RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 44, NUMBER 7 15 AUGUST 1991-I

# Many-body vertex corrections on quasiparticle properties of two-dimensional electron systems

I. K. Marmorkos and S. Das Sarma
*Joint Program for Advanced Electronic Materials, Department of Physics, University of Maryland, College Park, Maryland 20742*
(Received 15 May 1991)

We calculate theoretically the lifetime, the effective mass, the renormalization factor, and the exchange-correlation-induced band-gap renormalization for quasiparticles in two-dimensional electron systems. In our theory we go beyond the usual random-phase approximation by including many-body vertex corrections of the Hubbard type in the self-energy and the dielectric function of the electron gas. We find that in narrow quantum wells vertex corrections may be quantitatively significant, bringing calculated results close to the experimental data, especially for the case of the band-gap renormalization. In general, vertex correction is found to be more important for narrower quantum wells and for lower electron densities.

Many-body effects in two-dimensional (2D) electron systems have been studied extensively during the past years both theoretically and experimentally. There have been many[1-10] theoretical investigations of 2D quasiparticle properties including early calculations of renormalized effective mass (and $g$ factor) in Si inversion layers[1,8-10] and more recent calculations[2-7] of quasiparticle lifetimes and band-gap renormalization in GaAs quantum wells. Most of these calculations are done within the framework of random-phase approximation (RPA), leaving out higher-order vertex corrections. For example, quasiparticle scattering rates have recently been calculated[2] taking into account electron-electron and electron-phonon interactions. In these calculations the electron self-energy is obtained in the so-called $GW$ approximation[11] in which the noninteracting single-particle Green's function ($G$) is used, whereas the effective dynamically screened Coulomb interaction ($W$) is calculated within the RPA model and, consequently, vertex corrections are neglected. Even though some of the earlier calculations for the effective mass and the band-gap renormalization included in some *approximate* way the effects of vertex corrections (i.e., going beyond the $GW$ approximation), it is fair to say that there has not been much systematic work going beyond the RPA. For example, in Ref. 12 a *strictly* 2D calculation of the band-gap renormalization in a 2D electron-hole plasma was reported, taking into account vertex correction of the Hubbard type *only* in the dielectric function (i.e., leaving it out of the self-energy). A similar approximation[9] was made earlier in the calculation of electron effective mass in Si inversion layers. We know of *no* theoretical calculation of quasiparticle lifetimes including vertex corrections.

The purpose of this paper is to report a systematic investigation of many-body vertex corrections on 2D quasiparticle properties. In particular, explicitly obeying Ward identities we include vertex corrections both in the self-energy and in the dynamical dielectric function. The 2D system chosen for our calculation is the extensively experimentally studied modulation-doped GaAs quantum-well structure. We include the finite width of the quantum well within the infinite square-well approximation. When expressed in dimensionless units (i.e., density in units of effective $r_s$ and energy in units of effective Rydberg) our theoretical results should be valid for other 2D electron systems as well. We assume the validity of effective-mass approximation and take the bands to be isotropic and parabolic. All these are excellent approximations for the systems under consideration. In presenting our results (Figs. 1–3) we provide a comparison with the RPA results (where vertex corrections are neglected by putting the vertex function $\gamma=1$).

In this Rapid Communication we present zero-temperature calculations for the scattering rate, the effective mass, and the renormalization factor of quasiparticles in 2D and quasi-2D electron systems and for the exchange-correlation-induced band-gap renormalization in 2D and quasi-2D photoexcited electron-hole plasmas in GaAs quantum wells. For the band-gap renormalization calculation, the quantum well is taken to be undoped. In our calculations we include local-field corrections (vertex corrections) of the Hubbard type in the self-energy and in the dielectric function as well within the $GW\Gamma$ approximation.[11,13] In this approximation the self-energy $\Sigma(k,E)$ is given by

$$\Sigma(k,E)=i\int\frac{d^2q}{(2\pi)^2}\int\frac{d\omega}{2\pi}\frac{V_q}{\epsilon(q,\omega)}\gamma(q,\omega)\times G^0(|\mathbf{k}-\mathbf{q}|,E-\omega)\,, \qquad (1)$$

with

$$\epsilon(q,\omega)=1-V_q\chi^0(q,\omega)\gamma(q,\omega) \qquad (2)$$

and

$$\gamma(q,\omega)=\frac{1}{1+G(q)V_q\chi^0(q,\omega)}\,, \qquad (3)$$

where $\chi^0(q,\omega)$ is the noninteracting 2D polarizability for electrons, and $G(q)$ is a local-field correction given in the Hubbard approximation in the two-dimensional limit[8] by

$$G(q)=\frac{q}{2(q^2+k_F^2)^{1/2}}\,. \qquad (4)$$

We take $V_q=2\pi e^2/q\epsilon_\infty$ as the two-dimensional Fourier transform of the Coulomb potential with $\epsilon_\infty$ as the high-frequency dielectric constant of the semiconductor (here

