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Band-gap renormalization in photoexcited semiconductor quantum-wire structures in the *GW* approximation

E. H. Hwang and S. Das Sarma
Department of Physics, University of Maryland, College Park, Maryland 20742-4111
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We investigate the dynamical self-energy corrections of the electron-hole plasma due to electron-electron and electron-phonon interactions at the band edges of a quasi-one-dimensional (1D) photoexcited electron-hole plasma. The leading-order *GW* dynamical screening approximation is used in the calculation by treating the electron-electron Coulomb interaction and the electron–optical-phonon Fröhlich interaction on an equal footing. We calculate the exchange-correlation-induced band-gap renormalization (BGR) as a function of the electron-hole plasma density and the quantum-wire width. The calculated BGR shows good agreement with existing experimental results, and the BGR normalized by the effective quasi-1D excitonic Rydberg exhibits an approximate one-parameter universality. [S0163-1829(98)50528-0]

A highly dense electron-hole plasma (EHP) can be generated in a wide variety of semiconductors by optical pumping. The band structure and the optical properties of highly excited semiconductors differ from those calculated for noninteracting electron-hole pairs due to many-body exchange-correlation effects arising from the EHP.[1,2] One of the important many-body effects in high-density EHP is a density-dependent renormalization of the fundamental band gap of the semiconductor, which causes an increasing absorption in the spectral region below the lowest exciton resonance. The exchange-correlation correction of the fundamental band gap due to the presence of free carriers (electrons in the conduction band and holes in the valence band) in the system is referred to as the band-gap renormalization (BGR) effect. Optical nonlinearities, which are strongly influenced by Coulomb interaction in the EHP, are typically associated with the band-gap renormalization phenomenon. Band-gap renormalization has been widely studied in bulk and quasi-two-dimensional (quantum well) semiconductors.[1–3] In recent years, quasi-one-dimensional semiconductor quantum wires (QW) have been fabricated with atomic scale definition, and QW optical properties have been studied for their potential device applications, such as semiconductor lasers. There has, however, been little work on the BGR in QW systems, both experimentally[4] and theoretically.[5,6] Until now most calculations have been done in the static screening approximation or in the simple plasmon-pole approximation, which is a simplified version of the random-phase approximation (RPA). The plasmon-pole approximation consists of ignoring the weight in the single-particle excitations and assuming that all free-carrier contributions to the dynamical dielectric function lie at the effective plasma frequency ω_p. The advantages of the plasmon-pole approximation are its mathematical simplicity and simple physical meaning. However, a certain degree of arbitrariness in the choice of the effective plasmon-pole parameters that are needed to satisfy the f-sum rule and the static Kramers-Kroning relation leads to considerable difficulties in applying the theory to semiconductors with complex band structures. In this paper, we calculate the BGR of the quantum-wire structures based on the RPA dynamical screening *GW* scheme by taking into account the full frequency dependent dielectric response in the *two component* one-dimensional (1D) EHP.

Most high quality QW structures of our interest are fabricated in weakly polar III-V semiconductors. In a polar semiconductor, free carriers couple to the longitudinal-optical (LO) phonons of the underlying lattice through the long-range polar Fröhlich interaction. The carrier–LO-phonon interaction leads to polaronic many-body renormalization of the single-particle free-carrier properties. Even though the weakly polar III-V materials have rather small Fröhlich coupling constants, the electronic properties can still be substantially modified by the Fröhlich interaction. Thus, inclusion of dynamical electron-phonon interaction in the theory is important since, in the quantum wires made of weakly polar materials, the Fröhlich interaction produces observable many-body corrections. In spite of substantial current interest in the properties of polar quasi-one-dimensional QW systems existing in GaAs quantum wires, the full many-body problem that includes dynamical screening and treats electron-electron and electron-phonon interactions on an equal footing has not yet been worked out.

