Electron correlations in semiconductor heterostructures

Umbelino de Freitas
Departamento de Física, Universidade Federal da Paraíba, 58000 João Pessoa, Paraíba, Brazil

Nelson Studart*
Departamento de Física, Universidade Federal de Pernambuco, 50739 Recife, Pernambuco, Brazil
(Received 19 March 1987)

The theory of a two-dimensional electron gas is reexamined in the case of GaAs-$Al_xGa_{1-x}As$ heterojunctions and quantum wells. A new and accurate method was employed to calculate the static structure factor within the mean-field approximation. The influence of the finite width of the electron layer was investigated by calculation of the plasmon dispersion, the local-field function, and exchange and correlation energies in the random-phase approximation (RPA), the Hubbard approximation, and the self-consistent Singwi-Tosi-Land-Sjölander approximation.

Since the seminal paper of Stern,[1] a lot of theoretical work has been devoted to describe the many-body properties of the two-dimensional (2D) interacting electron system in a uniform positive background. This study has been motivated by the abundance of experimental results on metal-oxide-semiconductor inversion layers, electrons at the surface of liquid helium, and recently heterojunctions and quantum wells in artificially fabricated semiconductor heterostructures.[2-4] Although these systems are really three dimensional, there is ample evidence that the electrons are dynamically confined in a plane. A major part of the research is concerned with the electron gas interacting via the Coulomb e^2/r interelectron potential. However, for a realistic description of the system one has to include the effect of the third dimension, i.e., the actual width of the electronic layer. This effect can be incorporated by making an approximation in which the dynamics of electrons is still two dimensional, but a suitable average over the electron wave function in the third dimension is introduced.[5] On the other hand, most of the theoretical calculations of many-body properties have been performed using the random-phase approximation (RPA) which gives the exact results in the high-electron-density limit. However, previous studies have proved[5-7] that the inclusion of short-range correlations is much more important in the 2D case than the three-dimensional (3D) case. So, in order to obtain a good description of the electron gas in quasi-2D systems, it is necessary to include short-range correlations and the effect of the finite extension of the wave function in the third dimension.

This report presents a straightforward calculation of the effects of correlation and finite thickness of the layer in the static and dynamical properties of the electron system in semiconductor heterostructures. The novelty in the approach discussed here is a direct calculation of the static structure factor by an analytical continuation of the density-density response function in the fluctuation-dissipation theorem and a suitable and simple form to write the 2D noninteracting response function.

We consider an $Al_xGa_{1-x}As$-GaAs single heterojunction and multiple quantum wells (MQW's) composed of alternating layers of these two materials. In the former system, the electrons move into the GaAs side and form 2D subbands. The lowest one is well described by the Fang-Howard variational function

$$\Psi_0(z)=\left[\frac{b^3}{2}\right]^{1/2} z\exp(-bz/2)\ , \tag{1}$$

where the variational parameter b is related to the average electron extension from the interface and is determined by minimizing the total energy.[2] In MQW's the electrons are confined in 1D quantum wells with width d and potential barrier V_0. If the $Al_xGa_{1-x}As$ barriers are thick and the potential barriers are high (large Al concentration), the penetration of the wave functions in the barriers can be neglected and the quantum wells are decoupled. In this case the system can be modeled by a single quantum well with an infinitely deep potential barrier. The lowest-subband envelope function is taken in this approximation as

$$\Psi_0(z)=\left[\frac{2}{d}\right]^{1/2}\sin\left[\frac{\pi z}{d}\right]\ . \tag{2}$$

The bare interparticle potential $V(\mathbf{r}_1,\mathbf{r}_2,z_1,z_2)$ results from the direct Coulomb interaction between the electrons, since the dielectric constants of the two materials are close enough that the image forces are negligible. In quasi-2D systems, the electron-electron interaction can be written as

$$V(\mathbf{r}_1-\mathbf{r}_2)=\frac{e^2}{\epsilon}\int dz\int dz'\frac{|\Psi_0(z)^2|\Psi_0(z')|^2}{[r^2+(z-z')^2]^{1/2}}\ . \tag{3}$$

The Fourier transform of the effective potential is given by

$$V(q)=\frac{2\pi e^2}{\epsilon q}F(q)\ , \tag{4}$$

where the form factor to the Coulomb interaction due to layer thickness can be easily evaluated.[2,8] A strictly 2D

electron gas with δ-function density distribution is obtained by setting $F(q)=1$ in Eq. (4).

