Simplified calculations of band-gap renormalization in quantum-wells

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Non-linear optical properties of photoexcited semiconductor quantum-wells are of interest because of their opto-electronic device application possibilities. Band-gap renormalization arising from the many-body interactions of optically created electrons and holes is an important ingredient to understand the absorption spectra of such systems. Screening in the electron-hole system leads to a renormalization of the single-particle energies. In particular, the Coulomb interaction between the carriers results in a decrease in the average charge density felt by individual particles. These many-body interactions along with the Pauli exclusion principle reduce the energy of charge carriers in valence and conduction bands. The narrowing of the band-gap affects the luminescence properties with interesting consequences for the semiconductor lasers [1].

The full many-body calculations of the band-gap renormalization make use of the perturbation theory to calculate the electron and hole self-energies at the conduction and valence band edges. The contribution to the self-energy may be split into a screened-exchange and a Coulomb-hole term. The former is calculated using the screened Coulomb potential in which various models and approximations for the dielectric function is employed. The Coulomb-hole term, on the other hand, describes the charge-density fluctuations around individual carriers. The general conclusions drawn from numerous studies [2–4] are such that for bulk materials the band-gap renormalization exhibits a universal density dependence [5], whereas the quantum-well systems show marked dependence on the well-width.

The main purpose of this communication is to extend the recent calculations of Ninno et al. [6] to quantum-well systems, and explore the well-width and temperature dependence of the band-gap renormalization to make more realistic contact with experiments. We demonstrate that the simple approach of calculating the band-gap renormalization, which neglects the exchange-correlation effects but fully accounts for the Coulomb-hole contribution, yields reasonable agreement with experiments.
mental results, provided well-width and temperature dependences are included. This is chiefly due to the fact that the Coulomb-hole part of the self-energy becomes dominant for not too high densities, as also noted by Haug and Schmitt–Rink [2]. Similar model calculations [7] based on the Coulomb-hole contribution have proven quite useful in bulk systems. Microscopic calculations [8–10] taking the finite well-width and temperature dependence for quasi-two-dimensional (Q2D) systems are generally in good agreement with the experimental results [11–13]. Various simplified approaches [14–16] for 3D and 2D systems provide understanding for the basic mechanisms of band-gap renormalization.

In the following, we calculate the energy of a free electron-hole pair interacting only with plasmons for a Q2D system. We include the well-width and finite temperature dependences. The resulting band-gap renormalization shows satisfactory agreement with the experiments.

We express the Hamiltonian of an electron-hole pair interacting with the collective modes (plasmons) as [6,17].

\[
H = \sum_{i=e,h} \frac{p_i^2}{2m_i} + \sum_{q} \omega_q \left( a_q^\dagger a_q + \frac{1}{2} \right) + \sum_{i=e,h} \sum_{q} M_i^p(q)(a_q e^{iq.x} + a^\dagger_x e^{-iq.x}),
\]

in which we have neglected the direct electron-hole Coulomb interaction (we take \(h = 1\)). In the above expression, \(M_i^p(q)\) is the matrix element describing the interaction of \(i\)th carrier (electron or hole) with plasmons for a \(D\)-dimensional system, and \(\omega_q\) is the \(q\)-dependent plasma dispersion. Since this Hamiltonian is formally identical to that of the polaron problem, straightforward application of the Lee–Low–Pines variational scheme [18] gives

\[
E_g = -\sum_{i=e,h} \int \frac{d^Dq}{(2\pi)^D} |M_i^p(q)|^2(\omega_q + \frac{q^2}{2m_i})^{-1},
\]

for the energy of the electron-hole pair interacting with plasmons. The carrier-plasmon interaction matrix element for a \(D\)-dimensional system is found to be \(|M_i^p(q)|^2 = |V^p_i|^2 Nq^2 / (2\pi \omega_q)\), where \(V^p_i\) is the Coulomb interaction. For a 3D system \(V_q = 4\pi e^2 / (\varepsilon_0 q^2)\), and for a 2D system \(V_q = 2\pi e^2 f(q) / (\varepsilon_0 q)\), where \(\varepsilon_0\) is the static dielectric constant of the semiconductor material. In the 2D Coulomb interaction, we have allowed for a form factor \(f(q)\) arising from the subband quantization. An infinite square-well model with width \(a\) yields

\[
f(q) = \frac{8}{(qa)^2 + 4\pi^2} \left[ \frac{3}{8} qa + \frac{\pi^2}{qa} - \frac{4\pi^4}{(qa)^2} \right].
\]

The plasma dispersion \(\omega_q\) is evaluated within the static plasmon-pole approximation [17]

\[
\omega_q^2 = \omega_{p,q}^2(q) \frac{\varepsilon(q)}{\varepsilon(q)-1},
\]

where \(\varepsilon(q)\) is the static dielectric function (i.e. \(\varepsilon(q) = \varepsilon(q,\omega = 0)\)). We use the random-phase approximation (RPA) at zero and finite temperature for \(\varepsilon(q)\). (The explicit forms we use may be found in the references cited.) \(\omega_{p,q}^2(q)\) is the long-wavelength limit of the plasma frequency which reads \(\omega_{p,q}^2 = 4\pi e^2 N/(\varepsilon_0 \mu)\) and \(\omega_{p,q}^2(q) = 2\pi e^2 Nq / (\varepsilon_0 \mu)\) for 3D and 2D systems, respectively. Here \(\mu\) is the reduced mass of the electron-hole pair.

