Band-gap renormalization in semiconductor quantum wells

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We develop a theory for the many-body electron-electron- and electronphonon-interaction-induced band-gap renormalization of quasi-two-dimensional electron systems by calculating the electron and hole dynamical self-energy corrections at the band edges of semiconductor quantum-well structures. The self-energy calculations are performed within the randomphase approximation (RPA) by treating the electron-electron Coulomb interaction and the electron-optical-phonon Fröhlich interaction on an equal footing. We calculate the band-gap renormalization as a function of the carrier density and the quantum-well width and obtain good agreement with existing experimental results. We find that, when the carrier density and the well width are expressed in terms of effective dimensionless variables by scaling them with the effective Bohr radius for the material, the dimensionless-band-gap renormalization expressed in units of effective rydberg shows a universality, independent of the band-structure details of the material and dependent only on r_s , the dimensionless interparticle separation, and on the dimensionless well width. We show that this two-parameter universality can be reduced to an approximate oneparameter universality by choosing suitable quasi-two-dimensional Bohr radius and effective rydberg as effective length and energy scaling units, respectively. Finally, our complete RPA calculation shows that the popular and easy-to-use plasmon-pole approximation may not be quantitatively accurate in quasi-two-dimensional systems whereas the usual ϵ_0 approximation employed to include approximately the effects of Fröhlich interaction in the theory works extremely well for the weakly polar III-V compound semiconductor materials studied in this paper.

I. INTRODUCTION

A useful feature of quantum wells is that their band gaps can be tailored over a wide range by changing the well widths and well heights. This flexibility makes them very suitable systems for investigating and exploiting optical nonlinearities. It is well known that semiconductor band gaps are "renormalized" (by up to tens of meV's) by many-body effects arising from the presence of free carriers (electrons in the conduction band and/or holes in the valence band) in the system. In particular, exchangecorrelation corrections due to the presence of free carriers in the system reduce the band gap and this reduction in the band gap is usually referred to as the "bandgap renormalization" effect. Optical nonlinearities are typically associated with the band-gap renormalization phenomenon because one can induce substantial freecarrier population by optical excitation and the consequent band-gap renormalization can act as a "feedback" mechanism affecting the excitation process itself. In this paper we investigate the band-gap renormalization phenomenon in quasi-two-dimensional semiconductor quantum wells. In bulk semiconductors, the exchangecorrelation energy is known to be almost independent of band characteristics-in appropriate rescaled units it depends only on the interparticle distance r_s in a universal manner.¹ Thus, in the light of the great practical interest in quantum wells, it is natural to ask whether similar universality should hold for quantum wells as well. The

main objective of the present study is to investigate how the quantum-well band-gap renormalization depends on band characteristics, well width and carrier density, and, then, to relate these parameters to the band gap in a simple and universal way. Also, the band-gap renormalization will be computed as accurately as possible, rendering a comparison with experimental results more meaningful and fruitful.

There are already a number of studies $^{2-4}$ on the bandgap renormalization in quantum wells, both experimental and theoretical. Tränkle et al.² have found experimentally that the dependence of the band-gap renormalization on the interparticle distance r_s is universal when the band gap is expressed in two-dimensional (2D) rydbergs and the electron-hole density in the 2D r_s parameter. However, they find no appreciable well-width dependence of the band gap. It is clear that since quantum wells have a finite thickness, they are not strictly two-dimensional systems and, thus, as the well width increases threedimensional characteristics must eventually become dominant. So the above-mentioned simple universality of the dependence of the band gap only on the interparticle distance must be extended and reexamined. The purpose of this study is to provide a theoretically improved calculation of the band-gap renormalization in quantum wells. The following improvements over previous calculations⁴ are made: (i) The full random-phase-approximation (RPA) dielectric function is used. So far most calculations have been done in the simple plasmon-pole approximation.⁴ In the present work we compare our results with those of the plasmon-pole approximation and find significant deviations. (ii) The full dynamical Fröhlich electron-LO-phonon interaction is included. Inclusion of dynamical electron-phonon interaction in the theory is important since quantum wells are made of weakly polar materials where Fröhlich interaction produces quantitative many-body corrections.^{5,6} We will treat both electron-electron and electron-phonon interactions on an equal footing. (iii) The finite-size effect of quantum wells is incorporated, i.e., the well-width dependence is taken into account.