In order to describe the static and dynamical properties of these quasi-2D electron systems, we use the dielectric formulation of the many-body problem in the mean-field approximation. In this approach, the density-density response function is written as

$$\chi(q,\omega)=\frac{\chi_0(q,\omega)}{1+V(q)[1-G(q)]\chi_0(q,\omega)} , \tag{5}$$

where $\chi_0(q,\omega)$ is the noninteracting response function. $G(q)$ is the so-called local-field correction, which is responsible by the short-range effects among electrons caused by the exchange-correlation hole. The simplest approximation consists in taking $G(q)$ to be zero, which corresponds to RPA. So, RPA neglects all short-range exchange-correlation effects. Despite this failure, the RPA has been widely used in evaluating many-body properties in semiconductor heterostructures. In most self-consistent theories, $G(q)$ is expressed as a functional of the structure factor $S(q)$, the Fourier transform of the pair correlation function. For instance, in the theory of Singwi *et al.*,[9] (hereafter referred to as STLS) which has been found to give good results in several quantum systems, $G(q)$ is given as

$$G(q)=-\frac{1}{n}\int \frac{d\mathbf{k}}{(2\pi)^2}\frac{V(k)}{V(q)}\frac{\mathbf{k}\cdot\mathbf{q}}{q^2}[S(\mathbf{q}-\mathbf{k})-1] . \tag{6}$$

This expression is obtained by truncating the hierarchy of the equation of motion for higher-order Wigner distribution function with the use of a simple ansatz for the two-particle Wigner distribution function. The scheme is made self-consistent through the fluctuation-dissipation theorem, which relates the structure factor to the density-density response function in Eq. (7) as[10]

$$S(\mathbf{q})=-\frac{\hbar}{2\pi n}\int_{-\infty}^{+\infty}\chi(\mathbf{q},i\omega)d\omega . \tag{7}$$

Equations (5)–(7) must be solved self-consistently. As it is well known, $\chi(q,\omega)$ possesses singularities in ω plane associated with the continuum of the electron-hole pair excitation and the plasmon pole. This fact requires an awkward self-consistent calculation of the integral in Eq. (7). As discussed in Ref. 7, this problem can be elegantly handled by writing the 2D free density-density response function, which appears in Eq. (5), in terms of a new coordinate system defined by

$$\frac{2k_F}{q}=\cosh\xi\sin\theta , \tag{8a}$$

$$\frac{2m\omega}{\hbar q^2}=\sinh\xi\cos\theta , \tag{8b}$$

where $0\le\theta\le\pi/2$, $0\le\xi\le\infty$, and $k_F=(2\pi n)^{1/2}$ is the Fermi wave vector. Using this transformation, $\chi_0(q,i\omega)$ assumes a very simple form

$$\chi_0(\theta)=-\frac{m}{\pi\hbar^2}(1-\cos\theta) . \tag{9}$$

Using Eqs. (5) and (9) in Eq. (7) one gets the following expression for the structure factor

$$S(q)=\frac{q}{\pi k_F^2}\int_0^{\alpha(q)}\left[(4k_F^2-q^2\sin^2\theta)^{1/2}+\frac{4k_F^2\cot^2\theta}{(4k_F^2-q^2\sin^2\theta)^{1/2}}\right]\frac{(1-\cos\theta)d\theta}{1+V(q)[1-G(q)](1-\cos\theta)m/\pi\hbar^2} , \tag{10}$$

where

$$\alpha(q)=\begin{cases}\pi/2, & q\le 2k_F\\ \sin^{-1}(2k_F/q), & q>2k_F .\end{cases} \tag{11}$$

