneous emission from a quantum well in dielectric multilayer structures, especially the influence of dielectric geometry on the relative intensities of guided and radiation modes and on polarization, is presented. We first discuss a relatively simple three-layer case, and subsequently a technologically more interesting five-layer structure that has been proposed for a high-power laser. The expression for the partial as well as total emission rates is derived within a broader framework of coupled Heisenberg equations of motion for charge carriers and the quantized electromagnetic field. Thereby, explicit mode decomposition of the Green tensor is avoided. Still, the beta factor for individual guided modes, which is a relevant quantity for the lasing threshold of a device, can be identified and a competition between modes is shown to exist in specific cases.

Index Terms—Multilayer structures, spontaneous emission rate.

I. INTRODUCTION

AS the size of small semiconductor light-emitting devices approaches the optical wavelength regime, these devices become increasingly more interesting for emitting light with nonclassical signatures [1]–[4]. This situation asks for a fully quantum mechanical description of both the active charge carriers and the electromagnetic field in the corresponding dielectric environment. Here we consider a quantum mechanical Hamiltonian formulation of such a theory, specifically for a spatially extended source within a dielectric embedding that gives rise to guided and radiation modes with their corresponding polarization dependence. To focus on just these points and keep the presentation as transparent as possible, we neglect all complications of the electronic dynamics in operating semiconductor devices, such as saturation, many-body, and temperature effects and exciton formation which have been dealt with in extensive work by other authors [5], [6]. We, therefore, adopt here for the electrons just Bloch states in a simple two-band model to study the dependence of the spontaneously emitted radiation, its distribution among guided and radiation modes and its polarization, on device properties such as the thickness of the cladding layer in which a quantum

well is embedded and the position of the well within that layer. We show how the computational scheme, which avoids explicit mode decomposition of the electromagnetic field by making use of the Green tensor, allows the partial emission rates into a specific (guided) mode to be calculated as a fraction of the total spontaneous emission rate (beta factor). This is an important factor for the onset of lasing into that mode.

The general quantum mechanical Hamiltonian framework and derivation of equations of motion is presented in Section II. In Section III, we use this formalism to derive an expression for the spontaneous emission rate for a finite source of active charge carriers within a passive dielectric environment and, more specifically, for a quantum well in a multilayer semiconductor. In Section IV, we present results of several applications. First, a three-layer case is discussed to elucidate the essential features of its physical properties and of the calculation. Next, a more complicated structure for a high-power laser with a high catastrophic optical damage (COD)-limit [7] is analyzed. For both cases, we give an estimate of the beta factor β_{sp} for individual guided modes separately as a function of the geometrical parameters of the structure. A short summary is given in Section V. The methods presented here have also been applied in a study of the interior mode density of a multilayer structure that exhibits properties of an omnidirectional mirror [8], [9] and was shown to be a highly directional waveguide [10].

II. QUANTUM MECHANICAL HAMILTONIAN: EQUATIONS OF MOTION

A. Hamiltonian in Generalized Coulomb Gauge

We make a distinction between charge carriers within a limited active region and involved in the optical transitions and bound charges that form a dielectric background. The presence of the latter will be represented by a dielectric function $\epsilon(\mathbf{x}) = \epsilon_0 \epsilon_r(\mathbf{x})$, which depends on the space coordinate $\mathbf{x}$. Here, $\epsilon(\mathbf{x})$ is taken to be real; an acceptable approximation for the range of optical frequencies in most practical applications. Quantization of the field for complex-valued $\epsilon(\mathbf{x})$ received quite some attention in recent literature [11], [12] but is left outside the scope of the present work. Quantization of the electromagnetic radiation field in homogeneous space or vacuum is discussed in detail in text books, e.g., [13]. For inhomogeneous dielectric space, a detailed presentation was given in [14]. We briefly recall the essentials of this method here, to introduce the equations of motion that lead to an expression for the spontaneous emission rates in the next section.

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The canonical field variables to be used in a quantum Hamiltonian are obtained by imposing the *generalized* Coulomb gauge condition for the vector potential $\mathbf{A}(\mathbf{x}, t)$

$$\nabla \cdot (\varepsilon_r(\mathbf{x}) \mathbf{A}(\mathbf{x}, t)) = 0. \quad (1)$$

The scalar potential $\Phi(\mathbf{x}, t)$ can then be expressed as a function of the coordinates of the charge carriers and is therefore not an independent variable. It describes the instantaneous Coulomb interaction. The vector potential $\mathbf{A}(\mathbf{x}, t)$ describes the propagating (radiation) field. To stress this property, we shall henceforth express this by an index p . This propagating field satisfies the equation

$$\left\{ \mu_0 \varepsilon_0 \varepsilon_r(\mathbf{x}) \frac{\partial^2}{\partial t^2} + \nabla \cdot \nabla \right\} \mathbf{A}_p(\mathbf{x}, t) = \varepsilon_r(\mathbf{x}) \int d^3 x' \mathbf{J}(\mathbf{x}', t) \cdot \delta^\varepsilon(\mathbf{x}, \mathbf{x}') \quad (2)$$

where $\mathbf{J}(\mathbf{x}, t)$ is the free current density in the active region $\delta^\varepsilon(\mathbf{x}, \mathbf{x}')$ is the *generalized* transverse delta function which takes care of the selection of the subspace of propagating, generalized-transverse modes $\mathbf{g}_{p,\lambda}(\mathbf{x})$

$$\delta^\varepsilon(\mathbf{x}, \mathbf{x}') = \sum_\lambda \frac{\mathbf{g}_{p,\lambda}(\mathbf{x}) \mathbf{g}_{p,\lambda}^*(\mathbf{x}')}{\sqrt{\varepsilon_r(\mathbf{x})} \sqrt{\varepsilon_r(\mathbf{x}')}}. \quad (3)$$

This is a Cartesian tensor. The transverse vector functions $\mathbf{g}_{p,\lambda}(\mathbf{x})$ are the solutions, with eigenvalue $\omega_\lambda \neq 0$, of the Hermitian quadratic operator

$$\left\{ \sqrt{\varepsilon_r(\mathbf{x})} \right\}^{-1} \nabla \cdot \nabla \cdot \left\{ \sqrt{\varepsilon_r(\mathbf{x})} \right\}^{-1} \mathbf{g}_{p,\lambda}(\mathbf{x}) = \frac{\omega_\lambda^2}{c^2} \mathbf{g}_{p,\lambda}(\mathbf{x}). \quad (4)$$

They may be grouped in complex conjugate pairs with eigenvalues $\pm \omega_\lambda$ and satisfy the generalized transverse condition

$$\nabla \cdot \sqrt{\varepsilon_r(\mathbf{x})} \mathbf{g}_{p,\lambda}(\mathbf{x}) = 0. \quad (5)$$

