Quantum Kinetics of Semiconductor Light Emission and Lasing

K. Henneberger
Physics Department, University Rostock, Universitätsplatz 3, 18051 Rostock, Germany

S. W. Koch
Department of Physics and Materials Sciences Center, Philipps University, Renthof 5, 35032 Marburg, Germany
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Semiconductor light emission is analyzed as a paradigm of a nonequilibrium quantum mechanical many-body problem. The medium excitations and the quantized light field inside and outside a semiconductor slab are treated consistently. Splitting the photon density of states into a medium and a vacuum induced contribution the arbitrarily strong semiconductor emission is described as spontaneous emission into the vacuum induced part. With increasing gain narrowing peaks of growing intensity evolve for each propagation direction, whereas under laser conditions one propagation direction is favored by the cavity.

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The microscopic description of laser action in general and particularly laser action in semiconductors is one of the challenging topics in theoretical physics. A variety of models for semiconductor lasers has been developed in the past decades, many of which are summarized in modern textbooks [1,2]. However, relatively little work has been published which can be regarded as rigorous microscopic quantum theory. An exception is the work by Korenman [3], where the technique of nonequilibrium Green's functions (GF) [4,5] has been applied to lasers. However, the fundamental property of a laser as an optically inhomogeneous, energetically open many-body system was not considered.

The goal of this Letter is to address these problems by describing the semiconductor laser as a well-defined quantum-mechanical problem. Analyzing an excited semiconductor slab in vacuum with the excited electron-hole plasma inside the slab and an abrupt index change at the surface, the slab simultaneously serves as gain medium and laser cavity. Therefore we describe this system solely by the Hamiltonian of the electron-hole plasma interacting with the quantized light field plus appropriate boundary conditions. We assume steady state conditions and use the isotropic long wavelength limit for the optical functions of the semiconductor. To have a well-defined model we start by considering a semiconductor slab, which is homogeneously excited and infinitely extended in the transverse (y,z) direction, having a thickness L in the x direction. This system has been chosen since, due to homogeneity in the transverse direction, the three-dimensional (3D) light propagation problem can be solved exactly. However, using an infinite slab as gain medium is exotic in the sense that in the transverse direction an arbitrarily strong light amplification occurs. However, due to symmetry reasons the transverse energy currents cancel and do not contribute to the output loss of the slab, which remains only in the x direction. This way one forces output losses (but not light propagation) in only one direction. For this system we obtain an exact relation between the emitted intensity and the radiative loss in the carrier kinetics, which is valid for arbitrary excitation strengths (emission intensities).

Generalizing a classical analysis by Henry [6] we first investigate the wave propagation problem in the semiconductor cavity. The medium boundary conditions imply an abrupt change of the interband polarization from the inside to the outside,

$$\epsilon(\mathbf{r},\omega) = \theta\left(\frac{L}{2} - |x|\right)\epsilon(x,\omega) + \theta\left(|x| - \frac{L}{2}\right). \quad (1)$$

For notational simplicity we restrict our analysis here to TE-polarized light propagating freely in the transverse direction, which is described by the vector potential in Coulomb gauge, $\mathbf{A}(\mathbf{r},\omega) = \mathbf{e}_{\mathrm{TE}}(\mathbf{q}_\perp)e^{i\mathbf{q}_\perp\cdot\mathbf{r}}A(x,\mathbf{q}_\perp,\omega)$. The average field satisfies Maxwell's equation

$$\left\{\frac{\partial^2}{\partial x^2} + q^2(x)\right\}A(x) = 0\,, \quad (2)$$

where the wave number $q^2(x) = (\omega^2/c^2)\epsilon(x,\omega) - q_\perp^2$. The general solution is $A(x) = c_1A_+(x) + c_2A_-(x)$, where $A_+(x)$ and $A_-(x) = A_+(-x)$ correspond to waves propagating from left to right and vice versa, respectively. Up to a normalization factor, which we choose as the amplitude A_t of the forward propagating solution (2) $A_+(x)$, for $x > L/2$ (transmitted wave), $A_\pm$ is uniquely defined by the boundary conditions at the cavity facets. The analysis shows that there is no average or classical field which describes lasing, so that we have to focus on the next higher field average, i.e., the correlation function

$$D_{ij}^{>}(\mathbf{r},t,\mathbf{r}',t') = \frac{1}{4\pi ihc}\langle A_i(\mathbf{r},t)A_j(\mathbf{r}',t')\rangle = D_{ji}^{<}(\mathbf{r}'t',\mathbf{r}t)\ . \quad (3)$$

