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Quantum Description of Light Emitted from Semiconductor Microstructures

Abstract

We present a quantum mechanical formalism to study the interaction between the active region in a semiconductor device and the electromagnetic field. The method explicitly avoids decomposition into modes. Instead, use is made of the classical Green tensor for the passive structure. We derive an expression for the spontaneous emission rate generally valid for localized and delocalized interactions. As an application, we calculate the spontaneous emission factor β_{sp} for an edge-emitting three-layer (waveguide) structure with a quantum well as a function of the width of the middle layer and the position of the quantum well in it.

In view of apparent developments towards miniaturization of semiconductor devices as well as realization of schemes where semiconductor lasers emit light with non-classical properties [1, 2, 3, 4], there is an obvious need for a general quantum mechanical framework in which one is able to treat the electromagnetic field, the electron dynamics and the interaction between electrons and the electromagnetic field in a quantized way for general geometries. Such a framework could already today be necessary to understand the basic operation of quantum optical devices (noise properties, photon statistics and correlations). It should also allow for a straightforward integration with existing quantum mechanical models for the full electron dynamics in the active region [5] and in semiconductors in general [6].

The present paper reports on our approach towards such a general framework and the results obtained thus far. A key role in our quantum mechanical theory is played by the *classical* Green tensor of the passive dielectric structure, i.e., the full device with its active constituents like quantum wells removed. Most of the existing semiconductor light emitting devices can be described in this manner. In our approach we deal directly with the electromagnetic field operators, rather than creation and annihilation operators for the natural modes of the structure. Thus we avoid certain complications connected to the lossy character of a mode as a consequence of the open nature of any dielectric structure. The problem is formulated by defining the Hamiltonian in a generalized Coulomb gauge and the basic commutation relations. Then in the Heisenberg picture the equations of motion for the relevant operators are straightforwardly derived. An important position is taken by the inhomogeneous operator wave equation for the electromagnetic vector potential in which the source term reflects the field-matter interaction. This equation can be implicitly solved

for the vector potential in terms of the classical Green tensor pertaining to the dielectric structure that remains after removing the active constituents. From here on it is possible to build further towards a more comprehensive theory that includes the analysis of higher order correlation functions, stimulated emission, squeezing and lasing. In the present paper we focus on the application of the theory developed so far to the fundamental problem of spontaneous emission.

A general formula for the spontaneous emission rate is derived that, unlike the usual result based on localized electric dipole interaction, takes the delocalized character of the electron states fully into account (electric current rather than electric dipole interaction). Moreover, the orientation of the current matrix element, i.e., the polarization associated with the transition, is taken into account. Next, we apply this formula to a multilayer dielectric configuration with a quantum well and we obtain explicit results for three-layer waveguide structures, a problem that received significant attention recently, both theoretical and experimental [7, 8, 9]. Not only can we demonstrate the strength and elegance of our method [10], and completely confirm the theoretical results obtained in [9], but we also calculate the spontaneous emission factor β_{sp} for a selected mode in a three-layer edge emitter.

An important advantage of our method is that it allows a consistent Hamiltonian formulation of the problem, without running into difficulties associated with the open character of the system. The field is quantized directly, without invoking a modal decomposition, while the electromagnetic features are separated, in a way, from the quantum-mechanical ones. It is assumed that the (classical) Green tensor for the full device geometry without the active carriers is known. In practice it may not be an easy task to calculate the Green tensor for a realistic multilayer device. On the other hand, for a given structure, it needs only be done once. This Green tensor is then used as input for the quantum mechanical equations of motion.

1 Derivation of equations of motion

In this section the Heisenberg equations of motion for the relevant operators in a light emitting dielectric device will be derived. The Hamiltonian for such a device and the commutation relations for the operators need to be identified. For the charge carriers the well known fermion anti-commutation relations hold. For the field operators the situation is not so straightforward [11, 12, 13, 14] and indeed is different from the vacuum case. We distinguish two interacting parts in the light-emitting device. One part consists of the free charge carriers (the electrons in the conduction band and the holes in the valence band) the quantum transitions of which produce or absorb (incoming) light. Usually these occur only in a small subregion of the system, e.g. a quantum well. The other part is passive and constitutes all the rest of the device, including the various interfaces that give rise to reflection like in a cavity or to guided, radiation and substrate modes like in a waveguide. Here only bound charges interact with the field. We neglect absorption in this part, which is a reasonable approximation in the optically relevant regime. The dielectric properties (that arise due to the interaction with the bound charges) are then accounted for by a real dielectric function $\varepsilon(\mathbf{r})$ that is only space-dependent. This dielectric space may be considered as an effective vacuum, in which the electromagnetic field may be quantized in a similar way as in the true

vacuum. This is shortly summarized in the next subsection.