The solution of (2) for the propagating field $\mathbf{A}_p(\mathbf{x}, t)$ can be written by means of a propagating Green tensor $G_p(\mathbf{x}, \mathbf{x}', t, t')$

$$\mathbf{A}_p(\mathbf{x}, t) = \mu_0 \int d^3 x' dt' \mathbf{G}_p(\mathbf{x}, \mathbf{x}', t, t') \cdot \mathbf{J}(\mathbf{x}', t') + \mathbf{A}_{p,\text{free}}(\mathbf{x}, t). \quad (6)$$

Using (4), one verifies that the Green tensor can be expressed in terms of the vector functions $\mathbf{g}_{p,\lambda}(\mathbf{x})$; its Fourier transform is

$$\mathbf{G}_p(\mathbf{x}, \mathbf{x}', \omega) = \sum_\lambda \frac{\mathbf{g}_{p,\lambda}(\mathbf{x}) \mathbf{g}_{p,\lambda}^*(\mathbf{x}')}{\sqrt{\varepsilon_r(\mathbf{x})} \sqrt{\varepsilon_r(\mathbf{x}')}} \frac{c^2}{\omega_\lambda^2 - \omega^2}. \quad (7)$$

This Green (Cartesian) tensor will play a central role in the calculations presented in this paper. In (6), the full current density $\mathbf{J}(\mathbf{x}, t)$ may be used since the propagating Green tensor automatically selects the propagating part in the integration over $\mathbf{x}'$.

The propagating part, as distinct from the Coulomb field, of the electric field strength $\mathbf{E}_p(\mathbf{x}, t) = -(\partial/\partial t)\mathbf{A}_p(\mathbf{x}, t)$, is an independent variable in the Hamiltonian [13], [14]. In fact, $\varepsilon_0 \varepsilon(\mathbf{x}) \mathbf{E}_p(\mathbf{x}, t)$ plays the role of the canonical conjugate of

$\mathbf{A}_p(\mathbf{x}, t)$. The (equal time) quantization condition is, therefore, given by the commutation relation for the field operators

$$[\hat{\mathbf{E}}_p(\mathbf{x}, t), \hat{\mathbf{A}}_p(\mathbf{x}', t)]_- = \frac{\hbar}{i} \delta^\varepsilon(\mathbf{x}, \mathbf{x}') \quad (8)$$

where the hat above a symbol indicates field *operators* and the generalized transverse delta function (tensor) reflects the restriction to propagating fields only. As we focus in this paper on the influence of the dielectric structure on the (spontaneous) emission of radiation, we shall adopt a simple model for the Hamiltonian of the charge carriers in the semiconductor. We adopt the independent-electron model in which the electron wave functions $\varphi_{n,\mathbf{k}}$ are Bloch states with band index n , wavevector $\mathbf{k}$, and energies $E_{n,\mathbf{k}}$. The model quantum Hamiltonian then reads

$$\hat{H} = \int d^3 x \frac{1}{2} \left[\varepsilon_0 \varepsilon_r(\mathbf{x}) (\hat{\mathbf{E}}_p(\mathbf{x}, t))^2 + \frac{1}{\mu_0} (\nabla \cdot \hat{\mathbf{A}}_p(\mathbf{x}, t))^2 \right] + \sum_\gamma E_\gamma \hat{c}_\gamma^\dagger(t) \hat{c}_\gamma(t) - \int d^3 x \hat{\mathbf{J}}(\mathbf{x}, t) \cdot \hat{\mathbf{A}}_p(\mathbf{x}, t) \quad (9)$$

in which the operators $\hat{c}_\gamma$ and $\hat{c}_\gamma^\dagger$ are the annihilation and creation operators for an electron in the state $\gamma = (n, \mathbf{k})$.

The current density operator is also expressed in terms of creation and annihilation operators for the electrons

$$\hat{\mathbf{J}}(\mathbf{x}, t) = \sum_{\gamma\gamma'} \mathbf{j}_{\gamma\gamma'}(\mathbf{x}) \hat{c}_\gamma^\dagger(t) \hat{c}_{\gamma'}(t) - \frac{e^2}{2m} \hat{\mathbf{A}}_p(\mathbf{x}, t) \quad (10)$$

with

$$\mathbf{j}_{\gamma\gamma'}(\mathbf{x}) = \frac{-i\hbar e}{2m} (\varphi_\gamma^*(\mathbf{x}) \nabla \varphi_{\gamma'}(\mathbf{x}) - \varphi_{\gamma'}(\mathbf{x}) \nabla \varphi_\gamma^*(\mathbf{x})). \quad (11)$$

The last term in (10) that gives rise to a Hamiltonian term quadratic in $\hat{\mathbf{A}}_p(\mathbf{x}, t)$ can often be neglected when the strength of the radiation field is small compared to that of the Coulomb field. It is, however, essential in the description of two-photon processes and the study on nonclassical light. It can be treated in various ways involving canonical transformations [13]. In the derivation of the spontaneous emission rate in the next section, it does not contribute.

B. Heisenberg Equations of Motion

In the Heisenberg representation of quantum mechanics [15], [16] the equations for the quantum mechanical operators resemble most closely those for the classical variables. Indeed, (2) for the classical field and current density also holds for the corresponding field *operators*. This implies that also the field *operator* can be expressed as an integral over the current *operator* density and the same *classical* Green function as in (6)

$$\hat{\mathbf{A}}_p(\mathbf{x}, t) = \mu_0 \int d^3 x' dt' \mathbf{G}_p(\mathbf{x}, \mathbf{x}', t, t') \cdot \hat{\mathbf{J}}(\mathbf{x}', t') + \hat{\mathbf{A}}_{p,\text{free}}(\mathbf{x}, t) \quad (12)$$

with the free-field operator

$$\hat{\mathbf{A}}_{p,\text{free}}(\mathbf{x}, t) = \sum_\lambda \left\{ \frac{\hbar}{2\varepsilon_0 \varepsilon_r(\mathbf{x}) \omega_\lambda} \right\}^{1/2} \cdot (\hat{b}_\lambda \mathbf{g}_{p,\lambda}(\mathbf{x}) e^{-i\omega_\lambda t} + \hat{b}_\lambda^\dagger \mathbf{g}_{p,\lambda}^*(\mathbf{x}) e^{i\omega_\lambda t}). \quad (13)$$

Here, b_λ and $b_\lambda^\dagger$ are the annihilation and creation operators for a photon in the propagating mode $\mathbf{g}_{p,\lambda}(\mathbf{x})$, and they satisfy the boson commutation relations. The equation of motion for the electron polarization operator $\hat{c}_\gamma^\dagger(t)\hat{c}_\gamma(t)$ is

$$\begin{aligned} \frac{d}{dt} (\hat{c}_\gamma^\dagger(t)\hat{c}_\gamma(t)) &= + \frac{i}{\hbar} (E_\gamma - E'_\gamma) \hat{c}_\gamma^\dagger(t)\hat{c}_\gamma(t) \\ &+ \frac{i}{\hbar} \int d^3x \hat{\mathbf{A}}_p(\mathbf{x}, t) \left[\hat{\mathbf{J}}(\mathbf{x}, t), \hat{c}_\gamma^\dagger(t)\hat{c}_\gamma(t) \right]. \end{aligned} \quad (14)$$

Equations (12) and (14) form a set of coupled equations of motion for which a tractable approximation must be based on the physical properties of the system.

