LETTER TO THE EDITOR

Collective Excitations in Realistic Quantum Wires

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Abstract. We have used the Hartree-Fock Random Phase Approximation (HF-RPA) to study the interacting electron gas in a quantum wire. The spectra of intersubband spin-flip excitations reveal a considerable red shift with respect to single-particle HF energies. That signals on appearance of collective intersubband spin-density excitations due to the exchange interaction. The long wavelength dispersions of the intrasubband collective spin-density excitations are linear, but the sound velocities are renormalised due to the exchange interaction and screening. The in-phase intrasubband charge-density excitation has the long wavelength form \( q(−\ln(q))^{1/2} \). We found good qualitative agreement of our results with experimental observations.

A semiconductor quantum wire can be fabricated by applying a voltage with a microstructured gate to a 2D electron gas. The single-particle energy (SPE) spectrum typically consists of subbands separated by several meV. At a 1D electron density about \( 10^6 \text{cm}^{-1} \) more than one subband can be occupied. In recent years progress has been made in spectroscopic study of such systems. In angular resolved Raman spectra of GaAs quantum wires\(^1, 2, 3\), collective spin-density excitations (SDE) and charge-density excitations (CDE, or plasmons) were observed. The measured spectra cover from low to high frequency, and for low-frequency intrasubband excitations, the wave-vector dependence of the spin-wave energy was found to be linear. The correct interpretation of these experiments allows us not only to understand the interesting physical processes, but also to access important physical parameters.

The exchange interaction is crucial to the collective intrasubband and intersubband SDE. Similar to the direct long range Coulomb interaction which leads to the depolarisation shift of single-particle excitations and to the appearance of collective plasma modes, exchange interaction gives rise to the red-shift of SPE. If the red-shift is sufficiently large, the collective SDE with a sizable oscillator strength splits off the continuum of SPE. For semiconductor quantum wells, such split-off appears in the Hartree-Fock Random Phase Approximation (HF-RPA)\(^4, 5, 6, 7\). Thus, it is important to perform a HF-RPA analysis on collective electron excitations in a realistic GaAs quantum wire with full Coulomb interaction, and compare the results with measured spectra\(^8, 9, 10\). The selfconsistent and conserving\(^8\) HF-RPA is suitable for this task, because we will calculate the two-particle spectra but not single-particle properties. As in using any approximation, the HF-RPA calculation also contains error. However, our HF-RPA results agree very well with experimental measurements.

In this Letter we will first outline the HF-RPA method to express the spin or charge correlation functions in terms of the corresponding spin- or charge-density induced...
matrix, which satisfies an eigenvalue matrix equation. In a realistic quantum wire, for high energy intrasubband excitations and for excitation spectra when more than one subband is occupied, the self-consistent equations have to be solved numerically. However, for the case that only one subband is occupied, the analytical expressions of SDE and CDE are derived. With additional approximation applied to the HF-RPA analytical solutions, they reduce to known results. This may be coincidental, but is outside the central theme of this Letter.

To define the quantum wire, let us start from an electron gas in a narrow quantum well with interfaces parallel to the x-y plane, and the well width shorter than any other relevant length scales. We consider the realistic experimental situation that only the lowest subband in the quantum well is occupied, so the motion of electrons in the z direction can be ignored. By applying a properly designed gate potential, a quantum wire along the x axis is fabricated with a longitudinal constant electrostatic potential, but a transverse parabolic one \( V_C(y) = m^* \omega_0^2 y^2 / 2 \) along the y axis, where \( m^* \) is the electronic effective mass. The quantum wire has a finite length \( L_x \), and we assume periodic boundary conditions. In the absence of electron-electron interaction, the single particle eigenfunctions are simply \( \psi_{nk}(x, y) = \exp(ikx) \psi_{nk}(y) \), with the corresponding eigenenergies \( \epsilon_{nk} = \hbar \omega_0 (n + 1/2) + (\hbar^2 k^2) / (2m^*) \), where \( n \) is the subband index, \( k = \text{integer} \times 2\pi / L_x \), and \( \psi_{nk}(y) \) the harmonic oscillator wave function. The transverse confinement length of the electrons is \( l_0 = \hbar / (m^* \omega_0)^{1/2} \).