1.1 Quantization of the electromagnetic field in a lossless dielectric structure

For the quantization of the field in the passive part we follow the lines of the extensive discussions by Knöll, Vogel and Welsch [11, 12], Glauber and Lewenstein [13], and Tip [14]. Note that this part of the system contains no free charges or currents. We introduce the vector potential field in the usual way as (in SI units)

$$\mathbf{B}(\mathbf{r},t) = \nabla \times \mathbf{A}(\mathbf{r},t) \tag{1}$$

$$\mathbf{E}(\mathbf{r},t) = -\frac{\partial \mathbf{A}(\mathbf{r},t)}{\partial t}. \tag{2}$$

In (2) one normally expects a scalar potential as well. However, this term is chosen to be zero due to the absence of free charges. For the vector potential we choose the generalized Coulomb gauge [11, 12, 13, 14]:

$$\nabla \cdot (\varepsilon(\mathbf{r})\mathbf{A}(\mathbf{r},t)) = 0. \tag{3}$$

Note that this is compatible with $\nabla \cdot \mathbf{D} = 0$, where $\mathbf{D} = -\varepsilon_0 \varepsilon(\mathbf{r})\dot{\mathbf{A}}$. Identification of the proper canonical momentum density as the conjugate variable to $\mathbf{A}$ for quantization of the field requires special care, since the independent variables are non-trivial components of the vector field because of the generalized transversality condition (3). It can be shown that the canonically conjugate momentum density is given by [12]:

$$\Pi(\mathbf{r},t) = \varepsilon_0 \varepsilon(\mathbf{r})\dot{\mathbf{A}}(\mathbf{r},t) = -\varepsilon_0 \varepsilon(\mathbf{r})\mathbf{E}. \tag{4}$$

The Hamiltonian for the electromagnetic field then reads:

$$H_{diel} = \int d^3r \frac{1}{2}\left[\frac{(\mathbf{\Pi}(\mathbf{r},t))^2}{\varepsilon_0 \varepsilon(\mathbf{r})} + \frac{(\nabla \times \mathbf{A}(\mathbf{r},t))^2}{\mu_0}\right], \tag{5}$$

the integration extending over all space, with $\varepsilon(\mathbf{r}) \equiv 1$ everywhere outside the dielectric light emitting device. The canonical quantization condition is more complicated than in the usual Coulomb gauge, where it involves the transverse delta function [15]. Here, because of the generalized transversality condition (3), one obtains the equal-time commutators [12]:

$$[\hat{\mathrm{A}}_\alpha(\mathbf{r}), \hat{\mathrm{E}}_\beta(\mathbf{r}')] = -\frac{i\hbar}{\varepsilon_0}\delta^\varepsilon_{\alpha\beta}(\mathbf{r},\mathbf{r}'). \tag{6}$$

where $\delta^\varepsilon_{\alpha\beta}(\mathbf{r},\mathbf{r}')$ is the generalized transverse delta function [12, 13]. For a transverse vector field $\mathbf{X}^T(\mathbf{r})$ one has the relation:

$$\sum_\beta \int d^3r' \varepsilon(\mathbf{r})\delta^\varepsilon_{\alpha\beta}(\mathbf{r},\mathbf{r}')X^T_\beta(\mathbf{r}') = X^T_\alpha(\mathbf{r}), \tag{7}$$

while for a longitudinal vector field $\mathbf{X}^L(\mathbf{r})$:

$$\sum_{\beta} \int d^3r' \delta^{\varepsilon}_{\alpha\beta}(\mathbf{r},\mathbf{r}')\varepsilon(\mathbf{r}')X^L_{\beta}(\mathbf{r}') = 0. \tag{8}$$

Note that with this definition the generalized transverse delta function differs by a constant factor $\varepsilon(\mathbf{r}) = \varepsilon$ from the usual transverse delta function when $\varepsilon(\mathbf{r})$ is independent of $\mathbf{r}$. In a number of recent papers [16, 17, 18, 19] it has been stressed that a real $\varepsilon(\mathbf{r})$ unequal to 1 violates the Kramers-Kronig relations and therefore causality. However, as a model valid for the limited frequency range of optical waves in a dielectric material it should be acceptable [8, 13, 19].

1.2 Hamiltonian

The *total* Hamiltonian for the system has to be derived by determining the energy associated with all the processes in the system. The active particles and the interaction are confined to the active region. The part of the Hamiltonian concerned with the electromagnetic field is given in (5). Now consider the free charge carriers in the active region. The particle Hamiltonian is split into a part which contains only the canonical variables of the particles, now written in terms of the electron field operators $\hat{\Psi}(\mathbf{r},t)$ as

$$\begin{aligned} \hat{H}_{el} &= \int\limits_{act.reg.} d^3r \hat{\Psi}^{\dagger}(\mathbf{r},t)\left(\frac{-\hbar^2}{2m_e}\nabla^2 + eU(\mathbf{r})\right)\hat{\Psi}(\mathbf{r},t) \\ &\quad + \frac{1}{2}\int\int\limits_{act.\,reg.} d^3r d^3r' \hat{\Psi}^{\dagger}(\mathbf{r},t)\hat{\Psi}^{\dagger}(\mathbf{r}',t)V(\mathbf{r},\mathbf{r}')\hat{\Psi}(\mathbf{r}',t)\hat{\Psi}(\mathbf{r},t) \end{aligned} \tag{9}$$

(in which $U(\mathbf{r})$ is the lattice potential and $V(\mathbf{r},\mathbf{r}')$ is the instantaneous Coulomb interaction), and the electron-field interaction Hamiltonian

$$\hat{H}_{int} = -\int\limits_{act.reg.} d\mathbf{r}\hat{\mathbf{A}}(\mathbf{r},t)\cdot\hat{\mathbf{J}}(\mathbf{r},t) \tag{10}$$

with, in the case of a generalized Coulomb gauge (3), an operator $\hat{\mathbf{J}}(\mathbf{r},t)$ defined as:

$$\begin{aligned} \hat{\mathbf{J}}(\mathbf{r},t) &= \frac{-i\hbar e}{2m_e}\left\{\hat{\Psi}^{\dagger}(\mathbf{r},t)\nabla\hat{\Psi}(\mathbf{r},t) - \left(\nabla\hat{\Psi}^{\dagger}(\mathbf{r},t)\right)\hat{\Psi}(\mathbf{r},t)\right\} \\ &\quad + \hat{\Psi}^{\dagger}(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t)\left\{\frac{i\hbar e}{2m_e}\frac{\nabla\varepsilon(\mathbf{r})}{\varepsilon(\mathbf{r})} - \frac{e^2}{2m_e}\hat{\mathbf{A}}(\mathbf{r},t)\right\}. \end{aligned} \tag{11}$$

The third term in this expression originates from $\nabla\hat{\mathbf{A}}$ and the condition (3). Note that $\hat{\Psi}(\mathbf{r},t)$ and therefore the region of integration extends in practice only over the active region to which the free charge carriers are confined.

