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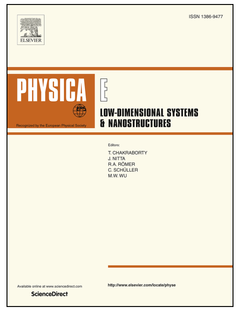

Current in nanojunctions: Effects of reservoir coupling

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Current in nanojunctions : Effects of reservoir coupling

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Abstract

We study the effect of system reservoir coupling on currents flowing through quantum junctions. We consider two simple double-quantum dot configurations coupled to two external fermionic reservoirs and study the net current flowing between the two reservoirs. The net current is partitioned into currents carried by the eigenstates of the system and by the coherences between the eigenstates induced due to coupling with the reservoirs. We find that current carried by populations is always positive whereas current carried by coherences are negative for large couplings. This results in a non-monotonic dependence of the net current on the coupling strength. We find that in certain cases, the net current can vanish at large couplings due to cancellation between currents carried by the eigenstates and by the coherences. These results provide new insights into the non-trivial role of system-reservoir couplings on electron transport through quantum dot junctions. In the presence of weak coulomb interactions, net current as a function of system reservoir coupling strength shows similar trends as for the non-interacting case.

Keywords: Nanojunctions, Electron transport, System-reservoir coupling strength

1. Introduction

Transport properties of quantum junctions have been studied for over two decades motivated not only by their technological relevance but also the opportunities they provide to explore fundamental physics. For example quantum dot junctions provide a good platform for verification of fundamental concepts, like fluctuation theorems [1, 2] . There have also been a lot of technologically relevant proposals of diodes [3], transistors [4], heat engines [5, 6], which can be realized using quantum junctions made of single molecules or quantum dots. Quantum dot junctions can also serve as promising candidates for realizing quantum computers [7].

Current flowing through quantum dot junctions [8] and molecular junctions [9, 10, 11, 12, 13] have been measured experimentally and studied using various theoretical formulations like quantum master equations (QME) [14], scattering matrix (SM) [15], and non equilibrium Green's function (NEGF) method [16]. QME and SM approaches are valid within a certain parameter regime, but NEGF method is exact and can be applied in all regimes, although analytically tractable results can be obtained only for non-interacting systems.

Although a good amount of theoretical work on quantum conduction exists in the literature [15], however the role of system-reservoir coupling has not been explored much, except for few works. For example in experiments performed with carbon nanotube junctions reported in Ref.[17], the importance of non-point like contact of reservoir system coupling was observed. The effect of finite contact length was studied in Ref. [18] using tight binding models, and it was demonstrated that the transmission can be enhanced at lower system reservoir coupling strengths by increasing the contact length. Further, in Ref.[19], the effect of reservoir induced coupling between quantum dots on the current was studied. It is important to note that the system-reservoir coupling strength can be tuned in several ways. For example, external gate potentials can be used to manipulate system-reservoir coupling in quantum dot junctions [8]. In molecular junction set-up [20], reservoir coupling can be varied by tuning the density of states of metal near Fermi-energy [21, 22, 23], orbital overlaps of metal and molecule [24], or by chemical gating [25].

To gain more understanding on the role of system reservoir coupling strength, we ask the question, "How does the current vary as system-reservoir coupling is changed?". To answer this question, we note that, in a simple scattering picture, the system-reservoir coupling offers (contact) resistance to the tunneling electrons. Within the quantum master equation formulation (Lindblad quantum master equation), the current increases monotonically as the coupling is increased. However, this does not present the complete picture and it is not at all obvious what happens as one goes beyond the regime of QME or simple scattering picture. In Ref.[26], scattering formalism under weak reservoir coupling was used to study the effect of reservoir induced coherences on the net current through a coupled double-quantum dot model.

In this work we explore the effect of strong system-reservoir couplings on the net current flowing through quantum junctions using NEGF formulation. The advantages of the NEGF formulation over the other formulations discussed above are two folds. First, in most practical cases, it provides an exact method to compute the current in molecular junctions. Secondly, this is a standard well established method to include effects arising due to many-body interactions, as we shall discuss in the later part of this paper.

In the following, we find that the net current is not always