When the electron-electron interaction is turned on, we will use the HF approximation

\[
\begin{align*}
\{ - \frac{\hbar^2}{2m^*} \nabla^2 + V_C(y) + \frac{2\epsilon^2}{\kappa} \int d\vec{r} \sum_b f_b |\psi_b(\vec{r})|^2 & \} \psi_a(\vec{r}) \\
- \frac{\epsilon^2}{\kappa} \int d\vec{r} \sum_b f_b \frac{\psi_b^* (\vec{r}) \psi_b(\vec{r})}{|\vec{r} - \vec{r}'|} \psi_a(\vec{r}') &= \epsilon_{HF}^a \psi_a(\vec{r})
\end{align*}
\]

to derive a complete orthonormal basis \( \{ \psi_a(\vec{r}) \} \) of quasi-particle Hartree-Fock states, where \( \epsilon_{HF}^a \) is the Hartree-Fock energy, \( f_a \) is the Fermi occupation factor and \( \kappa \) the dielectric constant of the surrounding medium. In terms of this basis set, we will use the corresponding time dependent HF (HF-RPA) to calculate the charge-density and the spin-density correlation functions, which describe the self-consistent linear response of the electron gas to an external perturbation. In this Letter, we restrict ourselves to the nonmagnetic ground state.

For inelastic light scattering not close to the band gap resonance, the Raman intensities in polarised and depolarised scattering geometries are proportional, respectively, to the imaginary parts of the charge-charge correlation function and spin-spin correlation function [9]. If we define \( \hat{\rho}(\vec{q}, t) \) as the Fourier transform of the charge-density operator and \( \hat{\sigma}(\vec{q}, t) \) the Fourier transform of the spin-density operator along the spin quantisation axis, then, these correlation functions are \( \chi^\nu(\vec{q}, \omega) = -\frac{\epsilon}{\hbar} \int_0^\infty dt e^{i\omega t} \langle [\hat{\rho}(\vec{q}, t), \hat{\sigma}(-\vec{q}, 0)] \rangle \) with \( \nu = \sigma, \rho \), where \( \langle \ldots \rangle \) denotes a thermodynamic average. In HF-RPA, they can be expressed as \( \chi^\nu(\vec{q}, \omega) = \sum_{cd} K_{cd}^\nu(\vec{q}, \omega) \langle c | \exp(-i\vec{q} \cdot \vec{r}) | d \rangle \) in terms of the \( \nu \)-density induced matrix \( K^\nu \). The charge-density induced matrix satisfies

\[
K_{\nu ab}^\nu(\vec{q}, \omega) = \frac{f_b - f_a}{\hbar \omega + i0^+ - (\epsilon_{HF}^b - \epsilon_{HF}^a)} |2 \langle a | e^{-i\vec{q} \cdot \vec{r}} | b \rangle^*|
\]

for high energy intrasubband excitations and for excitation spectra when more than one subband is occupied, the self-consistent equations have to be solved numerically. However, for the case that only one subband is occupied, the analytical expressions of SDE and CDE are derived. With additional approximation applied to the HF-RPA analytical solutions, they reduce to known results. This may be coincidental, but is outside the central theme of this Letter.

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\]
where $V_{abcd} = \int d\vec{r} \int d\vec{r}' \psi^*_a(\vec{r}) \psi_d(\vec{r}) \psi^*_b(\vec{r}') \psi_c(\vec{r}') / |\vec{r} - \vec{r}'|$. $K_{cd}(q, \omega)$ is the Coulomb matrix element in the basis of the HF single-particle states. When $\nu = \sigma$, there is no direct Coulomb interaction (Hartree term) between the electron spins. If the exchange term (Fock term) is neglected, the spin-density excitation spectra are simply given by the quasiparticle Hartree-Fock energies. In HF-RPA, the spin-density excitations are shifted from the quasiparticle Hartree-Fock energies due to the exchange terms. As a result, collective spin-density excitation may appear in the spectra. This shift is a measure of the effective strength of the exchange term in the system.