GaAs). The corresponding expressions for the quasi-2D system are obtained by the replacement of $V_q$ by $V_q f(q)$ where $f(q)$ is the subband form factor.[1,6] Our incorporation of vertex corrections in the self-energy accounts for the correlation between the position of the electron and the positions of the other local electrons in the screening cloud, whereas the local-field factor $G(q)$ in the dielectric function accounts for similar correlations between the electrons responsible for screening. Note that by substituting $G(q)=0$, or equivalently $\gamma(q)=1$, we recover the RPA theory which neglects vertex corrections.

Our main goal in this work is to determine over which density, wave vector, and well width range the exchange-correlation effects are quantitatively important so that vertex corrections should be included in the calculation. We find that over density regions of experimental interest (around $10^{11}$ cm$^{-2}$) calculations of the band-gap renormalization and of the scattering rates that include vertex corrections deviate from those in RPA by about 10%, and even more for lower densities (and/or larger wave vectors for the scattering rate). When the finite well width effect is included we find that a decrease of the well width enhances the effect of local fields.

First, we show in Fig. 1 the scattering rate $\Gamma(k) = |\mathrm{Im}\Sigma[k,\xi(k)]|$ of the quasiparticles in a 2D and in a quasi-2D electron gas as a function of the wave vector $k$ for low and high densities. Here $\xi(k)=\hbar^2k^2/2m$ is the electronic energy. The quasiparticle lifetime $\tau=\hbar/2\Gamma(k)$ along with the inelastic mean free path $l_k=k/2m\Gamma(k)$ are of direct experimental interest. From Fig. 1, we see that the inclusion of vertex corrections gives the same qualitative features as the RPA and that both approximations give the expected undamped quasiparticles at the Fermi surface. For wave vectors $k$ close to the Fermi wave vector our results are almost identical with those in RPA. For wave vectors away from the Fermi wave vector $\mathbf{k}_F$ (in and out of the Fermi disk), but not larger than some threshold wave vector $k_c$, damping rates including the vertex correction are higher from those in RPA by about 10%. This, in effect, slightly decreases the quasiparticle mean free path. When the wave vector crosses the threshold wave vector $k_c=q_c+k_F$ ($q_c$ being the wave vector at which the plasmon dispersion enters the electron-hole continuum), quasiparticles start to scatter through the plasmon excitation mechanism, an effect which manifests itself as a sharp increase of $\Gamma(k)$ in Fig. 1. In this large wave-vector regime, the contribution of vertex corrections is more drastic, giving a lower scattering rate than that obtained within the RPA. We also see that the inclusion of vertex corrections lowers the threshold wave vector $k_c$ for the onset of plasmon excitation. As the 2D electron density is decreased, RPA is expected to become less reliable. This is clearly seen in Fig. 1 where vertex corrections, in general, become quantitatively more important at lower densities (and, higher wave vectors). RPA seems to overestimate the scattering rate by 10–30% in the experimental density range. We note that the inclusion of finite width effect reduces the quantitative importance of vertex corrections. When the finite width of the well is included we have a steady decrease of the scattering rate as the well width increases, whereas the contribution of local fields becomes less pronounced.

