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Quantum Transport through Quantum Dot with Electron-Phonon Interaction

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ABSTRACT

We have studied the quantum transport through a quantum dot with electron-phonon interaction. For a generic model which is widely used to explain phonon coupled electron transport in quantum dots and single molecule junctions. We have shown that the system exhibit pronounced bistability even in out of equilibrium situations when the value of the bias is far from the linear response regime. The analysis revealed that the bistability increased for decreasing phonon frequency and depended on the electron-phonon coupling. We have developed an approach based on reduced density matrix formalism. The formalism is combined with the multilayer multi configuration time dependent Hartree method to numerically converge the memory Kernel at short times until it decays and infer from it the dynamics of the system at longer times and the approach to steady state. The relaxation to steady state and the appearance of the bistability depended on the phonon frequency and the strength of the electron-phonon coupling. We have found that the phenomenon persisted over time scale. The obtained results were found in good agreement with previously obtained results.

KEYWORDS

Quantum Transport, quantum dot, electron-phonon interaction, coupling, bistability, density matrix.

INTRODUCTION

The dependence of the steady state current on the initial occupation have been raised in the context of inelastic transport through nanoscale quantum dots[1-6]. Anders et al.[7], Schmittec Kert[8] and White[9] presented numerical brute force approaches, such as time dependent numerical renormalization group technique, eterative[10-12] or Stochastic[13-14] diagrammatic methods and wave function based approaches have been very fruitful but are limited in the range of parameters and time scales have

been studied. Doyon and Anderi[15] studied the existence of unique steady state in strongly correlated quantum systems out of equilibrium is a subject of great interest. For the case of the Anderson impurity model, it has been argued using the Bethe ansatz that single steady state solution existed. Kurth et al.[16] presented calculations of the nonequilibrium current based on time dependent density functional theory seem to indicate that at long times the system reached a dynamical state characterized by correlation induced current oscillations. Jee et al.[17] studied the role of coupling of electrons to longitudinal optical phonons in polar semiconductors on formation of long range bound states and this coupling leaded to acoustic phonons was reduced to the renormalization of the carrier effective mass.

Kumar and Singh[18] studied the quantum transport properties of two dimensional electron gases in Hall regimes. They determined the total current from the bulk Green function. This quantum mechanical property was exact result that holds as long as the high field expansion is applicable. They have numerically computed the hall conductance including self consistent equation which is independent of magnetic field. Sharma et al.[19] studied transport of a long quantum wire with one sided surface disorder in the presence of a perpendicular homogeneous magnetic field. It was found that irregular motion was induced by scattering at the disordered surface. In the corresponding mixed phase space they found direct regular and irregular motion, which were quantum mechanically coupled by dynamical tunneling. Kumari et al.[20] studied the transport properties of carbon wire between zig zag carbon nanotubes and armchair electrodes. The gap width between the electrodes was modulated and the corresponding conductance variation of the junction was calculated. It was found that transport properties of the junctions were significantly affected by the choice of chirality. For zig zag junctions ON and OFF states were observed. These corresponded to cumulence and polygene structures. Sah et al.[21] made systematic study of the electronic transport in realistic edge disordered graphene nanoribbons with zigzag and armchair edges. Three different defect topologies were examined. They found that the electron-electron interactions gave rise to charge redistribution towards the edges of th ribbons when gating shifted the ribbon Fermi energy away from the Dirac point. Cohen et al.[22] presented that memory kernel decays on much shorter time scales compared to the reduced density matrix. Pistolesi etal[23] studied the case for zero temperature and smaller bias voltage as predicted by approximate methods for a single phonon. Dzhioev and Kostov[24] studied adiabatic effective potentials for four frequencies and showed two distinct minima corresponding to two possible stable configurations[25]. The obtained results were compared with previously obtained results.