We will use the above HF-RPA analysis to investigate collective excitations in a multisubband system. This has to be done numerically, and the first step is to derive the quasiparticle basis set $\{\psi_i(\vec{r})\}$ by solving (1) self-consistently via iteration. The functional basis must be sufficient large in order to ensure the required accuracy for the quasiparticle energy spectra and the spatial electron density of the ground state. When using this self-consistent quasiparticle basis set to calculate collective excitations, the required accuracy for the peak position of an excitation energy is the experimental linewidth $\lesssim 0.1 \text{ meV}$.

The intrinsic materials parameters of a GaAs quantum wire required in our calculation are $m^* = 0.067 m_0$ and $\kappa = 12.4$, where $m_0$ is the electron mass. The extrinsic sample parameters are the total electron density $n$, the transverse potential $V_c(y)$, and the length of the quantum wire $L_x$. Our calculations are based on a sample with $n = 10.4 \times 10^5 \text{ cm}^{-1}$, which has been investigated experimentally in Ref. [3]. The transverse potential $V_c(y)$ is determined by the experimental conditions. Since the experimental sample does not have a parabolic potential as can be seen from the intersubband CDE, we will adjust $\hbar \omega_0$ to fit the subband electron occupations. When we set $\hbar \omega_0 = 7.9 \text{ meV} (l_0 = 120 \text{ Å})$, the derived self-consistent Hartree-Fock subband spacing between the two lowest subbands is 5.4 meV at the zone center and 5.6 meV at the Fermi level. The electron densities in the two occupied subbands are $n_0 = 6.4 \times 10^5 \text{ cm}^{-1}$ for the lowest subband (labeled by $i=0$), and $n_1 = 4.0 \times 10^5 \text{ cm}^{-1}$ for the second lowest subband (labeled by $i=1$). The physical properties of the quantum wire are insensitive to its length, provided that the wire is sufficiently long. Therefore, we set $L_x = 1.0 \text{ μm}$. The experiment[3] was done at a temperature 1.7 K, which is the temperature used in our calculation.

Let $k_i$ and $v_i$ be, respectively, the Fermi wave-vector and the Fermi velocity of the $i$th subband. In the limit of long wavelength $q \to 0$, the transverse excitation is forbidden (or allowed) if the excitation energy is low (or high), and so the corresponding physical processes are dominated by intrasubband (or intersubband) transitions. When $q$ increases to $k_0-k_1$, the low energy intersubband transitions are activated. However, collective excitations with large energy and/or large $q$ are strongly damped. To illustrate the main features of long wavelength excitations, let us consider a very simple case by neglecting the electron self-energies and the vertex correction. In this case we obtain analytical results for both the SDE and CDE energies. The SDE dispersion is linear in $q$, with sound velocities $v_0$ and $v_1$ for intrasubband excitations in the two lowest subbands. With two subbands occupied, the CDE dispersion has two branches. The in-phase mode is

$$\omega_p^+(q) = |q| \sqrt{2 (v_0 + v_1) V(q)} / \hbar \pi,$$

where $V(q)$ is the Fourier transform of the Coulomb potential $(e^2 / \kappa) [(x-x')^2 + (y-y')^2]$. However, collective excitations with large energy and/or large $q$ are strongly damped. To illustrate the main features of long wavelength excitations, let us consider a very simple case by neglecting the electron self-energies and the vertex correction. In this case we obtain analytical results for both the SDE and CDE energies. The SDE dispersion is linear in $q$, with sound velocities $v_0$ and $v_1$ for intrasubband excitations in the two lowest subbands. With two subbands occupied, the CDE dispersion has two branches. The in-phase mode is

$$\omega_p^+(q) = |q| \sqrt{2 (v_0 + v_1) V(q)} / \hbar \pi,$$
\(y/2\)\(^{-1/2}\), and the out-of-phase mode is

\[
\omega_r^-(q) = |q|\sqrt{v_0v_1}.
\]

(4)

Such two-band SDE and CDE dispersions are exactly the same results as Schulz\(^{10}\) obtained for a two-subband Tomonaga-Luttinger model (TLM)\(^{11}\).