The important findings of our study are the following: (i) the band-gap renormalization depends both on the interparticle distance r_s and the well width a. Thus the universality of the band-gap renormalization is a twoparameter universality for guasi-two-dimensional systems (it reduces to a one-parameter universality only when the well width vanishes, i.e., when the system is strictly 2D). This result contradicts² claims of the well-widthindependent universality of 2D band-gap renormalization. Furthermore, our results obtained using the full RPA dielectric function agree very well with recent experimental results. Our universal curve gives the calculated band-gap renormalization of quasi-2D systems within the accuracy of 10% in the reduced units. (ii) We have also discovered that this two-parameter dependence can be reduced to a novel single-parameter universality when the band gap and the interparticle distance are expressed, respectively, in the units of quasi-2D rydbergs and the quasi-2D Bohr radius. There is no longer an explicit dependence on the well width since it is now incorporated in the definitions of quasi-2D rydbergs and the Bohr radius. (iii) When the full dynamical Fröhlich electron-LO-phonon interaction is included in the theory, we find that the simple ϵ_0 approximation (where the high-frequency lattice dielectric constant ϵ_{∞} entering the definition of the Coulomb interaction is replaced by the low-frequency value ϵ_0 accounts for the effect of LO phonons surprisingly well, at least for the weakly polar III-V materials such as GaAs. The net band-gap renormalization is very close to the exchange-correlation correction calculated with the ϵ_0 -modified Coulomb interaction and without any LO-phonon correction. (iv) Another important theoretical finding is that the very successful and easy-to-use plasmon-pole approximation is not quantitatively very accurate for the calculation of the band-gap renormalization in quasi-2D systems. Consequently, the results of the plasmon-pole approximation do not agree well with the experimental results on bandgap renormalization.

The experimental measurement of the band-gap renormalization is done in an optically excited electron-hole plasma. The excitations are strong enough to achieve the high-density regime, where no bound (excitonic) states exist. The electron-hole plasma is obviously not an equilibrium system, but the laser pulse durations are of the order of 10-50 ns, much longer than the typical relaxation times in GaAs-Al_xGa_{1-x}As structures² permitting a quasiequilibrium description. The temperatures achieved are low enough to allow a zero temperature treatment of the electron-hole plasma. Also, effective mass approximation is expected to be fairly well-valid under the experimental conditions and we will assume that uncritically for our theory.

This paper is organized as follows. In Sec. II we give details of computing many-body self-energies where electron-electron and electron-phonon interactions are treated on equal footing. In Sec. III results for the undoped photoexcited case are presented. In Sec. IV the validity of the ϵ_0 approximation is studied as a function of the carrier density and the strength of the Fröhlich coupling. Section V deals with the band-gap renormalization for doped systems. Conclusions are given in Sec. VI. A preliminary account of some of our results have appeared in an earlier short publication.³

II. SELF-ENERGY CALCULATION

Our model system is as follows. We assume effective mass approximation throughout. We assume infinite square-well confinement for both electrons and holes in the quantum well. Only one kind of electrons and holes with isotropic, parabolic dispersion is assumed to exist, thus neglecting most of the band-structure complications of the valence subbands. We consider the T=0 K situation with only the lowest conduction subband (for the electrons) and the highest valence subband (for the holes) occupied. The electron-LO-phonon interaction is treated within the Fröhlich model of polar coupling. In Secs. III and IV we give results for the photoexcited undoped quantum wells with $N_e = N_h = N$, while in Sec. V we consider the doped case in which $N_e \neq N_h$.