METHOD

We have considered a generic model for charge transport through a quantum dot with electron-phonon interaction. According to this model we have

$$H = H_S + H_B + V_{SB}$$

where

$$H_S = \varepsilon_d d^\dagger d$$

is the system or quantum dot Hamiltonian fermionic creation / annihilation operators $d^\dagger / d$ and energy $\varepsilon_d, H_B = H_l + H_{ph}$,

where

$$H_l = \sum_{k \in L,R} \varepsilon_k a_k^\dagger a_k$$

represents the non interacting leads Hamiltonian with fermionic creation/ annihilation operators $a_k^\dagger / a_k$ and

$$H_{ph} = \sum_{\alpha} \omega_{\alpha} \left(b_{\alpha}^{\dagger} b_{\alpha} + \frac{1}{2} \right)$$

Represents the phonon bath bosonic creation / annihilation operators $b_{\alpha}^{\dagger} / b_{\alpha}$ for phonon mode α with energy ω_{α}. The coupling between the system and the bath is given by $V_{SB} = V_l + V_{ph}$ where

$$V_l = \sum_{k \in L,R} \left(t_k d a_k^{\dagger} + t_k^{*} a_k d^{\dagger} \right)$$

is the coupling between the system and the leads with coupling strength and
$V_{ph} = d^{\dagger} d \sum_{\alpha} M_{\alpha} \left(b_{\alpha}^{\dagger} + b_{\alpha} \right)$

Is the coupling between the system and the phonon bath, where M_{α} is the electron-phonon coupling to mode α.

The coupling strengths were parameterized by various spectral functions. The dot leads coupling terms were determined from the spectral density

$$\Gamma_{L,R}(\varepsilon) = 2\pi \sum_{k \in L,R} |t_k|^2 \delta(\varepsilon - \varepsilon_k) = \frac{a^2}{b^2} \cdot \sqrt{\left(4b^2 - \varepsilon - \mu_{L,R} \right)}$$

where a tight binding model was employed with $a = 0.2 \text{ eV}$ and $b = 1\text{eV}.\mu_{L,R}$. is the chemical potential of the left (L) or right (R) lead. The electron-phonon coupling were determined from a phonon spectral function

$$J(\omega) = \pi \sum_{\alpha} M_{\alpha}^2 \delta(\omega - \omega_a) = \frac{\pi}{2} \eta \omega e^{-\frac{\omega}{\omega_C}}$$

taken to be of ohmic form. The dimensionless Kondo parameter $\eta = \frac{2\lambda}{\omega_C}$, determines the overall strength of the electron-phonon couplings, where $\lambda = \sum \frac{M_{\alpha}^2}{\omega_{\alpha}} = \frac{1}{\pi} \int \frac{d\omega}{\omega} J(\omega)$ is the reorganization energy and ω_C is the characteristic phonon bath frequency.

RESULTS AND DISCUSSION

Figure (1) shows the influence of the electron-phonon coupling strength λ and the dot energy ε_d on the non equilibrium dynamics. We have compared the time dependence of σ for four different initial conditions. In the upper panel, we have shown the corresponding adiabatic effective potentials for four values of λ. For small values of λ the bistability disappeared as shown in Figure (1). This is consistent with the adiabatic effective potential has a single minimum for $\lambda \leq 3000 \ cm^{-1}$. Comparing the relaxation time for $\lambda = 2000$ and $3000 cm^{-1}$, we have found the latter is slower for $\delta_a = 1$. When λ is further increased to 4000 cm^{-1} the relaxation time stretched more and the system decayed to a different steady state depending on the value of δ_a, again consistent with the appearance of two stable configurations in the corresponding adiabatic effective potential. While the reduced density matrix shows a distinct bistability. In the upper right panel as shown in Figure (1) show the results for the case when $\lambda = 2000 cm^{-1}$ and $\varepsilon_d = 0.25 \text{ eV}$. The effective adiabatic potential for this case

shows two distinct minima. The barrier is lower than for $\lambda = 4000\,\mathrm{cm}^{-1}$ and $\varepsilon_d = 0.5\ \mathrm{eV}$ comparing the two right panels of Figure (1), we found that as λ and ε_d are decreased and the time scale to relax to steady state also decreased, consistent with the adiabatic tunneling. The time dependent approach developed describes the non-equilibrium dynamics numerically exactly only over a certain time scale. The long ranged memory effects not captured by the cut off approximation resulted in switching between the different states and leaded to a unique steady state. This is for strong non equilibrium situations and or high temperature and preliminary results indicate that at higher bias voltages the bistability vanishes. This is also the case for zero temperature and smaller bias voltages as predicted by approximate methods for a single phonon. We have found that the bistability persists even for a finite bias assuming that beyond the cut off time the memory kernel decays as a power law. The obtained results were found in good agreement with previous results.