III. SPONTANEOUS EMISSION FROM A QUANTUM WELL IN A MULTILAYER STRUCTURE

A. Derivation of the Spontaneous Emission Rate

We apply (14) to derive an expression for the spontaneous emission rate Γ_{SE} from the decay rate of the occupation probability $\langle \hat{c}_{\mathbf{ck}}^\dagger \hat{c}_{\mathbf{ck}} \rangle$ for a Bloch state in the conduction band, which we indicate with the label $\gamma = (\mathbf{ck})$. States in the valence band will be labeled as $(v\mathbf{k})$. Following [17], [18] the field operator $\hat{\mathbf{A}}_p(\mathbf{x}, t)$ is split into a positive and negative frequency part $\hat{\mathbf{A}}_p(\mathbf{x}, t) = \hat{\mathbf{A}}_p^-(\mathbf{x}, t) + \hat{\mathbf{A}}_p^+(\mathbf{x}, t)$. For $\hat{\mathbf{A}}_{\text{free}}(\mathbf{x}, t)$, this splitting is already explicit in the mode decomposition (13), but for the first term in (12), it is less obvious. We note, however, that we are only interested in components of the field operator with optical frequencies. This means that we retain in the source only those terms that move an electron from a conduction band to a valence band or vice versa. Since the energy differences between these bands will be close to the energy of the emitted light quanta, one may safely adopt for $\hat{\mathbf{A}}_p^-(\mathbf{x}, t)$ the expression, cf. (12)

$$\begin{aligned} \hat{\mathbf{A}}_{\text{opt}}^-(\mathbf{x}, t) &= \sum_\lambda \left\{ \frac{\hbar}{2\epsilon_0 \epsilon_r(\mathbf{x}) \omega_\lambda} \right\}^{1/2} \hat{b}_\lambda^\dagger \mathbf{g}_{p,\lambda}^*(\mathbf{x}) e^{i\omega_\lambda t} \\ &+ \sum_{\mathbf{k}, \mathbf{k}'} \int dt' \int d^3x' \mu_0 \mathbf{G}_p(\mathbf{x}, \mathbf{x}', t, t') \\ &\cdot \mathbf{j}_{\mathbf{ck}, v\mathbf{k}'}(\mathbf{x}') \hat{c}_{\mathbf{ck}}^\dagger(t') \hat{c}_{v\mathbf{k}'}(t') \end{aligned} \quad (15)$$

in which all parts have negative frequency. The other part is its Hermitian conjugate $\hat{\mathbf{A}}_{\text{opt}}^+(\mathbf{x}, t) = [\hat{\mathbf{A}}_{\text{opt}}^-(\mathbf{x}, t)]^\dagger$, in which all the terms have a positive frequency content. Like in [18], we associate $\hat{\mathbf{A}}_{\text{opt}}^-$ with a photon creation operator, while $\hat{\mathbf{A}}_{\text{opt}}^+$ is associated with a photon annihilation operator. We further adopt the rotating-wave approximation [19] in which creation of a photon is accompanied by the transition of an electron to an energetically lower state and the annihilation of a photon by

the opposite transition. Equation (14), for $\gamma = \gamma' = \mathbf{ck}$, then takes the form

$$\begin{aligned} \frac{d}{dt} (\hat{c}_{\mathbf{ck}}^\dagger(t)\hat{c}_{\mathbf{ck}}(t)) &= \frac{1}{i\hbar} \int d^3x \left(\hat{\mathbf{A}}_{\text{opt}}^-(\mathbf{x}, t) \cdot \hat{\mathbf{J}}_{\mathbf{ck}}^{\leq \dagger}(\mathbf{x}, t) \right. \\ &\quad \left. - \hat{\mathbf{J}}_{\mathbf{ck}}^{\leq}(\mathbf{x}, t) \cdot \hat{\mathbf{A}}_{\text{opt}}^+(\mathbf{x}, t) \right) \end{aligned} \quad (16)$$

in which

$$\hat{\mathbf{J}}_{\mathbf{ck}}^{\leq}(\mathbf{r}, t) = \sum_{\mathbf{k}'} \mathbf{j}_{\mathbf{ck}, v\mathbf{k}'}(\mathbf{x}) \hat{c}_{\mathbf{ck}}^\dagger(t) \hat{c}_{v\mathbf{k}'}(t). \quad (17)$$

Note that the current operator and the field operator $\hat{\mathbf{A}}_p(\mathbf{x}, t)$ commute at equal times (one can think of their interaction being switched on at $t = 0$); therefore, their order in (16) is arbitrary, but the order adopted in (16) is convenient in the derivation of the spontaneous emission rate. If one takes the expectation value of (16) in a state which contains no photons, the free parts $\hat{\mathbf{A}}_{\text{free}}^+(\mathbf{x}, t)$ and $\hat{\mathbf{A}}_{\text{free}}^-(\mathbf{x}, t)$ annihilate the vacuum states to the right and to the left, respectively [see (15)]. In this expectation value, then, only terms of the type $\mathbf{J} \cdot \mathbf{G}_p \cdot \mathbf{J}$ survive. Next, we assume that during the retardation time $t - t'$, the fermion operators of the current in (15) evolve in time as

$$\hat{c}_{\mathbf{ck}}^\dagger(t') \hat{c}_{v\mathbf{k}'}(t') = \hat{c}_{\mathbf{ck}}^\dagger(t) \hat{c}_{v\mathbf{k}'}(t) \exp[i\omega_{\mathbf{ck}, v\mathbf{k}'}(t - t')] \quad (18)$$

with $\omega_{\mathbf{ck}, v\mathbf{k}'} = 1/\hbar (E_{\mathbf{ck}} - E_{v\mathbf{k}'})$. Physically, this so-called adiabatic approximation [17] means that during the retardation time, the field oscillates much more rapidly than the particle motion. It is equivalent to the Wigner–Weiskopf approximation [17]. Substitution of (18) in (15) yields the Fourier transform of the Green function, now as a function of frequency. Taking expectation values, indicated by $\langle \rangle$, of (16) in a state with zero photons and arbitrary state of the electrons, one obtains (19), shown at the bottom of the page, with

$$\begin{aligned} I(\mathbf{ck}, v\mathbf{k}', v\mathbf{k}_1, \mathbf{ck}'') &= \mu_0 \int \int d^3x d^3x' \mathbf{j}_{\mathbf{ck}, v\mathbf{k}'}(\mathbf{x}) \\ &\cdot \mathbf{G}_p(\mathbf{x}, \mathbf{x}', \omega_{v\mathbf{k}', \mathbf{ck}_1}) \cdot \mathbf{j}_{v\mathbf{k}_1, \mathbf{ck}''}(\mathbf{x}'). \end{aligned} \quad (20)$$