Then, $S(q)$ is written in terms of a single integral over a finite domain, which can be performed very accurately by precise numerical methods. The structure factor in the Hartree-Fock approximation (HFA) and RPA are easily obtained by setting $G(q)=1$ and $G(q)=0$, respectively, in Eq. (10). A step forward to include correlations in the system can be taken by evaluating the local field $G(q)$ with $S(q)$ calculated in HFA. This approximation is equivalent to the Hubbard approximation (HA), which is usually obtained through the calculation of a certain class of particle-hole ladder diagrams. It neglects electron correlation but takes the exchange effects into account. For a more complete treatment of short-range correlations, we proceed to solve Eqs. (6) and (10) in a self-consistent way. The calculation was performed using standard iterative procedure. We calculated the functions $G(q)$, $S(q)$, and other physical quantities derived from them for a single heterojunction (SH), a quantum well (QW), and a purely 2D electron gas (2DEG) with several values of electron density $r_s=(\pi n a_B^2)^{-1/2}$, a_B being the effective Bohr radius. Results for $G(q)$ are plotted in Fig. 1. It is noted that $G(q)$ in HA for a SH does not show appreciable varia-

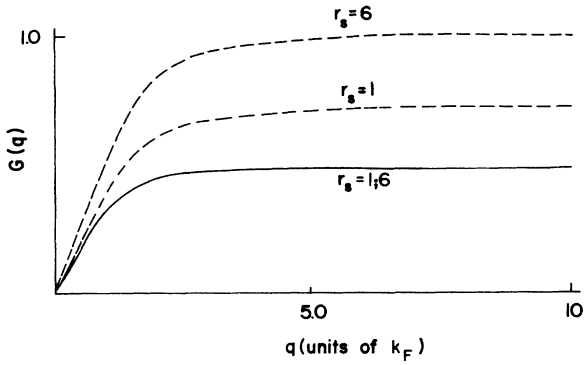

FIG. 1. Local-field correction $G(q)$ for a quasi-2DEG in a single heterojunction. Full curve, HA; broken curves, STLS.

tion as one changes the electron density and may be fitted by the well-known function which is obtained in the 2DEG

$$G_H(q)=\frac{1}{2}\frac{q}{(q^2+k_F^2)^{1/2}} . \tag{12}$$

On the other hand, $G(q)$ in the STLS approximation [Eq. (6)] shows a distinct behavior at different densities. In the long-wavelength limit one has

$$\lim_{q\to 0} G(q)=\gamma\frac{q}{k_F} , \tag{13}$$

where

$$\gamma=-\frac{1}{2}\int_0^\infty F(q)[S(q)-1]dq . \tag{14}$$

It is an important quantity which appears often in the calculations of the STLS scheme. In RPA, $\gamma=0$ and in HA, $\gamma=\frac{1}{2}$, if determined from $G(q)$ given in Eq. (12). For a QW system the effect of the spreading of the electron wave function is only observed at high densities. The STLS self-consistent results of $S(q)$ along with HA and RPA results are shown for a SH in Fig. 2. For comparison we plot $S(q)$ in RPA for the 2DEG. It is worthwhile to point out that greater values of $S(q)$ for all q are obtained as one improves the treatment of correlations in the system. So, the STLS value of $S(q)$ lies above that from HA, which in turn lies above that from RPA. The qualitative behavior of $S(q)$ for a SH is quite similar to that of QW. For small q, the following asymptotic limit is obtained

$$\lim_{q\to 0} S(q)=\gamma\frac{q^2}{k_F^2} . \tag{15}$$

The correlation energy is defined as the difference between the true interaction energy and the interaction energy in the HFA, which is called the exchange energy. The expression for E_c is given, in units of $R^*=me^4/2\epsilon^2\hbar^2$, as

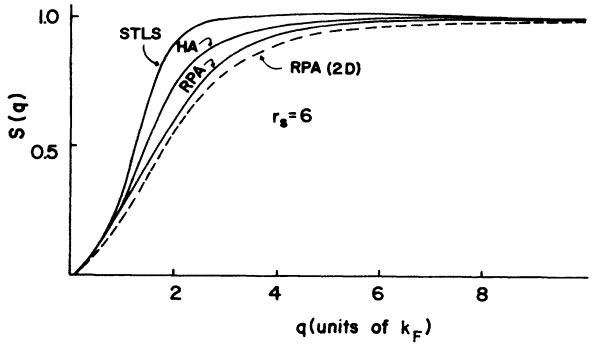

FIG. 2. Static structure factor $S(q)$ in STLS, HA, and RPA (full lines) for a quasi-2DEG in a single heterojunction. The dashed curve corresponds to $S(q)$ in RPA for a 2DEG.