When substituted in (10), the term in (11) proportional to $\hat{\mathbf{A}}(\mathbf{r},t)$ is often neglected on the basis of arguments that the electromagnetic radiation fields are weak compared to the

atomic field strengths [20, 21]. The term with the gradient of $\varepsilon(\mathbf{r})$ in (11) is also expected to be of minor importance, because the dielectric constant is by definition a macroscopic quantity, representing the effect of the average polarization of bound charges over a region that is large compared to atomic dimensions [22]. For the active layer it is a somewhat hypothetical quantity, referring to the system without the free carriers and will not differ very much from the dielectric constants of the surrounding layers. From now on, we will neglect these terms and identify $\hat{\mathbf{J}}(\mathbf{r},t)$ with the electromagnetic current:

$$\hat{\mathbf{J}}(\mathbf{r},t) \approx \hat{\mathbf{J}}_{EM}(\mathbf{r},t) \approx \frac{-i\hbar e}{2m_e}\left\{\hat{\Psi}^{\dagger}(\mathbf{r},t)\nabla\hat{\Psi}(\mathbf{r},t) - \left(\nabla\hat{\Psi}^{\dagger}(\mathbf{r},t)\right)\hat{\Psi}(\mathbf{r},t)\right\} \tag{12}$$

It is only the transverse current which acts as a source of the electromagnetic field. This follows from the the operator Maxwell equation, which can be expressed as:

$$\begin{aligned}\hat{\mathbf{J}}_{EM}(\mathbf{r},t) &= -\frac{\partial}{\partial t}\hat{\mathbf{D}}(\mathbf{r},t) + \nabla\times\hat{\mathbf{H}}(\mathbf{r},t) \\ &= -\frac{1}{i\hbar}[\varepsilon_0\varepsilon(\mathbf{r})\hat{\mathbf{E}}(\mathbf{r},t), \hat{H}_{int}],\end{aligned} \tag{13}$$

where the second equality in (13) follows from the Heisenberg equations of motion (see (15)) for the displacement operator. Using (6) and (7) one obtains:

$$\hat{J}_{EM,\alpha}(\mathbf{r},t) = \int_{act.reg.} d^3r'\varepsilon(\mathbf{r})\sum_{\beta}\delta^{\varepsilon}_{\alpha\beta}(\mathbf{r},\mathbf{r}')\hat{J}_{\beta}(\mathbf{r}',t) = \hat{J}^{T}_{EM,\alpha}(\mathbf{r},t), \tag{14}$$

where $\hat{J}_{\beta}(\mathbf{r}',t)$ is the β-component of $\hat{\mathbf{J}}(\mathbf{r},t)$ and $\alpha,\beta = x,y,z$. Since the current $\hat{\mathbf{J}}_{EM}(\mathbf{r},t)$ is transverse, we will denote it from here on as $\hat{\mathbf{J}}^{T}_{EM}(\mathbf{r},t)$.

1.3 Equations of motion

In the Heisenberg picture the operators are time-dependent, while the states are time-independent. An advantage of this picture is that the electromagnetic field operators satisfy equations that resemble as close as possible the classical electromagnetic field equations. By assuming the interaction switched on at $t = 0$, all expectation values can be evaluated in the free-field state of the system at $t = 0$. For an operator $\hat{F}$ that has no explicit time-dependence, the Heisenberg equation of motion is given by:

$$\frac{d}{dt}\hat{F} = \frac{1}{i\hbar}[\hat{F},\hat{H}]. \tag{15}$$

For the vector potential operator $\hat{\mathbf{A}}(\mathbf{r},t)$ one deduces the following vector wave equation, by application of (15) with the Hamiltonians (5) and (10), using relation (14) and the gauge condition (3):

$$\nabla\times\nabla\times\hat{\mathbf{A}}(\mathbf{r},t) + \frac{\varepsilon(\mathbf{r})}{c^2}\frac{\partial^2}{\partial t^2}\hat{\mathbf{A}}(\mathbf{r},t) = \mu_0\hat{\mathbf{J}}^{T}_{EM}(\mathbf{r},t). \tag{16}$$

After time-Fourier transformation of (16) the formal solution in terms of $\hat{\mathbf{J}}^T_{EM}(\mathbf{r}', \omega)$ is obtained as:

$$\hat{\mathbf{A}}(\mathbf{r}, \omega) = \hat{\mathbf{A}}_{free}(\mathbf{r}, \omega) + \int d^3r' \overleftrightarrow{G}(\mathbf{r}, \mathbf{r}', \omega) \cdot \hat{\mathbf{J}}^T_{EM}(\mathbf{r}', \omega), \tag{17}$$

in which the Green tensor satisfies the equation:

$$\sum_k \left[\partial^r_i \partial^r_k - \delta_{ik} \left(\Delta^r + \frac{\omega^2}{c^2} \varepsilon(\mathbf{r}) \right) \right] G_{kj}(\mathbf{r}, \mathbf{r}', \omega) = \mu_0 \delta_{ij} \delta(\mathbf{r} - \mathbf{r}') \tag{18}$$

and $\hat{\mathbf{A}}_{free}(\mathbf{r}, \omega)$ is a solution of the homogeneous equation, representing the electromagnetic field operator for the passive dielectric structure.

