Subbands, exchange, and correlation effects on collective excitations in parabolic-quantum-well wires

Antonio Newton Borges
Universidade Federal de Goiás and Universidade Católica de Goiás 74001-970 Goiânia, Goiás, Brazil

Salviano A. Leão and Oscar Hipólito
Departamento de Física e Ciência dos Materiais, Instituto de Física de São Carlos, Universidade de São Paulo, Caixa Postal 369, 13560-970 São Carlos, São Paulo, Brazil

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The plasmon collective excitations in quasi-one-dimensional quantum-well wires are calculated for two- and three-subband model by using the self-consistent-field approximation theory proposed by Singwi, Tosi, Land, and Sjölander [Phys. Rev. **176**, 589 (1968)] for the response function of the electron system. The present calculations are applied to GaAs-Ga$_{1-x}$Al$_x$As parabolic-quantum-well wires with the appropriate form factors that take into account the influence of the width of the electron layer. Quantities such as the effective potential, the static structure factor, the pair-correlation function, and the plasmon dispersion relation are calculated as a function of energy difference between subbands and electron density. We found that exchange and correlation effects may be quantitatively significant for quasi-one-dimensional electron gas with a parabolic confinement potential. In the case where more than one subband is occupied, we found an additional plasmonlike intersubband mode. We also found significant differences due to the presence of the local-field correction included in our model calculation when compared to the corresponding random-phase approximation results. [S0163-1829(97)04704-8]

Recent developments in the fabrication techniques such as molecular-beam epitaxy and lithographic deposition have increased the interest in the study of electronic properties of ultrathin semiconducting wires whose dimensions are of submicrometer size. In such structures based on the confinement of electrons, the electron gas is confined to have a quasifree motion along the length of the wire and is quantized on the two transverse directions. Recently, much theoretical work has been done to understand the behavior of electrons in such quasi-one-dimensional (quasi-1D) semiconductor structures.[1–5] Plasmon experiments[6] indicate that subband-quantization effects are important to the understanding of the collective motion in quantum-well wires. Most of the theoretical work to calculate the linear response of the quasi-1D electron gas was done in the framework of the random-phase approximation (RPA) theory.

Our aim here is to investigate the elementary excitation spectrum of the quasi-1D electron system by using a multisubband model. Within a self-consistent-field approximation, beyond the RPA, including correlation effects, we discuss the dispersion relations of both inter- and intrasubband excitations. We will show the importance of exchange and correlation as well as the subband effects on the collective excitations in GaAs quantum wires.

In the quasi-1D electron gas under study, the electrons are confined by a two-dimensional transverse potential $V(y,z)$ with a quasi-free motion parallel to the one-dimensional channel. It has been shown by a detailed self-consistent calculation[7] that, for the experimental system available, the confinement in one direction, say, the z direction, is stronger than that in the other one. In this case a reasonable approximation would be to separate the two-dimensional potential as a sum of two independent potential, say, $V_1(y)$ and $V_2(z)$.

In order to calculate the electronic properties of the quasi-1D electron gas we will assume that the energy separation between levels due to z confinement is much larger than that due to the y confinement and only the lowest subband in the z direction is occupied. For the sake of simplicity, we shall consider a quantum wire in which the electrons are located in a zero-thickness layer along the z direction, at $z=0$. In the y direction we will assume a parabolic confinement $V(y)=m\Omega^2y^2/2$.

From here to the end of this work we shall use the same notation as in Ref. 8. The self-consistent-field approximation method, as proposed by Singwi *et al.*,[9] has been applied successfully to several systems[10–13] Extending beyond the RPA, this method basically includes the short-range correlation through the local-field corrections to the Hartree mean-field theory. Here we give only the essentials of the Singwi-Tosi-Land-Sjölander (STLS) method, and we refer the interested reader to Ref. 9 for details. In the mean-field approximation, the generalized response function for a quasi-1D can be written as

$$\chi_{ijlm}(q_x,\omega)=\frac{\chi_{lm}(q_x,\omega)}{\delta_{il}\delta_{jm}-\Psi_{ijlm}(q_x)\chi_{lm}(q_x,\omega)}, \tag{1}$$

where the indices $ijlm$ indicate the subbands corresponding to the electron motion in the transverse direction and q_x is the wave vector in the x direction containing information on the collective effects. δ_{il} is the Kronecker symbol, $\chi_{lm}=P_{lm}$ if $l=m$ and $\chi_{lm}=P_{lm}+P_{ml}$ if $l\neq m$. $P_{kn}(q_x,\omega)$ is the RPA polarization function for the quasi-1D electron gas.

