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Band-gap renormalization in quasi-two-dimensional systems induced by many-body electron-electron and electron-phonon interactions

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Dynamical electron-electron and electron-phonon interaction corrections to the conduction- and valence-band edges of photoexcited quasi-two-dimensional quantum wells are calculated for arbitrary quantum-well widths and electron-hole densities. Band-gap renormalization, when expressed in Rydberg units, is shown to be an approximate universal function of the effective r_s parameter and the well width.

It has been known[1] for some time that electron-electron-interaction–induced exchange-correlation energy is quite insensitive to material parameters (e.g., details of the band structure, explicit values of the effective mass, and lattice dielectric constants, etc.) in three-dimensional systems. In particular, explicit calculations[1] of exchange-correlation energy of electron-hole liquids for a number of different bulk semiconductor systems show it to be independent of the band characteristics and to be a universal function of the electron-hole density when the energy is expressed in excitonic Rydberg and the density in the standard r_s parameter (which is basically the interparticle separation measured in effective Bohr radius). Very recently,[2] it has been claimed that similar results hold also in semiconductor quantum wells where the band-gap renormalization in the presence of optical excitation is claimed to be universal when expressed in two-dimensional (2D) Rydberg and the electron-hole density in the 2D r_s parameter.

For semiconductor quantum wells, most often made of polar compound semiconductor materials, one has the additional complication of the long-range dipolar Fröhlich interaction between the electrons and the LO-phonons which also renormalizes the band gap. Even though very extensive theoretical literature exists on the electron-LO-phonon-interaction effects in semiconductor microstructures, the full many-body problem that includes dynamical screening and treats electron-electron and electron-phonon interactions on equal footing has not yet been worked out. We provide results based on such a theory in this paper. We emphasize that the theory is quite sophisticated since a number of energy scales in the problem, namely, the electron and hole Fermi energies, the dynamical plasma frequencies, and the LO-phonon energy are all comparable and simple approximations can only be justified *a posteriori* after the full theory has been developed. For very weakly polar materials (e.g., GaAs), we provide such a justification for a specific simple approximation (namely, the so-called ϵ_0 approximation) which has been used in the literature to account for the electron-phonon interaction in polar semiconductors.

In this Rapid Communication we consider the band-gap renormalization in quasi-two-dimensional electron-hole liquids using a detailed quantitative theory based on the random-phase approximation (RPA). We calculate the self-energy corrections to the highest valence- and the lowest conduction-subband edges in the presence of a certain density $N_e = N_h$, of the electrons (N_e) and the holes (N_h) for quantum wells of various thicknesses and for a number of different semiconductor systems. We find, as one would expect, that the band-gap renormalization depends rather strongly on *both* the electron-hole density (i.e., the interparticle separation) and the quantum-well width. Thus, the universality of the band-gap renormalization in quasi two dimensions is, in fact, a two-parameter universality with both the electron-hole-density parameter r_s and the quantum-well-width parameter $a/a_{B,2D}$ (where a and $a_{B,2D}$ are, respectively, the well width and the 2D effective Bohr radius) being important. Our theoretical results while being completely consistent with recent experimental results[2] contradict claims of the *well-width-independent* universality of 2D band-gap renormalization.

We find that this two-parameter universality of 2D band-gap renormalization is approximately multiplicative in nature implying that when the renormalization Δ is expressed in the units of *quasi*-2D Rydberg and the Bohr radius is taken for a quantum well of *finite* thickness, a *single* universal curve gives the band-gap renormalization of quasi-2D systems within the accuracy of 20% (which is roughly the experimental accuracy within which Δ can be measured) in these reduced units. This is consistent with the earlier findings[3] of Schmitt-Rink, Chemla, and Miller in a different context. Another theoretical finding reported here is that the very successful and easy-to-use plasmon-pole approximation[4] does not work well for the calculation of the band-gap renormalization in quasi-2D systems.

