Realistic Electron-Electron Interaction in a Quantum Wire

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Abstract

The form of an effective electron-electron interaction in a quantum wire with a large static dielectric constant is determined and the resulting properties of the electron liquid in such a one-dimensional system are described. The exchange and correlation energies are evaluated and a possibility of a paramagnetic-ferromagnetic phase transition in the ground state of such a system is discussed. Low-energy excitations are briefly described.

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In three and two dimensional systems any interaction between electrons (in a forward scattering channel) appears to have a marginal property. This means that the low-energy dynamics of such systems is described by the Fermi liquid theory where quasi-particles are in a one-to-one correspondence with bare electrons. One-dimensional systems are very exceptional in this respect. The interaction between fermions is relevant and leads to a new collective type of a particle motion at low-energies. Such a system is described by the Luttinger liquid theory, according to which a spin-charge separation and an anomalous scaling take place.

A recent progress in nanofabrication enables to construct various one-dimensional structures, in which the Luttinger liquid theory can be experimentally tested. In such structures the effective interaction between the electrons is not a short-range one as in the standard Tomonaga-Luttinger (TL) model. Rather it must be of a long-range type because it originates from the Coulomb electrostatic forces between the charged particles. Accordingly, in such a case certain properties of the Luttinger liquid will be modified.

In this Brief Report we analyze theoretically the form of an effective interaction between the electrons in a one-mode quantum wire, and the corresponding new properties of the system. In particular, we are interested in how ground-state and excitation energies will be affected by a difference between the dielectric constants of the wire and its environment. Such a difference is large in the case of free standing wires, particularly of IV-VI semiconductors such as PbTe, characterized by a large static dielectric constant $\epsilon \approx 1000$. This very large dielectric constant is due to the proximity of this system to the ferroelectric phase transition. In those cases the electrostatic potential between the electrons is strongly modified because of the presence of image charges that assure the correct boundary conditions.

In order to determine the form of the interaction in such a system we consider a model, in which the electrons can propagate along an infinitely long cylinder of radius $a$, made of a material with a macroscopic dielectric constant $\epsilon_1$. This cylinder is embedded into a bulk system with a macroscopic dielectric constant $\epsilon_2$. Further, we assume that the single-electron wave function vanishes at the boundary of this cylinder. In other words, an electron moves
in a cylindrical potential well with infinite barriers. Eigenfunctions $\Psi_{nmk}$ in such a geometry are readily to find, and the result in the cylindrical coordinates $(\rho, \phi, z)$ is,

$$
\Psi_{nmk}(\rho, \phi, z) = \frac{1}{a\sqrt{\pi}J_{m+1}(X_{mn})} J_m \left( \frac{X_{mn}}{a} \rho \right) e^{im\phi} e^{\pm iqz} \sqrt{L},
$$

(1)

where $J_m(x)$ is the Bessel function, $X_{mn}$ are nodes of $J_m(x)$, $(n, m, q)$ is a set of quantum numbers.

In the following we are interested in properties of the quantum wire when only the lowest quantum level $(n = m = 0)$ is occupied. In this case the radial dependence of the wave function (1) can be approximated very well by the following parabola

$$
\psi(\rho) = \begin{cases} 
\sqrt{\frac{3}{\pi a^2}} (1 - \left(\frac{\rho}{a}\right)^2) & \text{for } \rho < a \\
0 & \text{otherwise.}
\end{cases}
$$

(2)

An electrostatic potential $V(r - r_0)$ between two electrons is determined by solving a Poisson equation $\nabla^2 V = -\frac{4\pi e}{\epsilon_1} \delta(r - r_0)$, where $e$ is an charge of an electron, with appropriate boundary conditions at $\rho = a$, i.e., $V_1 = V_2$ and $\epsilon_1 \partial_\rho V_1 = \epsilon_2 \partial_\rho V_2$. As a result we find that

$$
V(r - r_0) = \frac{e^2}{\epsilon_1} \sum_{m=-\infty}^{\infty} \int_0^\infty d\lambda e^{im(\phi - \phi_0)} \cos[\lambda(z - z_0)] \left[ I_m(\lambda \rho_\rho) K_m(\lambda \rho_\rho) + \frac{1}{\epsilon_1} \left( \frac{\rho_\rho}{\epsilon_1} \right) K'_m(\lambda \rho_\rho) I_m(\lambda \rho_\rho) - K_m(\lambda \rho_\rho) I'_m(\lambda \rho_\rho) + \frac{I_3(|\rho\rho|) K_3(|\rho\rho|)}{|\rho\rho|^4} \right],
$$

(3)

where $\rho_\rho \equiv \min(\rho, \rho_0)$, $\rho_\rho \equiv \max(\rho, \rho_0)$, $I_m(x)$, $K_m(x)$ are the modified Bessel functions and primes denote their derivatives. We have not considered here effects coming from electrodes, which are usually attached to the system, assuming that they are very far from each other and modify the system properties only very close to the edges. However, for short wires and quantum point contacts the electrodes may be important as well.

