Excitation spectrum of the quasi-one-dimensional electron gas with long-range Coulomb interaction

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Using ground-state energy calculations we calculate the density and width dependence of the spin susceptibility and the compressibility of the one-dimensional electron gas with long-range Coulomb interaction. An oscillator potential is used for the confinement. With the compressibility and the spin-susceptibility sum rule we describe charge-density and spin-density excitations in quantum wires as a function of the electron density and the wire-width parameter. Analytical results are presented. [S0163-1829(98)00831-5]

Spin-density excitations have been observed experimentally in two-dimensional systems[1] and recently in quasi-one-dimensional quantum wires as realized in doped $GaAs/Al_xGa_{1-x}As$ heterostructures.[2] The dispersion was found to be linear in wave number. Together with the experimental studies of charge-density excitations[2] the excitation spectrum of this model system for quasi-one-dimensional systems is known experimentally. The observed dispersion relation for charge-density excitation is in agreement with analytical results for plasmons in one-dimensional systems calculated within the random-phase approximation (RPA).[3] In the following we study many-body effects of electrons in quasi-one-dimensional quantum wires of finite width interacting via a long-range Coulomb potential.

The RPA describes many-body effects in systems with long-range Coulomb interaction. This theory is exact in the high-density limit and must be improved for intermediate and low density.[4] A very powerful approach was developed by Singwi, Tosi, Land, and Sjölander (STLS). For a review, see Ref. 5. This theory provides results for the ground-state energy in good agreement with quasi-exact Monte Carlo calculations. We have recently applied this theory and calculated the ground-state energy of quasi-one-dimensional systems as function of the density[6] and the spin polarization.[7] In fact, the ground-state energy as a function of the density determines the compressibility, while the ground-state energy as a function of the spin polarization determines the spin susceptibility. Using exact sum rules[4,8] one can calculate the collective modes of the system: one finds charge-density and spin-density excitations.

As the model we consider a quasi-one-dimensional electron gas with an effective mass m^* and with the wire axis in the z direction. The confinement in the xy plane is described by a width parameter b. The electron gas is characterized by the one-dimensional carrier density N and a positive background within the jellium model leads to a local neutrality. The Wigner-Seitz parameter r_s for one-dimensional systems is given by $r_s=1/2Na^*$. $a^*=\varepsilon_L/m^*e^2$ is the effective Bohr radius defined with the background dielectric constant ε_L, the electron charge e, and m^*. For Planck's constant we use $h=2\pi$. The energy is expressed in units of the effective Rydberg $\mathrm{Ry}^*=m^*e^4/2\varepsilon_L^2$. For GaAs with $m^*=0.067m_e$ and $\varepsilon_L=12.7$ the relevant parameters are $a^*=100$ Å and $\mathrm{Ry}^*=5.4$ meV. m_e is the electron mass in vacuum. The electron density N defines the Fermi wave number k_F via $N=2k_F/\pi$. The Fermi energy ε_F is given by $\varepsilon_F/\mathrm{Ry}^*=\pi^2/16r_s^2$ and the Fermi wave number k_F by $k_Fa^*=\pi/4r_s$. The Coulomb interaction potential $V(q)$ in the Fourier space depends on the confinement and is expressed as

$$V(q)=\frac{e^2}{2\varepsilon_L}f(qb). \tag{1}$$

For the oscillator confinement potential $U_c(\rho)=\rho^2/8m^*b^4$ with the width parameter b (and ρ is the distance from the wire axis) the interaction potential is given by $f(x)=2E_1(x^2)\exp(x^2)$.[9] $E_1(x)$ is related to the exponential-integral function $\mathrm{Ei}(x)$. We use in our calculation a one-subband model at zero temperature. This means that the Fermi energy must be smaller than the intersubband energy distance $\Delta E_{12}/\mathrm{Ry}^*=a^{*2}/b^2$, which leads for the oscillator confinement to $r_s>r_s^*=\pi b/4a^*$. For $r_s<r_s^*$ at least two subbands are occupied.

The dynamical response function for charge-density fluctuations $\mathbf{X}_c(q,\omega)$ and spin-density fluctuations $\mathbf{X}_s(q,\omega)$ are given in terms of the response function (Lindhard function) of the free electron gas $\mathbf{X}_0(q,\omega)$ by[4,8]

$$\mathbf{X}_{c,s}(q,\omega)=\frac{\mathbf{X}_0(q,\omega)}{1+V_{c,s}(q)\mathbf{X}_0(q,\omega)}. \tag{2}$$

