Quantum Transport in A Single Molecular Transistor at Finite Temperature

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Research Article

Keywords: transport, transistor, molecular, temperature

Posted Date: December 3rd, 2020

DOI: <https://doi.org/10.21203/rs.3.rs-112967/v1>

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Quantum transport in a single molecular transistor at finite temperature

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Abstract

We study quantum transport in a single molecular transistor in which the central region consists of a single-level quantum dot and is connected to two metallic leads that act as a source and a drain respectively. The quantum dot is considered to be under the influence of electron-electron and electron-phonon interactions. The central region is placed on an insulating substrate that acts as a heat reservoir that interacts with the quantum dot phonon giving rise to a damping effect to the quantum dot. The electron-phonon interaction is decoupled by applying a canonical transformation and then the spectral density of the quantum dot is calculated from the resultant Hamiltonian by using Keldysh Green function technique. We also calculate the tunneling current density and differential conductance to study the effect of quantum dissipation, electron correlation and the lattice effects on quantum transport in a single molecular transistor at finite temperature.

1. Introduction

With spectacular advances in the development of nano-fabrication techniques, recent years have witnessed unprecedented upsurge in research activity in the field of nano-electronics. In this context, the subject of moletronics has received particular attention. Aviram and Ratner [1] were the first to fabricate a molecular electronic device. They constructed, in 1974, a molecular rectifier using a single organic molecule. On the other hand, a single molecular transistor (SMT) appears to have been first devised in 2000 by Park et al. [2] who observed nano-mechanical oscillations in a single- C_{60} transistor. An SMT device normally consists of an arrangement in which a molecule or a quantum dot (QD) or any nanosystem constitutes the central part which is connected by metallic leads to a source one side and drain on the other. One of the important reasons for considering a QD or a nanosystem at the central part of an SMT device is that these systems have discrete energy levels. Tuning the gate voltage one can control the current through an SMT device [3, 4]. Research on single molecular transistors (SMTs) [5, 6] has lately grown by leaps and bounds for these devices hold immense promise in technological applications at the nanoscale. Indeed they can be used as spin filters [7], switching devices [8], sensors [9] and so on. Furthermore, an SMT device exhibits many important correlation effects like Kondo effect [10] due to magnetic impurity, Coulomb blockade [11] due to electron-electron (el-el) interaction and polaronic effects due to electron-phonon (el-ph) interaction. They can also have interesting non-equilibrium properties. Many research groups have theoretically studied using different techniques the phonon-assisted transport properties [12-18] of SMT devices with a single molecule or a quantum dot (QD) as the central molecule.

Chen et al. [19] have considered el-ph interaction in an SMT system and showed how the polaronic effects modify the transport properties. They have used the non-equilibrium Green function technique due to Keldysh and determined the spectral density, tunneling current and differential conductance. They have shown that el-ph interaction gives rise to phonon side bands in the spectral density function. The el-ph interaction has also been shown to reduce the current density and differential conductance. In a recent work, Raju and Chatterjee [20] have investigated the effect of quantum dissipation on the transport properties of an SMT device employing non-equilibrium Green function technique of Keldysh. To incorporate the damping effect arising from the interaction of the local QD phonon with the phonons of the substrate, they have added the Caldeira-Leggett term to the Anderson-Holstein Hamiltonian and called it the Anderson-Holstein-Caldeira-Leggett (AHCL) model. As expected, they have also demonstrated a reduction in the current density as well as the differential conductance due to the polaronic effect. Interestingly, however, the damping effect induced by the substrate has been shown to enhance the tunneling current. In a more recent work [21], the present authors have investigated the role of a magnetic field on the non-equilibrium transport in an SMT device in the presence of electron correlation, polaronic interaction and quantum dissipation due to the interaction between the QD phonon and substrate oscillator modes. Besides the spectral density, current density and differential conductance, we have also calculated the spin polarization. We have shown that the degeneracy in the electron energy due to the spin degree of freedom is removed in the presence of the external magnetic field and the device can be used as a spin filter.

