

Charging effects in a quantum wire with leads

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Abstract. We have found that a quantum wire in mesoscopic structures is charged as a result of the electron density redistribution between the wire and the reservoirs, which ones this wire connects. Charging of a wire is investigated in the frame of self-consistent field approach. The wire may be charged positively, negatively or be neutral as a whole. Correspondingly to these cases, a quantum well appear in the wire, a barrier arise between the wire and the leads or Friedel oscillations appear in the vicinity of the contacts. Charging of a quantum wire produces a variation in its conductance. This effect is especially important in non-linear transport regime.

Introduction

A great deal of interest is paid now to recent experiments on coherent electron transport in quantum wires [1, 2, 3]. Nonuniversality of conductance quantization [4] and especially the observation of $0.7 \cdot 2e^2/h$ conductance [5] show that new physical approaches based on many-body physics and exchange interaction should be attracted to understand these results. In this paper we draw attention to a charging effect of quantum wires which occurs in real quantum wire structures and, as far as we know, was not considered up to now. We show that together with an exchange interaction effect it has a profound impact on a conductance of mesoscopic quantum wires.

It is usually supposed, that the quantum wire has no charge as a whole (and in general, is locally neutral, if any impurity is absent there). In reality this is not the case. Certainly, a quantum wire (if it could be considered separately from the whole structure, it enters in which one) is neutral. However when a quantum wire is connected to the leads, which are bulky reservoirs of electrons, an equilibrium state of the whole system is established by means of the electron density redistribution between the wire and the leads. This results in charging the quantum wire. The analysis shows that three cases are possible depending on whether the chemical potential in the isolated wire is higher, lower or equal to that of the reservoirs.

(i) Electrons escape from the quantum wire when the equilibrium is established. In this case the wire is charged positively and a potential well for electrons appears there.

(ii) Electrons come into the quantum wire giving rise to a negative charge there. This charge creates a potential barrier appears which hinders the electrons to travel through the wire.

(iii) The electron density is not redistributed between the wire and the reservoirs when the equilibrium is established. In this case, the wire is not charged as a whole, though the Friedel oscillations of the electron density are presented near the contacts.

The charge, accumulated in a wire, and especially its change under the action the applied voltage produces an essential effect on the conductance. In particular, this may be a reason of anomalies observed experimentally.

1 The model

The approach we use here to study the charging effect in quantum wires is based on the consideration of a quantum wire and electron reservoirs as a unified quantum mechanical system with describing the electron-electron interaction within self-consistent Hartree–Fock approximation. Though this approximation underestimates correlation effects, it is very suitable to study charging effects, especially for nonlinear transport. The electron transport is described using one-dimensional Schrödinger equations while the electric field and the electron-electron interaction potential are determined from the solution of a three-dimensional Poisson equation with account of image charges induced on the lead surfaces [4]. For the sake of simplicity we restrict ourselves here with one-mode wires. The one-particle wave functions $\psi_{r,k}(x, t)$ are classified by quantum numbers k and $r = \pm$, where $r = +$ denotes the electrons incident on the wire from the left reservoir and $r = -$ does from the right one, k is wave vectors in the left and right reservoirs, where electron-electron interaction is screened owing to high conductivity. The wave functions are defined by equation

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi_{r,k}}{dx^2} + \left[U_0(x) - e\varphi_{\text{ext}}(x) - U_b(x) + U_H(x) + \hat{A} \right] \psi_{r,k} = \varepsilon_r(k) \psi_{r,k}, \quad (1)$$

where U_0 is the built-in potential due to lateral confinement in the quantum wire, $\varphi_{\text{ext}}(x)$ is an external potential, U_b is built-in potential of the positive background charge in the wire, $U_H(x)$ is the Hartree potential, \hat{A} is the exchange interaction operator,

$$\varepsilon_r(k) = U_0(-r \cdot \infty) + V_a \delta_{r,-} + \frac{\hbar^2 k^2}{2m}.$$

The electron density n_e (as well as an exchange density) in the wire is defined with using distribution functions in reservoirs $f_{\pm}(k)$ which are Fermi functions shifted in energy due to the applied voltage

$$n_e(x) = \frac{1}{\pi} \sum_{r=\pm} \int_0^{\infty} dk' f_r(k') |\psi_{r,k'}(x)|.$$

The potentials U_b , U_H and \hat{A} are defined in terms of Green's function $G(x, x')$ of the Laplace equation in the inter-reservoir space. Thus,

$$U_b(x) = \frac{e^2}{\epsilon a} \int_{-L/2}^{L/2} G(x, x') n_b dx',$$

where n_b is a positive background charge density. n_b should be compared with the density $n_0 = 2[2m(\mu_0 - U_0)]^{1/2}/\pi\hbar$. Depending on whether n_b is higher, lower or equal to n_0 , the chemical potential in the wire μ_w is higher, lower or equal to that in the reservoirs μ_0 .