$$E_c=\frac{\sqrt{2}}{r_s^2}\int_0^{r_s} dr_s'\int [S(q;r_s')-S^{\mathrm{HFA}}(q;r_s')]F(qd)dq . \tag{16}$$

The results of E_c in different approximations are listed in Table I along with the exchange energy for QW and SH systems. We must point out that the STLS approximation reduces drastically the RPA correlation energy values with decreasing density. For instance, E_c^{RPA} is reduced by 50% at $r_s=14$, while for $r_s=1$ the reduction is about 22%. The qualitative behavior of E_c does not differ very much from that obtained by Jonson in the SiO_2-Si inversion-layer problem.[5] For fixed r_s, E_c decreases as the QW becomes narrow.

Finally, we obtained the plasmon-dispersion relation $\omega_p(q)$ from the poles of the density-density response function:

$$1-V(q)[1-G(q)]\chi_0(q,\omega)=0 . \tag{17}$$

The solution of this equation is obtained with the use of the explicit expression of $\chi_0(q,\omega)$, evaluated first by Stern.[1] The result is[11]

$$\omega_p^2(q)=\frac{q}{2B(q)}\frac{[1+qB(q)]^2[4+2q^3B(q)+B^2(q)q^4]}{[1+qB(q)]/2} ,$$

where

$$B(q)=\{\sqrt{2}r_sF(q)[1-G(q)]\}^{-1} . \tag{18}$$

TABLE I. Exchange and correlation energy for the quasi-2DEG in heterojunctions and quantum wells. The energies are in units of $R^*\cong 5.25$ meV, and the well widths are in units of Å.

		Heterojunction		
r_s	$-E_x$	$-E_c^{\mathrm{RPA}}$	$-E_c^{\mathrm{HA}}$	$-E_c^{\mathrm{STLS}}$
1	0.710	0.079	0.062	0.061
2	0.396	0.089	0.074	0.071
3	0.282	0.090	0.074	0.069
4	0.221	0.090	0.073	0.065
5	0.183	0.089	0.072	0.061
6	0.155	0.088	0.070	0.056
8	0.122	0.087	0.068	0.051
10	0.100	0.086	0.066	0.046
14	0.174	0.081	0.064	0.040

		Quantum well			
r_s	d	$-E_x$	$-E_c^{\mathrm{RPA}}$	$-E_c^{\mathrm{HA}}$	$-E_c^{\mathrm{STLS}}$
1	50	0.825	0.159	0.126	0.138
	100	0.672	0.086	0.064	0.085
2	50	0.475	0.171	0.132	0.124
	100	0.413	0.116	0.094	0.099
3	50	0.336	0.168	0.128	0.106
	100	0.301	0.123	0.096	0.091
4	50	0.261	0.161	0.124	0.093
	100	0.234	0.124	0.096	0.082
5	100	0.197	0.123	0.095	0.075

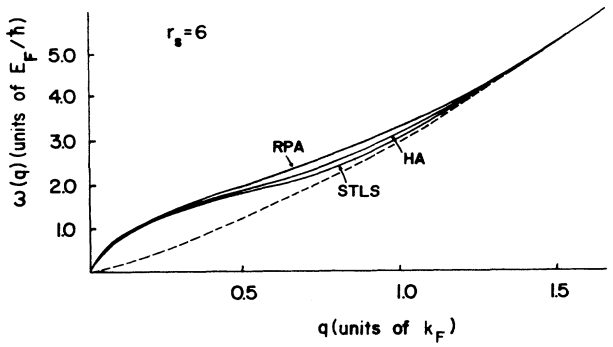

FIG. 3. Plasmon dispersion relation for a quasi-2DEG in a single heterojunction in SLTS, HA, and RPA (solid lines). The broken curve corresponds to the onset of the electron-hole continuum.

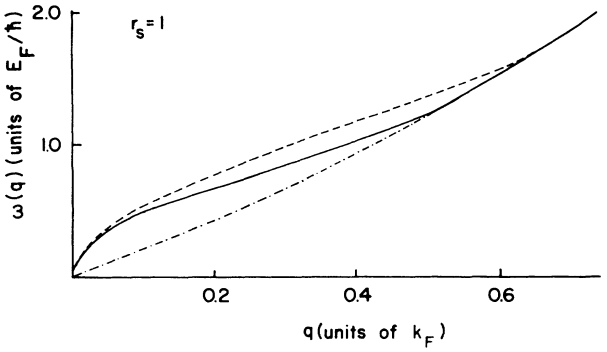

FIG. 4. Plasmon dispersion relation for a quasi-2DEG in a quantum well in STLS. The well widths are $d=20$ Å (— — —) and $d=400$ Å (——). The curve (—·—·—·) corresponds to the onset of the electron-hole continuum.