The temperature dependence of the transport properties of three terminal devices like single molecular transistor has been studied by several investigators [22-24] in recent years. However, the theoretical study has been few and far between [25]. In the present paper we make an attempt in this direction. We consider an SMT device in which the

central QD is assumed to have the onsite electron correlation and the Holstein el-ph interaction and use the AHKL model to investigate the effect of temperature and quantum dissipation on the non-equilibrium quantum transport in an SMT device employing the finite-temperature Green function technique of Keldysh.

2. Model

Fig. 1 describes an SMT device where QD refers to the central QD and S and D represent the conducting leads that play the roles of the source and the drain respectively. The QD molecule is considered to have a single vibrational mode that interacts with the charge carrier in QD through the el-ph interaction. The system of QD flanked

Fig.1 Schematic diagram of an SMT device showing a QD placed on a substrate and connected to source S and drain D . V_B is the bias voltage and V_G is the gate voltage.

by S and D is placed on an insulating substrate that plays the role of a heat reservoir. V_B and V_G are the bias voltage and the gate voltage respectively. The interaction between the local QD phonon and the substrate phonon modes is considered linear following the Caldeira-Leggett model. This interaction gives rise to a damping effect on the dynamics of the QD phonon. The Hamiltonian of the system is thus modeled by,

$$H = H_l + H_{QD} + H_t + H_B. \quad (1)$$

In the above equation, H_l represents the Hamiltonian for the source ($l = S$) and the drain ($l = D$) and is given by $H_l = \sum_{k\sigma \in S,D} \varepsilon_k n_{k\sigma}$, where $n_{k\sigma} (= c_{k\sigma}^\dagger c_{k\sigma})$ denotes the number operator for conduction electrons with wave vector $\mathbf{k}$ and spin σ in the continuum states of the S and D , $c_{k\sigma}^\dagger$ ($c_{k\sigma}$) representing the creation (annihilation) operator of the conduction electrons in the leads. H_{QD} describes the central QD and is modeled as

$$H_{QD} = \sum_{\sigma} (\varepsilon_d - eV_g) n_{d\sigma} + U n_{d,\sigma} n_{d,-\sigma} + \hbar\omega_0 b^\dagger b + \lambda \hbar\omega_0 (b^\dagger + b) \sum_{\sigma} n_{d\sigma}, \quad (3)$$

where $n_{d\sigma} (= c_{d\sigma}^\dagger c_{d\sigma})$ refers to the number operator for the localized electrons in the central QD which is assumed to have a single localized level of energy ε_d , $c_{d\sigma}^\dagger$ ($c_{d\sigma}$) representing the corresponding electron creation (annihilation) operator, U denotes the onsite repulsive coulomb correlation energy, $b^\dagger$ (b) stands for the creation (annihilation) operator for the localized QD phonon mode of wave-vector-independent frequency ω_0 and λ is the onsite e-p interaction strength in a QD. Throughout our calculation, we shall consider $\hbar = 1$ for the sake of simplicity. The Hamiltonian H_t represents the tunneling between the leads and the QD and is given by $H_t = \sum_{k\alpha \in S,D} (V_k c_{k\alpha}^\dagger c_{d\sigma} + h.c.)$, where V_k denotes the hybridization strength between the QD and the source or the drain. The substrate phonons can be described by the Hamiltonian: $H_{BO} = \sum_{j=1}^N [(p_j^2/2m_j) + (m_j\omega_j^2 x_j^2/2)]$, where x_j and p_j are respectively the position coordinate and the momentum of the j -th oscillator of mass m_j and frequency ω_j . The interaction of the QD phonon with the bath oscillators is taken as: $H_{vib-B} = \sum_{j=1}^N \beta_j x_j x_0$, following the Caldeira-Leggett model [26], where x_0 is the position coordinate of the QD oscillator, x_j is that of j^{th} bath oscillator and β_j is the corresponding coupling strength between the two. The spectral function of the bath phonon can be written as: $J(\omega) = \sum_{j=1}^N [\beta_j^2/(2m_j\omega_j)] \delta(\omega - \omega_j)$. The Hamiltonian corresponding to the bath and the bath-QD-phonon interaction is thus given by: $H_B = H_{BO} + H_{vib-B}$.