One new aspect of our work as mentioned earlier, is the inclusion of the full dynamical Fröhlich electron-LO-phonon interaction in the calculation of the band-gap renormalization. Inclusion of dynamical electron-phonon interaction in the theory is important since quantum wells are made of polar materials (e.g., GaAs, InAs) where Fröhlich interaction produces quantitative many-body corrections.[5] These electron-phonon renormalization corrections have so far been studied[6] only in *ad hoc* theoretical treatments where Coulomb interaction is ei-

ther neglected or included in a crude fashion through a screening term. To the best of our knowledge, this is the first calculation of electronic many-body correction in quasi-2D systems including full effects of both electron-electron and electron-phonon interactions treated on an equal footing. We find that the simple ϵ_0 approximation[7] (where the high-frequency dielectric constant ϵ_∞ entering the definition of the Coulomb interaction is replaced by the low-frequency value) accounts for the effect of LO-phonons surprisingly well and the net band-gap renormalization is very close to the exchange-correction calculated *with* the ϵ_0-modified Coulomb interaction and *without* any LO-phonon correction. This, however, is only a reflection of the fairly weak polar coupling in these materials and, for stronger polar coupling, the ϵ_0 approximation breaks down.

We assume infinite confining potential for both electrons and holes in the quantum well. Only one kind of electrons and holes with suitable effective masses, which has isotropic, parabolic dispersion, is assumed to exist; thus neglecting most of the band-structure complications of the quantum-well valence bands. We consider the $T=0$ situation with only the lowest conduction subband (for the electrons) and the highest valence subband (for the holes) occupied (i.e., we restrict ourselves to moderate excitation densities)—we give results here only for the photoexcited undoped quantum wells with $N_e=N_h=N$. We treat the electron-LO-phonon interaction within the Fröhlich model of polar coupling.[6]

We calculate the leading-order electron (and hole) self-energy correction in the RPA-screened total interaction ($\hbar=1$):

$$\Sigma(\mathbf{k},E)=i\int\frac{d^2q}{(2\pi)^2}\int\frac{d\omega}{2\pi}G_0(\mathbf{k}+\mathbf{q},E+\omega)\frac{V(q,\omega)}{\tilde{\epsilon}(q,\omega)},$$

where G_0 is the bare electron propagator, $V=v_C+v_{\rm ph}$, and $\tilde{\epsilon}=1-V\Pi_0$. For a strictly 2D electron gas, $v_C=2\pi e^2/\epsilon_\infty q$ and $v_{\rm ph}=|M_q|^2 D_{\rm LO}(\omega)$ are, respectively, the bare Coulomb and the bare LO-phonon-mediated electron-electron interactions. $|M_q|^2$ and $D_{\rm LO}(\omega)$ are the Fröhlich interaction and the unperturbed LO-phonon propagator, respectively, whereas, Π_0 is the noninteracting polarizability function. Since our system is a two-component system (electron and holes), the polarizability function is a sum of electron and hole polarizabilities ($\Pi_0=\Pi_{0e}+\Pi_{0h}$)—thus we include dynamical screening by both electrons and holes. The corresponding expressions for the quasi-2D electron gas are obtained[6,8] by multiplication of v_C and $v_{\rm ph}$ with the subband form factor $f(q)$ whereas the corresponding 3D expressions are standard.[9] Exchange-correlation corrections *without* electron-phonon interaction are obtained by setting $v_{\rm ph}=0$, whereas the ϵ_0 approximation consists[7] of replacing ϵ_∞ in v_C by ϵ_0 (still without any $v_{\rm ph}$) with the rationale that the main effect of the high-frequency optical phonons is to screen out the Coulomb interaction. Finally, the plasmon-pole approximation[10] consists of our replacing the full RPA dielectric function with suitable δ functions whose strengths and positions are determined by the f-sum rule and the static Kramers-Kronig relation. Since the many-body theory for an electron gas is described in the standard literature,[9] we do not provide any details except to note that the band-gap renormalization Δ is given by the diagonal self-energies $\Sigma_{e,h}$ for electrons and holes separately at the band edges ($k=0$, $E=0$): $\Delta=\mathrm{Re}\Sigma_e+\mathrm{Re}\Sigma_h$.