An effective Hamiltonian describing electrons in a 1D quantum wire with the lowest level occupied only $(n = m = 0)$ has a two-body matrix element (determined in a one-particle basis of states (2)) in the following form:

$$
V(aq) = \frac{36 e^2}{\pi \epsilon_1 |aq|} \left[ \frac{10}{10} - \frac{1}{3 |aq|^2} + \frac{1}{3 |aq|^4} - \frac{64}{|aq|^4} I_3(|aq|) K_3(|aq|) \right] + \frac{6 e^2 A_0(|aq|)}{\pi \epsilon_1 |aq|} \left[ I_1(|aq|) - \frac{4}{|aq|} I_2(|aq|) + \frac{8}{|aq|^2} I_3(|aq|) - 2 I_3(|aq|) + \frac{8}{|aq|} I_4(|aq|) + I_5(|aq|) \right],
$$

(4)
where
\[ A_0(|aq|) = \frac{(1 - \frac{\epsilon_2}{\epsilon_1})K'_0(|aq|)K_0(|aq|)}{\frac{\epsilon_2}{\epsilon_1}K'_0(|aq|)I_0(|aq|) - K_0(|aq|)I'_0(|aq|)}. \] (5)

The first part, which was found previously in Ref. 7, corresponds to the long range Coulomb interaction between the electrons moving in a quasi-1D constriction. The second part, which disappears when \( \epsilon_1 = \epsilon_2 \), describes the interaction between an electron and the image charges, which assures the proper boundary conditions.

In Fig. 1, we plotted the matrix element \( V(aq) \) as a function of \( aq \) for different ratios \( \epsilon_1/\epsilon_2 = 1, 10, 100 \). We see that \( V(aq) \) is a decreasing function of \( aq \) and for large values of \( aq \) becomes relatively small. Additionally, we find that the numerical values of \( V(aq) \) diminish when the dielectric constant \( \epsilon_1 \) increases and this reduction is very different when the image charges are taken into account as is shown in the inset to Fig. 1. For small \( aq \), however, the effective interaction is seen to diverge. We have been able to examine this limit analytically and found that at \( |aq| \ll 0 \) the matrix element behaves as
\[ V(aq) = \frac{e^2}{\pi \epsilon_2} \left\{ -\ln \frac{|aq|}{2} + \left[ \gamma \left( 2 \frac{\epsilon_2}{\epsilon_1} - 1 \right) - \frac{73}{120} \frac{\epsilon_2}{\epsilon_1} \right] + (aq)^2 \left[ \frac{\gamma^2}{2} \left( 1 - \frac{\epsilon_1}{\epsilon_2} \right) - \frac{\gamma}{16} \left( 1 + \frac{\epsilon_2}{\epsilon_1} \right) + \frac{1}{4} \right] \right. \]
\[ - \frac{89}{840} \frac{\epsilon_2}{\epsilon_1} + \left( \gamma \left( 1 - \frac{\epsilon_1}{\epsilon_2} \right) - \frac{1}{16} \left( 1 + \frac{\epsilon_2}{\epsilon_1} \right) \right) \ln \left| \frac{aq}{2} \right| + \frac{1}{2} \left( 1 - \frac{\epsilon_1}{\epsilon_2} \right) \ln^2 \left| \frac{aq}{2} \right| \left\} + \frac{\epsilon_2}{\epsilon_1} \right\}, \] (6)

so it diverges logarithmically (\( \gamma \) is the Euler constant). This behavior is characteristic for a 1D Fourier transform of the Coulomb interaction \( e^2/r \) (with \( a \) as a short-distance cut off). However, it is surprising that \( V(aq) \) for \( |aq| \to 0 \) does not depend on the dielectric constant \( \epsilon_1 \) of the wire but only on the dielectric constant \( \epsilon_2 \) of the environment. This means that as the wire is infinitely thin (or particles are very far from each other) a single electron interacts mainly with the image charges and not directly with the other electrons in the wire. We have checked explicitly that the disappearance of the dielectric constant \( \epsilon_1 \) in the first leading term takes place for both wave functions (1) and (2), which are separable in the cylindrical coordinates.

