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Dynamic regime of electron transport in correlated one-dimensional conductor with defect

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HIGHLIGHTS

- Boundary conditions for non-ideal contacts with a quantum wire, which take into account relaxation in the leads, are derived.
- New regime of conduction in which a dc current is supplemented by ac oscillations is predicted in the wire with impurity on a non-ideal contact.
- IV curves and noise spectrum are calculated in the limit of high voltages.
- Both spinless and spinful cases are studied

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ABSTRACT

The electron transport in a 1D conductor with an isolated local defect such as an impurity or a non-adiabatic contact is studied theoretically. A new regime of conduction in correlated 1D systems is predicted beyond the well-known regime of tunneling resulting in the power-law *I–V*-curves. In this regime a quantum wire becomes "opened" at a voltage bias above the threshold value determined by $2k_F$-component of impurity potential renormalized by fluctuations, giving rise to a rapid increase of the dc current, $\bar{I}$, accompanied by ac oscillations of frequency $f=\bar{I}/e$. Manifestations of the effect resemble the Coulomb blockade and the Josephson effect. The spin bias applied to the system affects the *I–V* curves due to violation of the spin-charge separation at the defect site. The 1D conductor is described in terms of the Tomonaga–Luttinger Hamiltonian with short range or long-range Coulomb interaction by means of the bosonization technique. We derive boundary conditions that take into account relaxation in the leads and permit to solve non-equilibrium problems. Charge fluctuations are studied by means of Gaussian model which can be justified strictly in the limit of large voltages or strong inter-electronic repulsion. Spin fluctuations are taken into account strictly by means of the refermionization technique applicable in the case of spin-rotation invariant interaction.

1. Introduction

It is well-known that in 1D systems the interaction between electrons cannot be considered as a small perturbation and the system is described as the Luttinger liquid (LL) that is an alternative to the Fermi liquid for 1D electronic systems (for a review see Refs. [1,2]), and Landau's Fermi-liquid picture where low-energy excitations are single-electron quasiparticles that in many respects behave like non-interacting electrons is not applicable. There are different realizations of 1D electronic systems demonstrating properties of the LL. The examples are semiconductor-based quantum wires in which dimensionality of the conduction electrons is reduced by dimensional quantization and carbon nanotubes, and such distinctive features of the LL as power-law suppression of tunneling into 1D systems and spin-charge separation have been confirmed experimentally, see e.g. Ref. [3].

Electron–electron interaction greatly affects electronic transport in 1D systems. In particular, the back-scattering component of the impurity potential in 1D systems with repulsive inter-electronic interaction scales to infinity under renormalization group transformations. Hence, even isolated impurities form effectively large barriers and strongly suppress conductance [4–6].

On the other hand, the limit of strong interaction between electrons in solids usually leads to the Wigner crystallization. However, in 1D systems the long-range order is destroyed by fluctuations [7]. So, strictly speaking, 1D Wigner crystals do not exist, but the density–density correlation functions of 1D gas with

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Coulomb repulsion contain the $4k_F$ oscillating part which decays extremely slowly [8], like $e^{-c\sqrt{\ln x}}$, that is slower than any power-law. As the period corresponding to $4k_F$ oscillations is exactly the average inter-electron spacing, such a system can be considered as a 1D Wigner crystal with pseudo-long-range order [8]. In the case of short range inter-electronic interaction (which takes place in gated quantum wires where the long-range part of the Coulomb interaction is screened by electrons in the metallic gate) the $4k_F$ density correlations decay slowly as well, as the power-law with a small exponent.

Sliding of electronic crystals contributes to conductance, the most studied case being quasi-1D CDW compounds [9]. Defects pin the CDW but when the driving electric field exceeds a threshold field the CDW starts to slide resulting in non-linear conductance and ac generation at washboard frequencies corresponding to a shift of the CDW by one period [9]. As long as the LL can be interpreted as a 1D form of the 1D Wigner crystal, one can expect a similar dynamic regime of depinning, sliding and ac generation in correlated 1D electron system as well. We show that such a regime does exist, at least, in the quasiclassical limit when quantum fluctuations at the impurity site are suppressed by strong electron–electron interaction. Such a scenario was addressed earlier in our letter [10] where the dynamic regime of conduction accompanied by oscillations of frequency $f=\bar{I}/e$ was predicted in a spinless LL.

