Collective excitation in GaAs-$Al_xGa_{1-x}As$ quantum wires: Multisubband model

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The effects of the potential barrier height on the collective excitations of an electron gas confined in a GaAs-$Al_xGa_{1-x}As$ quantum wire of rectangular cross section are investigated theoretically by using the self-consistent field approximation theory proposed by Singwi, Tosi, Land, and Sjölander (STLS) [Phys. Rev. **176**, 589 (1968)]. For several potential barrier heights, we calculated the effective potential, plasmon energy, structure factor, and pair-correlation function, considering a three-subband model with only the lowest subband populated by electrons. We verified that the intersubband plasmon is more sensitive to the potential barrier height variation than the intrasubband plasmon. We also observed that the confining potential effect decreases with the increasing of the wire width. The random-phase approximation results are also presented by comparison with the STLS results and significant differences were found. [S0163-1829(97)02631-3]

I. INTRODUCTION

In the last few years, due to the progress in fabrication techniques such as molecular-beam epitaxy (MBE) and lithographic deposition, there has been an increasing interest in the study of the electronic properties of ultrathin semiconducting wires, namely, quantum well wires (QWW), whose dimensions are of submicrometer size. In such quasi-one-dimensional systems (Q1D) the electrons have a quasifree motion along the length of the wire, while the motion normal to the wire is quantized in two directions. Following a suggestion by Sakaki,[2] Petroff, Gossard, Logan, and Wiegmann[1] were the first to fabricate these QWW of GaAs surrounded by $Al_xGa_{1-x}As$.

Recently, there has been considerable interest in the behavior of intrasubband and intersubband plasmons of Q1D semiconductor systems, from both the theoretical and experimental points of view. The intrasubband plasmon dispersion of Q1D electron gas in doped GaAs has been observed experimentally by Goñi *et al.*[3]. The results of this experiment are in agreement with the theoretical conclusions of Hu and Das Sarma,[4] both predicting that such systems behave as Fermi liquids.

In theoretical calculations[5,7–15] of the collective excitation of Q1D electronic systems, wires with different cross section geometry have been used. Cross section geometry effects on the intrasubband plasmon and intersubband plasmon of a quantum wire, with infinite height of the potential barrier, were theoretically considered by Bennett *et al.*,[5] within the two-subband random-phase-approximation (RPA) regime. They showed that the intrasubband plasmon is practically unaffected by a change in geometry. However, they also showed that the intersubband plasmon was more sensitive to the geometry. This happens because the energy separation between the ground state and the first excited state depends on the geometry. These results show the importance of considering more realistic geometries in the theoretical calculations of the plasmon excitations in Q1D systems when the multisubband model is used. In particular, a similar effect is expected to occur when the wire confining potential barrier height is varied. The intersubband plasmon energy results should be equally sensitive to the changes in the potential barrier height. Then, it is very important to consider a model of finite height for the wire confining potential barrier.

The local field corrections beyond the RPA have been used in the theoretical calculations[7–14] of the collective excitation of electronic systems. Camels and Gold[7] have calculated the local-field correction of a Q1D electron gas within the sum-rule version of the Singwi, Tosi, Land, and Sjölander[6] (STLS) theory. They found that the correlation effects increase with the decreasing of the carrier density and with the decreasing of wire width. Campos, Degani, and Hipólito[8] within the frame of the STLS theory, have studied the exchange and the correlation effects of a Q1D electron gas confined in a rectangular QWW, as a function of the electron density and thickness of the wire. In this calculation the authors have not explicitly taken into account the multisubband effects, which are very important for understanding the collective motion in QWW. For rectangular QWW of GaAs with infinite height to the potential barrier, the plasmon excitations were calculated by Borges, Leão, and Hipólito,[9] using the self-consistent-field approximation theory, proposed by STLS. The intrasubband excitation and the intersubband excitation were investigated in a two-subband model, and significant differences were found due to the presence of the local field correction when compared with the corresponding RPA results.

