Cumulant expansion approach to stimulated emission in semiconductor lasers

Witold Bardyszewski
Institute of Theoretical Physics, Warsaw University, ulica Hoża 69, 00-681 Warsaw, Poland

David Yevick
Department of Physics, University of Waterloo, 200 University Avenue, West Waterloo, Ontario, N2L 3G1 Canada

Mirosław Prywata
Institute of Theoretical Physics, Warsaw University, ulica Hoża 69, 00-681 Warsaw, Poland

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We present a simple model of absorption and gain spectra in highly excited semiconductor systems that incorporates interactions between electrons and holes. The scattering of the recombining electron-hole pair by charge fluctuations in the plasma is treated to infinite perturbation order by summing the corresponding cumulant series. We further show that the lowest cumulant in our expansion is simply related to the self-energy operator in the *GW* approximation. Our results therefore predict correctly the energy gap renormalization and the proper line shape of the emission spectra, including the exponential behavior of the spectral edge in the low-energy limit. Numerical results obtained within the plasmon pole approximation match experimental data in heterojunction lasers without adjustable parameters. Our procedure is sufficiently accurate and simple that it can be used in practical models of linear and nonlinear gain.

I. INTRODUCTION

In this paper, we investigate the response of many-body systems to electromagnetic fields with an emphasis on photon absorption and emission in semiconductor lasers. In particular, we describe the linear gain coefficient in the vicinity of the laser threshold as a function of photon energy and excitation level. In this regime the fundamental optical transitions between the valence and conduction bands are accompanied by low-energy excitations of the electron-hole plasma and phonons in the active layer. The interaction of the electron-hole pairs with this plasma leads to a substantial band-gap renormalization and spectral line asymmetry in the emission and absorption spectra.

Various theoretical models of gain and absorption spectra in semiconductor lasers or highly excited semiconductors take into account many-body effects such as band-gap renormalization, dephasing, excitonic enhancement or screening on different levels of approximation. A very popular approach consists in assuming that the basically two-particle interband excitations accompanying photon creation or annihilation can be described using the one-particle properties of the valence and the conduction band. Thus the band-gap renormalization is, for example, calculated as a difference of the separate shifts of those bands in the presence of the excited particles. Similarly the excitonic states are built from the combination of renormalized states of electron hole pairs interacting with a renormalized (screened) Coulomb potential.[1–4] Such models allow for a number of simplifications such as applying the plasmon pole model for calculating the energy-level renormalization or neglecting retardation in the screening of the electron hole-interaction (static screening approximation) providing a reasonable scheme for gain calculation. A microscopic description of the dephasing or spectral line-shape function usually required going beyond the Lorentzian approximation. The characteristic asymmetric shape of the spectral line was very often explained on the basis of the so-called ''no *k*-selection rule'' justified by an assumption of static disorder in the active material.[5,6] Such a disorder would be responsible for the fact that the interband transition with finite momentum change would become allowed. However, in the absence of lattice imperfections one should rather consider the time-dependent fluctuating potential due to, e.g., lattice vibrations or scattering by free carriers.[7,8] Realistic models of dephasing due to the coupling to phonons employ very often the cumulant expansion, i.e., the exponential resumation of the perturbation series. This method was used to explain the characteristic exponential low-energy tail of the absorption and gain spectra in intrinsic semiconductors.[9,10]

In our approach, an interband absorption process is divided into two distinct phases. First, an electron-hole pair is created by absorption of a photon with $E_\gamma \approx E_g$, the band-gap energy. This e-h pair then interacts with the electric field of the fluctuating plasma charge, gaining or losing energies that correspond to intraband transitions. We assume that only one interband particle-hole pair is created in the process and additionally neglect virtual interband transitions. The interaction of the electron-hole pair with the free-carrier plasma can be modeled by representing the eigenmodes of the plasma by a system of fictitious bosons corresponding to the potential fluctuations. For the one-electron spectra this procedure is equivalent to the *GW* approximation if the full boson dispersion relation and coupling potentials are replaced by effective quantities. We now extend this approach to the electron-hole pair which can be viewed as a composite particle coupled to the system of fluctuating potentials.[11]

Our paper is organized as follows. First we describe the fluctuating potential associated with plasma excitations within the random-phase approximation (RPA). Subsequently we derive the equation of motion for an exciton in the presence of fluctuating potentials. The approximate gain spectra is finally obtained by solving such an equation through an exponential (cumulant) resummation of the perturbation series.

II. ELECTRON-HOLE PLASMA MODEL

Under typical conditions in a semiconductor laser the electron-hole plasma is at quasi-equilibrium parametrized with conduction and valence band quasi-Fermi levels μ_c and μ_v respectively. The single-particle excitations of the system are generally modeled by the *GW* approximation in which the self-energy is calculated in the lowest order with respect to the fully screened potential *W*. This approximation yields the correct intensity and energy position of the quasiparticle resonances.

The mathematical structure of the *GW* self-energy expression is very similar to the analogous lowest order contribution from the electron-phonon interaction, e.g., the Fröchlich interaction with LO phonons, provided that the dispersive part of *W* is replaced by the phonon propagator.[12] The analytic properties of the screened interaction *W* in the random-phase approximation in fact permit the precise identification of the elementary plasma excitations as well as the exact form of the coupling potentials between these excitations and an external particle.