Full *I–V* curves of a single-channel LL with a single impurity were studied by means of a thermodynamic Bethe ansatz technique by Fendley et al. [11]. Egger and Grabert [12] calculated the *I–V* curves for a specific value of interaction parameter $K_\rho=1/2$ using the refermionization technique which makes the Hamiltonian quadratic and, hence, solvable exactly. But no non-stationary regime was found. The possibility of generation of self-sustained current oscillations in a quantum wire in a properly designed load circuit was considered in Ref. [13], but these oscillations are a consequence of instability induced by S-shaped *I–V* curves, and their origin is different from the mechanism discussed in the present work. We suppose that the main difference between our approach and Refs. [11–13] is that the equilibrium distribution of incident particles (non-interacting fermions, kinks and anti-kinks, etc.) was assumed in these papers. However, as the distribution of the particles transmitted through the defect is not the equilibrium one, the bosonic excitations of the LL are reflected from the leads to the quantum wire even in the case of adiabatic contacts since the reflection coefficient $r=(1-K_\rho)/(1+K_\rho)$ [14]. Then the incident waves consist in part of the particles reflected from the contact. So if the relaxation inside the conducting channel is small the distribution of the incident particles must not be necessarily the equilibrium one, and this applies equally to fermions derived from bosons after the refermionization. Therefore, one needs to calculate the distribution function of the incident particles, and we perform this by means of boundary conditions which take into account relaxation processes induced by coupling of the quantum wire to the Fermi liquid of the current leads considered as a heat bath. These boundary conditions are valid for non-ideal contacts, and they generalize the boundary conditions by Egger and Grabert [12] and the results of Safi and Schulz [14,15] were derived for expectation values and ideal adiabatic contacts.

We think that the results of Refs. [11–13] are applicable in the limit of conducting channels longer than the damping length of excitations due to coupling of electrons inside the wire to a dissipative bosonic bath (phonons, density fluctuations in a metallic gate, and so on). And we obtain the non-stationary regime of conduction for practically important case of the quantum wire which is shorter than the relaxation length, so that the relaxation is governed by boundary conditions.

The structure of the paper is as follows. In Section 2 we formulate the problem, derive boundary conditions at the contacts, and derive equations of motion for the displacement field at the impurity position. These equations resemble equations of motion of coupled quantum pendulums. In Section 3 we use our equations to study electronic transport in spinless LL. Using the Gaussian model to account for fluctuations, we study *I–V* curves, analyze noise spectrum, study non-Gaussian corrections and find that the Gaussian approximation is justified in the limit of strong interaction between electrons and large voltages. In Section 4 we consider the spinful LL with strong enough interaction between electrons when charge fluctuations at the defect position are small. However, spin fluctuations are large and they are taken into account strictly by means of the refermionization method in spin sector valid in the case of spin-rotation invariant interaction ($K_\sigma=1$). In Section 5 we show that non-adiabatic contacts induce non-stationary effects similar to those induced by impurities. In Section 6 we formulate conclusions.

Below we set e, $\hbar$ and k_B to unity, restoring dimensional units in final expressions when necessary.

2. General formulation

2.1. Problem formulation

We consider a correlated 1D conductor with an impurity at $x=0$ and connected to ideal Fermi-liquid reservoirs at $x=\pm L/2$. The Hamiltonian of the system with impurity consists of two terms $H=H_0+H_i$. The first one is the bosonized Tomonaga–Luttinger (TL) Hamiltonian that maps the 1D system of interacting electrons to free massless bosons described in terms of the displacement fields $\hat{\Phi}_\nu(t,x)$ and the conjugated momentum density $\hat{\Pi}_\nu(t,x)=\partial_x\hat{\Theta}_\nu/\pi$. Here $\nu=\rho,\sigma$ denotes charge and spin channels, respectively. The standard TL Hamiltonian in the Fourier transformed form reads [1,2]

$$\hat{H}_0=\frac{\pi v_F}{2}\sum_{\nu=\rho,\sigma}\int\frac{dq}{2\pi}\left\{\hat{\Pi}_\nu^2+\frac{1}{\pi^2K_\nu^2}q^2\hat{\Phi}_\nu^2\right\} \tag{1}$$

here the LL parameters K_ν, playing the role of the stiffness coefficients of the elastic string described by Hamiltonian (1), are related to the electron–electron interaction potential, and measure the strength of interaction between electrons. In the spin-rotation invariant case considered in our study, $K_\sigma=1$, $K_\rho(q)=1/\sqrt{1+g(q)/\pi v_F}$, where $g(q)$ is the Fourier transformed interaction potential. In the case of the short-range interaction the dependence of g on wave-vector q is usually neglected. For repulsive interaction $K_\rho<1$. In infinite 1D gas with long-range Coulomb interaction described by the approximate form $V_C(x)=e^2/\varepsilon\sqrt{x^2+d^2}$, where ε is a background dielectric constant and d is a diameter of quantum wire, one obtains $g(q)=2(e^2/\varepsilon)K_0(|qd|)$ [8]. Thus

$$K_\rho(q)=\frac{1}{\sqrt{1+\gamma K_0(|qd|)}},\quad \gamma=\frac{2e^2}{\pi\hbar v_F\varepsilon}\approx\frac{2}{137\pi}\left(\frac{c}{v_F}\right)\frac{1}{\varepsilon}, \tag{2}$$

where γ is the dimensionless parameter which measures the strength of the Coulomb repulsion between the electrons.

In the case of the long-range interaction and finite length of the conducting channel the Coulomb potential is modified by screening of the interaction by current leads. The exact form of the screening depends on the geometry of the system. We consider 3D metallic leads forming sheets of a plane capacitor connected by the quantum wire. Then the screening by the leads can be depicted in terms of the image charges, and the interaction potential between charges located at x and x' is described as

$$V(x,x')=\sum_{n=-\infty}^{\infty}[V_C(x-x'+2nL)-V_C(x+x'+2nL+L)], \tag{3}$$