Band-gap renormalization in quasi-one-dimensional electron - hole systems

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Band-gap renormalization in quasi-one-dimensional electron–hole systems

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Abstract. We study the band-gap renormalization (BGR) in semiconductor quantum wires. Assuming an electron–hole system in quasi-equilibrium, we employ the random-phase approximation (RPA) and beyond (e.g., local-field corrections) to calculate the electron and the hole self-energies. The plasmon-pole approximation to the static dielectric function $\varepsilon(q)$ agrees well with the RPA result. Our results for the BGR are compared with the recent experimental measurements and other theoretical calculations.

1. Introduction

A dense electron–hole plasma forms in a semiconductor under intense laser excitation. Because of the exchange effects and the screening of the Coulomb interaction, many single-particle properties in the system are renormalized. An interesting phenomenon is the band-gap renormalization (also known as the band-gap shrinkage) as a function of the plasma density which is important to determine the emission wavelength of coherent emitters as used in semiconductors [1]. Since a substantial carrier population may be induced by optical excitation, the renormalized band gap can affect the excitation process in turn and lead to optical nonlinearities. In this paper we investigate the density dependence of the band-gap renormalization (BGR) in quasi-one-dimensional (Q1D) photoexcited semiconductors. Under high optical excitation the band gap for 2D and 3D systems is found to decrease with increasing plasma density due to exchange–correlation effects. The observed band gaps are typically renormalized by $\sim$20 meV within the range of plasma densities of interest which arise solely from the conduction band electrons and valence band holes. In the Q1D structures based on the confinement of electrons and holes, the electron–hole plasma is quantized in two transverse directions, thus the charge carriers essentially move only in the longitudinal direction. Recent progress in the fabrication techniques such as molecular-beam epitaxy (MBE) and lithographic deposition has made possible the realization of such quasi-one-dimensional systems [2]. Band-gap renormalization as well as various optical properties of the electron–hole systems have been studied for bulk (3D) and quantum-well (2D) semiconductors [3–6], providing generally good agreement with the corresponding measurements [7].

Our main motivation comes from the recent experiments of Cingolani *et al* [8, 9] in which they investigated the carrier density dependence of a quasi-one-dimensional electron–hole plasma confined in GaAs quantum wires using luminescence spectra. Comparing the band-gap data with the available calculations, Cingolani *et al* [8] pointed out the need for a more realistic calculation. Density dependence of the BGR in Q1D systems was first

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considered by Benner and Haug [10] within the quasi-static approximation as previously employed for 2D and 3D systems [3–6]. In a detailed study that appeared recently Hu and Das Sarma [11] also calculated the BGR, neglecting the hole population and considering an electron plasma confined in the lowest conduction subband only. The results of Hu and Das Sarma [11] are rather close to the experimental data [8].

In this study our aim is to calculate the BGR using a statically screened approximation which is based on the RPA. We employ the temperature-dependent, static, RPA dielectric function and address the question of validity of using the plasmon-pole approximation to it. We investigate the temperature dependence of the BGR at various electron–hole plasma densities and quantum well widths. The density dependence of the renormalized chemical potential calculated using the exchange–correlation contribution is also given.

The rest of this paper is organized as follows. In the next section we give a brief outline of the static screening approximation (quasi-static approximation). In section 3 we present our results for the BGR in Q1D electron–hole plasmas and compare them with the experiments. Finally, we conclude with a brief summary of our main results.

2. Theory

For the Q1D system we consider a square well of width a with infinite barriers. It may be built from a Q2D quantum-well (grown in the z-direction) by introducing an additional lateral confinement. We assume that the effective-mass approximation holds and for GaAs take $m_e = 0.067m$, and $m_h = 0.2m$, where m is the bare electron mass. Note that we have chosen the hole effective mass to reproduce on average the dispersion of the four topmost 1D subbands to conform with the experimental analysis of [8]. The effective Coulomb interaction between the charge carriers is given by [11]

$$V(q) = \frac{2e^2}{\varepsilon_0}\int_0^1 \mathrm{d}x\, K_0(qax)\left[(1-x)[2+\cos(2\pi x)] + \frac{3}{2\pi}\sin(2\pi x)\right] \quad (1)$$

in which $K_0(x)$ is the zeroth-order modified Bessel function of the second kind, and ε_0 is the lattice dielectric constant. Due to the presence of an electron–hole plasma, assumed to be in equilibrium, the bare Coulomb interaction is screened. The equilibrium assumption is justified since the laser pulse durations are typically much longer than the relaxation times of the semiconductor structures under study. Defining the statically screened Coulomb interaction as $V_s(q) = V(q)/\varepsilon(q)$, we consider the dielectric function in the random-phase approximation (RPA)