To illustrate the above concepts, consider the retarded screened potential *W*,

$$W^R(q,\omega)=[1-v_q\chi_0^R(q,\omega)]^{-1}v_q. \quad (1)$$

Here $\chi_0^R(q,\omega)$ represents the susceptibility of the system, while v_q is the unscreened Coulomb potential in the wave-vector representation. Defining an analogous expression for the advanced potential

$$W^A(q,\omega)=v_q[1-\chi_0^A(q,\omega)v_q]^{-1}, \quad (2)$$

we can easily show that the spectral density function of $W^R(q,\omega)$ is given by

$$-\frac{1}{\pi}\mathrm{Im}\,W^R(q,\omega)=W^A(q,\omega)\left(-\frac{1}{\pi}\mathrm{Im}\,\chi_0^R(q,\omega)\right)\times W^R(q,\omega). \quad (3)$$

The continuous part of the spectrum of *W* is related to the elementary electron-hole (intraband) excitations in the noninteracting gas which according to the Lindhard formula provides the following contribution to $\mathrm{Im}\,\chi_0^R(q,\omega)$:

$$\begin{aligned}-\frac{1}{\pi}\mathrm{Im}\,\chi_0^R(q,\omega)=&\sum_{\mathbf{k}} f_c(\epsilon_c(\mathbf{k}))[\delta(\omega-\epsilon_c(\mathbf{k}+\mathbf{q})+\epsilon_c(\mathbf{k}))\\&-\delta(-\omega-\epsilon_c(\mathbf{k}+\mathbf{q})+\epsilon_c(\mathbf{k}))]\\&+\sum_{\mathbf{k}}[1-f_v(\epsilon_v(\mathbf{k}))][\delta(-\omega-\epsilon_v(\mathbf{k}+\mathbf{q})\\&+\epsilon_v(\mathbf{k}))-\delta(\omega-\epsilon_v(\mathbf{k}+\mathbf{q})+\epsilon_v(\mathbf{k}))].\end{aligned} \quad (4)$$

In the above expressions $\epsilon_c(\mathbf{k})$ and $\epsilon_v(\mathbf{k})$, respectively, denote the energies of the conduction and valence bands, while the corresponding Fermi-Dirac partition functions are $f_c(\epsilon_c(\mathbf{k}))$ and $f_v(\epsilon_v(\mathbf{k}))$. Since the electron and hole Fermi-Dirac functions in a degenerate gas are well approximated by a step function of energy, the intraband electron-hole excitations do not occur outside of a well-defined region in the (q,ω) plane and thus do not contribute to $\mathrm{Im}\,\chi_0^R(q,\omega)$. However, in the region where $\mathrm{Im}\,\chi_0^R(q,\omega)\approx 0$ discrete plasmons may still be emitted or absorbed if $\mathrm{Re}(1-v_q\chi_0^R(q,\omega))=0$ yielding the following contribution to the spectral density of the screened interaction:

$$-\frac{1}{\pi}\mathrm{Im}\,W^R(q,\omega)=\left|\frac{\partial\chi_0^R}{\partial\omega}\bigg|_{\omega=\omega_q^{\mathrm{pl}}}\right|^{-1}[\delta(\omega-\omega_q^{\mathrm{pl}})-\delta(\omega+\omega_q^{\mathrm{pl}})]. \quad (5)$$

in which ω_q^{pl} is the energy of a plasmon with momentum $\mathbf{q}$. Accordingly within this framework, the spectral density function for W^R can be expressed as

$$-\frac{1}{\pi}\mathrm{Im}\,W^R(q,\omega)=\sum_m\sum_{\mathbf{q}}V_q^m(V_{-q}^m)^*[\delta(\omega-\omega_q^m)-\delta(\omega+\omega_q^m)]. \quad (6)$$

The index *m* runs both over all possible electron-hole excitations $[m=(\nu,\mathbf{k})$, where $\nu=c$ or $\nu=v]$ with energies $\omega_q^m=\epsilon_\nu(\mathbf{k}+\mathbf{q})-\epsilon_\nu(\mathbf{k})$ and plasmon excitations $m=\mathrm{pl}$ with $\omega_q^m=\omega_q^{\mathrm{pl}}$. From the equations above, the coupling potentials for these excitations are

$$V_q^m=\begin{cases}W^R(q,\omega_q^m)\sqrt{1-f_v(\epsilon_v(\mathbf{k}))} & \text{for electron-hole pairs in the val. band,}\\ W^R(q,\omega_q^m)\sqrt{f_c(\epsilon_c(\mathbf{k}))} & \text{for electron-hole pairs in the cond. band,}\\ \left|\frac{\partial\chi_0^R}{\partial\omega}\bigg|_{\omega=\omega_q^{\mathrm{pl}}}\right|^{-1/2} & \text{for plasmons.}\end{cases} \quad (7)$$

III. SINGLE-PARTICLE SPECTRUM

Many properties of the one-particle spectrum of the electron-hole gas such as the change in the energy levels with carrier density can be immediately derived from the self-energy function in the *GW* approximation. This function can be generally represented as

$$\Sigma(q,\omega)=\Sigma^{\mathrm{HF}}(q)+M(q,\omega). \tag{8}$$

Here $\Sigma^{\mathrm{HF}}(q)$ is the time-independent Hartree-Fock contribution. The dispersive part $M(q,\omega)$, which is nonlocal in time, can be obtained by the Kramers-Krönig transformation from the spectral density function $-(1/\pi)M(q,\omega)$. The formulas of the previous section yield for the conduction band RPA spectral density

$$\begin{aligned}-\frac{1}{\pi}\mathrm{Im}\,M(q,\omega)=-\frac{1}{\pi}\mathrm{Im}\,\Sigma(q,\omega)\\ =\sum_m\sum_{\mathbf{q}}V_q^m(V_q^m)^*\{[1-f_c(\epsilon_c(\mathbf{k}+\mathbf{q}))\\ +N(\omega_q^m)]\delta(\omega-\omega_q^m-\epsilon_c(\mathbf{k}+\mathbf{q}))\\ +[f_c(\epsilon_c(\mathbf{k}+\mathbf{q}))+N(\omega_q^m)]\\ \times\delta(\omega+\omega_q^m-\epsilon_c(\mathbf{k}+\mathbf{q}))\},\end{aligned} \tag{9}$$

where $N(\omega_q^m)$ is the Bose-Einstein partition function. An analogous equation applies to the valence band. Note that Eq. (9) is virtually identical to the self-energy contribution from electron-phonon interactions with the coupling potentials V_q^m if we replace the phonon frequency by the plasmon frequency or electron-hole pair energy ω_q^m.