When we turn on the intrasubband and intersubband exchange interaction, as well as the screening, the SDE and CDE energies will be modified from the above expressions, and have to be derived numerically. In the polarised spectrum, the higher energy region is dominated by strong intersubband CDE. At \(q=0\), the calculated CDE spectrum consists of a single peak which is characteristic to transverse parabolic confinement potentials\(^{12}\). In the region of finite \(q\) the intersubband HF SPE energies show up at 5.5 meV. In the spin-flip depolarised Raman spectrum, we obtained the red shift of intersubband SDE with respect to HF SPE. The SDE has a dominant weight of the spectrum and appears at a resonance energy of 2.1 meV, which is shifted from the HF SPE, indicating the importance of vertex correction. These overall features of our numerical results have been observed experimentally\(^{2,3}\).

In Fig. 1 we show the calculated intrasubband SDE and CDE in the region of energy and frequency for which accurate experimental data are available. The mode with strong intensity is labeled as SDE0, and the next mode with weaker intensity is labeled as SDE1. The inset gives their dispersions, which are linear for small \(q\), with the corresponding sound velocities \(v_{\sigma,0}=0.9v_0\) and \(v_{\sigma,1}=0.7v_1\). These sound velocities are smaller than the respective Fermi velocities because of the exchange screening of SDE induced by the intersubband virtual transitions, and the renormalisation due to the intra- and intersubband exchange interaction. The experiments\(^{2,3}\) seem to have detected only \(v_{\sigma,0}\), which corresponds to the high energy SDE near the Fermi wave vector \(k_0\) of the lowest subband. It is probably the low electron density in the second lowest subband that causes the velocity \(v_{\sigma,1}\) of the SDE to be too small to be observed experimentally. The spin velocity \(v_{\sigma,0}\) agrees quantitatively with the experiment\(^{3}\). For sufficiently large \(q\), because of the finite length of our quantum wire, the Landau damping shows up in Fig. 1 in the form of enhanced intensities of satellite single-particle peaks around the SDE, instead of a broad band if the quantum wire is infinitely long. The mode SDE1 is not damped, since it does not enter the region of SPEs.

The dispersions of the CDE and SDE are also plotted in the inset in Fig. 1. In the long wavelength limit, the in-phase CDE+ can be well fitted with \(q[-\ln(q)]^{-1/2}\) according to \(3\), as expected for 1D electron gas\(^{10,13}\). The out-of-phase CDE- mode, corresponding to \(4\), with an expected linear dispersion\(^{10}\), appears in our calculation as a weak band with a sound velocity \(1.2(v_0v_1)^{1/2}\). This happens to be the same as the sound velocity of the SDE0, an accidental result for this specific sample. The CDE- mode has a much lower intensity compared to the CDE+ mode. Checking against the experiment\(^{2}\), we believe the the lower energy band observed in the low frequency polarised Raman spectrum is our calculated CDE- mode. The decay of the plasmon (CDE+) and the CDE- at higher \(q\) due to the Landau damping is stronger than the decay of SDE0 and SDE1, as shown in Fig. 1.

After the above complete study of a realistic quantum wire, perhaps it is worthwhile to mention some surprising findings for the special case that only the lowest subband occupied at zero temperature, namely, the pure 1D system including spin degrees of freedom. In this case we can drop the band index. For SDE, the
eigenvalue equation has the form

\[ K_x^f(q, \omega) = -\frac{f_{k-q/2} - f_{k+q/2}}{\hbar \omega - (\epsilon^{HF}_{k+q/2} - \epsilon^{HF}_{k-q/2})} \frac{1}{2\pi} \int dq' V(k - k') K_x^f(q, \omega), \]  

