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Coulomb interaction and charging effects in conductance of mesoscopic quantum wire structures

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Abstract. Electron transport in a quantum wire structure is investigated with comprehensive account of Coulomb interaction which includes both the direct interaction of electrons with each other and their interaction via the image charges induced on the leads. The Coulomb interaction is shown to change significantly the electron density distribution along the wire as compared with Luttinger liquid model. Under DC conditions, it causes the charge density to strongly increase near to the contacts with the leads. Together with a proximity effect, this may be a reason of nonuniversal conductance quantization. AC conductance shows a resonant behavior caused by charge waves. The charge wave velocity is renormalized due to the Coulomb interaction in a frequency-dependent manner: the velocity increases noticeably with decreasing the frequency. In the nonlinear regime, the conductance is significantly affected by the charge stored in the wire.

Introduction

Electron-electron (e-e) interaction becomes fundamentally important in one-dimensional structures. The interaction of 1D electrons turns out to be so significant that the Fermi liquid concept breaks down. More adequate becomes a strongly correlated state known as Luttinger liquid (LL) with boson-like excitations [1]. But there are important problems in application of this approach to actual quantum wire structures. First, the commonly used LL model treats the e-e interaction as a short-range one, though in reality the Coulomb interaction is essentially nonlocal. Second, the conductance of mesoscopic quantum wire structure is substantially determined by the wire contacts with leads, so the interaction of quantum wire electrons with leads is to be taken into consideration. Third, when applied voltage is compared with the Fermi energy, the balance of electron flows through the wire breaks down giving rise to a charging of the wire.

This paper aims to examine these problems and investigate phase coherent transport of electrons in a real situation of mesoscopic quantum wire structures with leads.

1 Electron-electron interaction potential

Mesoscopic structure under consideration consists of a quantum wire coupled to two bulky (2D or 3D) highly-conducting regions which serve as leads. The electron in the wire interacts with other ones both directly and via the surface charges which are induced by other electrons on the leads. The actual form of the e-e interaction potential $U(x, x')$ was obtained upon solving the Poisson's equation for electric potential generated by the charges localized inside the quantum wire with account of the highly conducting electrodes as equipotential surfaces.

The potential $U(x, x')$ decreases as $U \approx 1/|x - x'|$ when inter-electron distance is larger than the wire radius a . In the middle part of the quantum wire, $U(x = x') \sim L/a$, L being the wire length. In the vicinity of the contacts ($x, x' \rightarrow \pm L/2$) U goes to zero

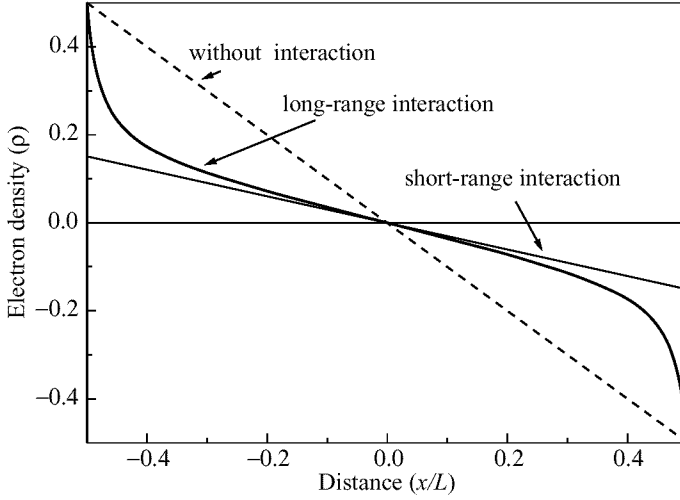


Fig 1. Distribution of the electron density (normalized by $2eV_a/(h\nu_F)$) along the quantum wire.

due to screening effect of the charges induced on the surfaces. The behavior of this kind is quite general for the interaction potential independently of the lead configuration.

2 Coulomb interaction effect on the charge distribution

Transport of the interacting electrons in a quantum wire structure was investigated with using the bosonization technique which is the most appropriate to describe the low-energy excitations of 1D electrons [1] and hence allows us to calculate the linear response to a voltage applied across the electrodes.

The equation of motion were obtained from the bosonized hamiltonian with direct inclusion of backscattering processes [1, 2]

$$H = \frac{1}{2\pi} \int dx v_F \left[(1 + g_1) \pi^2 \Pi^2(x, t) + (1 - g_1) (\partial_x \Phi)^2 \right] - e \int dx \rho(x, t) \varphi_{ext}(x, t) + \frac{1}{2\pi^2} \iint dx dx' (\partial_x \Phi) U(x, x') (\partial_{x'} \Phi) \quad (1)$$

were $\Phi(x, t)$ is the phase field corresponding to the charge excitations, $\Pi(x, t)$ is the momentum density conjugate to Φ , g_1 is the backscattering parameter, φ_{ext} is external potential. Φ is related to the long wave component of the electron density ρ via: $\rho = -\partial_x \Phi / \pi$.

We have developed [3] a method which allows one to solve *exactly* the equation of motion for the phase Φ in the case where the electrode surfaces are plains perpendicular to the wire. The exact solution shows that the Coulomb interaction affects significantly the charge density distribution along the wire, especially at low frequency. DC distribution of the electron density is shown in Fig. 1.