$$\varepsilon(q) = 1 - 2V(q)\sum_{i,k}\frac{f_i(k) - f_i(k+q)}{\varepsilon_i(k) - \varepsilon_i(k+q) + \mathrm{i}\eta} \quad (2)$$

where the index $i = e, h$, and $\varepsilon_i(k) = \hbar^2k^2/2m_i$ are the bare single-particle energies. In most previous studies, the dielectric function $\varepsilon(q)$ was further simplified by the plasmon-pole approximation. Here we use the full static RPA at finite temperature without resorting to any approximations and discuss in the following section the validity of the plasmon-pole approximation.

Assuming a homogeneously distributed electron–hole plasma in thermal equilibrium the electron and hole distribution functions are written as

$$f_i(k) = \frac{1}{\mathrm{e}^{\beta(\varepsilon_i(k)-\mu_i^0)} + 1} \quad (3)$$

where $\beta = 1/k_B T$ and μ_i^0 are the inverse carrier temperature and (unrenormalized) chemical potential of the different species, respectively. The plasma density N determines μ_i^0 through the normalization condition $N = 2\sum_k f_i(k)$.

Adopting the quasi-static approximation [3, 4] which amounts to neglecting the recoil effects relative to the plasma frequency in the full-frequency dependent expressions, we decompose [3, 4] the electron and hole self-energies into screened exchange (sx) and Coulomb hole (Ch) terms: $\Sigma_i(k) = \Sigma_i^{\rm sx}(k) + \Sigma_i^{\rm Ch}$, where

$$\Sigma_i^{\rm sx}(k) = -\sum_{k'} V_s(k-k') f_i(k') \tag{4}$$

and

$$\Sigma_i^{\rm Ch} = \frac{1}{2}\sum_{k'}[V_s(k') - V(k')]. \tag{5}$$

The above set of equations may be derived [3] from the dynamical self-energy expressions by neglecting all recoil energies with respect to the plasma frequency. As in the case of 2D and 3D calculations [3–6] we assume that the BGR results from rigid bandshifts; i.e., the self-energies depend only weakly on wave vector k. The band-gap renormalization is then given by

$$\Delta E_g = E_g' - E_g = \Sigma_e(0) + \Sigma_h(0) \tag{6}$$

namely the electron and hole self-energies calculated at the respective band edges. Within the same spirit, we calculate the renormalized total chemical potential of the electron–hole plasma using

$$\mu_T = \sum_i [\mu_i^0 + \Sigma_i(k_F)] \tag{7}$$

in which $k_F = \pi N/2$ is the Fermi wave vector. The self-energy part in the above expression is also called the exchange–correlation contribution $\mu_{\rm xc}$ to the chemical potential.

3. Results and discussion

In figure 1 we show the results of our calculation for the BGR (indicated by the solid curve) as a function of the electron–hole plasma density N. In order to make a ready comparison with the experimental results of Cingolani *et al* [8] (shown by full circles), we have evaluated ΔE_g for a quantum wire of width $a = 500$ Å, at $T = 100$ K. The investigated [8] quantum wires were fabricated by plasma etching from quantum-well structures with lateral widths of 600 ± 50 Å. The experimental data have been collected over a whole set of spectra at various carrier temperatures. As we shall demonstrate below the BGR is not very sensitive to the temperature and we obtain rather good agreement with the experimental results. The zero-temperature calculation of Hu and Das Sarma [11] also represents well the Cingolani *et al* [8] data, indicating the insensitivity of ΔE_g to temperature in the range of densities reported. The agreement between our calculated results and the experiment appears to be rather good. However, we caution that the experimental data points [8] were extracted from the observed luminescence spectra by assuming a free-carrier model. Our calculations indicate the importance of Coulomb effects. Thus a more refined line-shape analysis would be required to render the comparison more meaningful.

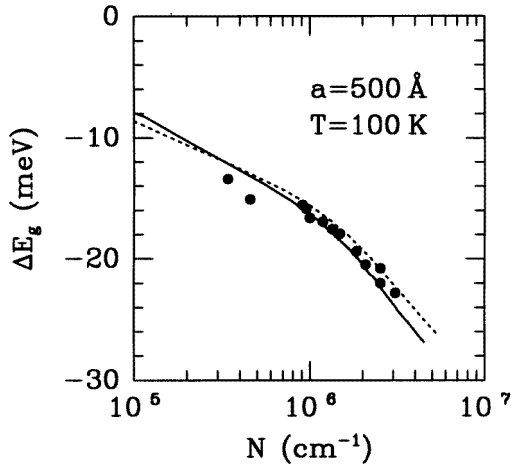

Figure 1. The calculated band-gap renormalization ΔE_g as a function of the electron–hole pair density. Full circles are the experimental results from [8]. Solid and dotted lines are calculated with the full RPA dielectric function and the plasmon-pole approximation to it, respectively.