Here q is in units of k_F and ω is in units of $E_F/\hbar$. Our results are shown in Figs. 3 and 4. The lower curve corresponds to the upper edge of the particle-hole excitation continuum which is left out. It is clearly noted that correlation effects reduce the plasmon frequency. With a decrease in density, the STLS approximation differs considerably from HA and RPA. In a very recent paper, Batke *et al.*[12] made an extensive experimental study of plasmon excitations in the electron space-charge layers on GaAs. They showed the importance of the corrections to the classical dispersion relation $\omega_c^2=2\pi ne^2q/m\epsilon$ with increasing q. These corrections are due to electron correlations, nonlocal effects and the finite thickness of the system. In order to make clear how the corrections appear in our calculation, we expand Eq. (18) for small q to get the dispersion relation in the long-wavelength limit

$$\omega_p(q)=\omega_c\left[1+\frac{3}{4}\frac{q}{q_s}-\frac{1}{2}\beta\frac{q}{k_F}-\frac{1}{2}\gamma\frac{q}{k_F}+O(q^2)\right], \tag{19}$$

where $\beta=\frac{15}{8}b$ for SH and $\beta=(\frac{1}{3}-\frac{5}{4}\pi^2)d$ for QW. q_s is the Thomas-Fermi wave number. The second term of Eq. (19) corresponds to nonlocal effects due to the higher-order terms in a series expansion of $\chi_0(q,\omega)$.[1] This correction is positive, independent of the electron density and leads to an increase in the plasmon frequency. The third term is a first correction coming from the finite thickness of the electron layer and it reduces the plasmon frequency. The last term is the contribution of correlation and finite thickness effects which again lowers the plasmon-dispersion relation. If $\gamma=\frac{1}{2}$, we recover the correction in HA.[13] Since the sample configuration in Ref. 12 is different from the model used here, the comparison with experiment is not straightforward. However, the correlation and finite thickness effects are shown to be very important in describing plasmon excitations in realizable 2D systems.

The authors wish to express their sincere gratitude to L. Ioriatti, Jr., for valuable discussions. This work was partially supported by Conselho Nacional de Desenvolvimento Científico e Tecnológico and Coordenacão de Aperfeiçoamento de Pessoal do Ensino Superior. The authors acknowledge support of the Instituto de Física e Química de São Carlos where the major part of the research was developed.

*Permanent address: Departamento de Física, Universidade Federal de São Carlos, 13560, São Carlos, (SP) Brazil.

[1] F. Stern, Phys. Rev. Lett. **18**, 546 (1967).
[2] T. Ando, A. B. Fowler, and F. Stern, Rev. Mod. Phys. **54**, 437 (1982).
[3] M. J. Kelly and R. J. Nicholas, Rep. Prog. Phys. **48**, 1699 (1985).
[4] N. Studart and O. Hipolito, Rev. Bras. Fis. **16**, 194 (1986).
[5] M. Jonson, J. Phys. C **9**, 3055 (1976).
[6] J. S. Thakur and K. N. Pathak, J. Phys. C **16**, 6551 (1983).
[7] U. de Freitas, L. Ioriatti, Jr., and N. Studart, J. Phys. C (to be published).
[8] P. J. Price, Phys. Rev. B **30**, 2234 (1984).
[9] K. S. Singwi, M. P. Tosi, R. H. Land, and A. Sjolander, Phys. Rev. **176**, 589 (1968).
[10] D. Pines, *Elementary Excitations in Solids* (Benjamin, New York, 1963).
[11] A. Czachor, A. Holas, S. R. Sharma, and K. S. Singwi, Phys. Rev. B **25**, 2144 (1982).
[12] E. Batke, D. Heitmann, and C. W. Tu, Phys. Rev. B **34**, 6951 (1986).
[13] A. Gold, Z. Phys. B **63**, 1 (1986).