The band-gap renormalization is given by the sum of the self-energies for electrons and holes at band edges (k=0, E=0)

$$\Delta = \operatorname{Re}\Sigma_{e}(\mathbf{0}, 0) + \operatorname{Re}\Sigma_{h}(\mathbf{0}, 0) . \tag{1}$$

We calculate the self-energy in the leading order in the effective dynamical interaction which is obtained within the RPA. Our bare Coulomb interaction includes e-e, e-h, and h-h interactions and the dynamical screening is due to both electrons and holes. The total electronic self-energy in a two-component electron-hole gas is

$$\Sigma_{e}(\mathbf{k}, E) = i \int \frac{d^{2}q}{(2\pi)^{2}} \int \frac{dE'}{2\pi} G_{e}^{0}(\mathbf{k} + \mathbf{q}, E + E') \frac{V(\mathbf{q}, E')}{\tilde{\epsilon}(\mathbf{q}, E')} ,$$
(2)

where the noninteracting electron Green's function, the total bare interaction, and the total dielectric function are, respectively,

$$G_{e}^{0}(k,E) = \frac{1}{E - \frac{\hbar^{2}k^{2}}{2m} + i\delta \, sgn(k - k_{F})},$$
(3)

$$V(\mathbf{q}, E) = V_C(q) + V_{\rm ph}(q, E)$$
, (4)

$$\widetilde{\epsilon}(q,\epsilon) = 1 - V(q,E)\pi_0(q,E) .$$
⁽⁵⁾

The parameters m_e and k_F are, the electron mass and the Fermi wave vector, respectively. For a strictly two-

dimensional electron gas (2D EG), $V_C = 2\pi e^2/\epsilon_{\infty} q$ 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. The bare LO-phonon propagator is given by $D_{\rm LO}^0(\omega) = -2\omega_{\rm LO}/(\omega_{\rm LO}^2 - \omega^2)$ where $\omega_{\rm LO}$ is the LO-phonon frequency. The electron-phonon matrix element is given⁶ by $M_q^2 = (2\pi\alpha(\hbar\omega_{\rm LO})^{2/3}/\sqrt{2m})1/q$, where the Fröhlich (or polaron) coupling constant is defined as $\alpha = e^2/\hbar(m/2\hbar\omega_{\rm LO})^{1/2}(1/\epsilon_{\infty} - 1/\epsilon_0)$. ϵ_{∞} and ϵ_0 are the optical and static dielectric constants of the semiconductor. The polarizability function $\pi_0 = \pi_{0e} + \pi_{0h}$ is a sum of electron and hole polarizabilities⁷ because our system is a two-component plasma. We are thus including dynamical screening by both, electrons and holes.

In the quasi-2D EG, V_C and $V_{\rm ph}$ should be multiplied with the appropriate form factor f(q) arising from the subband quantization.^{6,7} For an infinite square well of width a,

$$f(q) = \frac{8}{[(qa)^2 + 4\pi^2]} \times \left[\frac{3}{8}qa + \frac{\pi^2}{qa} - \frac{4\pi^4}{(aq)^2}\frac{(1 - e^{-qa})}{[(qa)^2 + 4\pi^2]}\right].$$
 (6)

The corresponding 3D expressions are standard⁸ and will not be given here. The formalism for holes, within our parabolic band approximation, is the same as that for electrons and the only modification needed in (2)-(5) is the substitution of m_e by m_h . We now proceed to sketch how the self-energies, and then the band-gap renormalization, can be computed numerically. The self-energy can be written as the sum of an exchange (Hartree-Fock) and a correlation contribution. Following the usual procedure we calculate the correlation contribution using the line-plus-pole decomposition^{8,9}

$$\Sigma(k,\epsilon) = \Sigma^{\mathrm{HF}}(k) + \Sigma^{L}(k,E) + \Sigma^{P}(k,E) .$$
⁽⁷⁾

For the strictly 2D case the Hartree-Fock contribution is given by $\Sigma_{\rm HF}(0) = -e^2 k_F / \epsilon_{\infty}$. The pole contribution is obtained⁹ after doing a one-dimensional integral and the line contribution after doing a two-dimensional integral. Band-gap renormalization is obtained by calculating Σ_e and Σ_h at k = 0. The self-energy calculation is standard and more details can be found in the literature (Ref. 8 for 3D calculations and Ref. 9 for 2D calculations).