We now discuss our results for the case of GaAs, for which the material parameters are: \(m_e = 0.067\ m\), \(m_h = 0.62\ m\), where \(m\) is the bare electron mass, and \(\varepsilon_0 = 13.18\) (we use the same material parameters as Ref. [6]). The band-gap renormalization within the present approach in bulk GaAs at zero temperature was calculated by Ninno et al. [6]. It was found that the density dependence of \(E_g\) was reasonably accounted for. We first explore the temperature dependence of \(E_g\) in our
Fig. 1. Band-gap renormalization in bulk GaAs as a function of carrier temperature, for plasma densities $N=10^{14}$ cm$^{-3}$ (dotted), $N=10^{15}$ cm$^{-3}$ (dashed), and $N=10^{16}$ cm$^{-3}$ (solid). We use the effective Rydberg for the energy scale, i.e. $Ry^* = e^2 \mu/(2\varepsilon_0)$.

Fig. 2. Band-gap renormalization in Q2D GaAs as a function of plasma density. Solid line is for a strictly 2D system at $T=0$. Dotted and dashed lines indicate $E_g$ for a quantum-well of width $a=100$ Å, at $T=0$ and $T=300$ K, respectively. The solid circles and open squares are the experimental data of Tränkle et al. [11] and Lach et al. [12], respectively.
The renormalized band-gap energy in a Q2D GaAs system as a function of the plasma density $N$ is depicted in Fig. 2. The solid line is for a strictly 2D electron-hole system at zero temperature. For comparison we also show the experimental data by Tränkle et al. [11] (solid circles) and Lach et al. [12] (open squares). The former of these measurements were taken on GaAs/GaAlAs samples of quantum-well-widths 21–83 Å, at $T=2$ K. The dotted line shows $E_g$ for a 100 Å wide quantum-well at $T=0$, and the agreement with the data improves considerably. Lach et al. [12] data on the other hand, is for a 103 Å GaAs/GaAlAs quantum-well at 300 K, and cover a higher range of plasma densities. The dashed line shows $E_g$ calculated for a 100 Å quantum-well at 300 K is also in reasonable agreement with the experimental data [12]. Our simplified model demonstrates the importance of including the finite well-width and temperature dependences in the band-gap renormalization. Calculations of Ryan and Reinecke [10] have already shown the importance of Coulomb-hole contribution over the screened-exchange in quantum wells for carrier densities of $N<3 \times 10^{12}$ cm$^{-2}$.

Having identified the importance of well-width and temperature dependence of the band-gap renormalization, we show in Fig. 3, $E_g$ as a function of quantum-well width at a fixed 2D plasma density $N=10^{12}$ cm$^{-2}$. The solid, dashed, and dotted lines are for $T=0$, 100, and 300 K, respectively.

In the above simplified approach of band-gap renormalization, we have considered the interaction of a single electron-hole pair with plasma excitations. It is well-known that a two-component system (i.e. electron-hole liquid) also supports an acoustic-plasmon mode [19] other than ordinary plasmons. We have attempted to include the contribution of acoustic modes to $E_g$ within the present approach, and found their effect to be rather small. This is due to their relatively weak interaction.
strengths, and limited region of existence in the phase-space [19]. The effect of carrier-phonon interactions on the band-gap renormalization was investigated by Das Sarma et al. [9] in a many-body formalism. In our case, the phonon contribution to screening is treated in the so-called $\epsilon_{\infty}$-approximation. We have also neglected the intersubband contribution to the self-energy within the present approach. Extension of the present approach to take for instance the intervalence band transitions into account should be straightforward once the dielectric function is suitably modified [10]. We have attempted to apply similar ideas for a quantum-well wire. In this case, we found that the Coulomb-hole term does not represent the experimental results well, suggesting the importance of screened-exchange term in the self-energy. Another possible source of discrepancy is our use of the bulk effective masses for the conduction and valence bands. In a confined system such as a quantum-well or a quantum-wire more accurate band masses should be used.

In summary, we have studied the band-gap renormalization in GaAs quantum-well systems within a simple model of electron-hole pair interacting with collective plasma excitations. We have found that experimentally observed band-gap energies may be accounted for qualitatively if the quantum-well width and temperature dependences are considered. Our calculations indicate that Coulomb-hole term is more important than the screened exchange term, in the self-energy calculations, and it represents the experimental data reasonably well.

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References