The Kronecker delta in the first term on the right-hand side comes from the interchange of fermion operators $\hat{c}_{v\mathbf{k}'}(t)$ and $\hat{c}_{v\mathbf{k}_1}^\dagger(t)$. This term is proportional to the occupation probability $\langle \hat{c}_{\mathbf{ck}}(t)^\dagger(t) \hat{c}_{\mathbf{ck}}(t) \rangle$ and, therefore, the factor that occurs here is interpreted as the decay rate

$$\Gamma_{\text{SE}} = \frac{2}{\hbar} \sum_{\mathbf{k}'} \text{Im}[I(\mathbf{ck}, v\mathbf{k}', v\mathbf{k}', \mathbf{ck})]. \quad (21)$$

The second term on the right-hand side of (19) gives a reduction if the final state $v\mathbf{k}'$ is already occupied and, thereby, accounts for the Pauli principle; the last term contains combinations of four operators that give rise to quantum interference among multiple pathways, similar to those occurring in V-type

$$\begin{aligned} \frac{d}{dt} \langle \hat{c}_{\mathbf{ck}}^\dagger(t) \hat{c}_{\mathbf{ck}}(t) \rangle &= -\frac{2}{\hbar} \sum_{\mathbf{k}', \mathbf{k}_1} \text{Im} \left\{ I(\mathbf{ck}, v\mathbf{k}', v\mathbf{k}_1, \mathbf{ck}) \cdot \langle \hat{c}_{\mathbf{ck}}^\dagger(t) \hat{c}_{\mathbf{ck}}(t) (\delta_{\mathbf{k}'\mathbf{k}_1} - \hat{c}_{v\mathbf{k}_1}^\dagger(t) \hat{c}_{v\mathbf{k}'}(t)) \rangle \right\} \\ &- \frac{2}{\hbar} \sum_{\mathbf{k}', \mathbf{k}_1, \mathbf{k}_2 \neq \mathbf{k}} \text{Im} \left\{ I(\mathbf{ck}, v\mathbf{k}', v\mathbf{k}_1, \mathbf{ck}_2) \cdot \langle \hat{c}_{\mathbf{ck}}^\dagger(t) \hat{c}_{v\mathbf{k}'}(t) \cdot \hat{c}_{v\mathbf{k}_1}^\dagger(t) \hat{c}_{\mathbf{ck}_2}(t) \rangle \right\} \end{aligned} \quad (19)$$

Fig. 1. Multilayer structure with a quantum well embedded in one of its layers. Each layer has a constant index of refraction. The index of the quantum well, which is very thin, is set equal to ε_j of the cladding layer (with thickness d_j). The position of the quantum well is given by z_0 . The Green tensor for this configuration is given by (30).

atomic systems [20], [21]. Moreover, these terms will give important contributions when correlations between the charge carriers are taken into account [5], [6]. As we do not expect that all these corrections modify the dependence of the emission rates on the dielectric configuration in a major way, we identify (21) as the decay rate to be evaluated in the following sections. Note that the current densities extend only over the active region in which the generation of light takes place, so that the region of integration is limited to that domain.

B. Calculation of Γ_{SE} for a Multilayer Dielectric

We consider a multilayer structure consisting of n layers each with a constant index of refraction as illustrated in Fig. 1. The index steps are in the z -direction; there is no variation in dielectric constant in the x and y direction. A quantum well (active layer) is embedded in the j th layer with permittivity ε_j . The Green tensor relating an observation point $\mathbf{x} = (\boldsymbol{\rho}, z)$ and a source point $\mathbf{x}_0 = (\boldsymbol{\rho}_0, z_0)$ was derived by Tomaš [22]. It is given piecewise for each homogeneous layer, within which the fields are composed of transverse waves. The interface boundary connection conditions for the fields, resulting in Fresnel coefficients for reflection and transmission [23], [24], tie the solutions in all layers together. The components of the wave vector parallel to the boundaries are the same on both sides; therefore, the 2-D $\mathbf{k}$ -vector $\mathbf{k} \equiv (k_x, k_y)$ is a characteristic label for each propagating mode with a certain frequency ω . The symbol k now denotes the magnitude of this 2-D vector. The z -component of the wave vector is different for each layer

$$k_z = \pm\beta_j = \pm\sqrt{\varepsilon_j \frac{\omega^2}{c^2} - k^2} \quad (22)$$

and may become purely imaginary in some layers or on the outside of the structure (i.e., the outermost layers). In that case, the wave is totally reflected within a layer or bunch of layers and one has a “guided mode.” The Fresnel reflection coefficients depend on polarization. In case of E polarization, when the electric field vector $\mathbf{E}$ is parallel to the layers, the reflection coefficient at a single interface between two layers j and k , neglecting the effect of any other layer is

$$\tilde{r}_{jk}^E = \frac{\beta_j - \beta_k}{\beta_j + \beta_k}; \quad k = j \pm 1 \quad (23)$$

and, for H polarization, with magnetic field H parallel to the layers

$$\tilde{r}_{jk}^H = \frac{\varepsilon_k \beta_j - \varepsilon_j \beta_k}{\varepsilon_k \beta_j + \varepsilon_j \beta_k}; \quad k = j \pm 1. \quad (24)$$

In the case of more layers, the waves are reflected at all boundaries and these reflected amplitudes add up, yielding an effective reflection coefficient $r_{j,+}$ for the upper boundary of the j th layer, due to the stack of layers above it and $r_{j,-}$ at its lower boundary due to the stack of layers below it. These effective reflection coefficients may be expressed by a recursion relation, the label q , indicating $q = E$ or $q = H$ polarization

$$r_{j,\pm}^q = \frac{1}{D_{j\pm 1}^q} [\tilde{r}_{j,j\pm 1}^q + r_{j\pm 1,\pm}^q \exp(2i\beta_{j\pm 1}d_{j\pm 1})] \quad (25)$$

with

$$D_j^q = 1 - r_{j-}^q r_{j+}^q e^{2i\beta_j d_j}. \quad (26)$$

The quantity $1/D^q$ represents the sum of the multiple reflections at the upper and lower interfaces of the j th layer [25]. Within a layer j , one may distinguish waves coming from above and reflected at the lower interface

$$\varepsilon^<(\mathbf{k}, \omega; z) = \mathbf{e}_j^q(\mathbf{k})e^{-i\beta_j z} + r_{j-}^q \mathbf{e}_j^q(\mathbf{k})e^{i\beta_j(d_j - z)} \quad (27)$$

and those coming from below and reflected at the upper interface

$$\varepsilon^>(\mathbf{k}, \omega; z) = \mathbf{e}_j^q(\mathbf{k})e^{-i\beta_j(d_j - z)} + r_{j+}^q \mathbf{e}_j^q(\mathbf{k})e^{i\beta_j z} \quad (28)$$

with unit polarization vectors

$$\mathbf{e}_j^{H\mp} = \frac{c}{\sqrt{\varepsilon_j \omega}} (\pm\beta_j \hat{\mathbf{k}} + k \hat{\mathbf{z}}), \quad \mathbf{e}_j^{E\mp} = \hat{\mathbf{k}} \cdot \hat{\mathbf{z}}. \quad (29)$$

