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Simplified calculations of band-gap renormalization in quantum-wells

K. Güven, B. Tanatar
Department of Physics, Bilkent University, Bilkent, 06533 Ankara, Turkey

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Non-linear optical properties of photoexcited semiconductor quantum-wells are of interest because of their opto-electronic device application possibilities. Many-body interactions of the optically created electrons and holes lead to the band-gap renormalization which in turn determines the absorption spectra of such systems. We employ a simplified approach to calculate the band-gap renormalization in quantum-well systems by considering the interaction of a single electron-hole pair with the collective excitations (plasmons). This method neglects the exchange-correlation effects but fully accounts for the Coulomb-hole term in the single-particle self-energy. We demonstrate that the density, temperature, and well-width dependence of the band-gap renormalization for GaAs quantum-wells within our model is in good agreement with the experimental results.

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 experi-

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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].

$$H=\sum_{i=\mathrm{e,h}}\frac{P_i^2}{2m_i}+\sum_q\omega_q\left(a_q^\dagger a_q+\frac{1}{2}\right)+\sum_{i=\mathrm{e,h}}\sum_q M_i^D(q)(a_q e^{i\mathbf{q}\cdot\mathbf{r}}+a_q^\dagger e^{-i\mathbf{q}\cdot\mathbf{r}}), \tag{1}$$

in which we have neglected the direct electron-hole Coulomb interaction (we take $\hbar=1$). In the above expression, $M_i^D(q)$ is the matrix element describing the interaction of ith carrier (electron or hole) with plasmons for a D-dimensional system, and ω_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

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

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 $|M_i^D(q)|^2=[V_q^D]^2Nq^2/(2m_i\omega_q)$, where V_q^D is the Coulomb interaction. For a 3D system $V_q=4\pi e^2/(\epsilon_0 q^2)$, and for a 2D system $V_q=2\pi e^2 f(q)/(\epsilon_0 q)$, where ϵ_0 is the static dielectric constant of the semiconducting 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

$$f(q)=\frac{8}{(qa)^2+4\pi^2}\left[\frac{3}{8}qa+\frac{\pi^2}{qa}-\frac{4\pi^4}{(qa)^2}\frac{1-e^{-qa}}{(qa)^2+4\pi^2}\right]. \tag{3}$$

The plasma dispersion ω_q is evaluated within the static plasmon-pole approximation [17]

$$\omega_q^2=\omega_{\mathrm{pl}}^2(q)\frac{\varepsilon(q)}{\varepsilon(q)-1}, \tag{4}$$

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.) $\omega_{\mathrm{pl}}(q)$ is the long-wavelength limit of the plasma frequency which reads $\omega_{\mathrm{pl}}^2=4\pi e^2N/(\epsilon_0\mu)$ and $\omega_{\mathrm{pl}}^2(q)=2\pi e^2Nq/(\epsilon_0\mu)$ for 3D and 2D systems, respectively. Here μ 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: $m_e=0.067\,m$, $m_{\mathrm{h}}=0.62\,m$, where m is the bare electron mass, and $\epsilon_0=13.18$ (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

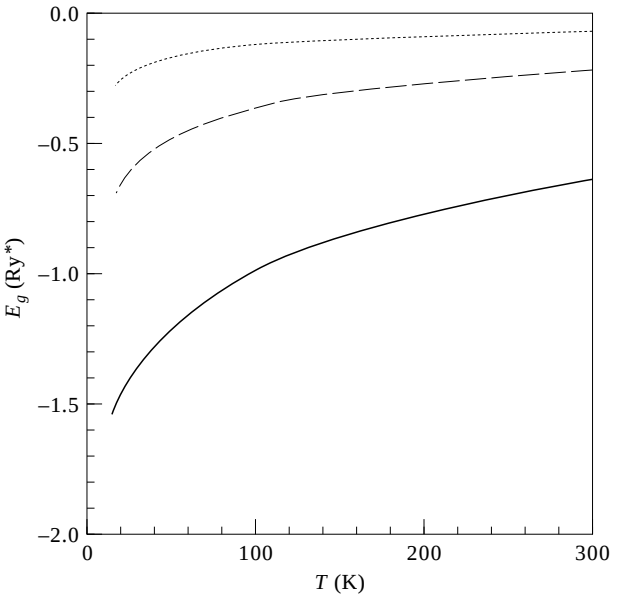

Fig. 1. Band-gap renormalization in bulk GaAs as a function of carrier temperature, for plasma densities $N=10^{14}$ cm^{-3} (dotted), $N=10^{15}$ cm^{-3} (dashed), and $N=10^{16}$ cm^{-3} (solid). We use the effective Rydberg for the energy scale, i.e. Ry* $=e^2\mu/(2\epsilon_0^2)$.