Our goal is to calculate the BGR of a coupled 1D electron-phonon many-body system, treating electrons and phonons on an equal footing. There has been no detailed quantitative study of 1D quasiparticle properties including both electron-electron and electron-phonon interactions. We provide such an analysis in this paper based on the leading-order many-body perturbation theory. We calculate the self-energy corrections to the band edges (the highest valence- and the lowest conduction-band edges) in the presence of the EHP density $n_e = n_h$ of the electrons (n_e) and the holes (n_h) for quantum well wires of various thicknesses and for a number of different semiconductor systems. To the best of our knowledge, this is the first calculation of electronic many-body BGR correction in QW systems including full effects of both the dynamical electron-electron and Fröhlich electron–LO-phonon interactions treated on an equal footing. We find that the calculated BGR using the full RPA dielectric function agrees very well with available experi-

mental results[4] and depends on both the electron-hole density and quantum-wire widths. Our calculated BGR in quantum wires shows an approximate materials independent two-parameter universality as a function of the *scaled* plasma density and wire width. We find that this two-parameter universality of the BGR can be reduced to a single universal curve when the BGR scaled in the units of the appropriate quasi-1D effective excitonic Rydberg is expressed as a function of the dimensionless 1D electron-hole density parameter $r_s = 1/(2na_B)$, with a plasma density n and an effective Bohr radius a_B.

We assume that our quasi-1D QW system has an infinite square-well confinement with a finite width (a) in the y direction and zero thickness in the z direction, which is one of the simplest 1D confinement models. Because of the universality mentioned above we believe that our results are valid for more general 1D confinement situations. Only one kind of electrons and holes with isotropic, parabolic dispersion in a direct gap semiconductor is assumed to exist, thus neglecting most of the band-structure complications of the valence subbands. This should be an adequate approximation for calculating the band-edge BGR. We consider here the $T = 0$ K situation with only the lowest conduction subband (for the electrons) and the highest valence subband (for the holes) occupied. The effective mass approximation is expected to be fairly well valid under the experimental conditions and we will assume that uncritically for our theory. Our main calculations use the GW approximation for the self-energy.[7,8] This is the leading term in an iterative expansion of the self-energy operator in powers of the dynamically screened effective electron-electron (including both Coulomb and Fröhlich couplings) interaction W, and has been shown to yield an excellent description of quasiparticle energies in semiconductors.[8–10]

The BGR is given by the sum of the self-energies for electrons and holes at band edges:

$$\Delta = \mathrm{Re}\,\Sigma_e(0,0) + \mathrm{Re}\,\Sigma_h(0,0). \tag{1}$$

The total electronic self-energy within the leading-order effective dynamical interaction in a two-component electron-hole plasma is

$$\Sigma_e(k,\omega) = i\int \frac{dq}{2\pi}\int \frac{d\omega'}{2\pi} G_0(k-q,\omega-\omega')\,\frac{V_t(q,\omega')}{\epsilon(q,\omega')}, \tag{2}$$

where G_0 is the Green's function for the noninteracting electron gas, $V_t = V_c + V_{\mathrm{ph}}$ is the total effective interaction, and $\epsilon(q,\omega) = 1 - V_t(q,\omega)\Pi_0(q,\omega)$ is the effective dynamical dielectric function. Here V_c, V_{ph}, and $\Pi_0(q,\omega)$ are the direct Coulomb interaction, the LO-phonon mediated electron-electron interaction, and the irreducible 1D noninteracting polarizability, respectively. In our extreme quantum limit model where only the lowest 1D subband is occupied by the electrons, we obtain the interaction matrix elements by taking the quantizing confinement potential to be of infinite square-well type[5,10] and the LO-phonon mediated electron-electron interaction is dependent on wave vector and frequency, $V_{\mathrm{ph}}(q,\omega) = M_q^2 D_0(\omega)$, where M_q is the effective 1D Fröhlich interaction matrix element and $D_0(\omega)$ the unperturbed retarded bare LO-phonon propagator.[10] Since our system is a two-component system (electron-hole plasma), the polarizability function is a sum of electron and hole polarizabilities $\Pi_0(q,\omega) = \Pi_{0e}(q,\omega) + \Pi_{0h}(q,\omega)$. The formalism for holes, within our parabolic band approximation, is the same as that for electrons and the only modification needed in Eq. (2) is the substitution of m_e by m_h. The self-energy calculation is standard and more details can be found in the literature.[10]