In Fig. 1 we show our calculated exchange-correlation-induced band-gap renormalization for 2D, quasi-2D, and 3D systems in the ϵ_0 approximation as a function of the free carrier density together with some of the experimental points from Ref. 2. The renormalization Δ is expressed in terms of the effective 2D excitonic Rydberg[11] whereas the free carrier density N is expressed in terms of

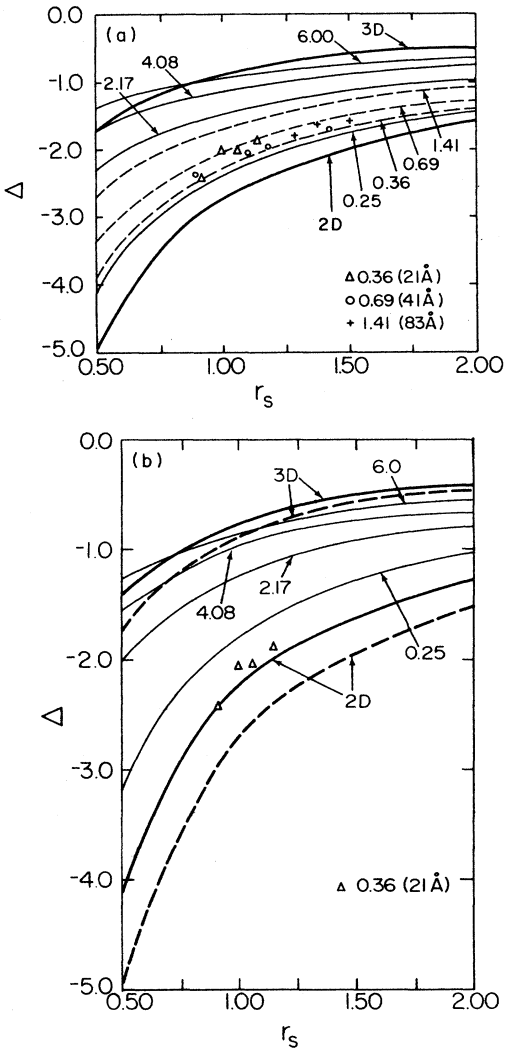

FIG. 1. (a) Band-gap renormalization calculated in RPA with ϵ_0 approximation (dashed lines correspond to the experimental well widths of Ref. 2); (b) band-gap renormalization calculated in plasmon-pole and ϵ_0 approximation (for comparison the 2D and 3D RPA results are given by the dashed lines). Δ is measured relative to the effective 2D excitonic Rydberg (Ref. 11). The density parameter r_s and the well widths are expressed in terms of the 2D Bohr radius for the 2D and quasi-2D cases. For the 3D case, r_s is expressed in terms of the 3D Bohr radius. The experimental points are taken from Ref. 2.

the 2D r_s parameter[11] (except for the 3D result where the abscissa corresponds to the 3D r_s parameter[11]). We show the band-gap renormalization for various quantum-well widths (expressed in the effective 2D Bohr radius[11]) in addition to the strictly 2D and 3D results. In Fig. 1(a) we show the RPA calculation whereas in Fig. 1(b) we show the plasmon-pole approximation. It is clear from a comparison with the RPA results the the plasmon-pole approximation is quantitatively not very accurate in 2D. From Fig. 1(b) we see that the *strictly* 2D plasmon-pole result gives good account of the experimental points. However, when we take into account the quasi-2D character of the confinement, this agreement is lost. On the other hand, the full RPA calculation approaches the experimental results when we include the *quasi*-2D character of the quantum-well wave functions. Another point to note is that the quasi-2D result for a very wide quantum well is *not* the same as the corresponding 3D result because of our approximation of keeping only one subband in the calculation. Thus our results are quantitatively inaccurate for very wide wells or for very high carrier densities with appreciable population of higher subbands.