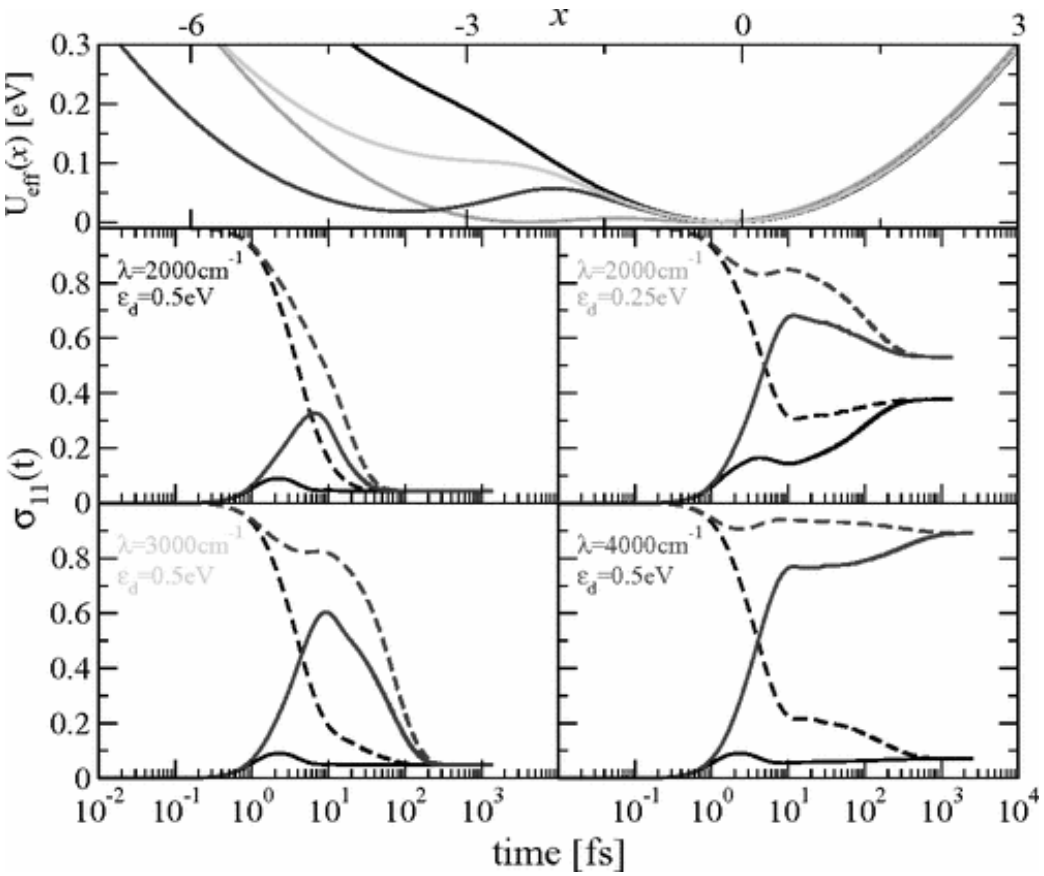

Figure 1: The adiabatic effective potentials for the different values of λ.

CONCLUSION

We have studied the problem based on bistability and the uniqueness of the steady state in a system with electron-phonon interaction under nonequilibrium conditions caused by a finite bias voltage. We have developed a approach based on a reduced density of state matrix formalism. We have considered a generic model for charge transport through a quantum dot with electron-phonon interaction. Our approach offered exact dynamics of quantum system driven out of equilibrium on time scale not previously accessible. The reduced density of state matrix formalism provided means to prove analytically that if a steady state exists then it must be unique. We have found that relaxation to steady state and appearance of the bistability depends on the phonon frequency and the strength of the electron-phonon couplings. We have found a unique steady state that existed regardless of the initial electronic preparation of the quantum dot, consistent with the converged numerical results. We

have also found that the bistability persists even for a finite bias assuming that beyond the cutoff time the memory Kernal decays as a power law. The obtained results were compared with previously obtained results of theoretical and experimental works and were found in good agreement.

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