3. Formulation

3.1 Decoupling of the bath phonons

The QD-phonon-bath interaction can be eliminated exactly by a canonical transformation which essentially renormalizes the phonon frequency of QD to $\tilde{\omega}_0 = (\omega_0^2 - \Delta\omega^2)^{1/2}$, where $\Delta\omega^2$, the change in ω_0^2 driven by the interaction with the bath phonons, is given by: $\Delta\omega^2 = \sum_{j=1}^N [\beta_j^2 / (m_0 m_j \omega_j^2)]$. The vibrational part of the total SMT Hamiltonian reduces to

$$H_{vib} + H_B = \left(\frac{p_0^2}{2m_0} + \frac{1}{2} m_0 \tilde{\omega}_0^2 x_0^2 \right) + \sum_{j=1}^N \left(\frac{\tilde{p}_j^2}{2m_j} + \frac{1}{2} m_j \omega_j^2 \tilde{x}_j^2 \right), \quad (4)$$

where $\tilde{x}_j = [x_j + (\beta_j/m_j \omega_j^2) x_0]$ and $\tilde{p}_j = -i \hbar (\partial/\partial \tilde{x}_j)$. Eq. (4) shows that the QD and the substrate phonons are now decoupled. If N is very large, the j -summation in the expression of $\Delta\omega^2$ can be replaced by an integration over ω . Thus, $\Delta\omega^2$ can be written as: $\Delta\omega^2 = 2 \int_0^\infty [J(\omega)/m_0 \omega] d\omega$, $J(\omega)$ being the spectral density. Following the Lorentz-Drude model, we make the choice for $J(\omega)$ as: $J(\omega) = 2m_0 \gamma \omega / [1 + (\omega/\omega_c)^2]$, where γ denotes the rate of damping and ω_c refers to the cutoff frequency which is much greater than the other characteristic frequencies of the SMT system. The change in the QD phonon frequency can be finally written as: $\Delta\omega^2 = 2\pi\gamma\omega_c$.

3.2 Elimination of el-ph interaction

Next we eliminate the el-ph interaction applying the Lang-Firsov transformation [27] to the transformed QD Hamiltonian with the generator: $S = \lambda(b^\dagger - b) \sum_\sigma n_{d\sigma}$. The total effective Hamiltonian of the SMT system becomes

$$\tilde{H} = \sum_{k\alpha \in S,D} \varepsilon_k n_{k\alpha} + \sum_\sigma \tilde{\varepsilon}_{d\sigma} n_{d\sigma} + \tilde{U} n_{d,\sigma} n_{d,-\sigma} + \hbar \tilde{\omega}_0 b^\dagger b + \sum_{k\alpha \in S,D} (\tilde{V}_k c_{k\alpha}^\dagger c_{d\sigma} + h.c.), \quad (5)$$

where $\tilde{\varepsilon}_{d\sigma}$ is the phonon-induced modified energy of the QD system and is given by: $\tilde{\varepsilon}_{d\sigma} = \varepsilon_d - eV_g - \lambda^2 \hbar \tilde{\omega}_0$, $\tilde{U}$ is the renormalized on-site Coulomb interaction strength and is given by: $\tilde{U} = U - 2\lambda^2 \hbar \tilde{\omega}_0$, and $\tilde{V}_k$ is the effective tunneling strength and is given by: $\tilde{V}_k = V_k e^{-\lambda(b^\dagger - b)}$.