In the present work we investigate the effects of the potential barrier height on the plasmon dispersion relations, effective potential, structure factor, and pair-correlation function within the STLS approach, for GaAs-Al_xGa_{1-x}As quantum well wires of rectangular cross section for both intrasubband and intersubband plasmons. We employed a three-subband model at zero temperature and we assumed that only the first subband is occupied. The local field correction taken into account in the STLS theory is an important effect and significant differences were observed in comparison with the RPA results.We observed a measurable change in the intersubband plasmon results when the potential barrier height is varied. This paper is organized as follow. In Sec. II we describe our theoretical model and the calculation method. In Sec. III we present our numerical results and the discussions. Our conclusions are presented in Sec. IV.

II. THEORY

Let us consider a GaAs-Al_xGa_{1-x}As quantum-well wire, which is assumed to have rectangular cross section, where the electrons are confined in the y and z directions by a two-dimensional potential, with a quasifree motion along the wire length, x direction. The electron confining wave function of the ith subband has the following form:

$$\phi_i(y)=\begin{cases} A\dfrac{m_2}{m_1}\dfrac{K_1}{K_2}e^{K_2 y}, & y<0 \\ A\left(\sin K_1 y+\dfrac{m_2}{m_1}\dfrac{K_1}{K_2}\cos K_1 y\right), & 0<y<L \\ A\left(\sin K_1 L+\dfrac{m_2}{m_1}\dfrac{K_1}{K_2}\cos K_1 L\right)e^{K_2 L}e^{-K_2 y}, & y>L, \end{cases} \tag{1}$$

where A is the wave-function normalization factor, m_1 and m_2 are the electron effective masses in GaAs and in Al_xGa_{1-x}As,[16] respectively. The parameters K_1 and K_2 are determined by using the appropriate current-conserving boundary conditions for the wave functions at the interfaces and must satisfy the following relation:

$$\tan(K_1 L)=\frac{2(m_2/m_1)K_1/K_2}{[(m_2/m_1)K_1/K_2]^2-1}. \tag{2}$$

Thus, the subband matrix element of the Coulomb interaction has the following expression:

$$V^C_{ijlm}(q_x)=\int dy\int dy'\,\phi_i^*(y)\phi_j(y)\frac{2e^2}{\varepsilon}\times K_0[|q_x(y-y')|]\phi_l^*(y')\phi_m(y') \tag{3}$$

$$=\frac{2e^2}{\varepsilon}\int_0^\infty dk\frac{F_{ijlm}(k,q_x)}{\sqrt{k^2+q_x^2}}, \tag{4}$$

where $K_0(x)$ is the modified Bessel function of the second kind, q_x is the wave vector in the x direction containing information on the collective effects, and ε is the dielectric constant of the semiconductor. $F_{ijlm}(k,q_x)$ is the form factor that takes into account the finite thickness of the quantum wire that is given by

$$F_{ijlm}(k,q_x)=\int dy\int dy'\,\phi_i^*(y)\phi_j(y)\times\exp(-\sqrt{k^2+q_x^2}|y-y'|)\phi_l^*(y')\phi_m(y'), \tag{5}$$

where the indices $ijlm$ indicate the subbands corresponding to the electron motion in the transverse direction.

In the mean-field approximation, the generalized response function of the system can be written as[10]

$$\chi_{ijlm}(q_x,\omega)=\frac{\chi_{lm}(q_x,\omega)}{\delta_{il}\delta_{jm}-\Psi_{ijlm}(q_x)\chi_{lm}(q_x,\omega)}, \tag{6}$$

where δ_{ij} is the Kronecker delta, $\chi_{lm}=P_{lm}$ if $l=m$, and $\chi_{lm}=P_{lm}+P_{ml}$ when $l\neq m$. $P_{lm}(q_x,\omega)$ is the random-phase-approximation polarization function of the Q1D electron gas and $\Psi_{ijlm}(q_x)$ is the effective potential given by

$$\Psi_{ijlm}(q_x)=[1-G_{ijlm}(q_x)]V^C_{ijlm}(q_x), \tag{7}$$

where $G_{ijlm}(q_x)$ reads

$$G_{ijlm}(q_x)=\frac{1}{\pi\rho q_x V^C_{ijlm}(q_x)}\int_0^\infty dq_x' V^C_{ijlm}(q_x')q_x'\times[S_{ijlm}(q_x-q_x')-1]. \tag{8}$$