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Using the nonequilibrium GF technique [4,5] we obtain the propagation equation for $D_{ij}^{\gtrless}$. For the same assumptions and notations as used before the $D_{ij}^{\gtrless}$ reduce to scalars, and for given $\mathbf{q}_\perp$ and ω

$$\left\{\frac{\partial^2}{\partial x^2} + q^2(x)\right\} D^{\gtrless}(x,x') = P^{\gtrless}(x) D^{\mathrm{adv}}(x,x'). \tag{4}$$

Hence, the propagation of the correlations is governed by the same effective wave operator that enters Maxwell's equation, however, on the right hand side (RHS) of Eq. (4) an inhomogeneity occurs which has to be regarded as the source of correlation. The source contributions in Eq. (4) are given in terms of the generation ($P^>$) and recombination rates ($P^<$). In order to obtain the correct retarded photon GF of the vacuum for either $L \to 0$ or $\epsilon(\omega) \to 1$, the effective wave number q introduced in Eq. (4) has to become $\omega + i\delta/c$. Accounting for the identity $P^>(x,\omega) - P^<(x,\omega) = (2\omega^2/ic^2)\mathrm{Im}\,\epsilon(x,\omega)$ we have to add $\pm i\delta\theta(\pm\omega)(2\omega/c^2)$ to the rates of the medium, considering the vacuum outside as an infinitely weak absorber as is usually done to assure causality.

As usual, the propagation equation is solved using the retarded Green's function, $D^{\mathrm{ret}}(x,x')$ which is determined from Eq. (4) with the RHS replaced by $\delta(x - x')$. The retarded Green's function satisfying the boundary conditions can be constructed from the solutions of (2)

$$D^{\mathrm{ret}}(x,x') = \theta(x - x')A_+(x)A_-(x') + \theta(x' - x)A_+(x')A_-(x), \tag{5}$$

where $A_\pm(x)$ is to be normalized in such a way that the Wronskian $W = 1$. Splitting the resulting x integral in its medium and vacuum contributions we find

$$D^{\gtrless}(x,x') = S^{\gtrless}(x,x') \pm \theta(\pm\omega)\hat{D}_0(x,x'), \tag{6}$$

where the medium contribution is

$$S^{\gtrless}(x,x') = \int_{-L/2}^{L/2} D^{\mathrm{ret}}(x,x'')P^{\gtrless}(x'')D^{\mathrm{adv}}(x'',x')\,dx'' \tag{7}$$

and the vacuum contribution is

$$\hat{D}_0(x,x') = \frac{2\omega}{ic}|A_t|^2\{A_+(x)A_+^*(x') + A_-(x)A_-^*(x')\}, \tag{8}$$

respectively. The transmitted amplitude is given as

$$|A_t|^2 = \left| \frac{2\tilde{q}e^{i\bar{q}L}}{(1 - r^2)(\tilde{q} + q_0)^2} \right|, \tag{9}$$

where

$$r(\omega) = \frac{\tilde{q} - q_0}{\tilde{q} + q_0} e^{i\bar{q}L} \tag{10}$$

is the reflection coefficient for the waves propagating inside the cavity. q_0 is the wave number $q(x)$ outside, $\bar{q}$ is the average wave number inside the cavity, and

$$\tilde{q} = q\left(\frac{L}{2}\right) + \frac{q'(\frac{L}{2})}{2iq(\frac{L}{2})} \tag{11}$$

is given by the wave number $q(x)$ and its first derivative $q'(x)$ for $x \to L/2$ from the inside. For homogeneous excitation $\tilde{q} = \bar{q} = q$. For inhomogeneous excitation the difference between $\bar{q}$ and $q(L/2)$ as well as the gradient $q'(L/2)$ account, e.g., for spatial hole burning.

Only the diagonal quantities $D^{\gtrless}(x,x,\omega) \equiv D^{\gtrless}(x,\omega)$ enter into the photon kinetics, e.g., the locally defined photon density of states (DOS) is given as $\hat{D}(x,\omega) = D^>(x,\omega) - D^<(x,\omega)$. Using (6) we obtain $\hat{D}(x,\omega) = \hat{S}(x,\omega) + \hat{D}_0(x,\omega)$, i.e., a medium induced and a vacuum induced contribution to the DOS. We will show in the following that the complete optical output as well as the total radiative loss in the carrier kinetics are described by the vacuum induced contribution only,

$$\hat{D}_0(x,\omega) = \sum_{q_\perp} \frac{L\omega}{ic}|A_t|^2\{|A_+(x)^2|^2 + |A_-(x)^2|^2\}. \tag{12}$$