3.3 Tunneling current and Spectral function; The Keldysh method

The tunneling current [28, 29] passing through QD is given by

$$J = \frac{e}{2\hbar} \int (\{f_S \Gamma_S - f_D \Gamma_D\} A(\omega) + (\Gamma_S - \Gamma_D) G^<(\omega)) d\omega, \quad (6)$$

where $\Gamma_{S,D}(\varepsilon_k) = 2\pi \rho_{S,D}(\varepsilon_k) \tilde{V}_k V_k^*$, $\tilde{V}_k$ being the average of $\tilde{V}_k$ with respect to the phonon state of the system, $\rho_{S(D)}$, the density of states in the source (drain) channel, $f_{S,D}(\varepsilon) = (\exp[(\mu_{S,D} - \varepsilon)/k_B T] + 1)^{-1}$ are the Fermi distributions, S and D referring to the source and the drain respectively and $\mu_{S,D}$, the corresponding chemical potentials which are related to V_B and V_m as: $eV_b = (\mu_S - \mu_D)$, $eV_m = (\mu_S + \mu_D)/2$, $A(\omega)$ is the spectral function which describes the possible excitation energy spectrum and is related to the Green functions as: $A(\omega) = i[G_{dd}^r(\omega) - G_{dd}^a(\omega)] = i[G_{dd}^>(\omega) - G_{dd}^<(\omega)]$, where $G_{dd}^{r(a)}(\omega)$ describes the retarded (advanced) Green function and $G_{dd}^{<(>)}(\omega)$ describes the energy-dependent lesser (greater) Keldysh Green function for the QD electron. These Green functions can be obtained by performing Fourier transformations of $G_{dd}^{r(a)}(\tau = t - t')$ and $G_{dd}^{<(>)}(\tau = t - t')$ which are given by

$$G_{dd}^{r(a)}(t - t') = \mp i \theta(\pm t \mp t') \langle 0 | \{ \tilde{c}_d(t), \tilde{c}_d^\dagger(t') \} | 0 \rangle, \quad (7)$$

$$G_{dd}^{<(>)}(t - t') = i \langle 0 | \tilde{c}_d^\dagger(t') \tilde{c}_d(t) | 0 \rangle, \quad G_{dd}^{>}(t - t') = i \langle 0 | \tilde{c}_d(t) \tilde{c}_d^\dagger(t') | 0 \rangle, \quad (8)$$

with $c_{d\sigma}(t) = e^{-i\tilde{H}_{el}t} c_{d\sigma} e^{i\tilde{H}_{el}t}$, $\tilde{c}_d(t) = \hat{O} c_{d\sigma}$, and $|0\rangle$ represents the true ground state of the whole SMT system i.e., $|0\rangle = |0\rangle_{el} \otimes |0\rangle_{ph}$ and $\hat{O} = e^{-\lambda(b^\dagger - b)}$. We determine the average value of occupancy on QD employing the expression: $n_{d\sigma} = \int d\omega [(f_S \Gamma_S + f_D \Gamma_D) A(\omega) / 2\pi\Gamma]$. For the sake of simplicity, we assume the coupling between the central QD and the leads to be symmetric. We can then write: $\Gamma(\omega) = (\Gamma_S(\omega) + \Gamma_D(\omega))/2$, where invoke the approximation in which we replace $\Gamma_{S(D)}$ by its expectation value with respect to the phonon state. $\Gamma_{S(D)}$ is given by: We obtain: $\Gamma_{S(D)} = 2\pi\rho(0)|V_k|^2 \exp[-\lambda^2(f_{ph} + 1/2)]$, where $f_{ph} = [\exp(\hbar \tilde{\omega}_0/k_B T) - 1]^{-1}$ is the phonon distribution at finite temperature. To obtain the spectral function, we consider one particle Green functions. We obtain

$$G_{dd}^{<(>)}(\tau) = i \langle 0 | \tilde{c}_d^\dagger(0) \tilde{c}_d(\tau) | 0 \rangle = i \langle 0 | c_d^\dagger(0) c_d(\tau) | 0 \rangle_{el} \langle \hat{O}^\dagger \hat{O} \rangle_{ph} = \tilde{G}_{dd}^{<(>)}(\tau) e^{-\varphi(-\tau)} = \tilde{G}_{dd}^{<(>)}(\tau) \sum_{n=-\infty}^{\infty} L_n e^{in\tilde{\omega}_0\tau}, \quad (9a)$$