$V_c(q)=V(q)[1-G_c(q)]$ and $V_s(q)=-V(q)G_s(q)$ are the effective potentials including the local-field corrections for charge-density fluctuations $G_c(q)$ and spin-density fluctuations $G_s(q)$. The collective modes are defined by $1+V_{c,s}(q)\mathbf{X}_0[q,\omega_{c,s}(q)]=0$. For $V_c(q)$ one obtains the collective charge-density modes (plasmons) and $V_s(q)$ determines the collective spin-density modes. The dispersion relation $\omega_{c,s}(q)$ for one-dimensional systems is given by

$$\omega_{c,s}(q)=\left[\frac{\Omega_+(q)^2A_{c,s}(q)-\Omega_-(q)^2}{A_{c,s}(q)-1}\right]^{1/2} \tag{3a}$$

with

$$A_{c,s}(q)=\exp[\pi|q|/m^*V_{c,s}(q)] \tag{3b}$$

and

$$\Omega_\pm(q)=v_Fq[1\pm q/2k_F]. \tag{3c}$$

$v_F=k_F/m^*=2\,\mathrm{Ry}^*k_Fa^{*2}$ is the Fermi velocity. Equation (3) was derived to describe collective particle-density modes[10] and later generalized to describe collective spin-density modes[11] of a one-dimensional electron gas with a short-range interaction potential. $\Omega_\pm(q)$ describes the electron-hole spectrum $\omega_{eh}(q)$: $|\Omega_-(q)|\leqslant\omega_{eh}(q)\leqslant|\Omega_+(q)|$ with $\omega_{eh}(q\to0)=v_F|q|$. For small wave numbers one can use $A_{c,s}(q\to0)=1+\pi|q|/m^*V_{c,s}(q\to0)$ and we find

$$\omega_{c,s}(q\to0)=v_F|q|[1+\rho_FV_{c,s}(q\to0)]^{1/2}. \tag{4}$$

$\rho_F=2m^*/\pi k_F$ is the density of states of the free electron gas at the Fermi energy. The collective modes depend on $G_{c,s}(q)$. We note that $V_c(q\to0)>0$ and $V_s(q\to0)<0$ and we conclude that $\omega_s(q\to0)<v_F|q|<\omega_c(q\to0)$.

The long-wavelength behavior of the effective potentials is determined by sum rules for the compressibility κ_c and the spin-susceptibility κ_s via[4,8]

$$1-\kappa_0/\kappa_{c,s}=\lim_{q\to0}[\rho_FV(q)G_{c,s}(q)]. \tag{5}$$

$\kappa_0=16r_s^3a^*/\pi^2\mathrm{Ry}^*$ is the compressibility of the free-electron gas. These sum rules allow one to express the collective modes as a function of $\kappa_{c,s}$ as

$$\omega_c(q\to0)=v_F|q|[\rho_FV(q\to0)+\kappa_0/\kappa_c]^{1/2} \tag{6a}$$

and

$$\omega_s(q\to0)=v_F|q|[\kappa_0/\kappa_s]^{1/2}. \tag{6b}$$

Equation (6) is an essential result of the present paper. Using our numerical results for κ_c and κ_s we derive predictions for the collective modes.

For the oscillator confinement[9] with $f(q\to0)=4[\ln(1/|q|b)-C/2]$ ($C=0.577$ is Euler's constant) we find

$$\omega_c(q\to0)=v_F|q|[16r_s[\ln(1/|q|b)-C/2]/\pi^2+\kappa_0/\kappa_c]^{1/2} \tag{7}$$

and the leading term is $\omega_c(q\to0)\propto|q|[\ln(1/|q|b)]^{1/2}$.[12] For $r_s\to0$ the spin susceptibility is given by $\kappa_0/\kappa_s\approx1$ and we predict $\omega_s(q\to0)\approx\omega_{eh}(q\to0)=v_F|q|$. This is in agreement with experiments made with structures having a high electron density and large wire radius.[2] In the long-wavelength limit the charge-density modes are determined by the interaction potential $V(q\to0)$: the compressibility $\kappa_0/\kappa_c<1$ is only a correction term. The spin-density modes are determined by $\kappa_0/\kappa_s<1$: it is essential to know the spin-susceptibility including exchange *and* correlation.

In order to calculate κ_c and κ_s the ground-state energy $\varepsilon_0(r_s,\zeta)$ per particle as a function of the density parameter r_s and the spin polarization ζ must be known. It is expressed in terms of the ground-state energy of the free electron gas (0), the exchange (ex) and the correlation (cor) contribution.[4] The compressibility κ_c of the one-dimensional electron gas is given as $\kappa_0/\kappa_c=1+\kappa_0/\kappa_{c,\mathrm{ex}}+\kappa_0/\kappa_{c,\mathrm{cor}}$. Numerical results for κ_0/κ_c have been given in Ref. 6. The spin susceptibility κ_s is expressed as $\kappa_0/\kappa_s=1+\kappa_0/\kappa_{s,\mathrm{ex}}+\kappa_0/\kappa_{s,\mathrm{cor}}$. Recently, we derived an analytical expression for $\kappa_{c,\mathrm{ex}}$ and $\kappa_{s,\mathrm{ex}}$: $\kappa_0/\kappa_{c,\mathrm{ex}}=\kappa_0/\kappa_{s,\mathrm{ex}}=-2r_sf(2k_Fb)/\pi^2<0$.[7,13] In the mean-spherical approximation (MSA) the local-field correction is set to zero and we found before $\kappa_0/\kappa_{s,\mathrm{MSA}}=1/[1+4r_sf(2k_Fb)/\pi^2]^{1/2}$.[7] The MSA is very similar to the RPA, however, in the MSA an analytical expression for the static structure factor is used. In the Hartree-Fock approximation (HFA) correlation effects are neglected.