The energy balance of the semiconductor slab in steady state can be written as

$$I = -\frac{1}{2F}\int dV\langle \mathbf{j}(\mathbf{r},t)\mathbf{E}(\mathbf{r},t)\rangle, \tag{13}$$

where the output intensity I is the x component of the Pointing vector $\sim \langle \mathbf{E} \times \mathbf{B}\rangle$ at $x = L/2$ and $\mathbf{B} = \mathrm{curl}\,\mathbf{A}$, $\mathbf{E} = -d\mathbf{A}/dt$ in Coulomb gauge. F is the surface of the slab and the factor $2F$ results from integrating the Pointing vector over the back and front surfaces. The integral on the RHS of Eq. (13) is to be taken over the slab. Using the nonequilibrium GF technique we obtain for the correlation function

$$\langle \mathbf{j}(\mathbf{r},\underline{t})\mathbf{A}(\mathbf{r}',\underline{t}')\rangle = \int d\mathbf{r}''\,d\underline{t}''\,P_{ij}(\mathbf{r},\underline{t},\mathbf{r}'',\underline{t}'')D_{ij}(\mathbf{r}'',\underline{t}'',\mathbf{r}',\underline{t}'), \tag{14}$$

where P and D are the polarization function and the photon Green's function, respectively. The times $\underline{t}$ are defined on the Keldysh contour [4,5].

For our model system we obtain (assuming TE polarization)

$$I = \frac{L}{8\pi}\int d\omega(\hbar\omega)\int_{-L/2}^{L/2} dx\,[iP^<(x,\omega)][i\hat{D}_0(x,\omega)], \tag{15}$$

where the medium induced contributions connected with $S^{\gtrless}$ have canceled exactly. This way the emission from the semiconductor through its surface has the formal structure of a spontaneous emission, where, however, the total photon DOS $\hat{D}$ is replaced by its vacuum induced part $\hat{D}_0$. Note that, in contrast to $\hat{D}$ itself, $\hat{D}_0$ is a strictly positive quantity.

The quantum kinetic equation for the Wigner distribution $f(\mathbf{k}, \mathbf{r}, t)$ of carriers, e.g., in the conduction band, reads

$$\left\{\frac{\partial}{\partial t} + (\nabla_{\mathbf{k}}\varepsilon)\nabla_{\mathbf{r}} - (\nabla_{\mathbf{r}}\varepsilon)\nabla_{\mathbf{k}}\right\}f = \int_{-\infty}^{\infty} d\omega[\Sigma^{>}(\omega)G^{<}(\omega) - \Sigma^{<}(\omega)G^{>}(\omega)], \quad (16)$$

where ε, $\Sigma^{\gtrless}$, $G^{\gtrless}$ are the quasiparticle energy, self-energy, and carrier Green's function, respectively, all depending on $\mathbf{k}, \mathbf{r}, t$. Summing over k we obtain a rate equation for the carrier density at x

$$\frac{dn(x,t)}{\partial t} + \operatorname{div}\mathbf{j}(x,t) = -\int_{-\infty}^{\infty} d\omega\{P^{>}(x,\omega)D^{<}(x,\omega) - P^{<}(x,\omega)D^{>}(x,\omega)\} + \cdots. \quad (17)$$

Here, the only optical or transverse contributions Σ_D to the self-energy Σ with one photon GF involved have been considered explicitly and a general GF relation $\Sigma_D G = PD$ has been used [7]. As usual the local optical rate results from balancing the local absorption $P^{>}D^{<}$ with the spontaneous plus stimulated emission, according to $P^{<}D^{>} = P^{<}(\hat{D} + D^{<})$. Integrating over the cavity length and using Eq. (6) yields the total optical rate

$$\left.\frac{dN}{dt}\right|_{\text{opt}} = -\int_0^{\infty} d\omega \int_{-L/2}^{L/2} dx\,[iP^{<}(x,\omega)][i\hat{D}_0(x,\omega)]. \quad (18)$$

Thus, in radiative loss emission and absorption resulting from medium induced processes $S^{\gtrless}$ again cancel out and the net less has the character of a spontaneous emission into the vacuum induced density of states $\hat{D}_0$.