Having determined the analytical form of the electron-electron interaction matrix element we can calculate ground state properties of such a quantum wire. We assume that the
electrons propagate in a jellium environment with positive ion charges. This leads to the cancelation of a direct self-energy contribution, which otherwise brings about infinities in the perturbation expansion. Hence, the Hartree-Fock correction to the ground state energy has the simple form

\[ E_{HF}^x = -2 \int_{-k_F}^{k_F} \frac{dk}{2\pi} \int_{-k_F}^{k_F} \frac{dp}{2\pi} V(a|k - p|), \]  

(7)

and its numerical values are depicted in Figs. 2a and 2b, for the different radii \( a \) of the wire and the different RPA parameters \( r_s \equiv (2a_0^*n)^{-1} \), where \( n \) is the density of the 1D electron gas. All results below are presented in the atomic units where \( a_0^* = \frac{a_0}{m^*e^2} \) is the effective Bohr radius, and \( \text{Ry}^* = \frac{\text{Ry}}{2\pi} \) is the effective energy unit; so-called the effective Rydberg. Note that since in the leading term of the expansion (6) only the dielectric constant \( \epsilon_2 \) appears, we have defined the effective Rydberg and the effective Bohr radius with \( \epsilon_2 \). We see from Figs. 2 that, as expected, the absolute value of the exchange energy is smaller for either a wider wire \( (a = 10) \), a less dense electron gas in the wire \( (r_s = 4) \), and a greater dielectric constant \( \epsilon_1 \). However, the decay of \( E_{HF}^x \) with \( \epsilon_1 \) is significantly weaker in our model (4) than in the model of Ref. 7, in which no image charges were considered, \( A_0 = 0 \), as is shown in the inset to Fig. 2a. This comparison convincingly demonstrates the important influence of the image charges upon the ground state energy of the wire.

We have also evaluated a correlation energy \( E_c \), i.e., the correction to the Hartree-Fock energy originating from a linear screening of the electron-electron interaction due to electron-hole excitations. For that we calculate the effective (RPA) interaction, which in the static limit has the form

\[ V_{\text{RPA}}^{\text{eff}}(aq) = V(aq)/\epsilon(aq), \]

with the dielectric function \( \epsilon(aq) \) approximated as \( \epsilon(aq) \approx 1 + 2V(aq)/\pi v_F \), where \( v_F = \frac{\hbar k_F}{m^*} \) is the Fermi velocity. The correlation energies \( E_c \) are plotted in Figs. 3a and 3b for the various wire’s radii \( a \) and the parameters \( r_s \).

In order to estimate the transition line between the paramagnetic and the ferromagnetic ground states we compare the ground state energies for these two phases. Our results are shown in Fig. 4 for the two wire’s radii \( a = 1 \) and 10. The critical value of the RPA parameter
$r^c_s$, above which the system would be completely polarized, increases with increasing $\epsilon_1$. This increase is, however, sublinear which indicates that the effects of the Coulomb carrier-carrier interaction may remain important even in nanostructures with a large bulk dielectric constant. At the same time, if there was $\epsilon_1 \ll \epsilon_2$ then the critical value of $r^c_s$ would go rapidly to zero (c. f. the inset to Fig. 4). This result suggests that if a quantum wire with a small dielectric constant was deposited on a ferroelectric substrate, then the ferromagnetic phase instability would be even more likely.

It is tempting at this point to make a comment on the so-called 0.7 step in the quantized conductance, which is observed in the quantum point contacts of GaAs/AlGaAs,\textsuperscript{3} and also in PbTe.\textsuperscript{5} Our results make possible to evaluate electron concentrations at which the zero-temperature ferromagnetic instability might appear. However, we cannot exclude other types of instabilities, e.g., the charge- or the spin-densities-waves, which are not discussed in the present paper.

Finally, we briefly describe the low energy excitations in our model. As is known, arbitrary weak interaction destroys the Fermi liquid description in one dimensional systems. Instead, the Luttinger liquid theory emerges as the proper low-energy principle in this case.\textsuperscript{3}

The one-dimensional model of interacting electrons can be solved exactly in the low-energy limit by means of a bosonization.\textsuperscript{3} In our case we must linearized the dispersion relation $\epsilon_k - \epsilon_F = v_F(\pm k - k_F)$, where $v_F = h k_F/m^*$ is the Fermi velocity at the two Fermi points $\pm k_F$. Next, we introduce the so-called left and right moving operators corresponding to $\pm v_F$, respectively, and then define fluctuation density operators $\hat{\rho}_{q\sigma\alpha} = \sum_k c_{k+q\sigma\alpha}^\dagger c_{k\sigma\alpha}$ for each branch $\alpha = R, L$ separately. In terms of these operators the many body Hamiltonian is bilinear and can be diagonalized exactly because in the low-energy limit $\hat{\rho}_{q\sigma\alpha}$ obeys boson-like commutation relation.\textsuperscript{3}