The dotted curve in figure 1 gives the BGR calculated within the plasmon-pole approximation to the dielectric function using the same parameters. In the plasmon-pole approximation the static dielectric function is expressed as [10]

$$\varepsilon(q) = 1 + \frac{\omega_p^2}{Nq^2/\mu\kappa + (q^2/2\mu)} \tag{8}$$

where the plasmon frequency for the Q1D system is $\omega_p^2 = (N/\mu)V(q)$, and the screening parameter is $\kappa = \sum_i \partial N/\partial\mu_i^0$. Here $\mu^{-1} = m_e^{-1} + m_h^{-1}$ is the reduced mass. This is essentially the approach taken by Benner and Haug [10], where they use a parabolic confinement potential. The plasmon-pole approximation consists of ignoring the weight of single-particle excitations and assuming that all the weight of the dynamic susceptibility $\chi_0(q,\omega)$ is at an effective plasmon energy ω_p. It correctly describes the static and long-wavelength limits of the full RPA expression. Most BGR calculations [3–6] are performed in the plasmon-pole approximation and its justification is rarely addressed. Das Sarma *et al* [12] have found significant deviations of the plasmon-pole approximation from the full RPA results in quantum wells. The qualitative similarity of dotted and solid curves in figure 1 demonstrates the applicability of the plasmon-pole approximation in Q1D systems in contrast to Q2D systems as found by Das Sarma *et al* [12]. To assess the validity of the plasmon-pole approximation in Q1D systems, we display in figure 2 the static dielectric function $\varepsilon(q)$ calculated in the RPA and the plasmon-pole approximation. The RPA calculation (solid line) is performed using equation (2) at a finite temperature, since the thermal electron and hole distribution functions $f_i(k)$ are used. The temperature dependence of $\varepsilon(q)$ in the plasmon-pole approximation (dotted line) comes from the screening parameter κ, and as may be observed in figure 2 it reproduces the full RPA result satisfactorily. Our calculations indicate that the plasmon-pole approximation becomes better for large T.

In figure 3 we show the temperature dependence of the band-gap renormalization ΔE_g in the Q1D electron system. The solid lines indicate BGR for a system at $N = 10^5$ cm^{-1} with $a = 100$ Å (lower curve) and $a = 500$ Å (upper curve). The dotted lines are for $N = 10^6$ cm^{-1} with $a = 100$ Å (lower curve) and $a = 500$ Å (upper curve). The results shown in figure 3 were calculated using the full RPA dielectric function at finite temperature, but we found that the plasmon-pole approximation also works quite well. Hu and Das Sarma [11] have also investigated the temperature dependence of the BGR within

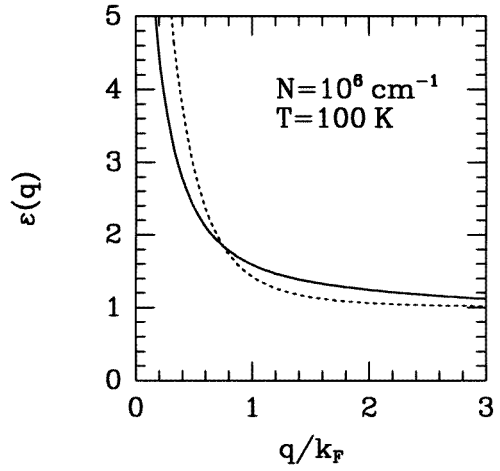

Figure 2. The static dielectric function of the 1D electron–hole system $\varepsilon(q)$ at $T = 100$ K and $N = 10^6$ cm^{-1}. The solid curve indicates the full RPA, and the dotted curve is the plasmon-pole approximation result.