Multiplied with $\exp(i\mathbf{k} \cdot (\boldsymbol{\rho} - \boldsymbol{\rho}_0))$, these are transversely polarized plane waves. The Green's function $\mathbf{G}_p(\mathbf{x}, \mathbf{x}', \omega)$ is composed of tensor products of these vector functions in a way similar to (7). For the calculation of the spontaneous emission coefficient Γ_{SE} , it is sufficient to know $\mathbf{G}_p(\mathbf{x}, \mathbf{x}', \omega)$ for arguments $\mathbf{x}$ and $\mathbf{x}'$, which are both within the active region cf. (20) and, therefore, both within the layer with dielectric constant ε_j . For this layer, with thickness d_j , Tomaš [22] obtained the expressions for $\mathbf{x}$ and $\mathbf{x}_0$, both in layer j

$$\begin{aligned} \mathbf{G}_{p,j}^{(j)}(\mathbf{x}, \mathbf{x}_0, \omega) = & \sum_{q=E,H} \frac{i}{4\pi^2} \int \frac{d^2 k}{2\beta_j} \zeta^q \frac{e^{i\beta_j d_j}}{D_j^q} \\ & \cdot \left[\varepsilon_j^{q>}(\mathbf{k}, \omega; z) \varepsilon_j^{q<}(-\mathbf{k}, \omega; z_0) \theta(z - z_0) \right. \\ & \left. + \varepsilon_j^{q<}(\mathbf{k}, \omega; z) \varepsilon_j^{q>}(-\mathbf{k}, \omega; z_0) \theta(z_0 - z) \right] \\ & \cdot e^{i\mathbf{k} \cdot (\boldsymbol{\rho} - \boldsymbol{\rho}_0)}, \quad 0 < z, z_0 < d_j \end{aligned} \quad (30)$$

with $\zeta^E = 1$ and $\zeta^H = -1$. Note that the 2-D k -integral in (30) should be restricted to (piecewise transverse) *propagating* waves only. The denominator D_j^q plays a similar role in this expression as the energy denominator in the general form of the Green function (7) and we shall use this in the following to identify the contributions of specific (sets of) guided modes to the emission rate and to calculate the beta factor (Section IV-C).

For the transition current density in the active region, which is the quantum well with negligible thickness at $z = z_0$, we adopt the form

$$\mathbf{j}_{v\mathbf{k}',c\mathbf{k}}(\mathbf{x}) = \frac{i\hbar e}{mS} \mathbf{K} e^{i(\mathbf{k}' - \mathbf{k}) \cdot \boldsymbol{\rho}} \delta(z - z_0) \quad (31)$$

with normalization area S . This corresponds to an independent-electron model, in which the initial and final electron wave functions are written as Bloch states $\varphi_c(\mathbf{x})e^{i\mathbf{k} \cdot \boldsymbol{\rho}}$ and $\varphi_v(\mathbf{x})e^{i\mathbf{k}' \cdot \boldsymbol{\rho}}$, respectively, with $\boldsymbol{\rho}$ the coordinate in the (x, y) direction, parallel to the layers, and $\mathbf{k}$ and $\mathbf{k}'$ the corresponding 2-D wave vectors. The 3-D vector $\mathbf{K}$ represents the dipole transition matrix elements between the lattice periodic functions of conduction and valence band. In a realistic model, this depends on whether a light- or heavy-hole band is the valence band with highest energy. Because of the symmetry of the electron and hole lattice periodic functions, H -polarized light couples to a transition from the conduction band to the light hole band *only*, while E -polarized light couples to a transition to the heavy hole valence band as well [5]. A pragmatic experimental approach is to deduce the relative size of the components of $\mathbf{K}$ from the measured ratios of E and H -polarized light.

The spontaneous emission coefficient (21) now takes the form

$$\Gamma_{SE} = \frac{2\mu_0}{\hbar} \sum_{\mathbf{k}_2} \text{Im} \left(\int \int d^2\rho d^2\rho' \mathbf{j}_{v\mathbf{k}_1,c\mathbf{k}_2}(\boldsymbol{\rho}) \cdot \mathbf{G}_p(\boldsymbol{\rho}, \boldsymbol{\rho}', z_0, \omega) \cdot \mathbf{j}_{c\mathbf{k}_2,v\mathbf{k}_1}(\boldsymbol{\rho}') \right). \quad (32)$$

with the Green tensor (30). Working out this expression, one obtains

$$\begin{aligned} \Gamma_{SE}^E &= \frac{\mu_0 \hbar q^2}{4\pi m^2} \text{Re} \cdot \left(\int_0^\infty dk \frac{k}{\beta_j} \frac{K_\perp^2}{D_j^2} (1 + r_{j+}^E \exp[2i\beta_j(d_j - z_0)]) \right. \\ &\quad \cdot (1 + r_{j-}^E e^{2i\beta_j z_0}) \Big) \\ \Gamma_{SE}^H &= \frac{\mu_0 \hbar q^2}{2\pi m^2} \text{Re} \int_0^\infty dk \\ &\quad \cdot \left(\frac{k^3}{k_j^2 \beta_j} \frac{K_\perp^2}{D_j^2} (1 + r_{j+}^H \exp[2i\beta_j(d_j - z_0)]) \right. \\ &\quad \cdot (1 + r_{j-}^H e^{2i\beta_j z_0}) + \frac{\beta_j k}{k_j^2} \frac{K_\perp^2}{2D_j^2} \\ &\quad \cdot (r_{j+}^H \exp[2i\beta_j(d_j - z_0)] - 1) \\ &\quad \cdot (r_{j-}^H e^{2i\beta_j z_0} - 1) \Big). \end{aligned} \quad (33)$$

Here $k_j^2 = \varepsilon_j \omega^2 / c^2$, and $\mathbf{K}_\perp$ is the component of $\mathbf{K}$ in the (x, y) -plane. Note that Γ_{SE}^H consists of a term proportional to $K_\perp^2$ and a term proportional to $K_\parallel^2$. In the following, we shall present these quantities separately and, therefore, use Γ_{SE}^H to indicate the part of Γ_{SE}^H that is proportional to $K_\perp^2$ and similarly Γ_{SE}^H to indicate the part that is proportional to $K_\parallel^2$. According to (33), the spontaneous emission rate depends on the reflectivity coefficients for the upper and lower layer stacks, the thickness of the j th layer, and the position of the quantum well within this layer.

Fig. 2. The three-layer structure. The different types of modes contributing to the spontaneous emission rate are indicated. Radiation modes (dotted line) couple out of the middle layer to both upper and bottom layer, substrate modes (long dashed line) couple out only to the bottom (substrate) layer, and guided modes (dashed line) propagate only in the middle layer due to total internal reflection.