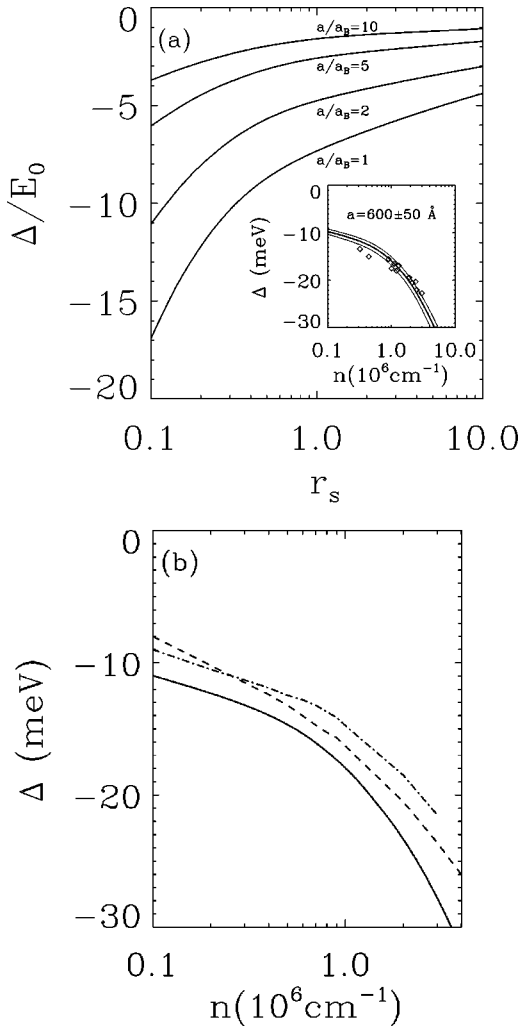

FIG. 1. (a) The calculated band-gap renormalization Δ as a function of the effective electron-hole pair density parameter $r_s = 1/(2na_B)$ for different quantum-wire widths, where a_B is the bulk effective Bohr radius. The BGR is scaled by the 3D exciton binding energy $E_0 = e^2/(2a_B\epsilon_0)$. In the inset we show the BGR for the quasi-1D GaAS-AlGaAs system as a function of the electron-hole plasma density n. The experimental points are taken from Ref. 4. The middle thick line is for confinement width $a = 600$ Å and the upper (lower) thin line for $a = 650$ Å ($a = 550$ Å). (b) Comparison of our calculated GW theory BGR with less sophisticated calculations (Refs. 5 and 6) for the quasi-1D GaAS-AlGaAs system ($a = 500$ Å). Here, the solid line represents our GW result, and the dashed (dot-dashed) line is from Ref. 6 (Ref. 5).

In Fig. 1(a) we show our calculated exchange-correlation-induced band-gap renormalization for quasi-1D quantum wires, which is scaled by the effective 3D Rydberg $E_0 = e^2/(2a_B\epsilon_0)$, as a function of the effective electron-hole plasma density parameter $r_s = 1/(2na_B)$. We also show in Fig. 1(a) the band-gap renormalization for various quantum-