If the e-e interaction is absent, the charge density is distributed linearly with the distance (the dashed line in Fig. 1). The long-range interaction forces the charges to neutralize each other in the middle part of the wire. The LL approach with short-range interaction gives a linear distribution of the density versus the distance, which never can

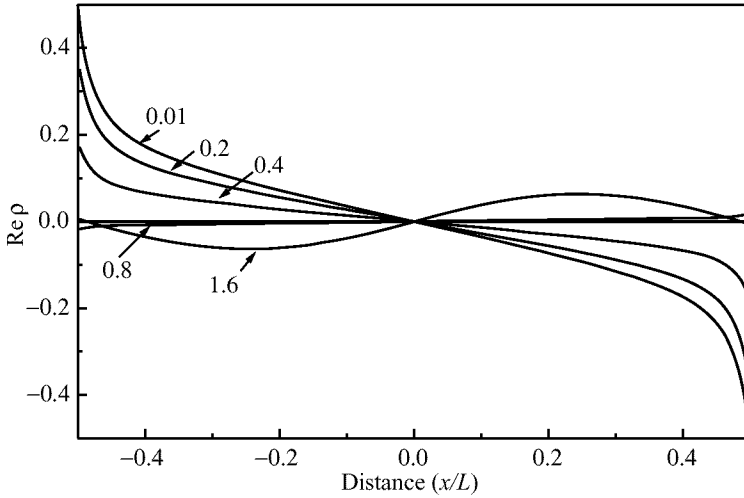


Fig 2. Electron density distribution along the wire for a variety of frequency. The curves are labeled by numbers those are the normalized frequency $\omega L / (2\pi v_F)$.

be fitted to the true result. Near to the contacts the actual value of $|\rho|$ is significantly larger and exponentially decreases with the distance from the contacts.

DC conductance turns out to be equal to the universal step e^2/h independently of the e-e interaction. However we have found that the conductance is determined by the electron density at the contacts with leads where this density is changed sharply. The proximity effect of the electron liquid inside the wire and the electrode should give rise to a change of boundary density. This can be a possible reason of nonuniversal conductance quantization observed in Ref. [4].

When the frequency is increased, charge waves appear (Fig. 2) which propagate along the wire. In contrast with the LL model with short-range interaction, the charge wave velocity we have found, is noticeably dependent on the frequency. This dependence is different from those obtained by Schulz [2] for infinite quantum wire. At low frequency the velocity renormalized by the Coulomb interaction is essentially larger than v_F . With increasing the frequency above a characteristic value, $\omega > [4\pi\lambda e^2 v_F / (\epsilon \hbar L^2)]^{1/2}$ (λ being a parameter determined by the interaction potential) the long-range interaction effect decays and $v \rightarrow v_F$.

3 Impedance of interacting quantum wire structure

AC conductance is characterized by an oscillating behaviour of the real part of the impedance, $\text{Re}Z$, versus the frequency Fig. 3. The oscillations are caused by the charge wave resonances along the wire length [5]. Under the resonance condition the standing wave appears inside the wire. The time-dependent evolution of the electron density consists in flowing the electrons inside the wire from one part to another without passing through the contacts. As a consequence, the electric current component in-phase with the applied voltage is absent and the real part of both admittance and impedance goes to a low value restricted by a possible dissipation. The resonance frequency spectrum shows that the charge wave velocity decreases with the frequency.

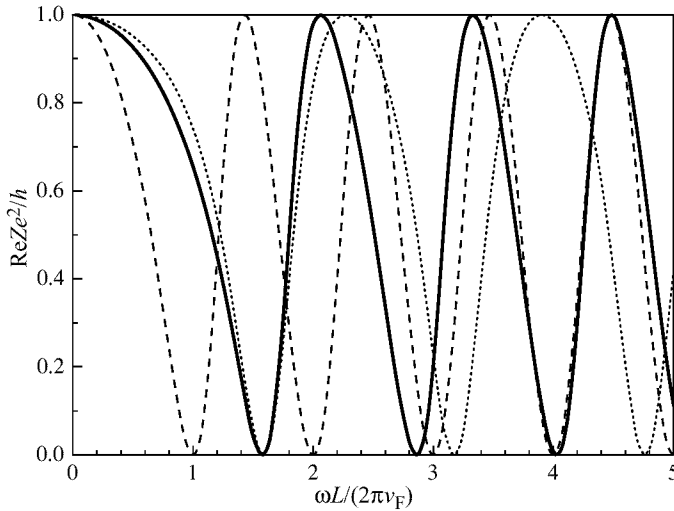


Fig 3. Real part of the impedance versus the normalized frequency for true long-range interaction (—), LL approach with $g = 0.63$ (---) and non-interacting electrons (···).

4 Nonlinear conductance due to charging of the quantum wire

When the applied voltage is compared with the Fermi energy, the conductance becomes essentially nonlinear due to the charging of the wire. The charge in the wire is a sum of the positive background charge and the charge of the electrons incoming from the left and right leads. Applied voltage suppresses the electron flow incoming from the anode lead which results in the positive charge becomes prevailing. The electric potential of the stored charge affects the electron flow injected from the cathode lead and incoming electron density. Nonlinear electron transport is investigated by the self-consistent solution of the Schrödinger equation with an effective potential and the Poisson equation.

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