The ϵ_0 approximation¹⁰ consists of replacing ϵ_{∞} by ϵ_0 in the Coulomb potential, $V_C^*(q) = 2\pi e^2/q\epsilon_0$, ignoring the electron-phonon interaction potential ($V_{el-ph}=0$) and adding the polaron shift (the self-energy correction due to Fröhlich interaction in the one-carrier limit). The rationale for this approximation is that the main effect of the high-frequency LO phonons is to screen the Coulomb interaction, which is suitably accounted for by the replacement of ϵ_{∞} by ϵ_0 .

The polaronic renormalization of the band edges (Δ_p) is given¹¹ by $(\pi/2)\alpha\hbar\omega_{\rm LO}$ in 2D and $\alpha\hbar\omega_{\rm LO}$ in 3D (for GaAs we have $\alpha_e = 0.07$ and $\alpha_h = 0.18$) systems. In the quasi-2D case an analytic expression cannot be obtained and the polaron shift is obtained as a one-dimensional integral. This polaronic renormalization is always present

and is, therefore, irrelevant from the experimental point of view. We should, therefore, subtract it out from our calculated many-body band-gap renormalization since it is *not* an observable correction. We concentrate on the calculation of the measurable band-gap renormalization $\Delta = \Delta_t - \Delta_p$ [where Δ_t is the total calculated renormalization, as given by (2) without the ϵ_0 approximation]. Another feature of the ϵ_0 approximation is that the electron effective mass is usually replaced by the polaron effective mass (renormalized mass due to Fröhlich interaction in the one-carrier limit). Since this correction is very small (less than 1%) for weakly polar semiconductors, we will neglect it here.

Finally, the plasmon-pole approximation¹² consists of ignoring the weight in the single-particle excitation and assuming that all the weight of $\text{Im}\pi_0$ lies at an "effective" plasmon energy given by $\tilde{\omega}_p^2 = \omega_p^2 + \beta^2 q^2$. ω_p is the plasmon energy and the parameter β is chosen to satisfy the *f*-sum rule and the static Kramers-Kroning relation. In the following section we calculate the band-gap renormalization in the ϵ_0 approximation, using the full RPA, and the plasmon-pole approximation.

III. PHOTOEXCITED UNDOPED SEMICONDUCTOR QUANTUM WELL $(N_e = N_h)$

In Fig. 1 we show our calculated exchangecorrelation-induced band-gap renormalization for 2D, quasi-2D, and 3D systems in the ϵ_0 approximation as a function of the free carrier density (expressed in r_s units) together with some of the experimental points from Ref. 2. The renormalization Δ is expressed in terms of the effective 2D excitonic rydberg,¹³ whereas the free carrier density N is expressed in terms of the 2D r_s parameter¹³ (except for the 3D result where the abscissa corresponds to the 3D r_s parameter¹³). We show the band-gap renormalization for various quantum-well widths (expressed in units of the effective 2D Bohr radius¹³) 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 corresponding results using the plasmon-pole approximation. It is clear from a comparison with the RPA results that 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 a good account of the experimental points. However, when we take into account the quasi-two-dimensional 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 model is valid only when the Fermi energy is below the second subband energy $E_F < E_1$, where $E_1 = 2\hbar^2 / ma^2$, i.e., when $r_s > a / a_{2D} / \sqrt{2\pi}$.

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 ex-



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 (effective) rydberg (Ref. 13). 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.

pressed 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 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. It is well known that Δ in 3D semiconductors is a universal function of only the r_s parameter since exchange-correlation energy depends only on r_s in three dimensions. In 2D systems, on the other hand, Coulomb interaction and, consequently, exchange-correlation energy depend on both the electron density and the well width. The wellwidth independence of Δ as found in Ref. 2 may be due to their use of a limited range of well widths.