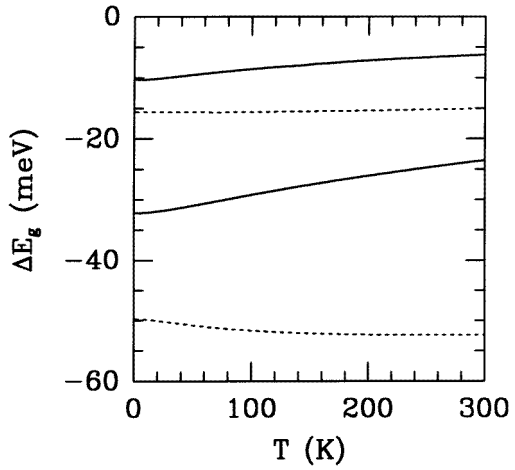

Figure 3. The temperature dependence of the band-gap renormalization for $N = 10^5$ (solid lines) and $N = 10^6$ cm^{-1} (dotted lines). The upper and lower curves are for $a = 500$ and $a = 100$ Å wide quantum-well wires.

the leading-order dynamical screening approximation (GW approximation). Our statically screened approximation yields qualitatively similar results suggesting dynamical screening is not significant in the range of plasma densities of experimental interest.

We have evaluated the renormalized chemical potential of the electron–hole plasma including the exchange–correlation contribution as set out in the previous section. In figure 4, we show the calculated total chemical potential μ_T (indicated by the solid curves) of the Q1D electron–hole system with well width $a = 600$ Å, for $k_BT = 8$ (lower curve) and 16 meV (upper curve) as a function of the plasma density (we scale the density using the effective Bohr radius $a_B^* = \varepsilon_0\overline{h}^2/\mu e^2$ in terms of the reduced mass μ and dielectric constant ε_0). Also displayed in the same figure by dotted curves are the unrenormalized chemical potentials $(\mu_e^0 + \mu_h^0)$ for $k_BT = 8$ (upper curve) and 16 meV (lower curve). Our calculations are to be compared with the experimental results of Cingolani *et al* [8] obtained for similar parameters (cf figure 4 of [8]). We observe that there is a quantitative disagreement with the experiment especially for large densities. This may be due to the subband effects which need to be investigated further. Comparison of the solid and dotted

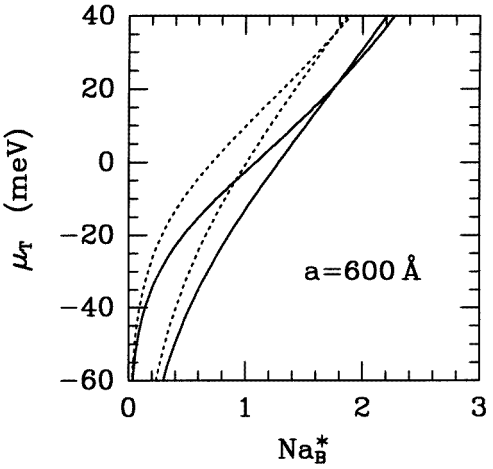

Figure 4. The chemical potential μ_T of the electron–hole system as a function of the plasma density for a 600 Å wide quantum well. The solid and dotted curves are the renormalized and unrenormalized $(\mu_e^0 + \mu_h^0)$ chemical potentials. Upper and lower curves are calculated at $k_B T = 16$ and 8 meV, respectively.

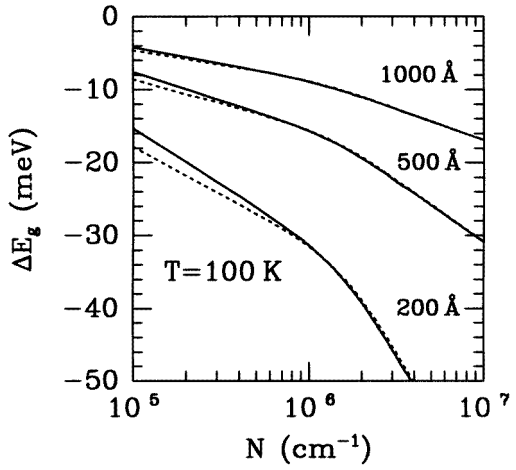

Figure 5. Effects of local-field corrections on the band-gap renormalization as a function of the plasma density at $T = 100$ K. Dotted and solid lines are calculated with and without local-field corrections, respectively.

curves in figure 4 gives some indication about the rigid-bandshift assumption. Using equation (8), we have calculated the exchange–correlation part of the chemical potential with both $\Sigma(k = 0)$ and $\Sigma(k = k_F)$ and found no notable difference which suggests that the bandshifts occur rigidly. It would be necessary to start from a fully dynamical model of the self-energy (i.e., using a frequency-dependent dielectric function) to test the rigid-bandshift assumption.