IV. APPLICATION

A. Three Layers

To demonstrate the main features of the expressions (33) for the spontaneous emission rate in a multilayer structure, we first examine a three-layer structure (see Fig. 2) in which the permittivity of the layer cladding the quantum well is ε_3 , the permittivity of the upper layer is ε_2 , and that of the lower one ε_1 . If $\varepsilon_3 > \varepsilon_1 \geq \varepsilon_2$, the propagating modes of the cavity field can be classified into radiation modes [26], whose wave vectors obey $0 < k < \sqrt{\varepsilon_2}(\omega/c)$, substrate modes with $\sqrt{\varepsilon_2}(\omega/c) < k < \sqrt{\varepsilon_1}(\omega/c)$, and guided modes with $\sqrt{\varepsilon_1}(\omega/c) < k < \sqrt{\varepsilon_3}(\omega/c)$. There is no contribution of the cavity evanescent waves ($k > \sqrt{\varepsilon_3}(\omega/c)$) to the spontaneous decay rate Γ_{SE} , because such waves do not propagate. The contribution of the guided modes requires special care. Consider r_-^E for $\sqrt{\varepsilon_1}(\omega/c) < k < \sqrt{\varepsilon_3}(\omega/c)$

$$r_-^E = \frac{\sqrt{\varepsilon_3 \frac{\omega^2}{c^2} - k^2} - i\sqrt{k^2 - \varepsilon_1 \frac{\omega^2}{c^2}}}{\sqrt{\varepsilon_3 \frac{\omega^2}{c^2} - k^2} + i\sqrt{k^2 - \varepsilon_1 \frac{\omega^2}{c^2}}} = e^{2i\varphi_-^E}. \quad (34)$$

Note that r_-^E is a complex quantity with modulus 1. This holds for all $r_q^\pm$ in this interval. In this region, the real part of the integrands in (33) is zero, apart from resonances when the following condition is satisfied:

$$\beta \left(k_{gm}^{(m)} \right) d - \varphi_-^q \left(k_{gm}^{(m)} \right) - \varphi_+^q \left(k_{gm}^{(m)} \right) = m\pi \quad (35)$$

in which the phases $\varphi_\pm^q$ are defined in similar fashion as in (34), and $k_{gm}^{(m)}$ is the wavenumber of the m th guided mode. This condition (35) shows that, for a certain thickness, a finite number of guided modes exist. In the Appendix, it is shown that for E polarization, one obtains the following summation over the guided modes:

$$\Gamma_{SE}^{E,gm} = \frac{\mu_0 \hbar q^2}{4\pi m^2} K_\perp^2 \cdot \sum_{g.m.} \frac{2\pi \cos^2 \left[\beta \left(k_{gm}^{(m)} \right) z_0 - \varphi_-^E \left(k_{gm}^{(m)} \right) \right]}{d + \frac{1}{\sqrt{k_{gm}^{(m)2} - \varepsilon_1 \frac{\omega^2}{c^2}}} + \frac{1}{\sqrt{k_{gm}^{(m)2} - \varepsilon_2 \frac{\omega^2}{c^2}}}} \quad (36)$$

and for H polarization, we have (37), shown at the bottom of the next page. Here, $\tilde{\beta}_j = \sqrt{k^2 - \varepsilon_j \omega^2 / c^2}$. We studied the behavior of (33) in the three-layer case as a function of the thickness of the cladding layer and the position of the quantum well. This is done by numerical integration for the continuous part of the integrand

Fig. 3. Dependence of the spontaneous emission rate for E polarization on the thickness d of the middle layer in a three-layer model with the quantum well in the middle of the middle layer. The width is in units $\lambda/2$ with λ the wavelength in vacuum. The contribution of the radiation modes and the guided modes is summed to give the total spontaneous emission rate. The upper layer of the system has index of refraction 3.2, the middle layer has index of refraction 3.6, and the bottom layer has index of refraction 3.4 (AlAs, GaAs, and $\text{Al}_{0.5}\text{Ga}_{0.5}\text{As}$ at 300 K near bandgap, respectively). The emission rates are normalized to the emission rate for the same quantum well in vacuum. The kinks in the guided-mode and the radiation-mode contribution are due to the conversion of radiation modes into a new guided mode.

Fig. 4. Dependence of the spontaneous emission rate for H -polarization on the thickness d of the middle layer in a three-layer model. Top: Γ_{SE}^H . Bottom: Γ_{SE}^H . (For further explanation, see the text and the caption of Fig. 3.)

to calculate the contribution of the radiation modes, while for the guided modes we look for all the zeros of D^q and then calculate the contribution of the poles using (36) and (37).

The results are shown in Figs. 3–5 for a three-layer case with values for the index of refraction taken from Saleh and Teich [26]. A striking feature is that the transition rates for the dif-

Fig. 5. Dependence of the spontaneous emission rate on the thickness d of the middle layer (top figure) and on the position z_0 of the quantum well in this layer at a fixed thickness of 0.75λ (bottom figure), in both cases for E -polarization and with the quantum well in the middle of the middle layer. The outer layers of the system have equal index of refraction 3.2 and the middle layer has index of refraction 3.6 (respectively AlAs and GaAs at 300 K near bandgap).

ferent types of modes exhibit a sharp cusp at the birth of a guided mode. Here, the derivatives of Γ_{SE}^E and Γ_{SE}^H are discontinuous, but the *total* decay rate shows a smooth behavior. For the symmetric case $\epsilon_1 = \epsilon_2$ and the quantum well in the middle of layer 3, it is seen by inspection of (35) and (36) that there is no contribution of the first, third, ... guided modes to Γ_{SE}^E because the quantum well is located in the nodes of these guided modes. Only the 0th, 2nd, ... guided modes do affect Γ_{SE}^E , as the quantum well is located in their antinode. Therefore, the kinks of Γ_{SE}^E for different modes only appear at $2d/\lambda = (2n\pi + \varphi_+(k_m))/\sqrt{\epsilon_3 - \epsilon_1}$. For Γ_{SE}^H the kinks appear for all modes. For Γ_{SE}^H , this behavior is similar to Γ_{SE}^E ; for Γ_{SE}^H , it is exactly the opposite. This can be understood from (37): the contribution for guided modes is proportional to a sin function which, for the even modes, has its node at the center. In this case, the contribution of the guided modes is small in Γ_{SE}^H as compared to that in Γ_{SE}^E .