IV. SPONTANEOUS AND STIMULATED EMISSION

The linear gain in a semiconductor laser can be immediately derived from the Fourier transform of the time-dependent electron-hole pair correlation function describing the spontaneous recombination:

$$iG^<_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_1'\mathbf{k}_2'}(t)=\langle a^\dagger_{c\mathbf{k}_1'}(0)a_{v\mathbf{k}_2'}(0)a^\dagger_{v\mathbf{k}_2}(t)a_{c\mathbf{k}_1}(t)\rangle. \tag{10}$$

The expectation value in Eq. (10) is taken with respect to the quasiequilibrium state of the excited semiconductor. The creation operator for a conduction-band electron with momentum $\mathbf{k}$ at time t and the corresponding annihilation operator for a valence-band electron are denoted by $a^\dagger_{c\mathbf{k}}(t)$ and $a_{v\mathbf{k}}(t)$, respectively.

The coupling of electron-hole pairs to the electromagnetic field with polarization σ is proportional to the matrix element of the σ component of the momentum operator between the valence and conduction band states:

$$\hat{P}_{\sigma,\mathbf{k}_1\mathbf{k}_2}=\langle c,\mathbf{k}_1|\hat{p}_\sigma|v,\mathbf{k}_2\rangle\delta_{\mathbf{k}_1,\mathbf{k}_2}. \tag{11}$$

Applying the standard definition of the scalar product:

$$\langle P|P'\rangle=\sum_{\mathbf{k}_1\mathbf{k}_2}P^*_{\mathbf{k}_1\mathbf{k}_2}P'_{\mathbf{k}_1\mathbf{k}_2}, \tag{12}$$

we obtain the following compact expression for the linear gain at a light frequency ω:

$$\alpha(\omega)=\frac{2\pi}{cn_r\omega\mathcal{V}}(1-e^{\beta(\omega-\mu_x)})\langle P_\sigma|i\hat{G}^<(\omega)|P_\sigma\rangle. \tag{13}$$

Here $\mu_x=\mu_c-\mu_v$ corresponds to the chemical potential for interband electron-hole pair excitations, $\hat{G}^<(\omega)$ represents the Fourier transform of $G^<(t)$, $\beta=1/k_BT$, n_r and $\mathcal{V}$ are the the refractive index and volume of the system, and c is the vacuum speed of light. Atomic units are used throughout the paper.

In order to calculate $G^<(t)$ we introduce a correlation function on the imaginary time path $t=-i\tau$ where $0\leqslant\tau\langle\beta$:

$$\mathcal{G}_{\mathbf{k}_1'\mathbf{k}_2'\mathbf{k}_1\mathbf{k}_2}(\tau)=\langle a^\dagger_{c\mathbf{k}_1'}(-i\tau)a_{v\mathbf{k}_2'}(-i\tau)a^\dagger_{v\mathbf{k}_2}(0)a_{c\mathbf{k}_1}(0)\rangle, \tag{14}$$

so that $iG^<_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_1'\mathbf{k}_2'}(t)$ is obtained by the analytic continuation of $\mathcal{G}_{\mathbf{k}_1'\mathbf{k}_2'\mathbf{k}_1\mathbf{k}_2}(-i\tau)$ to the real time axis at the end of our calculations.[13]

Applying next the coherent-state representation for bosonic excitations which here include intraband electron-hole pair excitations, plasmons, and phonons, we may cast the expression for $\mathcal{G}(\tau)$ into a functional integral with respect to the fluctuation amplitudes (coherent coordinates) $b_{\mathbf{q}}(\tau)$ and $b^*_{\mathbf{q}}(\tau)$ of the bosonic fields for the $\mathbf{q}$ wave-vector components of the potential. The resulting expression reads

$$\begin{aligned}\mathcal{G}(\tau)=\frac{1}{Z}\int\mathcal{D}[b^*_{\mathbf{q}}(\tau')b_{\mathbf{q}}(\tau')]\\ \times e^{-S_{\mathrm{bos}}[b^*_{\mathbf{q}}(\tau)b_{\mathbf{q}}(\tau);\tau']}g([b^*_{\mathbf{q}}(\tau')b_{\mathbf{q}}(\tau')];\tau).\end{aligned} \tag{15}$$

The correlation function $g(\tau)$ which depends on the the given time-dependent fluctuations of the classical amplitudes $b_{\mathbf{q}}(\tau)$ and $b^*_{\mathbf{q}}(\tau)$ can be expressed as the following thermal average solely with respect to electron variables in the Hartree-Fock approximation:

$$g_{\mathbf{k}_1'\mathbf{k}_2'\mathbf{k}_1\mathbf{k}_2}(\tau)=\langle a^\dagger_{c\mathbf{k}_1'}(-i\tau)a_{v\mathbf{k}_2'}(-i\tau)a^\dagger_{v\mathbf{k}_2}(0)a_{c\mathbf{k}_1}(0)\rangle_{\mathrm{el}\text{-}H\text{-}F}. \tag{16}$$

The effective action $S_{\mathrm{bos}}[b^*_{\mathbf{q}}b_{\mathbf{q}}]$ for boson fields is assumed to be bilinear with respect to $b_{\mathbf{q}}$ and $b^*_{\mathbf{q}}$ (Gaussian approximation) and the standard periodicity conditions $b_{\mathbf{q}}(\beta)=b_{\mathbf{q}}(0)$ and $b^*_{\mathbf{q}}(\beta)=b^*_{\mathbf{q}}(0)$ are applied.[14] According to Eq. (6) the effective interaction between electron-hole pairs and bosons of the type m can then be described by the Hamiltonian

$$H_{el\text{-}bos}=\sum_{\mathbf{k}}\sum_{\mathbf{q}}(a^{\dagger}_{c\mathbf{k}+\mathbf{q}}a_{c\mathbf{k}}+a^{\dagger}_{v\mathbf{k}+\mathbf{q}}a_{v\mathbf{k}})\times[V^m_q b^m_{\mathbf{q}}+(V^m_{-q})^*(b^m_{-\mathbf{q}})^*]. \tag{17}$$