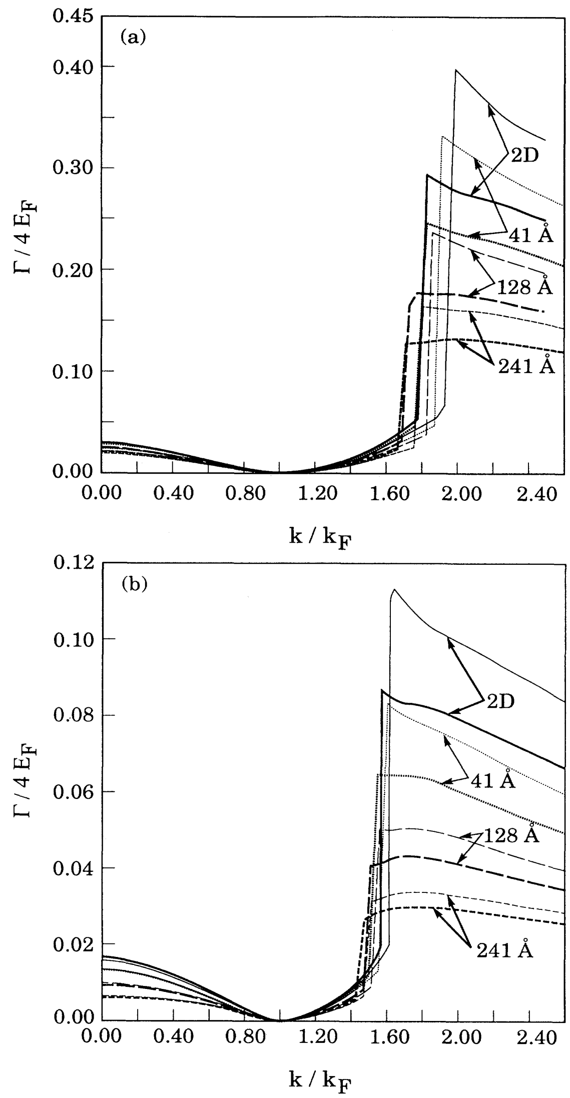


FIG. 1. Quasiparticle scattering rates (measured in units of $4E_F$) as a function of wave vector (measured in units of $k_F$) at densities (a) $2\times10^{11}$ cm$^{-2}$ and (b) $1\times10^{12}$ cm$^{-2}$ for quantum wells of 0, 41, 128, and 241 Å. Thick lines correspond to calculations with vertex corrections, whereas thin ones to RPA.

In Fig. 2 we report results on the exchange-correlation-induced band-gap renormalization in 2D and quasi-2D photoexcited electron-hole plasmas. Again we show, for the sake of comparison, corresponding results obtained within the RPA. We calculate the self-energy corrections, with the use of Eqs. (1)–(4), to the highest valence and the lowest conduction subband edges for quantum wells of various thicknesses. We consider a relatively low-density electron-hole plasma with equal electron ($N_e$) and hole ($N_h$) densities ($N_e=N_h$), so that we can consider[3] only the lowest conduction and the highest valence subbands as populated with band masses $m_e=0.067m_0$ and $m_h=0.45m_0$ for the electrons and holes, respectively. Since our system is a two-component system the polarizability