$$G_{dd}^>(\tau) = -i\langle 0|\tilde{c}_d(0)\tilde{c}_d^\dagger(\tau)|0\rangle = -i\langle 0|c_d(0)c_d^\dagger(\tau)|0\rangle_{el}\langle \hat{O}\hat{O}^\dagger\rangle_{ph} = \tilde{G}_{dd}^>(\tau) \sum_{n=-\infty}^{\infty} L_n e^{in\tilde{\omega}_0\tau}, \quad (9b)$$

with

$$\varphi(\mp\tau) = \lambda^2 \left[(2f_{ph} + 1) \mp [f_{ph}(1 + f_{ph})]^{1/2} 2\cos(\hbar\tilde{\omega}_0(\mp\tau + i/2k_B T)) \right], \quad (10)$$

$$L_{\pm n} = \exp[-\lambda^2(2f_{ph} + 1) + (n\tilde{\omega}_0/2k_B T)] I_n \left(2\lambda^2 [f_{ph}(1 + f_{ph})]^{1/2} \right). \quad (11)$$

where, I_n is Modified Bessel function of second kind and $L_{\pm n}$ is the spectral weights of the $+n$ th and $-n$ th phonon side bands as mentioned in [19]. Fourier transform of Eq. (9) gives the spectral function of SMT as

$$A(\omega) = \sum_{n=-\infty}^{\infty} iL_n(z) [\tilde{G}^>(\omega - n\tilde{\omega}_0) - \tilde{G}^<(\omega + n\tilde{\omega}_0)] = \sum_{n=-\infty}^{\infty} L_n(z) \left[\frac{2\tilde{\Gamma}}{(\omega \mp n\tilde{\omega}_0 - \tilde{\varepsilon}_d - \tilde{U}\langle n_{d,-\sigma} \rangle)^2 + \tilde{\Gamma}^2} \right], \quad (12)$$

where, n is the number of phonons and $\tilde{\Gamma} = \Gamma e^{-\lambda^2(f_{ph}+1/2)}$. The analytical continuation rule of Langreth is now applied to the Dyson equations for the Keldysh Green functions to obtain: $\tilde{G}^{>(<)}(\omega) = \tilde{G}_{dd}^r(\omega) \tilde{\Sigma}^{>(<)}(\omega) \tilde{G}_{dd}^a(\omega)$, where $\tilde{\Sigma}^<(\omega) = i\tilde{\Gamma}[f_S(\omega) + f_D(\omega)]$, $\tilde{\Sigma}^>(\omega) = -i\tilde{\Gamma}[2 - (f_S(\omega) + f_D(\omega))]$. The Green functions $\tilde{G}_{dd}^{r,a}(\omega)$ are determined by making use of the equation of motion method and subsequently $\tilde{G}^{>(<)}(\omega)$ and $A(\omega)$ are obtained and hence the tunneling current is finally obtained.

3.3 Differential conductance

The differential conductance G is given by : $G = dJ/dV_b$. Straight-forward calculation gives

$$G = \frac{e^2\Gamma}{2h} \sum_{n=-\infty}^{\infty} L_{\pm n} \int_{-\infty}^{\infty} d\omega F_n(\omega) A(\omega - n\tilde{\omega}_0), \quad (13)$$

where

$$F_n(\omega) = \frac{1}{2k_B T} \{f_S(\omega)[1 - f_S(\omega)] + f_D(\omega)[1 - f_D(\omega)]\} \{1 + \frac{1}{2} (e^{-\frac{n\tilde{\omega}_0}{k_B T}} - 1)[f_S(\omega - n\tilde{\omega}_0) + f_D(\omega - n\tilde{\omega}_0)]\} \\ + \frac{1}{4k_B T} (e^{-\frac{(n\tilde{\omega}_0)}{k_B T}} - 1)[f_S(\omega) - f_D(\omega)] \{f_S(\omega - n\tilde{\omega}_0)[1 - f_S(\omega - n\tilde{\omega}_0)] - f_D(\omega - n\tilde{\omega}_0)[1 - f_D(\omega - n\tilde{\omega}_0)]\} \quad (14)$$