$S_{ijlm}(q_x)$ is the structure factor, which is defined by

$$S_{ijlm}(q_x)=-\frac{\hbar}{\pi\rho}\int_0^\infty d\omega\,\mathrm{Im}\chi_{ijlm}(q_x,\omega), \tag{9}$$

where $\rho=1/L_x$ is the one-dimensional density of electrons in this system. The pair-correlation function is obtained from the structure factor by the relation

$$g_{ijlm}(x)=1+\frac{1}{\pi\rho}\int_0^\infty dq_x[S_{ijlm}(q_x)-1]\cos(q_x x). \tag{10}$$

III. RESULTS AND DISCUSSIONS

In our numerical calculation we have considered a GaAs-Al_xGa_{1-x}As rectangular quantum wire with $L=300$ Å, and with an electronic density $\rho=3.27\times10^5\ \mathrm{cm}^{-1}$. We

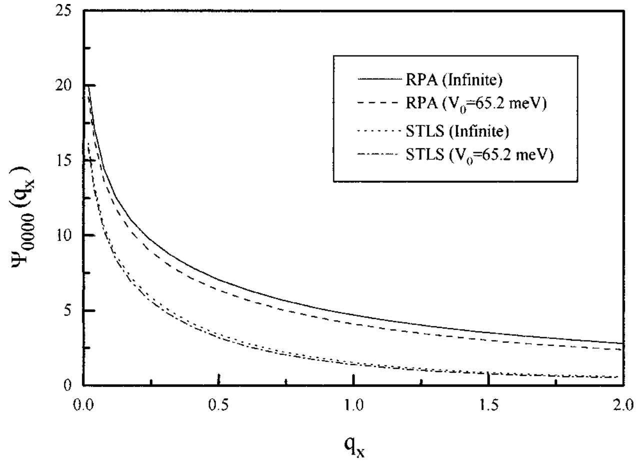

FIG. 1. Intrasubband electron-electron effective potential for the the lowest subband as a function of the dimensionless one-dimensional wave vector for infinite potential barrier height and $V_0 = 65.2$ meV.

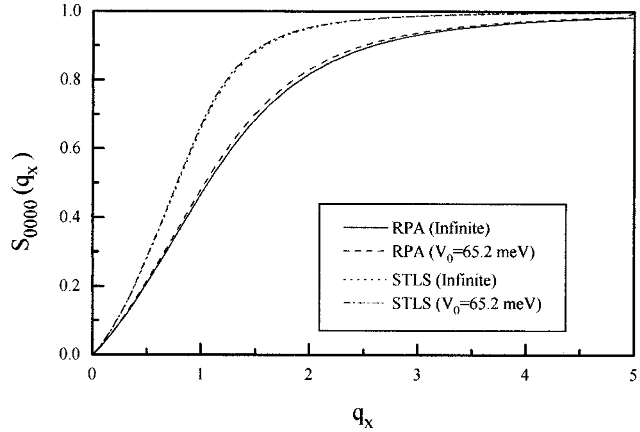

FIG. 3. Intrasubband (0-0) static structure factor as a function of the one-dimensional wave vector, considering the three-subband model with only the lowest subband populated. The RPA and STLS results are presented for infinite and finite (256 meV) potential barrier height.

have considered two heights of the confining potential, 65.2 and 212.6 meV, which correspond to aluminum concentrations $x = 0.1$ and $x = 0.3$, respectively. The infinite potential barrier height results are also included in the figures for comparison. We have calculated the electron-electron effective potential, plasmon energy, structure factor, and pair-correlation function within the STLS theory, assuming the three-subband model with only the first subband occupied. In this formalism we have self-consistently solved Eqs. (6), (7), and (9) and the collective excitation spectrum is obtained from the poles of the imaginary part of the generalized response function given by Eq (6). We can note that if we set $G_{ijlm}(q_x) = 0$ in Eq. (7), the RPA results are recovered. For comparison, these results (RPA) are shown in all the figures, where all the lengths and energies are taken in units of effective Bohr radius (a^*) and effective Rydberg (R_y^*) for the GaAs, which have the values 101.9 Å and 5.50 meV, respectively.