The operator for the electron field is expanded in a basis set:

$$\hat{\Psi}(\mathbf{r}, t) = \sum_\gamma \hat{c}_\gamma(t) \varphi_\gamma(\mathbf{r}). \tag{19}$$

where the label γ indicates quantum numbers of Bloch states, i.e., band index n and wave vector $\mathbf{k}$ [6]. For the operator $\hat{c}_\gamma(t)$ the Fermion anti-commutation rules hold:

$$\hat{c}_\gamma(t) \hat{c}_{\gamma'}(t) = -\hat{c}_{\gamma'}(t) \hat{c}_\gamma(t), \tag{20}$$

$$\hat{c}_\gamma(t) \hat{c}^\dagger_{\gamma'}(t) = \delta_{\gamma\gamma'} - \hat{c}^\dagger_{\gamma'}(t) \hat{c}_\gamma(t). \tag{21}$$

In the same representation the current operator (14) can be expressed as:

$$\hat{J}^T_{EM,\alpha}(\mathbf{r}, t) = \sum_{\gamma,\gamma'} \hat{c}^\dagger_\gamma(t) \hat{c}_{\gamma'}(t) j^T_{\alpha,\gamma\gamma'}(\mathbf{r}), \tag{22}$$

with

$$j^T_{\alpha,\gamma\gamma'}(\mathbf{r}) = \int_{act.reg.} d^3r' \varepsilon(\mathbf{r}) \sum_\beta \delta^\varepsilon_{\alpha\beta}(\mathbf{r}, \mathbf{r}') j_{\beta,\gamma\gamma'}(\mathbf{r}'), \tag{23}$$

and

$$j_{\beta,\gamma\gamma'}(\mathbf{r}) = \left\{ -\frac{i\hbar e}{2m_e} \left(\varphi^*_\gamma(\mathbf{r}) \nabla_\beta \varphi_{\gamma'}(\mathbf{r}) - \left(\nabla_\beta \varphi^*_\gamma(\mathbf{r}) \right) \varphi_{\gamma'}(\mathbf{r}) \right) \right\}. \tag{24}$$

If the adopted basis representation $\varphi_\gamma(\mathbf{r})$ is that of the mean-field (Hartree-Fock) solutions, the many-body Hamiltonian for the electrons (9) is represented as [23, 24, 25]:

$$\hat{H}_{el} = \sum_\gamma E_\gamma \hat{c}^\dagger_\gamma(t) \hat{c}_\gamma(t) + \frac{1}{4} {\sum_{\beta\beta'\gamma\gamma'}}' V_{\beta\beta'\gamma\gamma'} \hat{c}^\dagger_\beta(t) \hat{c}^\dagger_{\beta'}(t) \hat{c}_{\gamma'}(t) \hat{c}_\gamma(t).$$

The prime on the summation in (1.3) indicates that Coulomb interaction terms already included in the mean-field energies E_γ must be discarded in order to avoid double counting.

The equation of motion for the current density (22) is determined by Heisenberg equations of motion for a pair of electron creation and annihilation operators:

$$\begin{aligned}\frac{d}{dt}(\hat{c}^\dagger_\gamma(t)\hat{c}_{\gamma'}(t)) &= -\frac{1}{i\hbar}\sum_\alpha \int_{el.ext} d^3r \left\{\hat{c}^\dagger_\gamma(t)\hat{c}_\alpha(t)\hat{\mathbf{A}}(\mathbf{r},t)\cdot\mathbf{j}^T_{\gamma'\alpha}(\mathbf{r}) - \hat{c}^\dagger_\alpha(t)\hat{c}_{\gamma'}(t)\hat{\mathbf{A}}(\mathbf{r},t)\cdot\mathbf{j}^T_{\alpha\gamma}(\mathbf{r})\right\} \\ &+\frac{1}{i\hbar}(E_{\gamma'}-E_\gamma)\hat{c}^\dagger_\gamma(t)\hat{c}_{\gamma'}(t) \\ &+\frac{1}{i\hbar}\left[\hat{c}^\dagger_\gamma(t)\hat{c}_{\gamma'}(t), \frac{1}{4}{\sum_{\beta\beta'\alpha\alpha'}}' V_{\beta\beta'\alpha\alpha'}\hat{c}^\dagger_\beta(t)\hat{c}^\dagger_{\beta'}(t)\hat{c}_{\alpha'}(t)\hat{c}_\alpha(t)\right]. \end{aligned} \tag{25}$$

The last term in this expression entails the many-electron problem and can be approximated in various ways to obtain a closed set of equations that can be solved [6]. In the next section, which is intended to illustrate the use of the Green tensor, we shall treat (25) only in its simplest (free-carrier) approximation, i.e., we disregard the last term.