wire widths. The BGR increases with decreasing wire width. The QW BGR depends rather strongly on the wire width because the 1D Coulomb interaction matrix element is a sensitive function of the width even in the long wavelength limit. We have carried out the calculation of BGR as a function of carrier density and wire width for a number of III-V semiconductor materials. We find that when expressed in suitable dimensionless units (the effective 3D Rydberg and the effective 1D density parameter r_s) as shown in Fig. 1(a), the band-gap renormalization in quasi-1D systems is an approximate two-parameter universal function, i.e., a universal function of the effective density and the wire confinement width. (Since the lowest exciton state is not well defined in the ideal zero width limit of the 1D electron-hole system,[11] we use the effective 3D Rydberg to scale the band-gap renormalization.) The inset in Fig. 1(a) shows the BGR for the quasi-1D GaAS-AlGaAs system as a function of the electron-hole plasma density n together with the available experimental data from Ref. 4, in which the BGR is measured in confined quantum well structures with lateral widths of 600 ± 50Å. For GaAs we use the parameters $m_e=0.067m_0$, $m_h=0.45m_0$, and the background dielectric constant $\epsilon_0=13$. We find that the calculated BGR using the full RPA dielectric function agrees well with the available experimental data.[4] The comparison of our full GW calculation result with less sophisticated approximations[5,6] is shown in Fig. 1(b). We find that the BGR in GW dynamical approximation including both carrier-carrier Coulomb and carrier–LO-phonon interaction increases about 10%. Since the BGR as shown in Fig. 1(a) depends strongly on the lateral width, the qualitative comparisons for different widths may give different results. However, the only exchange-correlation-induced BGR's in all different models show the quantitatively similar dependence of a density and a confinement width, that is, BGR's increase as the density increases or the width decreases. It is very difficult to directly compare the theories with the existing experiments[4] because the experimental data for BGR are extracted from the observed luminescence spectra by neglecting the phase-space filling effects (population of higher subbands) and the electron-hole Coulomb correlation effects. Thus, to get better quantitative agreement between experiment and theory we need to include not only the exchange-correlation effects due to the screening of the interaction but the higher subband filling effects, which have been neglected in this calculation.

In bulk semiconductors the exchange-correlation energy is essentially independent[12,3] of band-structure details when expressed in appropriate dimensionless units. This leads to a universal form for the BGR when the self-energy corrections and the carrier density are expressed in appropriate rescaled units of the effective excitonic Rydberg and the normalized interparticle separation r_s, respectively.[12] A similar universality holds for two-dimensional (2D) systems when the band gap is expressed in effective 2D Rydberg and the electron-hole density in the 2D r_s parameter.[13] In quasi-2D quantum well systems, however, the BGR depends on the well width and is found to be a two-parameter universal function of the effective 2D r_s parameter and well width. It was shown[3] that this two-parameter universality can be reduced to an approximate one-parameter universality by choosing a suitable *quasi*-2D Bohr radius and an effective

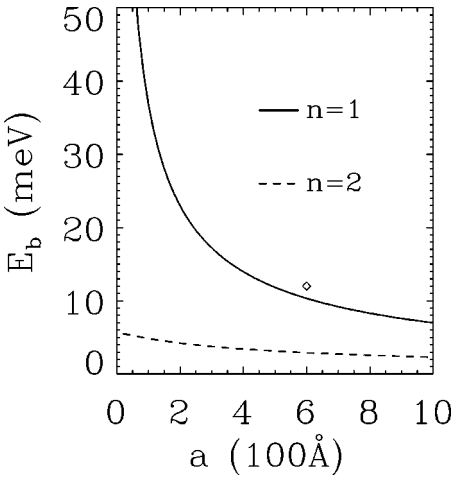

FIG. 2. The two lowest effective exciton binding energies of a quasi-1D GaAs QW system as a function of the confinement width a. $n=1$ ($n=2$) is for the ground (the first excited) state. The diamond represents a data point from Ref. 15.