The function $\Psi_{ijlm}(q_x)$ is the effective potential, given by

$$\Psi_{ijlm}(q_x)=[1-G_{ijlm}(q_x)]V^c_{ijlm}(q_x), \tag{2}$$

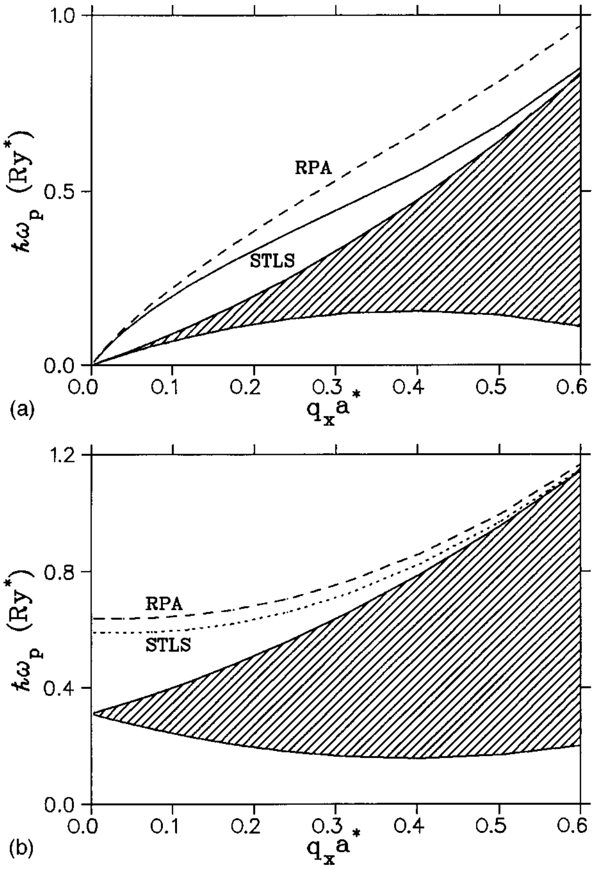

FIG. 1. (a) Dispersion relation of the intrasubband collective excitation for the lowest subband $\hbar\omega_{00}^p$, calculated according to the two-subband model with only one populated as a function of the wave vector $q_x a^*$. The dashed line represents the RPA result without the local-field corrections. The hatched area corresponds to the intrasubband single-particle excitation spectrum. The parameters used in the calculation are $\hbar\Omega = 1.7$ meV and $\rho = 2.45\times10^5$ cm^{-1} and the constants of the material are those of GaAs. (b) Intersubband collective excitation between the first and the second subband $\hbar\omega_{10}^p$, calculated in a two-subband model where only one is populated as a function of the wave vector $q_x a^*$. The dashed line is the RPA result, the dotted line is the STLS result, and the hatched area corresponds to the intersubband single-particle excitation spectrum. The parameters and semiconductor material constants are the same as in (a).