2 Application to spontaneous emission

2.1 Derivation of the spontaneous emission rate

The method we use to derive the spontaneous emission rate is adapted from the methods commonly used in quantum optics [26] and in particular inspired by [27]. On the basis of the equation of motion (25), we will derive an expression for the occupation number of the conduction band ($\gamma = \gamma' = 2, \mathbf{k}$) of the form:

$$\frac{d}{dt} < \hat{c}^\dagger_{2\mathbf{k}}(t)\hat{c}_{2\mathbf{k}}(t) >= -\Gamma_{SE} < \hat{c}^\dagger_{2\mathbf{k}}(t)\hat{c}_{2\mathbf{k}}(t) > + \cdots \tag{26}$$

in which the brackets indicate expectation values, the factor Γ_{SE} is interpreted as the coefficient of spontaneous emission and the dots represent terms of more complicated form. From inspection of (25) it is clear that, neglecting the electron-electron interaction, a result of the form (26) must be obtained from the first line on the right hand side of (25) which contains the field operator $\hat{\mathbf{A}}(\mathbf{r},t)$. This field operator, which describes the creation of a photon in the process that we consider, consists according to (17) of a free part and a part generated by the (transverse) electromagnetic current. Since we are interested in optical transitions, only terms with optical frequencies of the current $\hat{\mathbf{J}}^T_{EM}(\mathbf{r},t)$ are relevant here. These are the terms of (22) for which γ and γ' refer to different bands. For them, we use the zero-order expression for the elements of the density operator:

$$\hat{c}^\dagger_{n\mathbf{k}}(t)\hat{c}_{n'\mathbf{k}'}(t) = \hat{c}^\dagger_{n\mathbf{k}}(0)\hat{c}_{n'\mathbf{k}'}(0)\mathrm{e}^{-i\omega_{n'n}t}; \quad (n \neq n') \tag{27}$$

with $\omega_{n'n} = \frac{1}{\hbar}(E_{n'\mathbf{k}'} - E_{n\mathbf{k}})$. Then substitution of the current (22) into (17) yields:

$$\hat{\mathbf{A}}(\mathbf{r},t) = \hat{\mathbf{A}}_{free}(\mathbf{r},t) + \sum_{n'\neq n,\mathbf{k}'\mathbf{k}} \int_{act.reg.} d^3r' \overleftrightarrow{G}(\mathbf{r},\mathbf{r}',\omega_{n'n})\hat{c}^\dagger_{n\mathbf{k}}(t)\hat{c}_{n'\mathbf{k}'}(t)\cdot\mathbf{j}^T_{nn'}(\mathbf{r}',\mathbf{k},\mathbf{k}'), \tag{28}$$

with $\mathbf{j}^T_{nn'}(\mathbf{r},\mathbf{k},\mathbf{k}') \equiv \mathbf{j}^T_{n\mathbf{k}n'\mathbf{k}'}(\mathbf{r})$. The use of (27) in the intermediate step implies a limitation to lowest order in the field operator $\hat{\mathbf{A}}(\mathbf{r},t)$ (note that the fermion operators are coupled via (25) to the field operator) and thereby higher order processes such as the re-absorption of emitted photons are neglected.

The summation in (28) splits in two parts, one in which all terms have a negative frequency content ($E_q < E_p$):

$$\hat{\mathbf{A}}_{opt}{}^{-}(\mathbf{r},t) = \hat{\mathbf{A}}_{free}{}^{-}(\mathbf{r},t) + \sum_{q<p,\mathbf{k}_q,\mathbf{k}_p} \int_{act.reg.} d^3r \overleftrightarrow{G}(\mathbf{r},\mathbf{r}',\omega_{qp}) \cdot \mathbf{j}^T_{pq}(\mathbf{r}',\mathbf{k}_p,\mathbf{k}_q)\hat{c}^\dagger_{p\mathbf{k}_p}(t)\hat{c}_{q\mathbf{k}_q}(t) \quad (29)$$

and the other part which is its Hermitian conjugate $\hat{\mathbf{A}}_{opt}{}^{+}(\mathbf{r},t) = [\hat{\mathbf{A}}_{opt}{}^{-}(\mathbf{r},t)]^\dagger$, in which all the terms have a positive frequency content. The former can be associated with a photon creation operator while the latter is associated with a photon annihilation operator. Calculation of the spontaneous emission is most easily performed by normal ordering of the operators [27, 28, 29, 30], which implies that these photon creation operators are put on the left and the photon annihilation operators are put on the right in operator-product expressions. In this way one loses all vacuum expectation values containing factor $\hat{\mathbf{A}}^{\pm}_{free}$; i.e, contributions of the free field, and the spontaneous emission is regarded as the radiation reaction of the current source back on itself. Moreover we adopt the familiar rotating wave approximation [29], in which creation of a photon is accompanied by transition of an electron to an energetically lower state and the annihilation of a photon by the opposite transition. Substitution of (28) into (25) for $\gamma = \gamma' = (n,\mathbf{k})$ and omitting the last commutator in (25) then yields the Heisenberg equation of motion:

$$\frac{d}{dt}\left(\hat{c}^\dagger_{n\mathbf{k}}(t)\hat{c}_{n\mathbf{k}}(t)\right) = \frac{1}{i\hbar}\int d^3r \quad \Big[\hat{\mathbf{A}}^{-}(\mathbf{r},t)\cdot\hat{\mathbf{J}}^{<\dagger}_{n\mathbf{k}}(\mathbf{r},t) - \hat{\mathbf{J}}^{<}_{n\mathbf{k}}(\mathbf{r},t)\cdot\hat{\mathbf{A}}^{+}(\mathbf{r},t)$$
$$-\hat{\mathbf{A}}^{-}(\mathbf{r},t)\cdot\hat{\mathbf{J}}^{>\dagger}_{n\mathbf{k}}(\mathbf{r},t) + \hat{\mathbf{J}}^{>}_{n\mathbf{k}}(\mathbf{r},t)\cdot\hat{\mathbf{A}}^{+}(\mathbf{r},t)\Big], \quad (30)$$