In Fig. 1 we show the results for the intrasubband electron-electron effective potential for the lowest subband as a function of the one-dimensional wave vector for infinite potential barrier height and $V_0 = 65.2$ meV. From this figure, we can note that the screening effects are more pronounced in the STLS results than in the RPA results. However, the RPA results are more sensitive to the potential barrier height variation than are the STLS results. We can also observe that the higher the potential barrier height, the more repulsive is the effective potential, for both the RPA and STLS results plotted in Fig. 1. The differences between the two methods (STLS and RPA) are significant and show the importance of the local-field correction for the intrasubband plasmon.

For the intersubband plasmon the differences between the results RPA and STLS (not shown in figures) for the effective potential are not too relevant. They are smaller for the transition of the first to the third subband (0-2) than for the transition of the first to the second subband (0-1), as expected. The STLS results for the effective potential are more sensitive to the confinement potential variation in this case.

The importance of the STLS theory is that it takes into account the local-field correction in contrast with the RPA approach. This fact can be better observed from the pair-correlation function $g(x)$ [Eq. (10)], which remains positive for all distances in the STLS theory. However, as is well known the RPA intrasuband results, for $g(x)$, became negative when $x \to 0$.

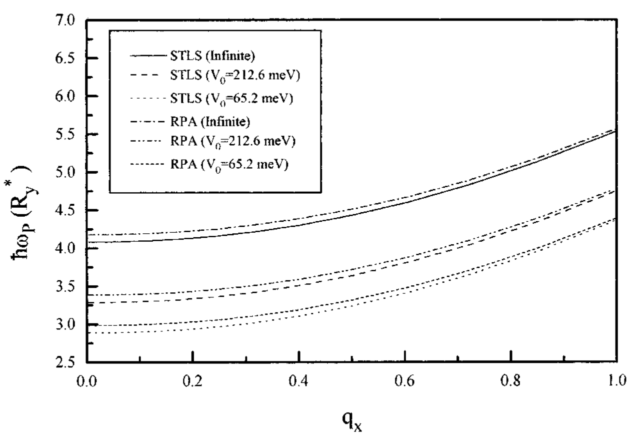

FIG. 2. Intersubband collective excitation energy, from the first to the second subband (1-0), as a function of the parameter q_x, in both the RPA and STLS approaches, for three different potential barrier heights.

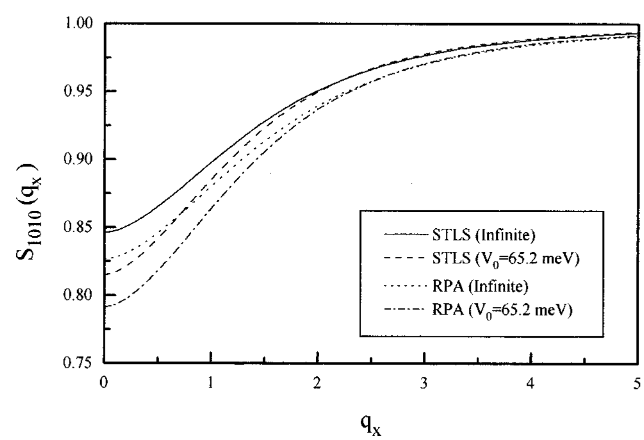

FIG. 4. Same as Fig. 3 but for the intersubband (0-1) case.

The potential barrier height effects on the intersubband collective excitation, from the first to the second subband (1-0), are shown in Fig. 2. As we can see the collective excitation energy is very sensitive to the variation of the potential barrier height. The differences between the results obtained with the simplest model of infinite height for the potential barrier and the more realistic one considering the barrier potential height as finite are remarkable, and cannot be neglected. For example, for $q_x = 0.5$, the values of the energy are 3.24, 3.63, and 4.43 for $V_0 = 65.2$ meV, $V_0 = 212.6$ meV and infinite height of the potential barrier, respectively. However, the effects of the confining potential are weak for the intrasubband (0-0) collective excitation energy for both the results STLS and RPA. Nevertheless, the differences between the results obtained with these two methods are pronounced and show that for the intrasubband plasmon the local-field correction is very important.