4. Results and Discussions

In our numerical computation, the phonon energy $\hbar\omega_0$ is set as the scale of energy and the following values for the SMT parameters are considered (unless we specify otherwise): $\varepsilon_d = 0$, $eV_g = 0$, $\Gamma = 0.2$, $eV_m = 0.5$, $U = 3$. In order to examine the role of temperature on the transport properties of an SMT device, we investigate the behaviour

Fig.2 $A(\omega)/A(0)$ as a function of ω for different values of $k_B T$ at $\lambda = 0.6$, $\gamma = 0.02$, $eV_b = 2.5$, $eV_m = 0.5$.

Fig.3 $A(\omega)/A(0)$ vs ω for different values of γ at $\lambda = 0.6$, $k_B T = 0.6$, $eV_b = 2.5$, $eV_m = 0.5$.

of Spectral density function A , Current density J and differential conductance G with respect to SMT parameters for different values of temperature. We also study the behaviour of these quantities directly as a function of temperature. In Fig. 2 we study the behaviour of the spectral function $A(\omega)$ with respect to energy ω at $\lambda = 0.6$, $eV_m = 0.5$, $eV_b = 2.5$. The inset shows the result for $\lambda = 0$ and $k_B T = 0$. The Lorentzian peak at zero resonant energy is clearly visible. The main plots in Fig. 2 show the behaviour of $A(\omega)$ as a function of energy ω for different values of temperature (T) in the presence of el-ph interaction. Fig. 2 also shows that at $T = 0$, as the el-ph interaction is switched on, the polaronic effect comes into play that causes renormalization of the SMT parameters and consequently the central peak in the spectral density undergoes a red shift and side peaks appear at: $\omega \mp n\tilde{\omega}_0$ in it. This was already shown in [20, 21]. The phonon side bands correspond to the excitation of phonons. The tunneling of electrons into the QD and out of it can occur by emitting or absorbing a phonon which shows up in the spectral function in the form of side bands. Higher-order phonon processes are less likely to happen and so the heights of the side bands decrease as the energy increases. The scenario becomes more interesting at nonzero temperature. At $T \neq 0$, the central peak becomes sharper, greater in height and undergoes a blue shift. Also the temperature has a diminishing effect on the phonon side bands in the negative energy region while in the positive energy region, the side bands tend to grow with temperature.

In Fig.3 we show the behavior of $A(\omega)$ as a function of ω for different values of the damping rate γ at a certain finite temperature ($k_B T = 0.6$) and finite el-ph coupling constant ($\lambda = 0.6$). One may notice that with increasing dissipation, the spectral function peak reduces in height and broadens in width. As discussed in [20], this implies that the role of dissipation is to reduce the occupancy of the phonon side bands.

Fig. 4 L_n vs λ for different $k_B T$ at $\gamma = 0.02$.

Fig.5 L_n vs $k_B T$ for different γ at $\lambda = 0.6$.

In [22], the authors have shown the behavior of the spectral weight at zero temperature for different values of n . To see the temperature dependence of the spectral weight, we plot in Fig.4 the spectral weight versus el-ph interaction

Fig.6 J/J_0 vs eV_b for different values of $k_B T$ at $\lambda = 0.6$, $eV_m = 0.5$, $\gamma = 0.02$.