in which

$$\hat{\mathbf{J}}^{<}_{n\mathbf{k}}(\mathbf{r},t) \equiv \sum_{m<n,\mathbf{k}'} \mathbf{j}^T_{nm}(\mathbf{r},\mathbf{k},\mathbf{k}')\hat{c}^\dagger_{n\mathbf{k}}(t)\hat{c}_{m\mathbf{k}'}(t),$$
$$\hat{\mathbf{J}}^{>}_{n\mathbf{k}}(\mathbf{r},t) \equiv \sum_{m>n,\mathbf{k}'} \mathbf{j}^T_{mn}(\mathbf{r},\mathbf{k}',\mathbf{k})\hat{c}^\dagger_{m\mathbf{k}'}(t)\hat{c}_{n\mathbf{k}}(t). \quad (31)$$

Since the integrand in (30) is anti-Hermitian, one obtains for the expectation value of this equation, in any state of the form $|\varphi_{el}> |0_{field}>$ with arbitrary electronic state and vacuum photonic state,

$$\frac{d}{dt} < \hat{c}^\dagger_{n\mathbf{k}}(t)\hat{c}_{n\mathbf{k}}(t) >=$$
$$-\frac{2}{\hbar}\left\{\sum_{m>n,\mathbf{k}'}\sum_{q<p,\mathbf{k}_p\mathbf{k}_q} \mathrm{Im}\left[I(n,\mathbf{k},m,\mathbf{k}',p,\mathbf{k}_p,q,\mathbf{k}_q) < (\hat{c}^\dagger_{p\mathbf{k}_p}(t)\hat{c}_{q\mathbf{k}_q}(t)\hat{c}^\dagger_{n\mathbf{k}}(t)\hat{c}_{m\mathbf{k}'}(t)) >\right]\right.$$
$$\left. + \sum_{m<n,\mathbf{k}'}\sum_{q>p,\mathbf{k}_p\mathbf{k}_q} \mathrm{Im}\left[I(n,\mathbf{k},m,\mathbf{k}',p,\mathbf{k}_p,q,\mathbf{k}_q) < (\hat{c}^\dagger_{n\mathbf{k}}(t)\hat{c}_{m\mathbf{k}'}(t)\hat{c}^\dagger_{p\mathbf{k}_p}(t)\hat{c}_{q\mathbf{k}_q}(t)) >\right]\right\} \quad (32)$$

where

$$I(n,\mathbf{k},m,\mathbf{k}',p,\mathbf{k}_p,q,\mathbf{k}_q) \equiv \int_{act.}\int_{reg} d^3r d^3r' \mathbf{j}^T_{nm}(\mathbf{r},\mathbf{k},\mathbf{k}')\cdot \overleftrightarrow{G}(\mathbf{r},\mathbf{r}',\omega_{qp})\cdot \mathbf{j}^T_{pq}(\mathbf{r}',\mathbf{k}_p,\mathbf{k}_q). \quad (33)$$

Equation (32) expresses the time evolution of the carrier number operator corresponding to band n and wave vector $\mathbf{k}$ in the first Brillouin zone as a net result of two contributions: transitions of electrons to band n and transitions from band n to other bands. We will now consider the simple case of just two bands, an upper band labeled 2 (conduction band) and a lower band 1 (valence band). Then (32) for the occupation operator of the conduction band can be written as:

$$\begin{aligned}\frac{d}{dt} &< \hat{c}^\dagger_{2\mathbf{k}}(t)\hat{c}_{2\mathbf{k}}(t) >= \\ &-\frac{2}{\hbar}\sum_{\mathbf{k}',\mathbf{k}_1} \mathrm{Im}\left\{ I(2,\mathbf{k},1,\mathbf{k}',1,\mathbf{k}_1,2,\mathbf{k}) < \hat{c}^\dagger_{2\mathbf{k}}(t)\hat{c}_{2\mathbf{k}}(t)(\delta_{\mathbf{k}'\mathbf{k}_1} - \hat{c}^\dagger_{1\mathbf{k}_1}(t)\hat{c}_{1\mathbf{k}'}(t)) > \right\} \\ &-\frac{2}{\hbar}\sum_{\mathbf{k}',\mathbf{k}_1,\mathbf{k}_2\neq\mathbf{k}} \mathrm{Im}\left\{ I(2,\mathbf{k},1,\mathbf{k}',1,\mathbf{k}_1,2,\mathbf{k}_2) < \hat{c}^\dagger_{2\mathbf{k}}(t)\hat{c}_{1\mathbf{k}'}(t)\hat{c}^\dagger_{1\mathbf{k}_1}(t)\hat{c}_{2\mathbf{k}_2}(t) > \right\}. \quad (34)\end{aligned}$$

