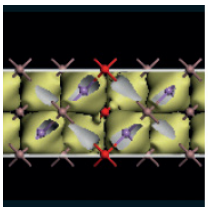

Dissipative NEGF methodology to treat short range Coulomb interaction: Current through a 1D nanostructure

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In this work a methodology describing Coulomb blockade within the Non Equilibrium Green Function formalism (NEGF) [1] is presented. The method incorporates the short-range coulomb interaction between two electrons [2] through the use of a two-particle Green's function (2pGF). Previous work [3] using the 2pGF in conjunction with NEGF has been carried out. However, the central region of the nanostructure or the quantum dot has no spatial resolution i.e. it is parameterized by the energy level and coupling constants of the dot. Our method intends to describe the effect of electron localization while maintaining an open boundary or extended wave function. It is of paramount importance that the methodology conserves the current through the nanostructure to ensure charge conservation.

The method developed here can be extended to describe recent results [4] on charge transport in polymer semiconductors, where the presence of crystalline and amorphous domains lead to a confinement of charge carriers in nanometer scale crystallites [5].

In standard NEGF, the potential energy of the electron is calculated in the mean field approximation. The 2pGF[2] incorporates the short-range electron-electron interaction3.

We have tested the methodology using a simple 1D nanostructure. Ballistic and dissipative (phonon scattering) current calculations have been carried out. A current increase is demonstrated when the 2pGF is incorporated. This is due to the shift and splitting of the energy levels caused by electron repulsion inside the structure. The increase of mobility [4] in polycrystalline polymers increases as electron occupation in the nanocrystalites increases. This has been associated with electron-electron coulomb interaction.

Fig. 1 shows the local density of states (LDOS) with and without considering the 2pGF. The short-range Coulomb energy [3] is 100 meV for a case of two electrons occupying the nanostructure. When the 2pGF is neglected, the ground state energy of the structure is lower than the source potential energy. In addition the next confined state energy is too high in energy to influence the current. In the upper panel the 2pGF is considered and as a consequence the ground state energy is lifted over the source potential and enters into the bias bandwidth. This substantially enhances the current by more than 100% as shown in Fig. 2. We have also studied the impact of inelastic phonon scattering. Phonon scattering reduces the current substantially when the 2pGF is included but the impact lessens when it is not included. As mentioned before our calculation conserves the current locally. This can be seen in figure 3 for inelastic electron phonon scattering.

Finally it is important to note that the LDOS show the two poles related to the 1 or 2 electron occupation, both poles are shown at an intermediate occupation number. Figures 4 and 5 show the LDOS for 0.01 eV^2 and 0.1 eV^2 electron-phonon couplings. Note the increase in broadening with increasing coupling.

This preliminary work demonstrates that coulomb blockade like effects can be integrated in a phenomenological way into the standard NEGF formalism. However, the issue of how to address the transition between localization and delocalization of electrons inside an open nanostructure is still unsolved as well as the self-consistent calculation of the local coulomb interaction in the nanostructure.

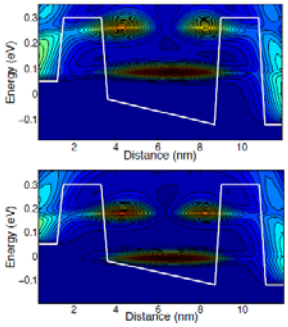

Fig.1 Upper panel: The LDOS including 2pGF. Lower panel: The LDOS without considering the 2pGF, when the electron occupation in the well is 2.

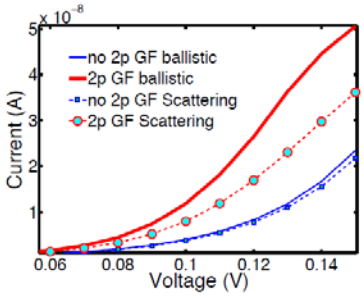

Fig.2 The current voltage characteristics for ballistic and scattering simulations. The simulations shown in red include the 2pGF and the blue neglects it.

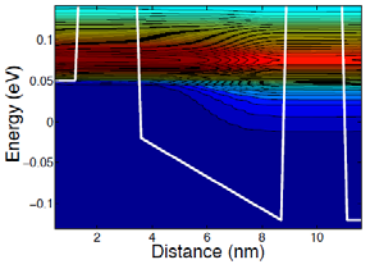

Fig 3. Current spectra through the nanostructure. The current is conserved as can be seen from the figure. The broadening of the distribution on the drain is due to inelastic phonon scattering.

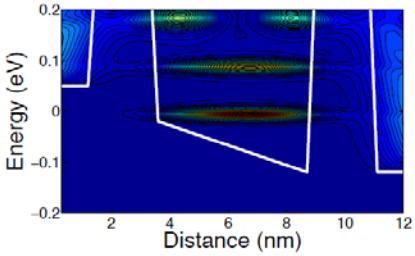

Fig. 4 LDOS for intermediate well occupation (0<occupation<2). For an electron interaction coupling strength of 0.01eV². The two poles of the LDOS are shown simultaneously in the G^R function.

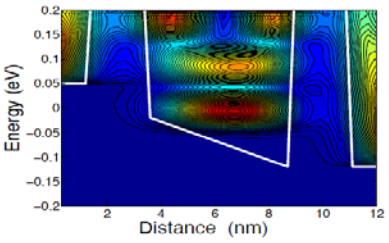

Fig. 5 LDOS for intermediate well occupation (0<occupation<2). For an electron interaction coupling strength of 0.1eV². The large broadening of the energy levels are a result of strong electron phonon coupling

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