In Figs. 3 and 4, we show the results for the intrasubband (0-0) and intersubband (0-1) static structure factor, respectively, as a function of the wave vector. The structure factor shown in the figures has the same qualitative behavior as that presented previously in Ref. 10, for the case of infinite potential barrier height. The differences between both the results (RPA and STLS) are more pronounced in Fig. 4 as expected. As we can note in Fig. 3 the potential barrier height effects are weak for the intrasubband collective excitation. However, for the intersubband (0-1) transition (Fig. 4) the effect of the confining potential height plays an important role, and is more pronounced for small wave vector value ($q_x < 2$).

IV. CONCLUSION

In conclusion, we have used the self-consistent field approximation, which includes the local-field correction within the STLS theory to calculate the intrasubband and the intersubband excitation of a quasi-one-dimensional electron gas confined in a GaAs-Al$_x$Ga$_{1-x}$As quantum well wires of rectangular cross section, considering the finite height for the potential confining. We employed a three-subband model at zero temperature and we assume that only the first subband is occupied. We calculated the intrasubband and intersubband effective potential, pair-correlation function, plasmon energy, and structure factor for several potential barrier heights, as a function of the one-dimensional wave vector. The STLS results were compared with the corresponding RPA results and significant differences were found due to the presence of the local field correction. We show that the potential barrier effects are important for the intersubband plasmon. We verified that the intersubband collective energies are reduced about 25% for wires with aluminum concentration $x = 0.1$ in comparison with wires with infinite height potential barrier. Then we conclude that the model of the infinite height for the potential barrier is not a good approximation to treat the quasi-one-dimensional intersubband plasmon.

[1] P.M. Petroff, A.C. Gossard, R.A. Logan, and W.W. Wiegman, Appl. Phys. Lett. **41**, 635 (1992).
[2] H. Sakaki, Jpn. J. Appl. Phys. Part 2 **19**, L735 (1980).
[3] A.R. Goñi, A. Pinczuk, J.S. Weiner, J.M. Calleja, B.S. Dennis, L.N. Pfeiffer, and K.W. West, Phys. Rev. Lett. **67**, 3298 (1991).
[4] Ben Yu-Kuang Hu and S. Das Sarma, Phys. Rev. Lett. **68**, 1750 (1992); Phys. Rev. B **48**, 5469 (1993).
[5] C.R. Bennett, B. Tanatar, N.C. Constantinou, and M. Babiker, Solid State Commun. **12**, 947 (1994).
[6] K.S. Singwi, M.P. Tosi, R.H. Land, and A. Sjölander, Phys. Rev. **176**, 589 (1968).
[7] L. Camels and A. Gold, Solid State Commun. **92**, 619 (1994).
[8] V.B. Campos, M.H. Degani, and O. Hipólito, Superlattices Microstruct. **17**, 85 (1995).
[9] A.N. Borges, S.A. Leão, and O. Hipólito, Phys. Rev. B **55**, 4680 (1997).
[10] A.N. Borges, M.H. Degani, and O. Hipólito, Superlattices Microstruct. **13**, 51 (1993).
[11] A. Gold and A. Ghazali, Phys. Rev. B **41**, 7626 (1990); **41**, 8318 (1991).
[12] M. Jonson, J. Phys. C **9**, 3055 (1976).
[13] V.B. Campos, O. Hipólito, and R. Lobo, Phys. Status Solidi B **81**, 657 (1977).
[14] A.N. Borges, O. Hipólito, and V.B. Campos, Phys. Rev. B **52**, 1724 (1995).
[15] L. Wendler and V.G. Grigoryan, Phys. Rev. B **49**, 14 531 (1994).
[16] F.A.P. Osório, Marcos H. Degani, and O. Hipólito, Phys. Rev. B **37**, 1402 (1988).