Very recently Bongiovanni and co-workers¹⁴ observed a band-gap reduction as the QW narrows, consistent with our calculations and contradicting the well-width independence of Ref. 2. The values of the band-gap renormalization of Bongiovanni and co-workers are somewhat lower than the ones of our calculation and of the ones of Ref. 2. The two sets^{2.14} of experimental data, therefore, differ in the value of the band-gap renormalization and in its well-width dependence. This may be due to the fact that band-gap renormalization cannot be directly measured, but is extracted from optical spectroscopic data after considerable spectral analysis. It is quite possible that the detailed quantitative result depends on the details of this analysis, making a quantitative comparison between theory and experiment somewhat difficult.

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 achieved between our theory and the experimental results (for the narrower wells) of Ref. 2. The fortuitous agreement between² 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.

In Fig. 2 we investigate whether the two-parameter universality of Fig. 1 can be reduced to a one-parameter universality by suitably rescaling energy and length units. A reasonable expectation is that if we use rydberg and Bohr units corresponding to the quasi-2D system, we may obtain a one-parameter universality as one finds in strictly 3D and 2D systems. The energy and length units in Fig. 2 for the ordinate and the abscissa respectively are quasi-2D effective excitonic rydberg and quasi-2D Bohr radius. The excitonic binding energy¹⁵ E(a) for a quantum well with finite width a is used to define the quasi-2D rydberg and the quasi-2D Bohr radius a_B^* is defined to be $a_B^* = e^2 / [2\epsilon_0 E(a)]$ if the well width *a* is larger than the effective 3D Bohr radius, whereas $a_B^* = e^2 / [\epsilon_0 E(a)]$ otherwise. The rationale for such a definition is that the spatial confinement of the excitons is not important once their Bohr radius becomes smaller than the well width. Obviously this scaling is not satisfactory near the transition $(a/a_{B,2D}=2)$ from one regime to the other, where a_B^*



FIG. 2. Rescaling of Fig. 1(a) as described in the text, showing an approximate one-parameter universality.

should be a smooth function of a (and is not in our approximation). E(a) has been calculated for GaAs-AlGaAs quantum wells between 20 and 300 Å by Greene and Bajaj.¹⁵ We use their infinite-well numerical results for our scaling. As one can see from Fig. 2, this rescaling of units in terms of quasi-2D effective parameters produces an approximate (to within 20%) one-parameter universality. One can see that the result for $a/a_{B,2D}=2.17$ shows the largest departure from the universality in Fig. 2. This is due to the artificial definition of a_B^* as explained above. If the correct a_B^* for the quasi-2D system (smoothly interpolating between 2D and 3D limits) were known, we believe that Fig. 2 would show better one-parameter universality. In the absence of the "correct" a_B^* for the quasi-2D system, Fig. 2 should be taken only as indicative of a possible oneparameter universality for band-gap renormalization in quantum wells.

IV. VALIDITY OF THE ϵ_0 APPROXIMATION

In order to check the accuracy of the ϵ_0 approximation we calculate the full dynamical band-gap renormalization (without making the ϵ_0 approximation) including both electron-electron and electron-phonon interactions and compare them with the results of the ϵ_0 approximation. In Fig. 3 we show our results for the total interaction correction to Δ as well as the ϵ_0 -approximation results. We take the Fröhlich constant $\alpha_e = 0.07$ (corresponding to GaAs) for these calculations. In Fig. 3(a) we show the total self-energy corrections to the band gap of 2D, quasi-2D, and 3D systems whereas in Fig. 3(b) we subtract out¹¹ the *purely* polaronic corrections (Δ_p). Thus Fig. 3(b) is the more physical result since the purely polaronic renormalization of the band edges (obtained by 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 included¹¹ in the definition of the nominal band edges without any carrier renormalization effect. From Fig. 3, we conclude that for weakly polar materials (e.g., GaAs, InAs, GaSb, InSb, Ge, Si, AlAs, AlSb) the band-gap renormalization is very well approximated in 2D and quasi-2D systems by the ϵ_0



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



FIG. 4. Band-gap renormalization for 2D systems and different Fröhlich coupling constants as a function of the carrier density. Dashed lines correspond to the ϵ_0 approximation and solid lines to the full RPA calculation.

approximation and the approximate universality of Figs. 1 and 2 holds.