Fig.7 J/J_0 vs eV_b for different values of λ at $eV_m = 0.5$, $\gamma = 0.02$, $k_B T = 0.6$.

strength λ for different temperatures at $n = 1$. One can observe that the height of the spectral weight increases with increasing temperature T up to a certain value of λ after which the temperature dependence of the spectral weight becomes marginal. With respect to λ , the spectral weight initially shows an increasing behaviour, then attains a maximum at a certain value of λ and finally decreases smoothly. We have also studied the behaviour of the spectral weight for higher values of n and observed the same qualitative behavior as $n = 1$. But quantitatively, the value of the spectral weight undergoes significant reduction with increasing n . (We have not shown this here to save space). To see the effect of damping rate at $n = 1$, we plot in Fig.5, the spectral weight L_1 with respect to T for different values of damping rate. One can clearly see that the spectral weight L_1 increases sharply with T at low T , develops a maximum at a certain value of T beyond which it decreases with further increase in T . It is also visible that the spectral weight L_1 increases with dissipation up to a certain temperature beyond which it decreases with T .

The variation of current density J with the bias voltage V_B at a particular el-ph coupling constant λ is displayed in Fig. 6 for different values of T . The inset in the figure which presents the result for $\lambda = 0$, $T = 0$, $\gamma = 0$, suggests that the current density increases linearly with the bias voltage before it saturates. The main figure reveals that for a given set of SMT parameters, J decreases with increasing T . In Fig.7, we present the variation J with respect to V_B for different values of λ . At a particular finite temperature, the current density is reduced by the el-ph interaction because of the formation of polarons. However, for the range of electron-phonon coupling considered in the present analysis, the reduction is only marginal.

Fig.8 J/J_0 vs eV_b for different values of γ at $\lambda = 0.6, eV_m = 0.5, k_B T = 0.6$

Fig.9 J/J_0 vs λ for different values of $k_B T$ at $eV_b = 2.5, eV_m = 0.5, \gamma = 0.02$

Fig.10 J/J_0 vs $k_B T$ for different values of λ with $eV_b = 3.6, \gamma = 0.02, U = 3$.

Fig. 11 G/G_0 vs eV_b for different values of $k_B T$ at $\lambda = 0.6, eV_m = 0.5, \gamma = 0.02$.

To see the damping effect on the bias-voltage-dependence of current density, we plot in Fig.8, J with respect to V_B for different values of the damping rate γ with $\lambda = 0.6$ and $k_B T = 0.6$. J increases only marginally with increasing γ . We have also studied the variation of J as a function of eV_b for different values of eV_m (not shown here) and observed that at low bias voltage, V_m -dependence of J is essentially insignificant while at higher bias voltage, J shows a small

but observable increase with V_m . Fig.9 shows the behavior of J as a function of λ . It is clearly visible that the el-ph interaction reduces the current density. Indeed the current density becomes zero at a certain value of λ . The figure also shows that J decreases as T increases. Fig. 10 shows directly the plot of J versus T for different values of λ . As expected, the current density decreases with increasing temperature and el-ph interaction strength. This is in conformity with Figs. 6 and 7.

In Fig.11 we present the variation of differential conductance G with respect to the bias voltage V_B for different values of temperature T . The inset in Fig.11 shows the plot at $T = 0K$ for $\lambda = 0$ and $\gamma = 0$. It is clear that in the absence of dissipation and the el-ph interaction and at zero temperature ($T = 0$), G exhibits a single central peak that is symmetric in nature. The main figure shows that the el-ph interaction splits the central peak into two symmetric peaks around $\lambda=0$ and also gives rise to a few phonon side bands due to polaronic effect. One can observe that temperature in general reduces the differential conductance.

Fig. 12 G/G_0 vs λ for different values of $k_B T$ at $\lambda = 0.6$, $eV_m = 0.5$, $\gamma = 0.02$.

Fig. 13 G/G_0 vs eV_b for different values of $k_B T$ with $\lambda = 0.6$, $eV_m = 0.5$, $\gamma = 0.02$.