We have carried out the calculation of Δ as a function of carrier density for a number of different semiconductor materials (GaAs, InAs, GaSb) and for a number of different quantum-well widths. We find that, when expressed in suitable dimensionless units (namely, the effective Rydberg and the effective Bohr radius) as shown in Fig. 1, they all fall within 10% of the curves shown in Fig. 1. It is obvious from Fig. 1 that the dimensionless band-gap renormalization in a quasi-2D system is an approximate universal function of *two* parameters, namely the effective r_s parameter (i.e., the interparticle separation, or, equivalently the carrier density) and the effective dimensionless well width. The well-width independence of Δ as found in Ref. 2 is due to their use of a limited range of well widths. It will be helpful to have more detailed experimental results particularly in wider (larger than 100 Å for GaAs) wells to directly test our theoretical predictions. This is particularly true in view of the good agreement between our theory and the experimental results of Ref. 2. The fortuitous agreement between[2] the experiment and the *strictly 2D* plasmon-pole theory which was found in Ref. 2 disappears when the finite extent of the quantum-well confinement is included in the theory.

We find that the two-parameter universality of Fig. 1 can be reduced to an approximate one-parameter universality by suitable rescaling of the energy and length units with *quasi*-2D Rydberg and *quasi*-2D Bohr radius, respectively. This is consistent with the earlier finding of Ref. 3. This universality is, however, quite approximate (correct to only 20%) and probably not of great significance since the accurate parameters for really quasi-2D excitons[12] are not known.

In order to check the accuracy of the ϵ_0 approximation, we calculate the full dynamical band-gap renormalization including *both* the electron-electron and the electron-phonon interactions. For large values of the electron-phonon coupling constant, the universality of the band-gap renormalization is completely destroyed since Δ now depends explicitly on the Fröhlich coupling α of each material in a significant way. For small α ($\ll 1$), however, we find that the results obtained with the total interaction ($v_C + v_{ph}$) are very close to the exchange-correlation correction calculated with the ϵ_0 approximation.[7] In Fig. 2 we show our results for the *total* interaction correction to Δ as well as the ϵ_0-approximation results. We take the Fröhlich constant $\alpha = 0.07$ (corresponding to GaAs) for these calculations. In Fig. 2(a) we show the *total* self-energy corrections to the band gap of 2D, quasi-2D, and quasi-3D systems whereas in Fig. 2(b) we subtract out[13] the *purely* polaronic corrections to Δ. Thus, Fig. 2(b) is the more physical result since the purely polaronic renormalization of the band edges (obtained by our putting $v_C = 0$ and by assuming only one carrier to be present in the system so that the Fermi factors are all zero) is *always* present and should be included[13] in the definition of the nominal band edges without any carrier renormalization effect. From Fig. 2, we conclude that for weakly polar materials (e.g., GaAs, InAs, GaSb, InSb, Ge, Si, AlAs,