The coupling constants V_q^m for interaction with plasma fluctuations are defined in Eq. (7) while the polar coupling to the longitudinal-optical (LO) phonons is given by the Fröchlich expression:

$$V_q^{\mathrm{LO}}=-i\left[\frac{2\pi e^2\hbar\omega_0}{\mathcal{V}}\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right)\right]^{1/2}\frac{1}{q}, \tag{18}$$

in which $\hbar\omega_0$ denotes the LO phonon energy and ϵ_∞ and ϵ_0 are high-frequency and static dielectric constants, respectively. Representing the Coulomb interaction between the electron and hole by U_q, the Hartree-Fock approximation for the electron-hole pair moving in a fluctuating field generates the equation of motion

$$\frac{\partial}{\partial\tau}g_{\mathbf{k}_1'\mathbf{k}_2'\mathbf{k}_1\mathbf{k}_2}(\tau)=[\epsilon_c(\mathbf{k}_1')-\epsilon_v(\mathbf{k}_2')]g_{\mathbf{k}_1'\mathbf{k}_2'\mathbf{k}_1\mathbf{k}_2}(\tau)+\sum_{\mathbf{k},\mathbf{q}}U_{\mathbf{q}}[\langle a^{\dagger}_{v\mathbf{k}}(-i\tau)a_{v\mathbf{k}_2'}(-i\tau)\rangle_{\mathrm{el}}g_{\mathbf{k}_1'+\mathbf{q}\,\mathbf{k}+\mathbf{q}\,\mathbf{k}_1\mathbf{k}_2}(\tau)$$
$$-\langle a^{\dagger}_{c\mathbf{k}_1'}(-i\tau)a_{c\mathbf{k}}(-i\tau)\rangle_{\mathrm{el}}g_{\mathbf{k}+\mathbf{q}\,\mathbf{k}_2'+\mathbf{q}\,\mathbf{k}_1\mathbf{k}_2}(\tau)]+\sum_m\sum_{\mathbf{q}}[V^m_q b^m_{\mathbf{q}}+(V^m_{-q})^*(b^m_{-\mathbf{q}})^*]$$
$$\times[g_{\mathbf{k}_1'+\mathbf{q}\,\mathbf{k}_2'\mathbf{k}_1\mathbf{k}_2}(\tau)-g_{\mathbf{k}_1'\mathbf{k}_2'-\mathbf{q}\,\mathbf{k}_1\mathbf{k}_2}(\tau)]. \tag{19}$$

In the presence of fluctuating potentials associated with intraband plasma excitations or phonons, the effective electron-hole interaction is modified through the one-particle density matrices $\langle a^{\dagger}_{v\mathbf{k}}(-i\tau)a_{v\mathbf{k}_2'}(-i\tau)\rangle_{\mathbf{el}}$ and $\langle a^{\dagger}_{c\mathbf{k}_1'}(-i\tau)a_{c\mathbf{k}}(-i\tau)\rangle_{\mathbf{el}}$ and the direct coupling to the fluctuating potentials given by the last term in Eq. (19). Thus in the context of the RPA, averaging with respect to fluctuating potentials reproduces the vertex corrections and dynamical screening. A commonly used approximation is thus to replace U_q by the statically screened potential. The density matrix elements are similarly approximated by the corresponding averages with respect to the fluctuating potentials and, therefore, adopt the form

$$\langle a^{\dagger}_{v\mathbf{k}}(-i\tau)a_{v\mathbf{k}_2'}(-i\tau)\rangle_{\mathbf{el}}=\delta_{kk_2'}f_v(\epsilon_v(k)) \tag{20}$$

and

$$\langle a^{\dagger}_{c\mathbf{k}_1'}(-i\tau)a_{c\mathbf{k}}(-i\tau)\rangle_{\mathbf{el}}=\delta_{kk_1'}f_c(\epsilon_c(k)). \tag{21}$$

The quasiparticle energies $\epsilon_v(k)$ and $\epsilon_c(k)$ now represent renormalized quantities within the RPA.

The equation of motion, Eq. (19) can be written as

$$\frac{\partial}{\partial\tau}g(\tau)=[\hat{H}_0+\hat{V}(\tau)]g(\tau). \tag{22}$$

$\hat{H}_0$ denotes an effective electron-hole Hamiltonian

$$\hat{H}_0=\hat{T}+\hat{F}\hat{U}, \tag{23}$$

in which $\hat{T}$ is the kinetic energy matrix, and the statically screened Coulomb interaction $\hat{U}$ is multiplied by the occupation factor represented by the matrix

$$\hat{F}_{\mathbf{k}_1'\mathbf{k}_2'\mathbf{k}_1\mathbf{k}_2}(\tau)=\delta_{\mathbf{k}_2\mathbf{k}_2'}\delta_{\mathbf{k}_1\mathbf{k}_1'}[f_v(\varepsilon_v(k_2))-f_c(\varepsilon_c(k_1))], \tag{24}$$

and the time-dependent coupling to the boson fields given by the last term in Eq. (19) is denoted by $\hat{V}(\tau)$.