Rydberg as the effective length unit and energy scaling unit, respectively. In order to investigate whether the two-parameter universality of the quasi-1D BGR in Fig. 1 can be reduced to a one-parameter universality by suitably rescaling energy and length units, we calculate the quasi-1D exciton binding energy, which would be used as a suitable energy rescaling unit. The exciton energy of the quasi-1D system has earlier been calculated in the cylindrical wire with a finite radius smaller than the bulk exciton radius.[14] However, in order to be consistent with our BGR calculation we use the quasi-1D Coulomb interaction of the quantum wire with a zero thickness in the z direction and a finite width a in the y direction to calculate the 1D excitonic binding energy within our confinement model. In this approximation and within the one subband extreme quantum limit the effective quasi-1D Coulomb interaction is given by

$$V_{q1d}(x-x')=\int\int dydy'V_{2D}(x-x',y-y') \times|\phi(y)|^2|\phi(y')|^2, \tag{3}$$

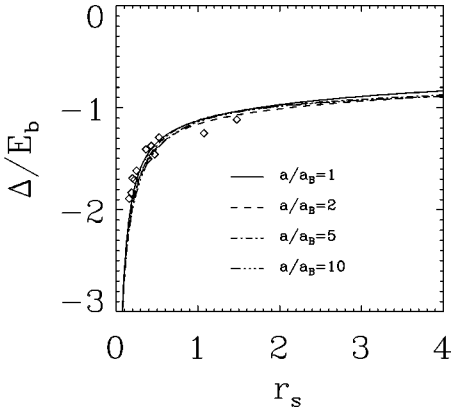

FIG. 3. The approximate one-parameter universality of the band-gap renormalization of the quasi-1D system as a function of the effective density parameter r_s. We rescale the BGR in Fig. 1 in the unit of the effective quasi-1D exciton binding energy of Fig. 2. The experimental points from Ref. 4 are also shown.

where $V_{2D}(x,y)=e^2/(\epsilon_0\sqrt{x^2+y^2})$ is the 2D Coulomb potential and $\phi(y)$ is the single-particle wave function in the unperturbed quantum well wire with infinite barriers. The Fourier transform of Eq. (3) is used as the bare Coulomb interaction to calculate the self-energy of the electron-hole plasma in Eq. (2). If we neglect the motion of carriers in the y direction, the relative motion of a quasi-1D electron-hole pair is described by the 1D Schrödinger equation with the effective quasi-1D Coulomb interaction given in Eq. (3). In Fig. 2 we show our numerically calculated two lowest excitonic binding energies $E_b(a)$ for a GaAs-AlGaAs quantum well wire as a function of the width a (the ground state $n=1$ and the first excited state $n=2$). Comparing with the measured exciton energy ($E_b \approx 12$ meV) for a GaAs quantum wire with the lateral width $a=600\pm 50$ Å,[15] our calculation gives reasonable agreement. Using the calculated effective exciton binding energy (Fig. 2) we rescale the calculated QW band-gap renormalization to investigate the applicability of a one-parameter QW BGR universality. In Fig. 3, we show the rescaled BGR in the unit of the effective binding energy of the exciton as a function of the density parameter r_s. As one can see from Fig. 3, this rescaling of units in terms of *quasi*-1D effective parameters produces an approximate one-parameter universality. (Note that we use the 3D Bohr radius a_B to rescale the lengths.) In order to check the general applicability of our universal BGR results, experimental data on different III-V quasi-1D semiconductor QW systems are needed. It would be interesting to verify our predicted one-parameter BGR universality by measuring the BGR in different III-V materials for QW of different widths.

In conclusion, we investigate the band-gap renormalization of quasi-1D electron-hole plasma systems in semiconductor QW structures including the full dynamical effects of both the electron-electron and electron-phonon interactions treating electrons and phonons on an equal footing. Our calculated BGR agrees well with the available experimental data. We derive an approximate one-parameter universality in the band-gap renormalization (rescaled by the effective quasi-1D excitonic Rydberg) as a function of the effective 1D density parameter r_s, which should be experimentally checked.

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