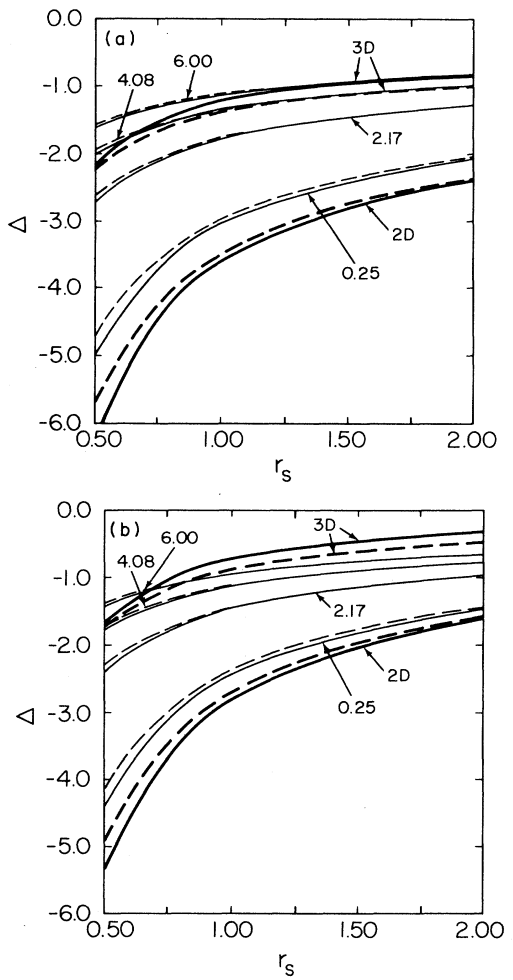

FIG. 2. (a) Total band-gap renormalization for 2D, quasi-2D, and quasi-3D systems; (b) band-gap renormalization with the polaronic correction subtracted. Dashed lines correspond to the ϵ_0 approximation. Full lines correspond to the full RPA calculation. The units are the same as in Fig. 1.

AlSb) the band-gap renormalization is very well approximated in 2D and quasi-2D systems by the ϵ_0 approximation and the approximate universality of Figs. 1 and 2 hold. We have verified, however, that for larger values of the Fröhlich coupling constant ($\alpha > 0.2$) the ϵ_0 approximation fails, giving results which are wrong by about 25% for $\alpha \approx 0.2$.

Before concluding, we point out that Kleinman had earlier calculated[14] exchange-correlation–induced band-gap renormalization in GaAs quantum wells. Instead of calculating the self-energy correction (as done in this paper), he followed Ref. 1 and calculated the exchange-correlation contribution to the total energy. Thus his calculation assumes a rigid-band shift, whereas we make no such assumption. In fact, our self-energy calculation shows that Δ calculated at k_F differs from that calculated at the band edge by about 10% for $N = 2\times10^{11}$ cm^{12}. He also used a model potential rather than using the matrix elements of the Coulomb interaction in the subband representation. Results on the universality, comparison with plasmon-pole approximation, and the inclusion of Fröhlich interaction are all completely new features of this work.

In conclusion, we obtain the band-gap renormalization of quasi-2D systems including full dynamical effects of both the electron-electron and electron-phonon interactions (within the RPA). We show that the plasmon-pole approximation is poor in 2D whereas the ϵ_0 approximation for the electron-phonon interaction works extremely well for weakly polar materials. We find an approximate universality in the band-gap renormalization of quasi-2D systems, but the universality is more subtle than that claimed in a recent publication.[2] Our results agree well with the limited experimental results available to date; however, we hope that our detailed predictions will motivate more vigorous experimental work on this important problem.

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[11]The 2D Rydberg and the effective Bohr radius are related to those of 3D values as follows: $R_{y,2D} = 4R_{y,3D}$ and $a_{B,2D} = \frac{1}{2} a_{B,3D}$, where $R_{y,3D} = e^2/2\epsilon_0 a_{B,3D}$, and $a_{B,3D} = \hbar^2\epsilon_0/me^2$, where m is the effective mass $m^{-1} = m_e^{-1} + m_h^{-1}$. For GaAs we used $m_e = 0.067m_0$, $m_h = 0.45m_0$, and $\epsilon_0 = 13$. We then have $R_{y2D} = 18.7$ meV and $a_{B,2D} = 59$ Å. The density N of 2D and 3D systems is related to the equivalent interparticle separation r_s by the formulas $\pi r_s^2 = (na_{B,2D}^2)^{-1}$ and $4\pi r_s^3/3 = (na_{B,3D}^3)^{-1}$, respectively.

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