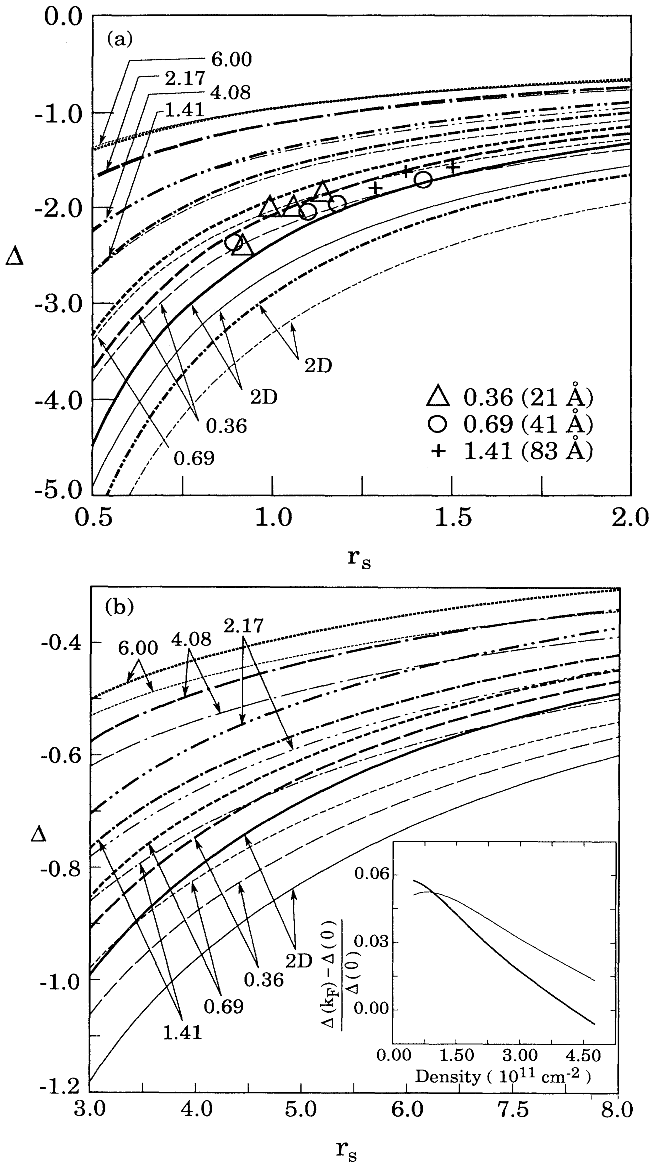


FIG. 2. Band-gap renormalization calculated in the $\epsilon_0$ approximation as a function of the density parameter $r_s$ (appropriate for GaAs) over different quantum-well widths (measured in units of the effective 2D Bohr radius in GaAs). Thick lines correspond to results obtained with vertex corrections, whereas thin ones to RPA. Available experimental data from Ref. 12 are also shown. In (a) the 2D result *without* any polaronic correction is shown by dashed lines for the sake of comparison. In the inset of (b) we show the difference of the band-gap renormalization obtained at zero and Fermi wave vectors as a function of density for the 2D limit in the $\epsilon_0$ approximation.

function is a sum of electron and hole polarizabilities, $\chi^0=\chi_e^0+\chi_h^0$. In this way we include the effect of dynamical screening from both electrons and holes.

The band-gap renormalization $\Delta$ is given by the diagonal self-energies $\Sigma_{e,h}$ for the electrons and the holes separately at the band edges ($k=0$, $E=0$): $\Delta=\mathrm{Re}\Sigma_e+\mathrm{Re}\Sigma_h$. With this definition of $\Delta$ we are not assuming a rigid shift of the band gap. In fact, we plot as an inset in Fig. 2 the difference in the band-gap renormalization at zero wave vector and at the Fermi wave vector $k_F$ as a function of density in both RPA and *GWΓ* approximations. We clearly see that this difference is small but nonzero, at least in the density range of interest. We take into account polaronic corrections to $\Delta$ through the $\epsilon_0$ approximation[3,14] which has been found to account very accurately for electron-LO-phonon interaction-induced band-gap renormalization in weakly polar semiconductors like GaAs.[3] In the $\epsilon_0$ approximation the explicit phonon interaction terms are neglected, whereas the high-frequency dielectric constant $\epsilon_\infty$ in the Coulomb potential $V_q$ is replaced by the static dielectric constant $\epsilon_0$ and the bare band mass of the carrier is replaced by the polaron mass. The validity of the $\epsilon_0$ approximation for the polaronic contribution to the band-gap renormalization in weakly polar semiconductors merely reflects the fact that the main effect of the high-frequency optical phonons is to screen the Coulomb interaction.

We express[3] the band-gap renormalization $\Delta$ in units of quasi-2D Rydberg, the density in terms of the effective 2D $r_s$ parameter and the well width in units of the 2D effective Bohr radius. The band-gap renormalization is approximately universal when expressed in these reduced units in quasi-2D systems[3,7] and, therefore, our results hold fairly well for other weakly polar semiconductors as well (vertex corrections do not destroy this universality).

From Fig. 2 we see that although vertex corrections give results which are qualitatively similar to RPA, there are quantitative differences, especially in narrow wells and at lower densities. More specifically, we see from Fig. 2(a) that in narrow wells (width $\sim$21 Å) vertex corrections give a band-gap renormalization of about 7%–8% higher than that of RPA. This difference is just enough to

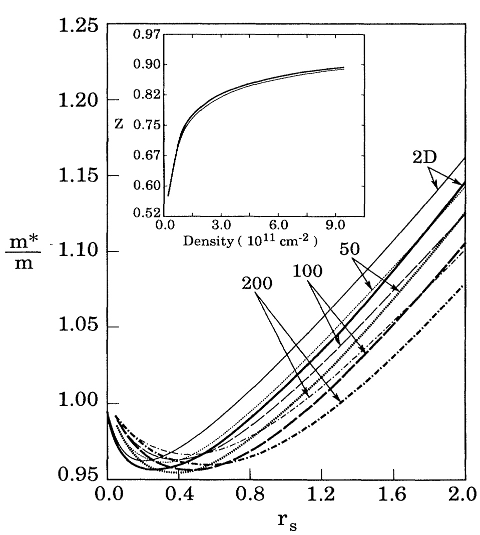


FIG. 3. Effective mass of quasiparticles normalized by the bare band mass in GaAs as a function of the density parameter $r_s$ for wells of widths 0, 50, 100, and 200 Å. Thick lines correspond to our calculations and thin ones to RPA. The inset gives the renormalization factor of quasiparticles as a function of density.

bring our results in better quantitative agreement with experimental data.[12] For wider wells (~41 Å) the difference with RPA becomes smaller and for widths larger than 128 Å we practically get the same results as the RPA. In the low-density region the difference with RPA is about 17% when the well width is around 21 Å, and drops (for the same density) to about 11% when the well width increases to 340 Å. This is expected since it is well known[8] that as the system approaches the three-dimensional limit the contribution of the vertex corrections becomes less important. We point out that our calculation predicts a well width dependence of the band-gap renormalization in agreement with the experimental results of Ref. 15.