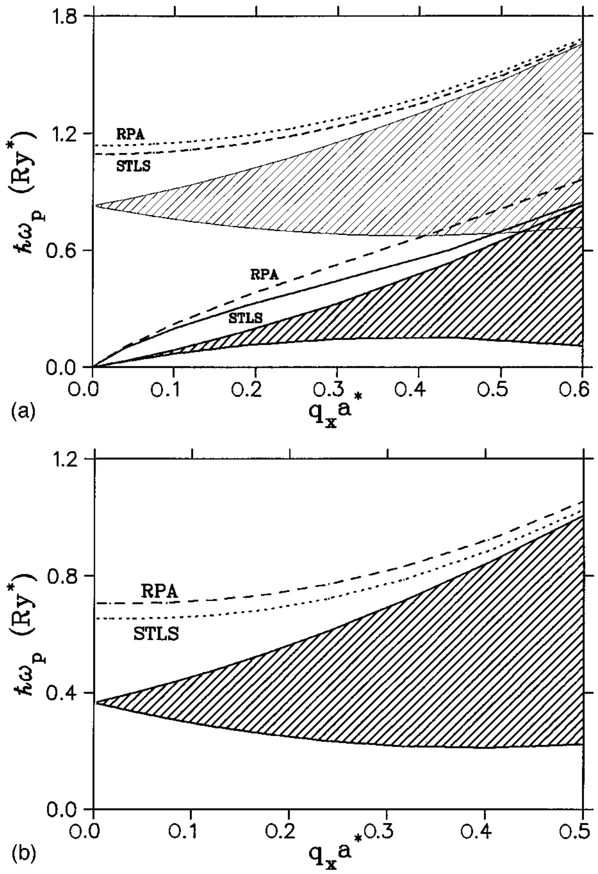

FIG. 2. (a) Dispersion relation of the mixed intrasubband collective excitation $\hbar\omega_{00}^p$ and intersubband collective excitation between the first and third subband, calculated in a three-subband model with only one populated as a function of the wave vector $q_x a^*$. The hatched areas in the $(\hbar\omega^p, q_x a^*)$ plane are the regions where the single-particle excitation occurs. The parameters used in the calculation are $\hbar\Omega = 2.0$ meV and $\rho = 2.5\times10^5$ cm^{-1} and the constants of the material are those of GaAs. (b) Dispersion relation of the nonmixed intersubband collective excitation between the first and the second subband $\hbar\omega_{10}^p$, calculated in a three-subband model where only one is populated as a function of the wave vector $q_x a^*$. The dashed line is the RPA result, the dotted line is the STLS result, and the hatched area corresponds to the intersubband single-particle excitation spectrum. The parameters and semiconductor material constants are the same as (a).

where

$$G_{ijlm}(q_x) = -\frac{1}{\pi\rho q_x V_{ijlm}^c(q_x)}\int_0^\infty dq_x' q_x' V_{ijlm}^c(q_x) \times [S_{ijlm}(q_x - q_x') - 1] \tag{3}$$

is the local-field correction, $\rho = 1/L_x$ is the one-dimensional density of electrons in the system, and L_x is the unit length of the wire in the x direction. $S_{ijlm}(q_x)$ is the structure factor and $V_{ijlm}^c(q_x)$ is the direct Coulomb interaction between the electrons,

$$V_{ijlm}^c(q_x) = -\frac{2e^2}{\epsilon_0}\int_0^\infty dk F_{ijlm}(q_x, k)(k^2 + q_x^2)^{-1/2}, \tag{4}$$

where F is the form factor, which takes into account the finite thickness of the wire,

$$F_{ijlm}(k, q_x) = \int d\eta \int d\eta' \Phi_i^*(\eta)\Phi_j(\eta) \times \exp[-(k^2 + q_x^2)^{-1/2}|\eta - \eta'|] \times \Phi_l^*(\eta')\Phi_m(\eta'), \tag{5}$$

$\Phi_i(\eta)$ is the confining wave function of the ith subband, and ϵ_0 is the background lattice dielectric constant. The structure factor is defined by

$$S_{ijkm}(q_x) = -\frac{\hbar}{\pi\rho}\int_0^\infty d\omega \, \mathrm{Im}\chi_{ijlm}(q_x, \omega). \tag{6}$$