The first term on the right hand side of (34) describes, apart from a correction due to a possible Pauli blocking of the final state $\mathbf{k}'$ in the valence band, the effect of decay by spontaneous emission of intial conduction band state $\mathbf{k}$. The second term on the right hand side of (34) contains combinations of $\hat{c}$-operators that give rise to quantum interference among multiple radiation pathways, some of which are similar to those occuring in $\bigvee$-type atomic systems [31, 32]. Such effects may lead, in principle, to much faster decay than resulting from the first term. However, in realistic situations the necessary coherences for such enhancement are most probably not observable. Therefore, we will neglect such effects here. We may now find the coefficient of spontaneous emission from the term on the right hand side of (34) that is proportional to $< \hat{c}^\dagger_{2\mathbf{k}}(t)\hat{c}_{2\mathbf{k}}(t) >$. This coefficient is:

$$\begin{aligned}\Gamma_{SE} &= \frac{2}{\hbar}\sum_{\mathbf{k}'} \mathrm{Im}[I(2,\mathbf{k},1,\mathbf{k}',1,\mathbf{k}',2,\mathbf{k})] = \\ &= \frac{2}{\hbar}\mathrm{Im}\sum_{\mathbf{k}'}\int_{act.} dr \int_{reg} dr' \mathbf{j}^T_{21}(\mathbf{r},\mathbf{k},\mathbf{k}')\cdot \overleftrightarrow{G}(\mathbf{r},\mathbf{r}',\omega_{2\mathbf{k},1\mathbf{k}'})\cdot \mathbf{j}^T_{12}(\mathbf{r}',\mathbf{k}',\mathbf{k}). \quad (35)\end{aligned}$$

The form of (35) is reminiscent of the traditional Fermi Golden Rule result for the spontaneous emission rate, which reads:

$$\Gamma_{SE,GR} = \frac{2\pi}{\hbar}| < f|H_{int}|i > |^2\rho(E). \quad (36)$$

The current densities $\mathbf{j}^T$ play parts similar to the transition matrix elements in (36), while the Green tensor takes account of the electromagnetic contribution to the density of final states $\rho(E)$. Our basic result has a simple interpretation in terms of the (self) radiation reaction energy of the emitting current in its own emitted field [33].

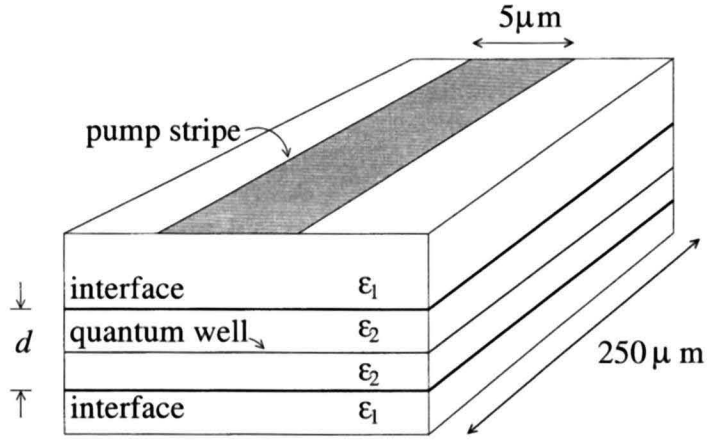

Figure 1: A typical edge-emitting laser. The pump stripe on the top determines the pumped region of the quantum well, and this in turn determines the opening angle of the laser mode.

3 The β_{sp}-factor

Applications of (35) to a quantum well in a dielectric multilayer configuration can be found elsewhere in these proceedings [34] as well as in [10]. These concern calculations of spontaneous emission rates and their variations as functions of width of the guiding layer and the position of the quantum well therein. As another application, we will present here a calculation of the spontaneous emission beta-factor, β_{sp}, for an edge-emitting structure. By its definition [35], this factor is the spontaneous emission rate into a given (laser) mode as a fraction of the total spontaneous emission rate. These emission rates may be calculated using (35), in which for the emission into a lasing mode the corresponding contribution to the total Green tensor should be retained as follows. For a dielectric configuration that occupies a finite region in space, the mode of interest for lasing will, in most cases, manifest itself by a simple pole of $\overleftrightarrow{G}(\mathbf{r},\mathbf{r}',\omega)$ in the complex ω-plane at $\omega = \omega_{mode}$. Then the propagator of this mode may be constructed by the prescription:

$$\overleftrightarrow{G}^{red}(\mathbf{r},\mathbf{r}',\omega) = \left[\lim_{\zeta\to\omega_{mode}} (\zeta - \omega_{mode})\,\overleftrightarrow{G}(\mathbf{r},\mathbf{r}',\zeta)\right]\frac{1}{\omega - \omega_{mode}}, \tag{37}$$

and the β_{sp}-factor is obtained as:

$$\beta_{sp} = \frac{\mathrm{Im}\sum_{\mathbf{k}'}\int_{act.} dr \int_{reg} dr' \mathbf{j}_{21}^{T}(\mathbf{r},\mathbf{k},\mathbf{k}')\cdot \overleftrightarrow{G}^{red}(\mathbf{r},\mathbf{r}',\omega_{2\mathbf{k},1\mathbf{k}'})\cdot \mathbf{j}_{12}^{T}(\mathbf{r}',\mathbf{k}',\mathbf{k})}{\mathrm{Im}\sum_{\mathbf{k}'}\int_{act.} dr \int_{reg} dr' \mathbf{j}_{21}^{T}(\mathbf{r},\mathbf{k},\mathbf{k}')\cdot \overleftrightarrow{G}(\mathbf{r},\mathbf{r}',\omega_{2\mathbf{k},1\mathbf{k}'})\cdot \mathbf{j}_{12}^{T}(\mathbf{r}',\mathbf{k}',\mathbf{k})}. \tag{38}$$

Since the Green tensor for a finite dielectric object such as, e.g., a VCSEL, is quite complicated and, in fact, at present not available to us, we have adopted the model of a multilayer