TABLE I. Inverse spin susceptibility $1/\kappa_s$ (in units of the inverse spin susceptibility of the free electron gas $1/\kappa_0$) within the VWN approach (Ref. 14) for various values of r_s and the oscillator confinement parameter b. In the last row we give the values for r_{sc}.

	κ_0/κ_s					
r_s	$b=a^*/5$	$b=a^*/2$	$b=a^*$	$b=2a^*$	$b=3a^*$	$b=4a^*$
0.6	0.758	0.911	0.970	0.991	0.996	0.998
1.0	0.501	0.748	0.891	0.964	0.983	0.990
2.0	0.001	0.314	0.581	0.803	0.890	0.931
3.0			0.266	0.577	0.729	0.815
4.0				0.347	0.543	0.665
5.0				0.132	0.357	0.505
6.0						0.345
7.0						0.191
[r_{sc}]	[1.46]	[2.14]	[2.98]	[4.25]	[5.29]	[6.20]

Some numerical results for the spin susceptibility obtained by using the Vosko, Wilk, and Nusair (VWN) approach[14] are given in Table I for $r_s<r_{sc}$ and different wire width. r_{sc} will be explained later. The results obtained within the VWN approach are in very good agreement with results obtained within the STLS approach.[7] We find $0<\kappa_0/\kappa_s<1$ for $0<r_s\leqslant r_{sc}$ and the spin susceptibility is enhanced near r_{sc}: $\kappa_s\approx4\kappa_0$. An approximating (A) expression for the spin susceptibility $\kappa_{s,A}$, which gives good agreement with our results obtained numerically, is given by

$$\frac{\kappa_0}{\kappa_{s,A}}=\frac{1}{2}\left[(1-p)\,\frac{\kappa_0}{\kappa_{s,\mathrm{HFA}}}+(1+p)\,\frac{\kappa_0}{\kappa_{s,\mathrm{MSA}}}\right]. \tag{8}$$

We get a very good fit to our data in Table I with Eq. (8) for $p=0.55$. $\kappa_0/\kappa_{s,A}$ has a large validity range: $r_s\leqslant r_{sc}$. We believe that $\kappa_{s,A}$ together with Eq. (6b) is useful for experimenters in order to analyze experimental results.

Numerical results for $\omega_c(q\to0)/v_Fq$ and $\omega_s(q\to0)/v_Fq$ versus r_s are shown in Fig. 1 and Fig. 2, respectively. Including only exchange effects we derive $\omega_c(q\to0)=v_F|q|[\rho_FV(q\to0)+1+\kappa_0/\kappa_{c,\mathrm{ex}}]^{1/2}$ and $\omega_s(q\to0)=v_F|q|[1+\kappa_0/\kappa_{s,\mathrm{ex}}]^{1/2}$. For charge-density modes correlation effects become important for larger q values only. For spin-density modes exchange effects are not sufficient to describe many-body effects and correlation effects must be taken into account; see Fig. 2. We suggest studying the collective modes by Raman spectroscopy. Quantum wires with

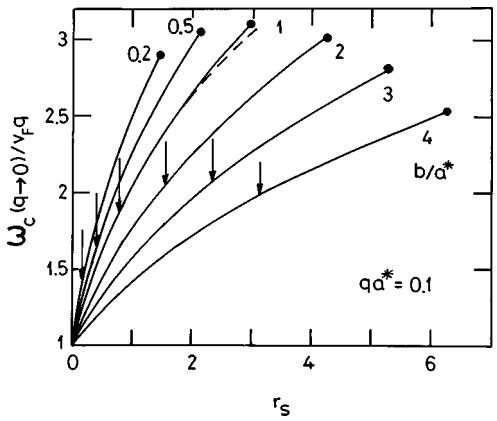

FIG. 1. Charge-density excitation energy $\omega_c(q)$ (in units of $v_F q$) r_s according to Eq. (6a) for different oscillator-confinement parameter b and for $qa^*=0.1$ ($q=1\times10^5$ cm^{-1} and a GaAs wire with $a^*=100$ Å). The solid lines contain exchange and correlation effects. For the dashed line only exchange effects are taken into account (only shown for $b=a^*$). The Wigner-Seitz parameter r_{sc} is shown as a full circle. For $r_s<r_s^*$ two subbands are occupied and r_s^* is indicated by an arrow.