The formal solution to Eq. (22) can be written as

$$g(\tau)=e^{\hat{H}_0\tau}\mathcal{T}\exp\left[\int_0^{\tau}e^{-\hat{H}_0\tau'}\hat{V}(\tau')e^{\hat{H}_0\tau'}d\tau'\right]g(0). \tag{25}$$

In the above expression, the time-ordering operator $\mathcal{T}$ is applied along the integration interval. Averaging with respect to the potential fluctuations and performing a cumulant expansion to the second order with respect to the coupling $\hat{V}(\tau)$ then yields

$$\mathcal{G}(\tau)=e^{\hat{H}_0\tau}\exp\left[\int_0^{\tau}d\tau_1\int_0^{\tau_1}d\tau_2 e^{-\hat{H}_0\tau_1}\langle\hat{V}(\tau_1)e^{\hat{H}_0(\tau_1-\tau_2)}\hat{V}(\tau_2)\rangle_{\mathrm{bos}}e^{\hat{H}_0\tau_2}\right]\mathcal{G}(0), \tag{26}$$

after factoring the average of the initial value $g(0)$ of $\mathcal{G}$ where $\mathcal{G}(\tau)=\langle g(\tau)\rangle_{\rm bos}$. Equation (26) can now be expanded in terms of the right and left eigenvectors of the Hamiltonian $\hat{H}_0$ defined by

$$\hat{H}_0|n\rangle=E_n|n\rangle \quad \text{and} \quad \langle\tilde{n}|\hat{H}_0=\langle\tilde{n}|E_n. \tag{27}$$

Retaining only diagonal elements in the $|n\rangle$ representation of the exponential in Eq. (26) and passing to the real time correlation function yields

$$iG^{<}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}'_1\mathbf{k}'_2}(t)=\sum_n e^{-iE_nt}e^{S_n(t)}\frac{1}{\langle\tilde{n}|n\rangle}\sum_{k''_1k''_2}\langle k'_1k'_2|n\rangle \times\langle\tilde{n}|k''_1k''_2\rangle iG^{<}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}''_1\mathbf{k}''_2}(0). \tag{28}$$

The time-dependent correlation function is, therefore, equal to a sum of terms that oscillate at a frequency given by the electron-hole pair eigenfrequencies $E_n/\hbar$ with additional time-dependent phase factors that both renormalize the e-h energies and are responsible for the dephasing of those oscillations. Since

$$\langle[b_{\mathbf{q}}(\tau)+b^*_{-\mathbf{q}}(\tau)][b_{-\mathbf{q}'}(0)+b^*_{\mathbf{q}'}(0)]\rangle_{\rm bos} =\delta_{\mathbf{qq}'}\{[N(\omega_{\mathbf{q}})+1]e^{-\omega_{\mathbf{q}}\tau}+N(\omega_{\mathbf{q}})e^{\omega_{\mathbf{q}}\tau}\}, \tag{29}$$

the time-dependent phase function is in our model given by

$$S_n(t)=\int_{-\infty}^{\infty}M_n^{<}(\omega+E_n)\left(\frac{e^{-i\omega t}+i\omega t-1}{\omega^2}\right)d\omega, \tag{30}$$

where

$$M_n^{<}(\omega)=\sum_m\sum_{n'}\sum_{\mathbf{q}}\frac{1}{\langle\tilde{n}'|n'\rangle}\langle\tilde{n}|V^m_{\mathbf{q}}|n'\rangle\langle\tilde{n}'|(V^m_{-\mathbf{q}})^*|n\rangle \times\{[N(\omega^m_{\mathbf{q}})+1]\delta(\omega+\omega^m_{\mathbf{q}}-E_{n'}) +N(\omega^m_{\mathbf{q}})\delta(\omega-\omega^m_{\mathbf{q}}-E_{n'})\}. \tag{31}$$

The contributions from the differing sources of the fluctuating potentials are labeled by *m*.

Finally, we turn our attention to the initial value, $\mathcal{G}(0)$ of $iG^{<}_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}'_1\mathbf{k}'_2}(0)$. From the cyclic property of the trace appearing in our expressions for thermodynamic averages of quasiequilibrium quantities we obtain

$$\langle(\mathcal{T}e^{\int_0^\beta[\hat{H}_0+\hat{V}(\tau)]d\tau}-1)g(0)\rangle_{\rm bos}=\mathcal{F}. \tag{32}$$

The matrix elements of $\mathcal{F}$ are

$$\mathcal{F}_{\mathbf{k}'_1\mathbf{k}'_2\mathbf{k}_1\mathbf{k}_2}=\delta_{\mathbf{k}_1\mathbf{k}'_1}\langle a^\dagger_{v\mathbf{k}_2}a_{v\mathbf{k}'_2}\rangle-\delta_{\mathbf{k}_2\mathbf{k}'_2}\langle a^\dagger_{c\mathbf{k}'_1}a_{c\mathbf{k}_1}\rangle. \tag{33}$$

Factorizing the average on the left-hand side of the Eq. (32) and defining an effective electron-hole Hamiltonian such that $e^{\beta\hat{H}_{\rm eff}}=\langle\mathcal{T}e^{\int_0^\beta(\hat{H}_0+\hat{V}(\tau))d\tau}\rangle_{\rm bos}$ yields

$$\mathcal{G}(0)=(e^{\beta\hat{H}_{\rm eff}}-1)^{-1}\mathcal{F}. \tag{34}$$

The linear gain can therefore be calculated as

$$\alpha(\omega)=\frac{2\pi}{cn_r\omega\mathcal{V}}(1-e^{\beta(\omega-\mu_x)})\sum_n|\langle P_\sigma|n\rangle|^2B_n\mathcal{L}(\omega-E_n). \tag{35}$$

In Eq. (35) the first term of the summation is the square of the optical transition-matrix element associated with the recombination channel σ for the eigenstate $|n\rangle$ of the excitonic Hamiltonian H_0, while the line-shape function $\mathcal{L}_n(\omega)$ is defined by

$$\mathcal{L}_n(\omega)=\mathrm{Re}\int_0^{+\infty}e^{S_n(t)}e^{i\omega t}dt. \tag{36}$$

Further, the statistical factor

$$B_n=\langle\tilde{n}|(e^{\beta\hat{H}_{\rm eff}}-1)^{-1}\mathcal{F}|\tilde{n}\rangle \tag{37}$$

corresponds to the distribution function of electron-hole pairs prior to recombination. If correlation effects in the electron hole pair are neglected, B_n accordingly reduces to the product of the Fermi-Dirac occupation factors for electrons in the conduction band and for holes in the valence band: $B_n=f_c(\varepsilon_c(k_e))[1-f_v(\varepsilon_v(k_h))]$.