Obviously the ϵ_0 approximation would become less appropriate with increasing carrier density since the Fermi energies become comparable to the LO-phonon energy. For higher values of the Fröhlich coupling constant the ϵ_0 approximation breaks down, especially for high carrier densities (Fig. 4). Therefore the universality with respect to the material parameters also breaks down because a new parameter (i.e., the Fröhlich coupling constant) dependence is established. In the calculations of Fig. 4 the higher values of the coupling constants α were obtained by suitably adjusting the static dielectric constant ϵ_0 and keeping fixed all the other parameters of the theory. These higher values of α do not correspond to any real material but are useful in giving us an idea about the trend at higher couplings constants. We conclude that for highly polar materials, one must include electron-phonon interaction explicitly in the calculation and the ϵ_0 approximation underestimates the band-gap renormalization.

V. DOPED SEMICONDUCTOR QUANTUM WELL

For the doped situation where the number of electrons and holes are not equal $(N_e \neq N_h)$ the formalism of Sec. II can still be applied to the calculation of the band-gap renormalization. It is important to realize that even in the case when no holes are present, the valence band is renormalized.¹⁶ This is due to the fact that all experiments measuring the band-gap shifts involve creation or annihilation of electron-hole pairs. We cannot simply put $N_h=0$ in our calculations. In Fig. 5 we present the band-gap renormalization (within the ϵ_0 approximation)



FIG. 5. Band-gap renormalization (in the ϵ_0 approximation of the *n*-type doped situation as a function of the majoritycarrier density N_e . Solid lines correspond to $N_h/N_e = 1$, dashed lines to $N_h/N_e = 0.1$, and dotted lines to $N_h/N_e = 0.01$.

for the strictly 2D case as a function of the electron density in *n*-doped situation for three density ratios: $N_h/N_e = 1$, $N_h/N_e = 0.1$, and $N_h/N_e = 0.01$.

VI. CONCLUSIONS

In conclusion, we obtain the band-gap renormalization of quasi-2D systems including full dynamical effects of both electron-electron and electron-phonon interactions (within the RPA). We show that the plasmon-pole approximation is inadequate 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 claimed² in a recent publication. 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.

We would like to point out that Kleinman had earlier calculated¹⁷ exchange-correlation-induced band-gap renormalization in GaAs quantum wells. Instead of calculating the self-energy correction (as done in the present work), 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 calculations show that Δ calculated at k_F differs from that calculated at the band edge by about 10% for $N = 2 \times 10^{11}$ cm⁻². Numerical calculations¹⁶ of band-gap renormalization in bulk GaAs by Sernelius show that the bands are far from being shifted rigidly, which is consistent with our finding

that $\Delta(k_F)$ differs by about 10% from $\Delta(0)$. Other differences with Kleinman's approach is that he used a model potential rather than using the actual matrix elements of the Coulomb interaction in the subband representation as done in this work, and did not consider the Fröhlich interaction effects at all.

In this work we have made extensive use of the RPA. The validity of this approach is then important for all our quantitative conclusions. Mahan and Sernelius¹⁸ have recently shown that vertex corrections, when properly incorporated, introduce a very small departure from RPA in the calculation of the bandwidth of metals (which is a calculation very similar to the one addressed here).