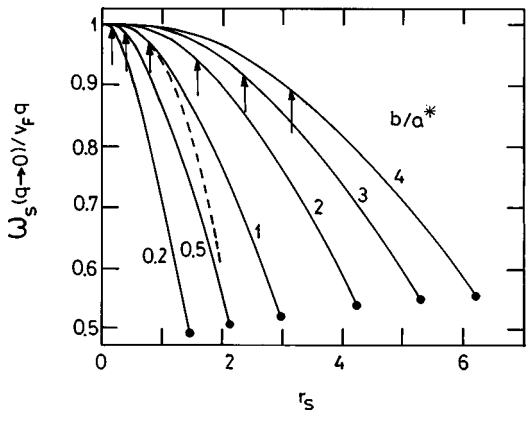

FIG. 2. Spin-density excitation energy $\omega_s(q\to0)$ (in units of $v_F q$) vs r_s according to Eq. (6b) for different oscillator-confinement parameter b. The solid lines contain exchange and correlation effects. For the dashed line only exchange effects are taken into account (only shown for $b=a^*$). The Wigner-Seitz parameter r_{sc} is shown as a full circle. For $r_s<r_s^*$ two subbands are occupied and r_s^* is indicated by an arrow.

a lower electron density than in current Raman experiments[2,15] should be used. We also note that within our theory electron-hole excitations are expected, due to $\mathbf{X}_0(q,\omega)$ in Eq. (2).

Collective modes in quantum wires have been discussed using the bosonization approach[16] and are described by unspecified parameters. The results are not predictive. Ground-state energy calculations are missing and the results for collective modes are not in agreement with our exact results in Eq. (6). This is most clearly seen by taking only exchange effects into account. Moreover, sum rules are not satisfied. We stress that Luttinger-liquid effects, for instance, critical exponents, are described by the STLS approach, which we used in our calculations. This was shown in Ref. 11 for a short-range interaction potential.[17]

In a recent paper we determined the validity range of the STLS approach for a short-range interaction potential.[18] Translated to the present model, this study implies that the STLS approach should give correct values for the compressibility and the spin susceptibility for $r_s<(1.\text{-}1.5)r_{sc}$. In fact, we found that the validity range for the compressibility and the spin susceptibility is larger than for the ground-state energy.[18] We conclude that r_{sc} is at the border of the validity range of the STLS approach. The value r_{sc} introduced in Table I is the largest r_s value for which our theory should be applied. We conclude that the validity range of our theory concerning the charge density excitations (compressibility) and the spin-density excitations (spin susceptibility) is given by

$$r_s^*<r_s<r_{sc} \tag{9}$$

and indicated in Fig. 1 and Fig. 2 by arrows (for r_s^*) and full circles (for r_{sc}). For $r_s>r_s^*$ only one subband is occupied. The results given in Fig. 1 and Fig. 2 for $r_s<r_s^*$ can be considered as guide to experimenters: in that case the number of charge-density (and spin-density) modes should be equal to the number of occupied subbands. We think that even for $r_s<r_s^*$ our prediction for the collective modes (of the lowest subband) should be correct if the electron density in the lowest subband is used to calculate r_s and v_F. We stress that the validity range for the exchange-only calculation for spin modes is $r_s<r_s^*$; see the dashed line in Fig. 2.

For r_{sc} we found[19] $\varepsilon_0(r_{sc},\zeta=0)=\varepsilon_0(r_{sc},\zeta=1)$ and for $r_s>r_{sc}$ we derived $\varepsilon_0(r_s,\zeta=1)<\varepsilon_0(r_s,\zeta=0)$. This would suggest that the electron gas undergoes a Bloch instability and a polarized state is expected for $r_s>r_{sc}$.[20] On the one hand it is not clear if this transition really occurs because the Bloch instability is in contradiction with a theorem predicting the absence of a magnetized state in one dimension.[21] We are not convinced that one can apply this theorem: see our discussion of this theorem in Ref. 7. On the other hand we note that experimental indications for the Bloch instability found in ballistic transport experiments with point contacts have been reported.[22,23] We believe that our finding that $\varepsilon_0(r_{sc},\zeta=1)=\varepsilon_0(r_{sc},\zeta=0)$ either means that for $r_s>r_{sc}$ a new phase is approached or that our calculated values of the ground-state energy cannot be trusted for $r_s>r_{sc}$. In any case our results should only be used for $r_s<r_{sc}$.

We calculated charge-density and spin-density excitations of quantum wires using exact sum rules. Exchange and correlation effects have been taken into account. Spin-density modes cannot be described by exchange-only calculations.

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