In a recent paper by Urbach and Rikken [27], a plot similar to that of Γ_{SE}^E is shown. These authors study the spontaneous emission rate of an atomic dipole in a dielectric slab embedded in two half spaces of different refractive index and use an explicit mode-decomposition of the electromagnetic field. We verified that the present method gives the same results for that case.

$$\Gamma_{SE}^{H, gm} = \frac{\mu_0 \hbar q^2}{4\pi m^2} \cdot \sum_{g.m.} \left(K_z^2 \frac{k_{gm}^2}{\epsilon_3} \frac{2\pi \cos^2 \left[\beta \left(k_{gm}^{(m)} \right) z_0 - \varphi_-^E \left(k_{gm}^{(m)} \right) \right]}{d + \frac{\epsilon_2 \epsilon_3}{\beta_2 ((\epsilon_3 + \epsilon_2) k^2 - \epsilon_2 \epsilon_3)} + \frac{\epsilon_1 \epsilon_3}{\beta_1 ((\epsilon_3 + \epsilon_1) k^2 - \epsilon_1 \epsilon_3)}} + K_\perp^2 \frac{\beta_{gm}^2}{\epsilon_3} \frac{2\pi \sin^2 \left[\beta \left(k_{gm}^{(m)} \right) z_0 - \varphi_-^E \left(k_{gm}^{(m)} \right) \right]}{d + \frac{\epsilon_2 \epsilon_3}{\beta_2 ((\epsilon_3 + \epsilon_2) k^2 - \epsilon_2 \epsilon_3)} + \frac{\epsilon_1 \epsilon_3}{\beta_1 ((\epsilon_3 + \epsilon_1) k^2 - \epsilon_1 \epsilon_3)}} \right) \quad (37)$$

Fig. 6. Structure of five layers for which the results in Fig. 7 are calculated. We concentrate on layer 3. The number x indicates the fraction of Al in the $\text{Al}_x\text{Ga}_{1-x}\text{As}$ compound. The vertical levels indicate the dielectric constant profile. From the x value, the dielectric constant can be inferred directly by linear interpolation, given that when $x = 0$, $\epsilon^{1/2} = 3.6$, and when $x = 1$, $\epsilon^{1/2} = 3.4$. In the actual structure proposed, the air layer was a metal one.

B. A Laser Structure with a High COD-limit

The case of more than three layers is quite similar to that explained in the previous section as long as the layer in which the active region is embedded has the highest refractive index. Only the effective reflection coefficients $r_{j\pm}^+$ are now influenced by the presence of a certain stack of layers instead of a single one above and below the central layer.

For a configuration as shown in Fig. 6, a new situation arises since now the layer in which the active region is embedded does *not* have the highest refractive index. Such a structure has been proposed [7] for high-power laser diodes to prevent extremely high light concentration in the active region and thereby premature breakdown of the device. Therefore, one aims at a small overlap of the active region with the laser field to increase the COD limit. In this case, guided modes can exist in layer 2, if it has a sufficient thickness, with their evanescent tails extending into the region of the quantum well. The contribution of spontaneous emission into these modes is again obtained as the sum of pole terms at the values of k for which the denominators D^q in (33) are zero. That is, when

$$1 - r_- r_+ \exp \left[-2\sqrt{k^2 - \epsilon_3} \frac{\omega^2}{c^2} d_3 \right] = 0. \quad (38)$$

The reflection coefficients r_+ and r_- are those seen from layer 3. Their formal expressions (25) are still valid, although they now pertain to evanescent waves and may have a modulus greater than 1. The contribution of the guided modes to Γ_{SE}^E is shown in (39), at the bottom of the page. This expression is derived in the Appendix.

The results calculated for the case of Fig. 6 are shown in Fig. 7. Both layers 2 and 4 are able to sustain a guided mode, but tunneling through layer 3 results in one guided mode with

Fig. 7. Top: spontaneous emission rate Γ_{SE}^E as a function of thickness d_2 of layer 2 in units $\lambda/2$, with thickness 0.57λ of layer 3. Bottom: spontaneous emission rate Γ_{SE}^E as a function of the position of the quantum well, for a thickness 0.35λ of layer 2. The point 0 corresponds to the quantum well on the interface between layer 2 and layer 3, and the point 0.5 corresponds to the quantum well on the interface between layer 3 and layer 4.

a peak in layer 2 and in layer 4. The peaks in the contribution of the guided modes in Fig. 7 can be attributed to the formation of new guided modes. The lower part of the figure shows the dependence of the contribution of the guided modes on the distance between the quantum well and layer 2, for a constant thickness of layer 3.

C. Estimate of the β_{sp} Factor

The spontaneous emission factor β_{sp} is defined [28] as the fraction of the total spontaneous emission rate that is emitted into a specific (laser) mode. We discuss this here for an edge-emitting multilayer structure. The emission into a nondegenerate discrete (laser) mode is isolated by selecting the term of the Green tensor corresponding to a simple pole at its value $\omega = \omega_\lambda$, of (7). Then this term may be selected by the prescription

$$G_p^{\text{red}}(\mathbf{x}, \mathbf{x}', \omega) = \left[\lim_{\zeta \rightarrow \omega_{\text{mode}}} (\zeta - \omega_{\text{mode}}) G_p(\mathbf{x}, \mathbf{x}', \zeta) \right] \cdot \frac{1}{\omega - \omega_{\text{mode}}} \quad (40)$$

and the β_{sp} factor is obtained as

$$\beta_{sp} = \frac{\mu_0}{\Gamma_{\text{SE}}} \cdot \text{Im} \sum_{\mathbf{k}' \text{ act. reg}} \int d^3x d^3x' \mathbf{j}_{\mathbf{ck}, \nu \mathbf{k}'}(\mathbf{x}) \cdot G_p^{\text{red}}(\mathbf{x}, \mathbf{x}', \omega_{\mathbf{ck}, \nu \mathbf{k}'}(\mathbf{x})) \cdot \mathbf{j}_{\nu \mathbf{k}', \mathbf{ck}}(\mathbf{x}'). \quad (41)$$

$$\Gamma_{\text{SE}}^{E, gm} = -\frac{\mu_0 \hbar q^2}{4m^2} K_{\perp}^2 \sum_{gm} \text{Im} \left(\frac{k_{gm}}{\beta_{gm}} e^{-2i\beta_{gm}d_3} \frac{(1 + r_+ \exp[2i\beta_{gm}(d_3 - z_0)]) (1 + r_- e^{2i\beta_{gm}(z_0)})}{\left\{ \frac{dr_+}{dk} r_- + r_+ \frac{dr_-}{dk} + 2ir_+ r_- d \frac{d\beta}{dk} \right\}_{k=k_{gm}}} \right) \quad (39)$$

Fig. 8. (a) Spontaneous emission factor β_{sp} of zeroth guided mode (solid), second guided mode (dotted), and fourth guided modes (dashed) versus width of the middle layer d , for a three-layer symmetric waveguide (AlAs/GaAs/AlAs) with the active quantum well at the center of the layer. (b) The same for guided modes in the configuration of Fig. 6. In both figures, the horizontal scale is in units $\lambda/2$ with λ the wave length in vacuum.

For the case of an infinite flat multilayer structure, the guided modes can be identified as residues of G_p at poles in the complex k plane, where k is the lateral wavenumber. All lateral directions of $\mathbf{k}$ contribute equally to that pole term; the technique to calculate the contribution of such a pole term in the spontaneous emission was discussed in Section IV-A and the Appendix. However, for a typical edge-emitting laser, lasing can only occur in lateral directions within the activated layer, roughly determined by the orientation of the pump stripe, which defines a selection of the relevant modes. For typical stripe dimensions of $5 \mu\text{m}$ by $250 \mu\text{m}$, this implies restriction of the lasing modes to an angle $\psi \simeq 2 \cdot 10^{-2}$ rad out of the 2π continuum of guided modes with a given k .

