Effects of Repulsive Dopants on Quantum Transport in a Nanowire

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We present an analysis of quantum coherent transport inside a nanowire in presence of a repulsive dopant [1]. In particular, we focus on the current that flows inside the nanowire and which depends on the potential energy of the dopant. The latter is modeled by a screened Coulomb potential centered in the middle of the wire. The electron evolution has been studied by using the Wigner transport equation:

$$\left[\frac{\partial}{\partial t}+\ \frac{\mathbf{p}}{m}\cdot\nabla_r\right]f_w(\mathbf{r},\mathbf{p},t)=\ \int d\mathbf{p}'\,V_w(\mathbf{p}-\mathbf{p}',\mathbf{r})f_w(\mathbf{r},\mathbf{p}',t)\ . \quad (1)$$

Pure states corresponding to Gaussian wave packets are injected from the bottom contact, which in particular avoids the decoherence effects characterizing ohmic contacts [2]. The chosen formalism allows to treat both the quantum and the classical evolution in the same framework, allowing to conveniently highlight the quantum effects. A stochastic reformulation of the Wigner transport model named the signed-particle approach is used [3]. In this formulation the Wigner function is modeled by numerical particles that evolve in the phase space along forceless Newtonian trajectories as suggested by the left-hand side of (1). The quantum effects are governed by the Wigner potential V_w, obtained from the electric potential of the dopant. V_w determines the generation of couple of particles, with opposite sign. The Wigner function in the phase space cells is given by the sum of the sign of the particles inside, legitimizing the annihilation of particles with opposite sign in the same cell. The current density inside the nanowire can be determined as the first order moment of the Wigner function,

$$\mathbf{J}(\mathbf{r},\mathbf{p},t)=n(\mathbf{r},t)\ \ \mathbf{v}(\mathbf{r},t)=\frac{1}{m}\int\mathbf{p}f_w(\mathbf{r},\mathbf{p},t)d\mathbf{p}\ . \quad (2)$$

Fig. 1a) and Fig 1b) show the current density inside the nanowire in the classical and in the quantum case, respectively, with a 0.35 eV dopant. In contrast to the classical case, where the current density after the dopant is established by the boundary reflection, the quantum current is distributed due to a complicated interplay of reflection, nonlocal action of V_w, and tunneling effects [1]. As a consequence, the total current inside the nanowire is higher in the quantum case, as shown in Fig. 2. However, both the classical and the quantum case offer lower currents as compared to the case where no dopant is present. In Fig. 3, we show the decrease of the current with the increase of the dopant potential. Fig. 4 shows the ratio between the quantum and the classical current that starts from 1.0, in absence of the dopant, to around 1.1 (a 10% increase) for a 0.35 eV dopant.

The research particularly illustrates why a global treatment is needed to model quantum current transport as the results can be different for closed physical setups as illustrated by the considered density and current behavior.

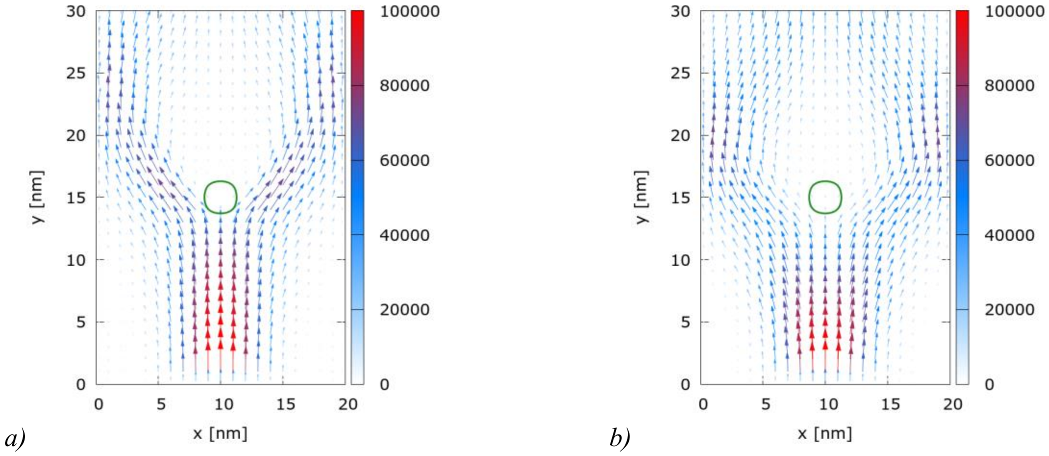

Fig.1: Current density around a dopant with a 0.35 eV peak potential energy, that is represented by the green 0.15 eV isoline: a) classical evolution, b) quantum coherent evolution.

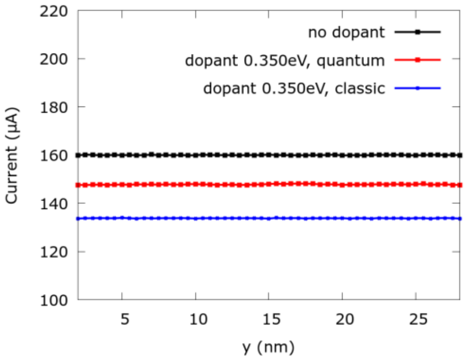

Fig.2: Current inside the nanowire without dopants (black) and with a 0.35 eV repulsive dopant placed in the center: quantum case (red), classical case (blue).

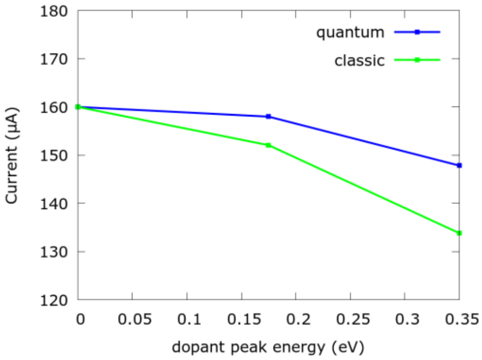

Fig.3: Classical and quantum current inside the nanowire as function of the potential energy of the repulsive dopant

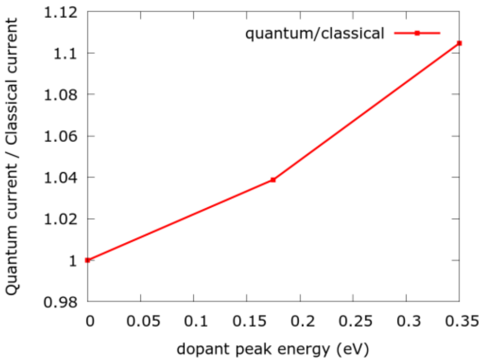

Fig.4: Ratio between quantum and classical current as function of the potential energy of the (repulsive) dopant.

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