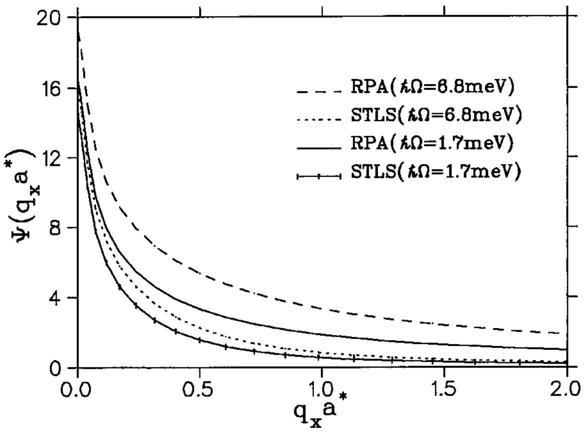

FIG. 3. Effective electron-electron potential for the first subband as calculated within the self-consistent-field approximation for differents subband separation energies $\hbar\Omega$ of GaAs quantum wires as a function of the wave vector $q_x a^*$. The RPA results are also shown for comparison.

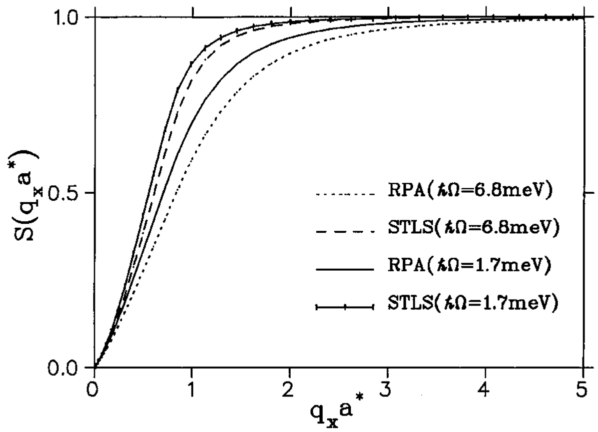

FIG. 4. Structure factor for a quasi-1D electron gas in a semiconductor GaAs quantum wire for the lowest subband calculated in a two-subband model where one subband is filled as a function of the wave vector $q_x a^*$. Sizable differences can be seen in comparison to the RPA results mainly for a subband separation energy of $\hbar\Omega = 6.8$ meV.

The RPA result is recovered if we set $G_{ijlm}(q_x) \equiv 0$ in Eq. (2), which means that short-range correlations are not present at the RPA level.

We have three equations [(1), (2), and (6)] that have to be solved self-consistently in order to obtain the STLS approximation. Using a two- and three-subband model in the case where one or two subbands are populated, we have numerically solved the set of self-consistent equations to obtain the properties of the quasi-1D electron gas. The collective excitation spectrum is obtained from the poles of the imaginary part of the generalized response function, which is given by Eq. (1). Quantities such as effective potential, structure factor, pair-correlation function, and plasmon dispersion relation are shown in graphical form as a function of the energy differences between subbands and the electronic density.

The results for the random-phase approximation are also presented for comparison with sizable deviation from STLS results. We have found that exchange and correlation effects may be quantitatively significant for a quasi-1D electron gas with a parabolic confinement potential. In the case where more than one subband is occupied, we find an additional plasmon like intersubband mode. The dispersion relation curves of the intrasubband plasmon, for the lowest subband ($\hbar\omega_{00}^p$) in a two-subband model, with only one occupied are plotted in Fig. 1(a), in units of effective Rydberg $\mathrm{Ry}^* = me^4/2\epsilon_0\hbar^2$, as a function of the wave vector along the wire length $q_x a^*$, where a^* is the effective Bohr radius $a^* = \epsilon_0\hbar^2/me^2$. We are using a GaAs-$\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ quantum wire with the subband separation energy $\hbar\Omega = 1.7$ meV and with a linear electronic density $\rho = 2.45\times 10^5\ \mathrm{cm}^{-1}$. For these parameters and for semiconductor materials only one subband is occupied. One sees from Fig. 1(a) that the effects of local-field correction are quite significant and cannot be neglected in any theory. It was also noted (although not shown in the figure) that the corrections arising from the correlation effects become smaller as the density increases and/or the subband energy separation $\hbar\Omega$ decreases.