Another complication is that in a real device the emission spectrum is not monochromatic but has a width $\Delta\omega_{sp} \simeq 3 \text{ THz}$ [29], while the selected longitudinal mode has a natural width $\Delta\omega_{\text{mode}} \simeq 30 \text{ GHz}$ due to outcoupling losses. Therefore, we take as an estimate of β_{sp} for a realistic structure the fraction $(\psi/2\pi)(\Delta\omega_{\text{mode}}/\Delta\omega_{sp}) \simeq 10^{-4}/\pi$ of the contribution of the fundamental guided mode, (i.e., the 0th) of the same layered configuration with infinite lateral extension. For the *relative* magnitudes of the β_{sp} values for different modes, this factor is of course irrelevant.

In Fig. 8(a), we plot the calculated β_{sp} factor, as described above, for a symmetric three-layer configuration consisting of $\text{Ga}_x\text{Al}_{1-x}\text{As}$ with $x = 0.50$, $x = 0$, and $x = 0.50$, respectively, and for E polarized light. The β_{sp} factor is shown not only for the fundamental guided mode, that is the first guided mode born with increasing width d of the middle layer, starting at $d = 0$, but also for two that come next. The second mode

appears to become competitive with the fundamental one when the width of the middle layer supersedes λ , the vacuum wave length associated with the electronic transition frequency gap ω_{gap} . The steep rise of β_{sp} of the fundamental mode as d increases from zero to the maximum at $d = \lambda/4$ is almost linear [30]. This is explained by the argument that the spontaneous emission rate into the mode of interest is proportional to the value of the mode intensity at the location of the emitter, i.e., the quantum well, whereas the total spontaneous emission rate does not change much with increasing width (see Section IV-A).

An interesting case of mode competition is found for the five-layer case discussed in the previous section. The β_{sp} factors of the first few modes are displayed in Fig. 8(b) as a function of the thickness d_2 of layer number 2 (see Fig. 6). For very small thicknesses of this layer, the spontaneous emission into the guided modes is only possible due to the evanescent tail of the mode in layer 4. With increasing d_2 , guided modes in layer 2 also become possible and the active region finds itself within a superposition of evanescent tails of modes in layers 2 and 4. The new guided mode that is born with further increases of d_2 has a larger β_{sp} factor than the first one as soon as $d_2 \geq 0.3\lambda$ (the scale is in units $\lambda/2$). So, the second mode will then become the lasing mode. For values of d_2 where two modes have an equal β_{sp} factor, a bistable situation may thus arise at laser threshold. Note that, as already expected from the total emission rates for the total of guided modes, the β_{sp} factors in Fig. 8(b) are an order of magnitude smaller than those for the three-layer case in Fig. 8(a), which again confirms that the configuration for the high COD-limit laser must have a high laser threshold.

V. SUMMARY AND CONCLUSION

We have presented a fully quantum mechanical scheme for the description of the emission of radiation from a region with active charge carriers within a passive inhomogeneous dielectric environment. Within this theoretical framework, we derived an expression for spontaneous emission rates in terms of the classical Green tensor of the dielectric structure and of transition current densities. This was applied to a few cases of plane multilayer structure with a thin active layer (quantum well). The formalism, which provides a tool to distinguish between emission rates into single (sets of) guided modes or into a continuum of radiation modes and to study their polarization dependence, was presented in detail.

The main features were first illustrated for a simple three-layer model. It was shown that the emission rate into radiation modes exhibits sudden drops with increasing thickness of the dielectric layer that is cladding the quantum well. These are compensated by an equally large sudden rise of the emission rate into guided modes, which is due to the birth of a new guided mode. The total spontaneous emission rate is a smooth function of the thickness of the cladding layer and is also insensitive to the precise positioning of the well within that layer. As a more practical example, a multilayer structure for a high-power laser with a high COD limit was considered. In this case, the quantum well is located in a layer with lower refractive index than surrounding layers and, as a consequence of this, it overlaps only with evanescent tails of guided modes. Here, the par-

tial emission rate into the fundamental mode as a fraction of the total spontaneous emission rate (β_{sp} factor) is found to be much smaller than when the well is embedded in a dielectric region with the largest index of refraction. This is a possible explanation for the observed high lasing threshold for such a laser with a high COD limit. We also found that depending on the thickness of the cladding layer, other (sets of) guided modes than the fundamental one may have the largest β_{sp} factor and are, consequently, expected to function as the lasing modes.

The quantum formalism presented here, resulting in coupled Heisenberg equations of motion for the electromagnetic field and the active charge carriers, provides a basis for the study of observables other than just spontaneous emission rates and polarization. Interesting items for future model investigations are photon correlations and statistics of the light emitted by small dielectric devices.

APPENDIX

CONTRIBUTION OF THE GUIDED MODES

Here, we discuss how to find the contribution of a pole to the spontaneous emission coefficient γ^q , as mentioned in Section IV. The factor D_j^q has zeros in the integration interval, coinciding with the k value of the guided modes k_{gm} . We expand D_j^q around $k = k_{gm}$ in a Taylor series as follows:

$$D^q(k) = D(k_{gm}) + (k - k_{gm}) \frac{dD^q(k)}{dk} \Big|_{k=k_{gm}} + \dots \quad (42)$$

where we have omitted all labels not relevant for this discussion for reasons of generality and readability. The first term on the right-hand side of (42) is zero; the derivative of $D^q(k)$ consists of three terms

$$\frac{dD^q(k)}{dk} = \left(\frac{dr_+}{dk} r_- + r_+ \frac{dr_-}{dk} + 2ir_+ r_- \frac{d\beta}{dk} \right) e^{2i\beta d}. \quad (43)$$

The factor $(k - k_{gm})$ in the denominator should now be interpreted as $(k - k_{gm} - i\eta)$ with η a positive infinitesimal, because we must use the *retarded* Green tensor. Then

$$\text{Im} \left(\lim_{k \rightarrow k_{gm}} \frac{1}{k - k_{gm} - i\eta} \right) = \pi \delta(k - k_{gm}). \quad (44)$$

Using (35), (38), and $D(k_{gm}) = 0$ in (26), one finds that the integral in (33) for Γ_{SE}^E can be rewritten as

$$\begin{aligned} \text{Re} \left(\int_{\sqrt{\epsilon_{\min}}\omega/c}^{\sqrt{\epsilon_{\max}}\omega/c} dk \frac{k}{\beta} \frac{(1 + r_+ e^{2i\beta(d-z_0)}) (1 + r_- e^{2i\beta(z_0)})}{D^q(k)} \right) \\ = - \sum_{gm} \frac{k_{gm}}{\beta_{gm}} \text{Im} \left(\frac{2 \cos^2(\beta_{gm} z_0 - \varphi_-)}{\frac{dD}{dk} \Big|_{k=k_{gm}}} \right) \end{aligned} \quad (45)$$

which results in the contributions of the guided modes given in (36). In the same way, one obtains (37) and (39).

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