(5)

where \( V(k) = (2e^2/\kappa)K_0(q_0) \) for the quasi-1D Coulomb potential \( (e^2/\kappa)[(x-x')^2 + l_0^2]^{-1/2} \), which has a logarithmic singularity \( (-2e^2/\kappa)\ln q_0 \) as \( q \to 0 \). Since the Hartree self-energy is canceled by the potential energy due to the positive background charges, the difference in exchange self-energy at the Fermi energy, \( \Delta_x(q) = \Sigma_x(k_0 + q/2) - \Sigma_x(k_0 - q/2) \) is

\[ \Delta_x(q) = \frac{1}{\pi} \int_{-q/2}^{+q/2} dq' \left[ V(k') - V(k' - 2k_0) \right]. \]

We define \( y(k) \) by \( K_x^f \equiv (f_{k-q/2} - f_{k+q/2})y(k) \), and at \( k = k_0 \) rewrite (5) as

\[ \int_{-q/2}^{+q/2} dq' \left[ V(k')y(k_0 + k') + V(k' - 2k_0)y(-k_0 + k') \right] \]

\[ = 2\pi [\hbar \omega - \hbar q v_0 - \Delta_x(q)] y(k_0). \]  

(6)

In the limit of long wavelength, by substituting \( y(k_0 + k') \approx y(k_0) \) and \( y(-k_0 + k') \approx y(-k_0) \) into the above equation, we see that the contributions of Coulomb potential in the exchange energy and the vertex corrections, both behave as \( q \ln(q) \), exactly cancelling each other. Hence, the \( q \ln(q) \) behaviour of low-energy single-particle excitation due to the exchange self-energy is removed from the SDE and the plasmon energies, and so only the exchange terms at momentum \( 2k_0 \) are important. An equation similar to (6) for \( y_\rho \) at \( k = -k_0 \) can also be derived. In the long wavelength limit, we find the SDE energy

\[ \omega_\rho(q) = |q|v_0 \sqrt{1 - 2g_0}, \]  

(7)

where \( g_0 = V(2k_0)/2\hbar \pi v_0 \). The sound velocity is reduced with respect to the bare Fermi velocity. We have also solved for the CDE and found the plasmon dispersion

\[ \omega_p(q) = |q|v_0 \sqrt{2V(q)}/\hbar v_f + 1 - 2g_0. \]  

(8)

For a long-range Coulomb potential \( V(q) \approx \ln q \), the plasmon energy is not affected by the exchange interaction within the HF-RPA. These results (3) and (5), derived with full Coulomb interaction, differ from those obtained by Schulz (10) for the TLM including a nonsingular backscattering matrix element at \( 2k_0 \), which mixes the right- and the left-traveling modes. Nevertheless, in (3), if we replace the Hartree-Fock energy by the bare single-particle energy, and omit the singular part around \( V(q=0) \) in the vertex correction, then our results exactly reduce to Schulz’s results for the SDE and the plasmon energies. Whether this finding, as well as (3) and (5), is simply a coincidence remains to be clarified.

To close this Letter, we should mention that according to our analysis, the frequency of the lowest energy SDE decreases as \( q \) increases towards \( k_1 \), and then vanishes at a value of \( q \) close to \( 2k_1 \). This behaviour suggests a low temperature intrinsic instability of the electron gas against the formation of spin-density waves (SDW), namely, the Peierls instability. When this instability emerges from our mean-field analysis, we must take into account the SDW long-range order in the ground state. On the other hand, the results of the TLM with backscattering predict the absence of SDW long-range order, but instead the appearance of a slowly decaying Wigner crystal at \( 4k_F \) (11). We guess that the TLM with backscattering describes the real ground state better than HF-RPA. Hence, we believe that our analysis based on
a ground state without SDW long range order is a better approximation than that including SDW in the ground state.

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Figure captions

Figure 1. Intensity of intrasubband SDE and CDE as a function of the frequency shift for different wave vectors $q$. The upper part shows the dispersion of intrasubband CDE and intrasubband SDE. The quantum wire is specified in the text.