We now specialize to a two-band model and further approximate the excitonic states by a product $|n\rangle=|\lambda\rangle|\mathbf{P}\rangle$ where $|\lambda\rangle$ describes the internal state of the exciton and $|\mathbf{P}\rangle$ is a plane-wave function of the center-of-mass momentum $\mathbf{P}$. Representing the internal energy and the total mass of the exciton by ϵ_λ and *M*, respectively, the energy of this state is

$$E_\lambda(\mathbf{P})=\epsilon_\lambda+\frac{P^2}{2M}. \tag{38}$$

After some algebra, the following expression for the function $M^{<}$ for an exciton in the state $|\lambda_0\rangle|\mathbf{P}=0\rangle$ can be derived, where $\mathbf{r}_e$ and $\mathbf{r}_h$ are the electron and the hole positions

$$M^{<}_{\lambda_0}(\omega)=\sum_\lambda\sum_m\sum_{\mathbf{q}}V^m_q(V^m_q)^*[(1+N(\omega^m_q)) \times\delta(\omega+\omega^m_q-E_\lambda(\mathbf{q})) +N(\omega^m_q)\delta(\omega-\omega^m_q-E_\lambda(\mathbf{q}))] \times\frac{1}{\langle\tilde{\lambda}|\lambda\rangle}\langle\tilde{\lambda}_0|e^{-i\mathbf{q}\cdot\mathbf{r}_e}-e^{i\mathbf{q}\cdot\mathbf{r}_h}|\lambda\rangle \times\langle\tilde{\lambda}|e^{i\mathbf{q}\cdot\mathbf{r}_e}-e^{-i\mathbf{q}\cdot\mathbf{r}_h}|\lambda_0\rangle. \tag{39}$$

Note that the matrix element $\langle\tilde{\lambda}|e^{i\mathbf{q}\cdot\mathbf{r}_e}-e^{-i\mathbf{q}\cdot\mathbf{r}_h}|\lambda_0\rangle$ is proportional to the probability amplitude of a scattering process in which the internal state of the exciton is transformed from $|\lambda_0\rangle$ to $|\lambda\rangle$, while its total momentum changes by $\mathbf{q}$. The first term in this expression corresponds to the electron and the second to the hole scattering amplitude. Since these two contributions are 180° out of phase, the negative quantum interference between the two processes, which vanishes in the absence of correlation between the electron and hole, partially cancels the contribution from the interaction with long-wavelength potential fluctuations. This, in turn, removes the singularity generated by the coupling potentials V^m_q in $M^{<}$. Indeed, for correlated (e.g., bound) electron-hole pairs the exciton has zero net charge and therefore couples only weakly to fluctuating electric fields.

V. RESULTS AND DISCUSSION

To illustrate our theoretical approach we now consider spontaneous recombination and emission in a 1.3 μm, $In_{0.727}Ga_{0.273}As_{0.58}P_{0.42}$/InP based heterostructure laser at room temperature.[15,16] For simplicity we neglect the Coulomb interaction between the valence and conduction band electrons in the Hamiltonian H_0. Since the motion of electrons in the conduction and valence band is then uncorrelated, the expression for $M^<$ can be divided into the sum of two seperate terms pertaining to each band separately. The time-dependent spectral density function of an e-h pair, $e^{S_n(t)}$ is given by the product of one-particle spectral densities since the line-shape function is then the convolution of two single-particle spectral densities.[8] In our calculations we include the scattering of electron-hole pairs by LO phonons and plasma fluctuations. To obtain an analytic expression for $M^<$ we describe the latter through the plasmon pole approximation in which all plasma excitations are represented by well-defined plasmons with frequency

$$\omega_q^2=\omega_p^2\left(1+\frac{q^2}{\kappa^2}\right)+\left(\frac{q^2}{2m_e}\right)^2. \tag{40}$$

Here m_e is the conduction band effective mass and κ is the screening parameter given in terms of the concentration of electrons and holes n_e and n_v by

$$\kappa^2=\frac{4\pi e^2}{\epsilon_\infty}\left(\frac{\partial n_e}{\partial \mu_c}+\frac{\partial n_h}{\partial \mu_v}\right). \tag{41}$$

The plasma frequency ω_p is then obtained from

$$\omega_p^2=n_e\left(\frac{\sqrt{m_H}+\sqrt{m_L}}{\sqrt{m_H^3}+\sqrt{m_L^3}}+\frac{1}{m_e}\right)\frac{4\pi e^2}{\epsilon_\infty}.$$

The coupling constant for this case is

$$V_q^{\rm PL}=\left(\frac{2\pi e^2\omega_p^2}{\epsilon_\infty\omega_q}\right)^{1/2}\frac{1}{q}, \tag{42}$$

where we have neglected the exciton scattering by low-energy intraband electron-hole excitations. Moreover, it is well known that plasmon excitations in the presence of free holes in III-V semiconductors are strongly damped due to intervalence band transitions.[17] As the associated plasmon spectral density is, therefore, broadened, the plasma contribution to the $M^<$ function is similarly damped. Finally, in order to further simplify the calculations we neglect the dependence of both $M^<$ and the line-shape function on initial state of the recombining electron-hole pair $|n\rangle$. Instead, we apply the line-shape function associated with the lowest energy transition to the entire spectrum. The details of this calculations are given in the Appendix.