As a result we find that spectra in the charge and the spin channels are different. Namely, the eigenvalue in the charge sector of the many-body theory is $\omega^c_q = v_F q \sqrt{1 + 2V(aq)/\pi v_F}$, whereas the spin degrees of freedom propagate with the free dispersion relation $\omega^s_q = v_F q$. We see that in the low-energy limit these degrees of freedom are completely separated as in
The model with the logarithmic divergence of $V(aq)$ leads to non-analytic properties of thermal quantities. For example, the specific heat of this system at low temperatures is $C = \gamma T + \beta T \ln T$ contrasting with the standard result in TL model where $C_{TL} = \gamma_{TL} T$. Additionally, a single-particle density of states vanishes at the Fermi level as $N(\omega) \sim \omega^x \ln^y \omega$ with $x$ and $y$ being non-universal constants. Again in TL model $N_{TL}(\omega) \sim \omega^\mu$. Also, as shown by Schultz, the long range correlation functions have logarithmic corrections, and this might drive the system into a Wigner crystal.

In conclusion, these results strongly suggest that the ground state and the low-energy properties of 1D electrons in a quantum wire with the realistic form of the interaction are very different from those expected in the framework of the standard TL-type models. In particular, the actual form of the potential $V(aq)$, and particularly, the screening effects due to the boundaries should modify transport properties in this system. It would, therefore, be very interesting to evaluate directly the conductivity.

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FIGURES

FIG. 1. Fourier transform of the electrostatic interaction, $V(aq)$ as a function of $aq$ for different ratios $\epsilon_1/\epsilon_2$ of the dielectric constants inside and outside the wire of the radius $a$. The inset shows $V(aq)$ as a function of $\epsilon_2/\epsilon_1$ for $|aq| = 0.1$ in our model (solid line) and in the model without the image charges (dashed line).

FIG. 2. Exchange energy as a function of $\epsilon_1/\epsilon_2$ for different: a) radius $a = 1, 2, 5, 10$ with $r_s = 1.0$, b) RPA parameters $r_s = 0.5, 1, 2, 4$ (from bottom to top) with $a = 1.0$. Energy and length units are given in the units of the effective Rydberg and Bohr radius calculated with the effective mass $m^*$ inside the wire and the dielectric constant $\epsilon_2$ outside the wire. The inset compares our model (Eq. 4) (solid lines) with the model without the image charges (dashed lines).

FIG. 3. Correlation energy as a function of $\epsilon_1/\epsilon_2$ for different: a) radius $a = 1, 2, 5, 10$ with $r_s = 1.0$, b) RPA parameters $r_s = 0.5, 1, 2, 4$ with $a = 1.0$.

FIG. 4. Critical value of the RPA parameter $r_s$ as a function of $\epsilon_1/\epsilon_2$ for $a = 1, 10$. Above $r_s^c$ the ferromagnetic phase is a stable ground state. Inset shows the behavior of $r_s^c$ for small $\epsilon_1 \leq 1$. 
Fig. 1, Byczuk & Dietl, PRB

![Graph showing the relationship between \( V(aq) \) and \( 1/\text{Dielectric Constant} \) for different values of \( aq \) with and without image charges. The graph includes a inset showing a comparison between the two cases at \( aq = 0.1 \).]
Fig. 2a, Byczuk & Dietl, PRB

![Graph showing exchange energy vs. dielectric constant](image)

- Horizontal axis: Dielectric Constant
- Vertical axis: Exchange Energy

- Curves labeled as 'a = 1' and 'a = 2' for different cases.
- Inset: Comparison between 'no image charges' and 'with image charges' scenarios.
Exchange Energy

Dielectric Constant

$r_s = 0.5, 1, 2, 4$
Correlation Energy

Dielectric Constant

Fig. 3a, Byczuk & Dietl, PRB

(a)
Dielectric Constant

Correlation Energy

Fig. 3b, Byczuk & Dietl, PRB
Fig. 4, Byczuk & Dietl, PRB

Dielectric Constant

Critical RPA Parameter

\[ a = 10 \]

\[ a = 1 \]

Inset: \[ a = 1 \]