In Fig. 1(b) the intersubband plasmon, between subbands 0 and 1 ($\hbar\omega_{10}^p$) are depicted, using the same parameters as those of Fig. 1(a). We also can note that the depolarization shift, which is the energy difference between the intersubband single-particle excitation ($\hbar\omega_{10}^p$) and the plasmonlike collective excitation at $q_x = 0$ is lowered due to the effects of local-field correction.

In Figs. 2(a) and 2(b) the full STLS dispersion relation curves of the three-subband model with only one subband populated are plotted. Figure 2(a) shows the dispersion relation curves of the mixed $\hbar\omega_{00}^p$ and $\hbar\omega_{20}^p$ plasmon, where $\hbar\omega_{20}^p$ is the intersubband plasmon between subbands 0 and 2. The shaded areas in the ($\hbar\omega^p, q_x a^*$) plane correspond to the regions where the single-particle excitations occur. In these regions, $\mathrm{Im}\chi_{ijlm}(q_x,\omega)$ is nonzero and the collective excitations are Landau damped. We will only investigate the modes outside these regions.

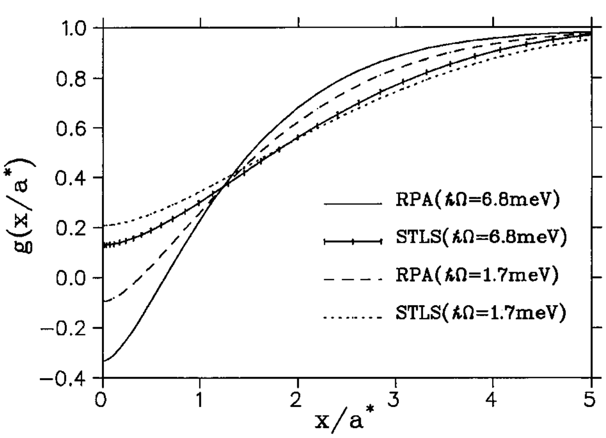

FIG. 5. Pair-correlation function for a quasi-1D electron system in a GaAs quantum wire in which only the lowest subband is occupied by electrons as a function of the wave vector $q_x a^*$. The RPA results are shown for comparison with the self-consistent-field approximation. For the subband separation energies $\hbar\Omega$ the STLS-gives a positive value, while RPA gives a negative nonphysical result for the pair-correlation function at $x=0$.

Figure 2(b) shows the dispersion relation curves' nonmixed intersubband collective excitation between the first and second subbands $\hbar\omega_{10}^{p}$, with the same parameters as those of Fig. 2(a). Once again one sees the effects of the local-field correction on the random-phase approximation data.

The results of our self-consistent approximation calculations for the electron-electron effective potential, structure factor, and pair-correlation function for the lowest subband and for two different values of the subband separation energies for the GaAs quantum wire are shown in Figs. 3–5. The RPA results are also plotted for comparison. From Fig. 3 we clearly see that the screening effects are much more significant in the STLS calculation. Also from Fig. 5 we note that while RPA gives a negative nonphysical result for the pair-correlation function at $x=0$, for both values of the energy separations, $\hbar\Omega=6.8$ meV and $\hbar\Omega=1.7$ meV, the STLS theory gives a positive value for all energy difference subbands. As we can note, even for large subband separation energy the STLS shows better results than the corresponding RPA. Finally, we also note that as the subband separation energy decreases the STLS results approaches those of the random-phase approximation, which means that correlation effects are no longer important.

In conclusion, we have used a self-consistent-field approximation that includes short-range correlations to calculate the intra- and intersubband collective excitations for a two- and three-subband model in the case where one subband is populated for a quasi-1D electron gas in a parabolic semiconductor quantum wire of GaAs. We discussed intra- and intersubband plasmon excitations, the effective electron-electron potential, the structure factor, and the pair-correlation function for different subband separation energies. We found significant differences between our model calculation and the corresponding RPA results, due to the inclusion of the local-field correction.

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