Note that Eqs. (15) and (19) for the emitted intensity and carrier loss together with the explicit expression (12) for $\hat{D}_0$ apply for any excitation strength ranging from the case of a nonexcited, i.e., absorbing semiconductor up to a highly excited gain medium. The frequency dependence of $\hat{D}_0(x,\omega)$ is, up to slowly varying functions, comprised in the Fabry-Pérot factor $|1 - r^2|^{-2}$ contained in $\hat{D}_0(x,\omega)$. Writing the complex reflectivity $r(\omega) = \varrho(\omega)e^{i\phi(\omega)}$, according to Eq. (10) the phase is given essentially by $\phi(\omega) = \text{Re}\{\overline{q}\}L = (\omega/c)\eta_{\text{eff}}(\omega)L$ selecting the Fabry-Pérot resonances according to $\phi(\omega_m) = m\pi$ with integer m, and the amplitude function is $\varrho|[(\tilde{q} - q_0)/(\tilde{q} + q_0)]|e^{-\text{Im}\{\overline{q}\}L} = e^{-[\kappa + (\omega/c)\alpha_{\text{eff}}L]}$, respectively. The Fabry-Pérot denominator $|1 - r^2|^2 = (1 - \varrho^2) + 4\varrho^2\sin^2\phi$ changes between $1 - \varrho^2$ for $\phi = m\pi$ (resonance) and $1 + \varrho^2$ for $\phi = (m + \frac{1}{2})\pi$ (antiresonance).

In the case of high excitation, where the semiconductor medium is partially inverted, one may reach a situation where for a resonance frequency $\omega_m = \omega_0$ near the gain maximum the gain nearly compensates the loss, i.e., $\kappa(\omega_0) + (\omega_0/c)\alpha_{\text{eff}}(\omega_0)L = \delta \ll 1$. Because $n(\omega)$ varies slowly due to the strong dephasing in the electron-hole plasma, we can approximate $n(\omega) \approx n(\omega_0)$ in the vicinity of ω_0 and obtain

$$\left.\frac{1}{|1 - r^2(\omega)|^2}\right|_{\omega\simeq\omega_0} = \frac{\omega_L^2}{4}\,\frac{1}{(\omega - \omega^2)^2 + \delta^2\omega_L^2},$$

where $\omega_L = c/n_{\text{eff}}(\omega_0)L$. Because of high gain-loss compensation ($\delta \ll 1$) a very narrow peak of width $\delta\omega_L \ll \omega_L$ and intensity $1/4\delta^2$ evolves contributing $\sim 1/\delta$ to the output.

So far our discussion is valid for any propagation direction characterized by a fixed wave number $\mathbf{q}_\perp$ in $q^2(x) = (\omega^2/c^2)\varepsilon(x,\omega) - q_\perp^2$. Only wave vectors $q_0 > 0$ contribute to the output, i.e., $q_\perp < \omega/c$, whereas for $q_\perp > \omega/c$ we have total internal reflection inside the cavity. Consequently, performing the $q_\perp$ integral in Eq. (12) results in strong broadening, since the resonance frequency $\omega_0(q_\perp)$ changes approximately from ω_0 for $q_\perp = 0$ up to $\omega_0\sqrt{\varepsilon_b/\varepsilon_b - 1}$ for $q_\perp = \omega_0/c$, where ε_b is the background dielectric constant. Hence, although the output occurs only in the x direction, the transverse degrees of freedom cause a large "directional" broadening, which is on the order of 10% of the optical frequency.

Addressing the problem of lasing one cannot expect the infinitely extended slab to be a good model for a lasing system due to its large directional broadening, which results from the original isotropic emission inside the cavity. However, in almost all existing semiconductor lasers this directional broadening is suppressed by the structural cavity design. Unfortunately for such realistic cavities an exact analytic investigation of the laser mode structure, as done here for the slab configuration, is out of reach. In order to avoid this problem, we approximately treat the cavity by assuming that only $q_\perp$ within a small opening angle $q_\perp < q_0\tan\vartheta$ contribute to the lasing modes in the x direction, whereas all $q_\perp$ with $q_\perp > q_0\tan\vartheta$ lead to transverse losses in the carrier kinetics. Restricting in Eq. (12) the $q_\perp$ integral and evaluating in the remaining integrand all functions at $q_\perp = 0$, one obtains

$$\hat{D}_0(x,\omega) \Rightarrow \frac{\omega^2}{c^2}\,\frac{\tan^2\vartheta}{4\pi}\,\hat{D}_{0,q_\perp=0}(x,\omega). \quad (19)$$

This way the general structure of Eqs. (15) and (18) is preserved with the only differences being that (i) the optical output in Eq. (15) as well as the radiative loss (18) are the ones due to the modes emitting in the x direction only, (ii) transverse losses are to be considered in a carrier kinetics, and (iii) a free parameter enters the theory, which describes the effect of the cavity design.

In summary, our microscopically consistent fully quantum-mechanical theory treats light emission from a semiconductor as a nonequilibrium many-body problem, where the electron-hole excitations are coupled to the quantum fields inside the cavity and in the surrounding vacuum. For the structure of a semiconductor slab the problem is solved exactly and it is shown that the conclusions are valid for semiconductor lasers in general.

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