Also, at high densities (small r_s) one expects RPA to be well-valid. A very recent calculation¹⁹ of band-gap renor-

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- ¹P. Vashishta and R. K. Kalia, Phys. Rev. B 25, 6492 (1982); G. Kirczenow and K. S. Singwi, Phys. Rev. Lett. 41, 326 (1978); T. L. Reinecke and S. C. Ying, *ibid.* 43, 1054 (1979). In these papers exchange-correlation contribution to the total energy was calculated whereas we directly calculate the self-energy correction.
- ²G. Tränkle *et al.*, Phys. Rev. Lett. **58**, 419 (1987); Phys. Rev. B **36**, 6712 (1987).
- ³S. Das Sarma, R. Jalabert, and S.-R. E. Yang, Phys. Rev. B **39**, 5516 (1989).
- ⁴S. Schmitt-Rink and C. Ell, J. Lumin. **30**, 585 (1985); S. Schmitt-Rink *et al.*, Solid State Commun. **52**, 123 (1984); H. Haug and S. Schmitt-Rink, J. Opt. Soc. Am. B **2**, 1135 (1985).
- ⁵U. Merkt, M. Horst, and J. P. Kotthaus, Phys. Scr. **T13**, 272 (1986), and references therein; M. A. Brummel *et al.*, Phys. Rev. Lett. **58**, 77 (1987).
- ⁶S. Das Sarma, Phys. Rev. B **27**, 2590 (1983); S. Das Sarma and B. A. Mason, *ibid.* **31**, 5536 (1985); Ann. Phys. (N.Y.) **163**, 78 (1985); S. Das Sarma and M. Stopa, Phys. Rev. B **36**, 9595 (1987); X. Wu *et al.*, Phys. Status Solidi B **133**, 229 (1986).
- ⁷T. Ando, A. B. Fowler, and F. Stern, Rev. Mod. Phys. **54**, 437 (1982).
- ⁸J. J. Quinn and R. A. Ferrell, Phys. Rev. **112**, 812 (1958); L. Hedin and S. Lundqvist, in *Solid State Physics*, edited by H. Ehrenreich, F. Seitz, and D. Turnbull (Academic, New York, 1969), Vol. 23, p. 1; G. Mahan, *Many-Particle Physics* (Plenum, New York, 1981).
- ⁹R. Jalabert and S. Das Sarma, Phys. Rev. B 40, 9723 (1989); R.

malization in quantum wells including vertex corrections shows that the RPA results presented in this paper are well-valid up to $r_s \approx 2-3$.

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- ¹⁰L. 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); G. Kawamoto *et al.*, Surf. Sci. **98**, 598 (1980).
- ¹¹B. A. Mason and S. Das Sarma, Phys. Rev. B **33**, 8379 (1986); M. Matsuura, *ibid.* **37**, 6977 (1988).
- ¹²B. I. Lundqvist, Phys. Condens. Mater. 6, 193 (1967); 7, 117 (1968); B. Vinter, Phys. Rev. B 13, 4447 (1976).
- ¹³The 2D effective 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 $R_{y,3D}=e^2/2\epsilon_0a_{B,3D}$ 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 $R_{y,2D}=18.7$ 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.
- ¹⁴G. Bongiovanni, J. L. Staehli, and D. Martin, Phys. Status Solidi B 150, 685 (1988); G. Bongiovanni and J. L. Staehli, Phys. Rev. B 39, 8359 (1989).
- ¹⁵R. L. Greene and K. K. Bajaj, Solid State Commun. 54, 831 (1983).
- ¹⁶B. E. Sernelius, Phys. Rev. B 33, 8582 (1986).
- ¹⁷D. Kleinman, Phys. Rev. B **33**, 2540 (1986); D. Kleinman and R. C. Miller, *ibid*. **32**, 2266 (1985).
- ¹⁸G. D. Mahan and B. E. Sernelius, Phys. Rev. Lett. **62**, 2718 (1989).
- ¹⁹I. K. Marmorkos and S. Das Sarma (unpublished).

Jalabert, Ph.D. thesis, University of Maryland, 1989 (unpublished).