In Fig. 1 the solid line represents the calculated energy dependence of the spectral density $M^<$ for an electron-hole pair concentration of $n=1.8\times10^{18}$ cm^{-3}. Observe the two pairs of singularities at energies corresponding to $\pm\omega_0=\pm35.8$ meV and $\pm\omega_{\rm pl}=\pm58$ meV. As a consequence, the resulting shape function shown as the solid line in Fig. 2 is asymmetric and posesses pronounced sidebands. Fitting this curve to a Lorentzian function with the same half width and height, displayed as the dotted curve in the figure, shows that the half width at half maximum of the main spectral line approximately equals $\Gamma=M^<(0)$.

Due to the plasmon frequency dependence on q [Eq. (40)] an electron hole pair with total momentum equal to zero cannot decay through plasmon absorption or emission. LO phonons, therefore, play a dominant role in broadening the emission and gain spectra. The resulting linewidth is solely determined by dispersionless LO phonon scattering, while the plasmon coupling simply yields the sidebands that appear on the low-energy side of the main peak in Fig. 2. The plasmon satellites are thus responsible for experimentally observed gain profile in the tail region.[16]

In Fig. 3(a) we display the material gain curves for 1.3 μm, $In_{0.727}Ga_{0.273}As_{0.58}P_{0.42}$/InP at several subthreshold concentrations at room temperature. The experimental modal gain spectra according to Ref. 16 are given in Fig. 3(b) for injection current values corresponding approximately to excess carrier densities used for theoretical calculations of Fig. 3(a). The evolution of the crossover and gain maximum with carrier concentration is quite well reproduced. Note that our model incorporates not only the screened exchange contribution to the energy level shift but also the ''Coulomb hole'' correction associated with low-energy intraband electron-hole plasma excitations within the RPA. Since the latter contribution properly shifts the maximum of the line-shape function with wavelength, our model correctly describes band-

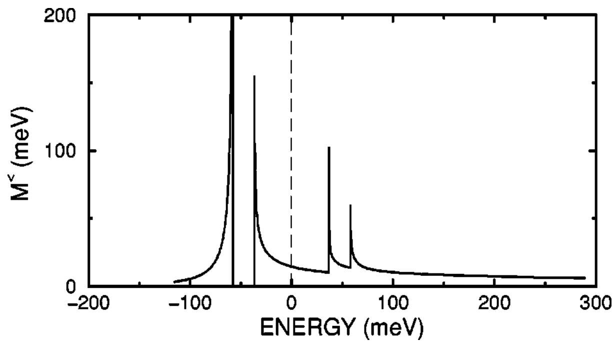

FIG. 1. $M^<(E)$ function at electron-hole concentration 1.8×10^{18} cm^{-3}.

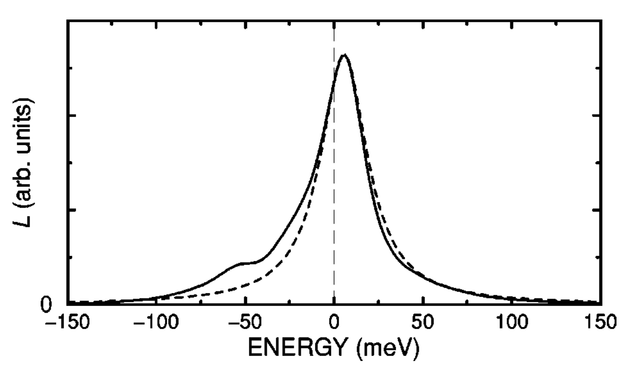

FIG. 2. Line-shape function for the lowest energy electron-hole pair excitation (solid line) and the Lorentzian function with HWHM$=M^<(0)$ (dashed line).

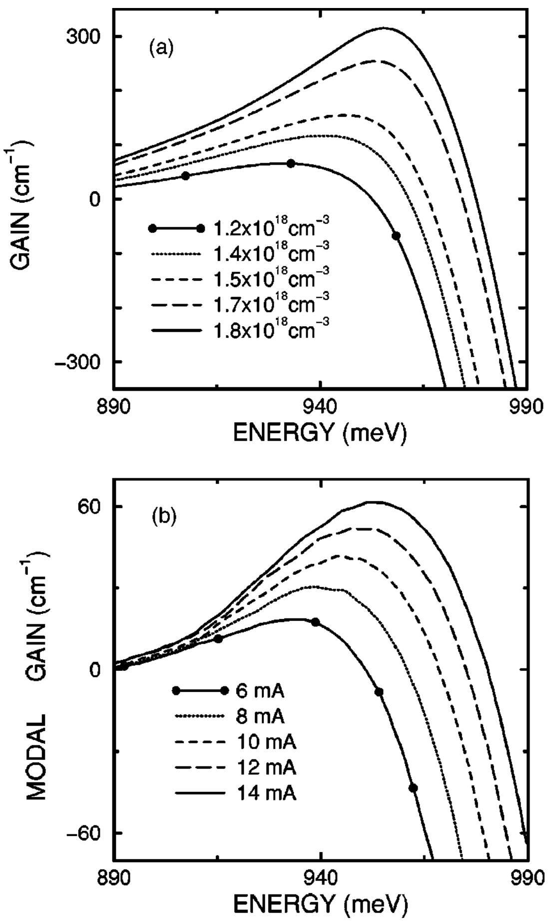

FIG. 3. (a) Theoretical material gain curves at electron-hole pair concentrations of 1.2×10^{18} cm^{-3}, 1.4×10^{18} cm^{-3}, 1.5×10^{18} cm^{-3}, 1.7×10^{18} cm^{-3}, and 1.8×10^{18} cm^{-3} for $In_{0.727}Ga_{0.273}As_{0.58}P_{0.42}$/InP at room temperature. (b) Experimental modal gain curves of a 1.3 μm, $In_{0.727}Ga_{0.273}As_{0.58}P_{0.42}$/InP heterostructure laser for currents values of 6, 8, 10, 12, and 14 mA, at room temperature (Ref. 16).

gap narrowing and hence the correct variation of the maximum gain with carrier concentration.