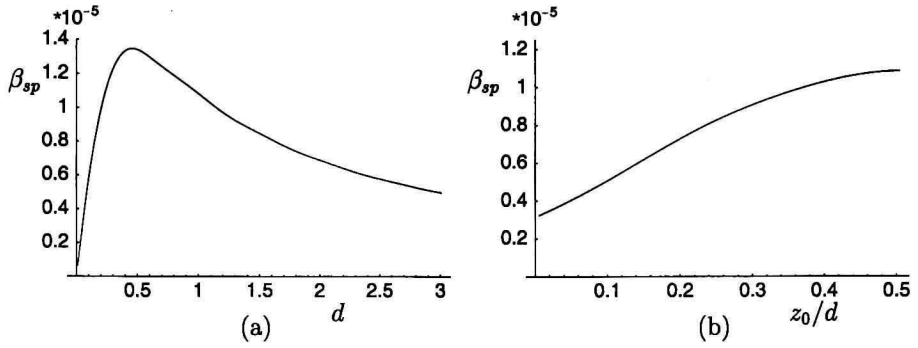

Figure 2: (a) β_{sp} of the fundamental guided mode versus width of the middle layer d, with the active quantum well at the center of the layer. (b) β_{sp} versus position of the quantum well z_0/d, for fixed width $d = \lambda/2$ ($z_0/d = 0$ means quantum well at the interface and $z_0/d = 1/2$ means quantum well at the center).

configuration with infinite extension in the lateral direction, for which the Green tensor is known in analytic form [8].

A complication that arises in the case of a dielectric structure with finite extent is that the mode spectrum has also guided modes which form continuous branches, so that the prescription (37) cannot be applied. However, we have shown in [10] that in this case the contribution of individual guided modes, for a given frequency ω_{gap} of the electronic transition between the conduction band and the valence band, can be identified as residues of $\overleftrightarrow{G}$ at poles in the complex k-plane, where k is the lateral wavenumber. The contribution of a single guided mode is then given by integration over all lateral directions of $\mathbf{k}$. For a typical edge-emitting laser, with structure as shown in Fig. 1, lasing can only occur in lateral directions within the activated layer, roughly determined by the orientation of the pump stripe. For typical stripe dimensions of 5 μm by 250 μm, this implies restriction of the lasing modes to an angle $\psi \simeq 2 \times 10^{-2}$ 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 $\Delta\omega_{sp} \simeq$ 3THz [36], while the selected longitudinal mode has a natural width $\Delta\omega_{mode} \simeq$ 30GHz due to outcoupling losses. Therefore, we take as an estimate of β_{sp} for a realistic structure the fraction $(\psi/2\pi)(\Delta\omega_{mode}/\Delta\omega_{sp}) \simeq 10^{-4}/\pi$ of the contribution of the fundamental guided mode of the same layered configuration with infinite lateral extension.

We previously calculated the total spontaneous emission rate as a function of layer width for a three-layer waveguide fabricated from $Al_xGa_{1-x}As$ with a quantum well embedded at the center of the middle layer [10, 34]. The quantum well is very thin and has dielectric constant equal to that of the middle layer. For the case of a three-layer waveguide fabricated from $Ga_xAl_{1-x}As$ with $x = 0.50$, $x = 0$ and $x = 0.50$ respectively, we now calculate the β_{sp}-factor, as described above, for the fundamental guided mode, i.e., the first guided mode to be born with increasing width d of the middle layer, starting from $d = 0$. The β_{sp}-factor as a function of d is plotted in Fig. 2(a). The width d is given in units of $\lambda/2$, where λ is the vacuum wavelength associated with the electronic transition frequency ω_{gap}. It is seen

that as d increases from 0, the β_{sp}-factor rises steeply, obtains a maximum near $d = \lambda/4$ and then decreases monotonously. This can be explained as follows. First it should be realized 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 [10]. One can show that for small d the intensity at the center of the middle layer scales as $I \propto \sqrt{k_{gm}^2(d) - \varepsilon_1 \frac{\omega^2}{c^2}}$, where $k_{gm}(d)$ is the pole in the complex k-plane associated with the mode of interest, given by [10]:

$$d\sqrt{\varepsilon_2 \frac{\omega^2}{c^2} - k_{gm}^2} - 2 \arctan\left(\frac{\sqrt{k_{gm}^2 - \varepsilon_1 \frac{\omega^2}{c^2}}}{\sqrt{\varepsilon_2 \frac{\omega^2}{c^2} - k_{gm}^2}}\right) = 0, \quad \sqrt{\varepsilon_1}\frac{\omega}{c} < k_{gm} \leq \sqrt{\varepsilon_2}\frac{\omega}{c}. \tag{39}$$

From this one finds that for small d, where k_{gm} is only slightly larger than $\sqrt{\varepsilon_1}\omega/c$, the mode intensity is proportional to d:

$$I \propto \frac{\omega^2}{2c^2}(\varepsilon_2 - \varepsilon_1)d, \tag{40}$$

which explains the initial linear increase of β_{sp} with d. In turn, for large d the mode intensity scales as $1/d$, which leads to the final $1/d$ decrease of the β_{sp}-factor.

The value of the β_{sp}-factor found here is on the order of 10^{-5}, depending on the width of the middle layer. This agrees well with estimates by others [35, 36, 37], based on various different approaches. Clearly, our technique provides a good approximation for the β_{sp}-factor and allows us to predict the general trends of its dependence on design parameters such as dielectric constants, quantum-well position, and width of the middle layer. As an example, we show in Fig. 2(b) the variation of β_{sp} with the position of the quantum well in the middle layer. Here the β_{sp}-factor clearly probes the mode intensity.

4 Acknowledgments

This research is supported by the 'Stichting voor Fundamenteel Onderzoek der Materie (FOM)', which is financially supported by the 'Nederlandse Organisatie voor Wetenschappelijk Onderzoek (NWO)'.

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