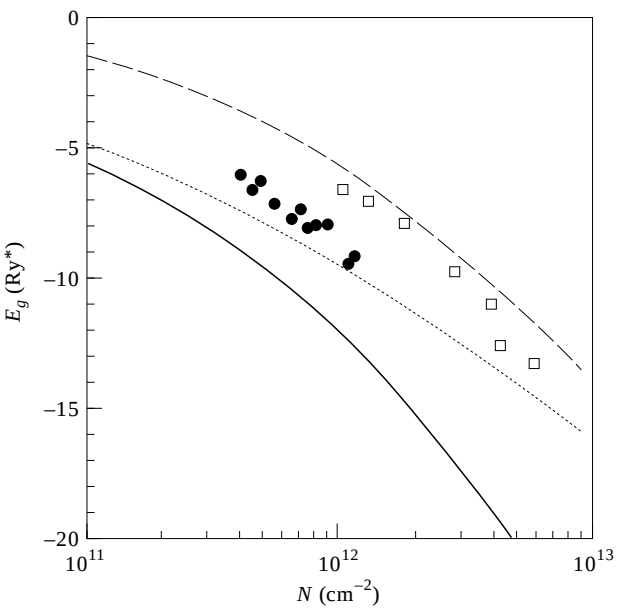

Fig. 2. Band-gap renormalization in Q2D GaAs as a function of plasma density. Solid line is for a strictly 2D system at $T=0$. Dotted and dashed lines indicate E_g for a quantum-well of width $a=100$ Å, at $T=0$ and $T=300$ K, respectively. The solid circles and open squares are the experimental data of Tränkle *et al.* [11] and Lach *et al.* [12], respectively.

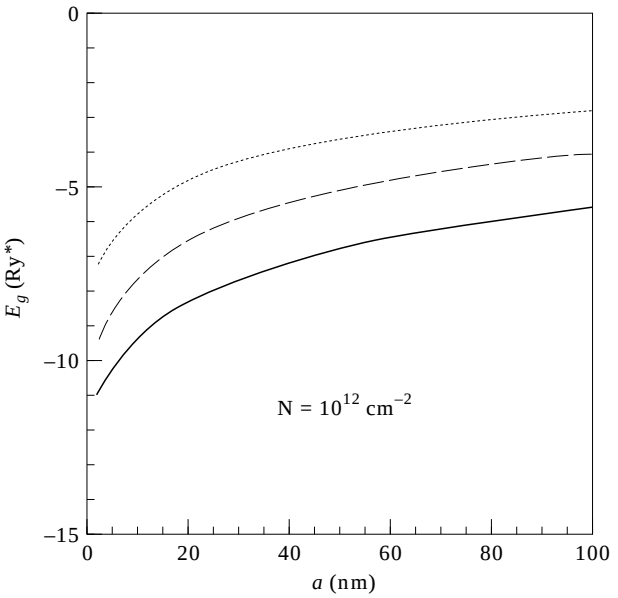

Fig. 3. Band-gap renormalization in Q2D GaAs as a function of the quantum-well width. Solid, dashed, and dotted lines indicate $T=0$, 100, and 300 K, respectively.

simplified scheme, for a 3D system. Figure 1 shows the band-gap renormalization in bulk GaAs as a function of carrier temperature for fixed plasma densities $N=10^{16}$ cm^{-3} (solid), $N=10^{15}$ cm^{-3} (dashed), and $N=10^{14}$ cm^{-3} (dotted). We observe that the temperature dependence of E_g is stronger for lower plasma densities. In so far as the population of higher subbands is neglected, such behavior is also obtained in more detailed calculations [8].

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 $N<3\times10^{12}$ 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 ϵ_0-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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