That the gain curve decreases more slowly on the low-energy side than on the high-energy side of its maximum is a consequence of multiphonon and multiplasmon scattering processes. However, neglecting interference effect resulting from quasiboson emission and reabsorption and employing the plasmon pole approximation in our model of uncorrelated electron-hole pairs results in an overestimation of the relative strength of such processes[18] in the low-energy part of the gain spectra.

Our theoretical gain spectra possess the characteristic shape described by the phenomenological k nonconservation rule with a maximum shifted slightly towards the crossover point in the gain spectrum. In the low-energy region, the measured gain decays exponentially.[8] This behavior has previously often been modeled by assuming a line-shape function of the form $\cosh^{-\nu}(\sigma(\omega-\omega^0))$ where the values of σ and ω^0 are determined empirically. Our technique clearly reproduces this exponential behavior as is evident from the logarithmic plot of the gain curves in the low-energy region, cf. Fig. 4.

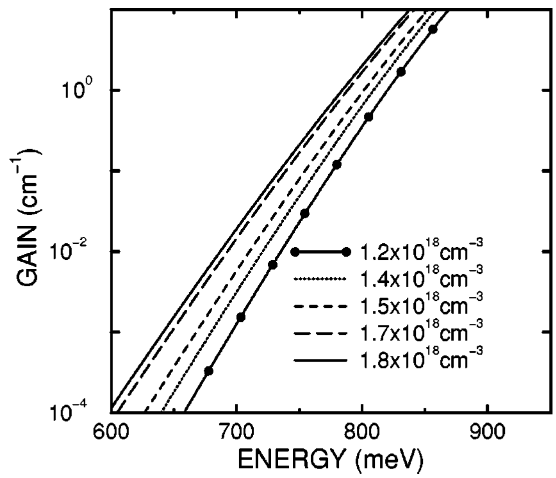

FIG. 4. The low-energy region of the gain curves of Fig. 3(a).

VI. CONCLUSIONS

In conclusion we have developed a consistent yet easily implemented procedure for describing many-body effects in highly excited semiconductors. Our model includes exciton scattering by both plasmons and electron-hole excitations. Applying the plasmon pole approximation to the inverse dielectric function generates a numerical description of semiconductor laser gain that is in good agreement with experiment. We believe that the theory is sufficiently efficient and compact that it can easily be incorporated into standard programs for, e.g., semiconductor laser gain and linewidth.

APPENDIX: EVALUATION OF THE SPECTRAL DENSITY

The wave function of an electron-hole pair with total momentum $\mathbf{P}$ is given in the independent particle model by

$$\Psi_{\mathbf{k},\mathbf{P}}(\mathbf{r}_e,\mathbf{r}_h)=\frac{1}{\mathcal{V}}e^{i\mathbf{P}\cdot\mathbf{R}}e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{A1}$$

in which $\mathbf{R}=(m_e\mathbf{r}_e+m_h\mathbf{r}_h)/(m_e+m_h)$ and $\mathbf{r}=\mathbf{r}_e-\mathbf{r}_h$ represent the center of mass and relative coordinates of the electron and hole. The corresponding energy is given by

$$E_{\mathbf{k}}(\mathbf{P})=\frac{\mathbf{P}}{2M}+\frac{\mathbf{k}}{2\mu}+E_g\,, \tag{A2}$$

where $M=m_e+m_h$ and $\mu^{-1}=m_e^{-1}+m_h^{-1}$.

The matrix element of Eq. (39) then becomes

$$\langle\mathbf{k}_0|e^{-i\mathbf{q}\cdot\mathbf{r}_e}-e^{i\mathbf{q}\cdot\mathbf{r}_h}|\mathbf{k}\rangle=\mathcal{V}(\delta_{\mathbf{k}-\mathbf{k}_0,\mathbf{q}m_h/M})-\delta_{\mathbf{k}_0-\mathbf{k},\mathbf{q}m_e/M}). \tag{A3}$$

Since the Kronecker delta functions are both equal to one only when $\mathbf{q}=0$ the cross products of the electron and hole scattering amplitudes in Eq. (39) that correspond to interference terms vanish. The $M^<$ function can thus be seperated into two terms which correspond to electron and hole contributions, namely

$$M^<_{\mathbf{k}_0}(\omega)=M^{e,<}_{\mathbf{k}_0}(\omega)+M^{h,<}_{\mathbf{k}_0}(\omega). \tag{A4}$$

Here we have defined

$$M_{\mathbf{k}_0}^{e,<}(\omega)=-\sum_m \frac{\gamma_m^2}{2\pi}\left[\sum_{\mathbf{q}_-}\frac{N(\omega_{\mathbf{q}_-}^m)}{\left|\frac{\mathbf{q}_-}{m_e}+\frac{d\omega_{\mathbf{q}_-}^m}{dq_-}\right|}+\sum_{\mathbf{q}_+}\frac{[1+N(\omega_{\mathbf{q}_+}^m)]}{\left|\frac{\mathbf{q}_+}{m_e}-\frac{d\omega_{\mathbf{q}_+}^m}{dq_+}\right|}\right]. \tag{A5}$$

The coupling constant to the mth boson branch is thus given by

$$\gamma_m^2=\begin{cases}2\pi e^2\hbar\,\omega_p^2\frac{1}{\epsilon_\infty\omega_q} & \text{for plasmons}\\ 2\pi e^2\hbar\,\omega_0\left(\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right) & \text{for LO phonons,}\end{cases} \tag{A6}$$

where the summation is performed with respect to the positive roots $q_\pm^2$ of the equation

$$\omega\pm\omega_q^m-\frac{q^2}{2m_e}=0. \tag{A7}$$

The hole contribution $M_{\mathbf{k}_0}^{h,<}(\omega)$ is finally obtained by replacing the electron mass m_e by the hole mass m_h in the above expressions.

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