There seems to be a discrepancy in the band-gap renormalization between theory and experiment at high densities for Q2D structures. The origin of this general disagreement is not well understood. Several attempts to improve the theory, particularly the multisubband population case, did not change the qualitative behaviour of the BGR. To explore the existence of similar behaviour it would be interesting to perform experiments in Q1D structures at higher densities.

We now discuss the effects of local-field correction to the BGR in quantum wires. Writing the dielectric function as $\varepsilon(q) = 1 - V(q)\Pi(q)[1 - G(q)]$, where $G(q)$ is the static local-field factor and $\Pi(q)$ is the static polarizability, we may account for the vertex corrections to $\Pi(q)$ in the mean-field sense. Recently, Schuster and co-workers

[13] considered finite-temperature vertex corrections in the form of second-order exchange contribution to the self-energy in 2D and 3D electron–hole plasmas. We use the equivalent of the Hubbard approximation for $G(q)$ in one dimension to obtain [14]

$$G(q) = \frac{1}{2}\frac{V(\sqrt{q^2 + k_F^2})}{V(q)}. \tag{9}$$

The physical nature of the Hubbard approximation is such that it takes exchange into account and corresponds to using the Pauli hole in the calculation of the local-field correction between the particles of the same kind. Coulomb correlations are omitted. In this simple form, the static local-field factor $G(q)$ is temperature independent. Figure 5 shows the BGR for quantum wires of various lateral widths at $T = 100$ K with and without the local field corrections. The solid curves are calculated with the local-field correction whereas the dotted curves give the RPA ($G(q) = 0$). We observe that, within the simple Hubbard approximation to $G(q)$, the BGR deviates from the RPA result as the quantum-well width decreases. The difference in BGR with and without $G(q)$ is more appreciable for lower densities. We argue that in general RPA is a good approximation for high densities, but requires modifications for low densities. In order to assess a reliable measure of corrections beyond RPA, better approximations to the local-field factor $G(q)$ are needed. Returning to the issue of discrepancy in the calculated ΔE_g and measurements for high densities in Q2D systems [13], it seems unlikely that improvements of RPA could yield satisfactory agreement. Elaborate calculations of Schuster *et al* [13] give an indication in this direction. Clearly, more experimental measurements of the type reported by Cingolani *et al* [8, 9] covering a wide range of plasma densities are necessary to resolve these questions.

As pointed out earlier, the band-gap renormalization accounts for the optical nonlinearities in the photoexcited semiconductor structures. The theoretical description of these phenomena in Q2D and 3D systems has been reviewed by Haug and Schmitt-Rink [15]. It would be interesting to examine the nonlinear optical properties of Q1D electron–hole systems using a similar approach. It is also possible to investigate the effects of electron–phonon interaction on the band-gap renormalization. Das Sarma *et al* [12] have treated a coupled electron (hole)–phonon system using many-body techniques. A similar attempt in Q1D systems would be worthwhile to determine the electron–phonon-interaction-induced BGR.

For the Q1D electron system we have used the model developed by Hu and Das Sarma [11] which introduces an additional confinement to an infinite square well. There are various other models of the quantum-well wire structures using parabolic confining potentials and geometrical reduction of dimensionality. The general trends obtained here for the plasma density and temperature dependence should be valid irrespective of the details of the model chosen.

Although we have carried out our numerical calculations for the material parameters of GaAs, the same formalism may be applied to other semiconductor structures such as InAs, GaSb and AlAs. It would be desirable to have experimental results of the BGR for different Q1D semiconductor materials to compare with theoretical calculations. In 2D and 3D, a somewhat universal dependence of ΔE_g on plasma density is established largely independent of the band structure details. Whether a similar general behaviour exists in Q1D electron–hole systems would be settled as more photoluminescence experiments become available.

4. Summary

We have found that the static plasmon-pole approximation to the dielectric function yields very close results to the full RPA expression. The temperature dependence of the BGR is weak for densities $N \sim 10^6$ cm^{-1}. Local-field corrections employed within the Hubbard approximation decrease the BGR at low densities especially when the lateral width of the quantum wire is small. The calculated renormalized chemical potential of the electron–hole plasma qualitatively differs from the measurement which may be attributed to the subband effects.

Extension of our calculations to cases where more than one subband is populated would be interesting for comparison with future experiments. It was recently found by Ryan and Reinecke [16] that in Q2D systems the intersubband interactions make significant contribution to the band-gap renormalization. More experimental results are needed in quantum wires to discuss fully the various aspects of BGR. Given the importance of the Coulomb interaction, it would be useful to analyse the experimental results with more refined line-shape models.

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