In Fig. 3 we give results for the calculated quasiparticle effective mass $m^*$ as a function of electron density for wells of various thicknesses. We see that vertex corrections give a value for $m^*$ lower by about 2% from that in the RPA. These lower values of the effective mass agree rather well with the experimental results in silicon inversion layers.[16] We mention that a recent attempt[17] was made in calculating the effective mass of a 2D system by including vertex corrections *only* in the dielectric function (and *not* in the self-energy also as we do here) within the plasmon-pole approximation. Finally, in the inset of Fig. 3, we plot the renormalization factor $Z$ of the quasiparticles as a function of density in the strictly 2D limit. We see that at high densities, $Z$ approaches unity, meaning the single-particle character of the quasiparticles is more pronounced. Here RPA and vertex corrections give practically the same quantitative results implying that an improved account of the many-body effects does not affect much the single-particle aspects of the quasiparticles obtained in RPA.

In summary, we have presented many-body calculations of 2D quasiparticle properties by going beyond the *GW* approximation of RPA and by calculating vertex corrections in the Hubbard approximation. We find that the inclusion of local-field corrections within the *GWΓ* approximation introduces 5%–30% corrections to various quasiparticle renormalizations compared with the RPA results, in general improving agreement between theory and experiment, particularly at lower densities (and/or narrower wells). We point out that the Hubbard approximation itself is a rather crude way of calculating the *GWΓ* self-energy because it solves the ladder-vertex integral equation in an approximate way within the Thomas-Fermi screened potential approximation. We do not, however, expect corrections beyond the Hubbard approximation to be quantitatively significant in the regime of our interest.

This work is supported by the U.S. Army Research Office and the U.S. Office of Naval Research.

[1] T. Ando, A. B. Fowler, and F. Stern, Rev. Mod. Phys. **54**, 437 (1982).

[2] R. Jalabert and S. Das Sarma, Phys. Rev. B **40**, 9723 (1989).

[3] S. Das Sarma, R. Jalabert, and E. Yang, Phys. Rev. B **39**, 5516 (1989); **41**, 8288 (1990).

[4] S. Schmitt-Rink *et al.*, Solid State Commun. **52**, 123 (1984).

[5] G. E. W. Bauer and T. Ando, Phys. Rev. B **31**, 8321 (1985); J. Phys. C **19**, 1537 (1986); D. A. Kleinman and R. C. Miller, Phys. Rev. B **32**, 2266 (1985).

[6] S. Das Sarma, Phys. Rev. B **27**, 2590 (1983); S. Das Sarma and B. A. Mason, *ibid.* **31**, 5536 (1985); X. Wu *et al.*, Phys. Status Solidi (b) **133**, 229 (1986).

[7] S. Schmitt-Rink, D. S. Chemla, and D. A. B. Miller, Phys. Rev. B **32**, 6601 (1985).

[8] M. Jonson, J. Phys. C **9**, 3055 (1976).

[9] C. S. Ting, T. K. Lee, and J. J. Quinn, Phys. Rev. Lett. **34**, 870 (1975).

[10] B. Vinter, Phys. Rev. Lett. **35**, 1044 (1975).

[11] L. Hedin and S. Lundqvist, Solid State Phys. **23**, 135 (1969).

[12] G. Tränkle *et al.*, Phys. Rev. Lett. **58**, 4119 (1986).

[13] G. D. Mahan and B. E. Sernelius, Phys. Rev. Lett. **62**, 2718 (1988).

[14] L. V. Keldysh and A. P. Silin, Zh. Eksp. Teor. Fiz. **69**, 1034 (1976) [Sov. Phys. JETP **42**, 525 (1976)]; G. Beni and T. M. Rice, Phys. Rev. B **18**, 768 (1978).

[15] V. D. Kulakovskii *et al.*, Phys. Rev. B **40**, 8087 (1989); G. Bongiovanni and J. L. Staehli, *ibid.* **39**, 8359 (1989); G. Bongiovanni, J. L. Staehli, and D. Martin, Phys. Status Solidi (b) **150**, 685 (1988).

[16] J. L. Smith and P. J. Stiles, Phys. Rev. Lett. **29**, 102 (1972).

[17] G. E. Santoro and G. F. Giuliani, Solid State Commun. **67**, 681 (1988).