We have solved Eq. (1) numerically considering $\psi_{r,k}(x)$ as a function of two continuous variables: x and k . The solution gives the self-consistent distribution of the electron density and the electric current.

2 The equilibrium state

The ground (equilibrium) state is obtained at $V_a = 0$. The potential energy of electrons $U = U_0 + U_b + U_H$, which includes the self-consistent Hartree potential, is shown in Fig. 1

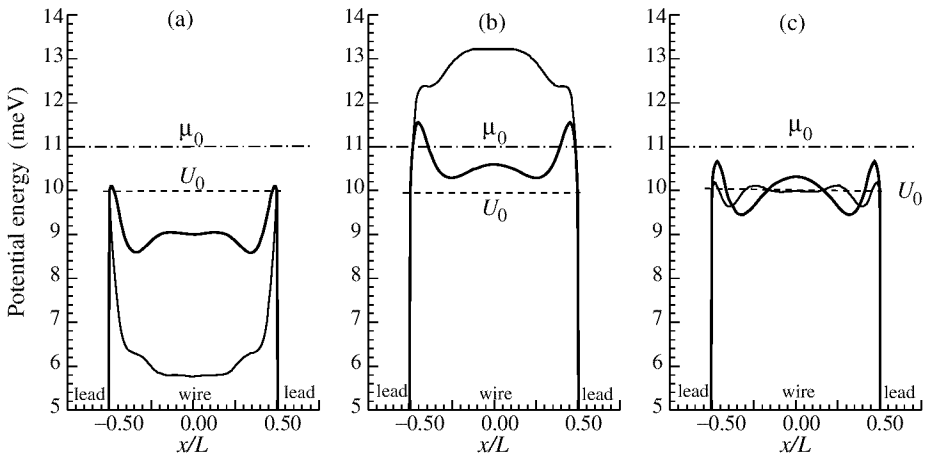


Fig. 1. Potential energy of an electron as a function of distance for cases (a), (b), (c) where $n_b/n_0 = 1.5, 0.5, 1.0$. Thick solid lines were obtained for $\mu_0 - U_0 = 1$ meV, dash-dotted line is the chemical potential, dotted line is U_0 energy. Thin solid lines show the potential energy for $\mu_0 - U_0 = 5$ meV. The parameters used in calculation were: the wire radius $a = 5 \cdot 10^{-7}$ cm, the wire length $L = 10^{-5}$ cm.

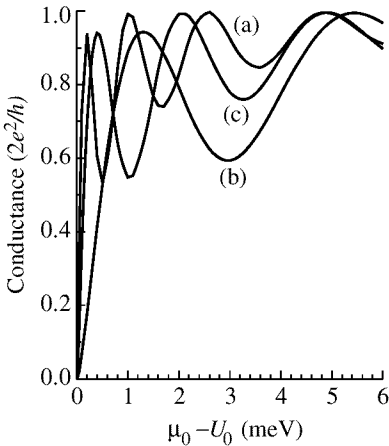


Fig. 2. The dependence of conductance on the chemical potential for the cases (a), (b), (c).

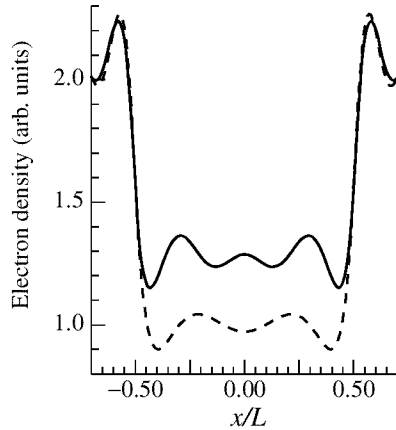


Fig. 3. The electron density distribution calculated with account of the exchange interaction (solid line) and ignoring it (dashed line).

as a function of the distance for three cases: (a) $\mu_w > \mu_0$, (b) $\mu_w < \mu_0$, (c) $\mu_w = \mu_0$. In the first case, the self-consistent potential causes a quantum well to appear in the wire. In the second case a barrier rises between the wire and the reservoirs. When the chemical potential μ_0 is close to U_0 this barrier may be higher than the chemical potential level. This means that the electrons have to tunnel through the self-consistent barrier. In the third case, the Friedel oscillations are only presented near the contacts.

3 The conductance

Figure 2 shows the dependence of the linear conductance upon the chemical potential μ_0 for cases (a), (b) and (c). The conductance is seen to depend on the self-consistent potential, which appear due to the electron density redistribution between the wire and the leads.

Variation of charge piled up in the wire with the applied voltage is a mechanism of non-linear conductance. Under certain conditions it may results in a current instability.

4 Exchange interaction effect

The above results were obtained without inclusion the exchange interaction. Exchange interaction gives rise to an effective electron-electron attraction which results in lowering the energy of the ground state and finally in electron density increase, as is demonstrated in Fig. 3.

Effect of exchange interaction is partially compensated by electron-electron correlation, however the main our result remains as before: the charging of a quantum wire really occurs and produces an essential effect on the conductance.

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