In Fig.12 we plot the differential conductance G as a function of el-ph coupling constant λ for different values of temperature T . At $T = 0K$, as λ increases, G initially decreases and then exhibits a shallow minimum. As λ increases further, G develops a peak and finally reduces to zero. It is interesting to note that if the temperature is increased from zero, the behaviour of G undergoes a qualitative change. To be more specific, at finite temperature, a double-peak structure is observed in the G vs. λ curves, one at (say) λ_1 and the other one at (say) λ_2 , where $\lambda_2 > \lambda_1$. The peak occurring at λ_1 is much broader in width than the one occurring at λ_2 . Furthermore, as T increases, the peaks at λ_1 shift towards higher values of λ while those at λ_2 shift toward the lower values. With increasing T , the height of the second peak reduces whereas that of the first peak remains unaffected. At low values of λ , one can clearly see that G decreases with increasing temperature.

Fig. 14 G/G_0 as a function of eV_b for different values of λ with $eV_m = 0.5$, $\gamma = 0.02$ at $k_B T = 0$

Fig. 15 G/G_0 as a function of eV_b for different values of λ with $eV_m = 0.5$, $\gamma = 0.02$ at $k_B T = 0.6$

In Fig.13, we plot G as a function of V_B for different values of T . We can clearly see that G decreases with increasing temperature as shown in Fig.1. However, we find that as temperature becomes high, the side bands completely disappear and the $G - eV_b$ curves exhibit only a single and broad maximum. As T is further increased, the curves become essentially flat independent of V_b .

Figs.14 and 15 display the variation of G with respect to V_B for different values of λ at $k_B T = 0$ and $k_B T = 0.6$ respectively. One can see that at zero temperature and in the absence of e-p interaction $G - V_b$ curve has a single central peak structure. Fig. 14 also shows that in the presence of e-p interaction, the central peak is split into two peaks giving rise to a central minimum. As λ increases, the peaks decrease in height and move away from each other, and the central minimum also moves down. At $\lambda = 0.8$, G becomes zero for small values of V_b on both sides of $V_b = 0$. Fig.15 shows that at finite temperature, even at $\lambda = 0$, the central peak of G undergoes a splitting and G remains zero over a range of values on either side of $V_b = 0$. As λ is increased but is still kept low, the peaks decrease in height and come closer to each other and the window of V_b values over which $G = 0$ decreases. Interestingly, if λ is increased beyond a critical value, the sharp double peak structure disappears and a single broad maximum with the maximum at $V_b = 0$, appears. As λ is further increased, an interesting structure with a flat maximum around $V_b = 0$ is observed.

Fig. 16 G/G_0 vs eV_m for different values of $k_B T$ at $eV_b = 3.6, \gamma = 0.02, U = 3$ and $\lambda = 1$.

Fig. 17 G/G_0 vs $k_B T$ for different values of λ at $eV_b = 2.5, eV_m = 0.5, \gamma = 0.02$.

In Fig.16, we show the behavior of G with respect to V_m in the presence of el-ph and el-el interactions at different temperature. It is clear that, in general, the differential conductance together with its peak heights decreases with increasing temperature. One can also observe that the peaks shift towards the positive voltage with increasing temperature. At the mid-voltage range 0-1, a sudden drop in current density occurs (not shown here), the differential conductance is almost zero. As we have already pointed out, the peaks in the differential conductance represent the availability of energy levels for transport. At finite temperature, most of the peaks scale down. So the differential conductance reduces with increasing temperature. To examine the role of temperature on differential conductance

Fig. 18 Three-dimensional plots for: (a) J/J_0 as a function of $k_B T$ and λ ; (b) G/G_0 as a function of $k_B T$ and λ (at $eV_b = 2.5$).

directly, we plot in Fig. 17, G versus T for different values of λ . We observe that at $\lambda = 0.4$, G initially increases with T , develops a peak at a certain value of T and then decreases smoothly with further increase in T . With the increase in λ , the peak broadens and shifts towards to higher values of T . A critical study of the G vs T and G vs λ reveal that the variation of G with respect to T or λ depends on the range of T or λ under consideration. The three-dimensional plots of J and G with respect to T and λ together are shown in Fig. 18.

Fig. 19 Map of J in the V_b - V_m -space for $\lambda = 0.6$ and $U = 3$ for (a) $k_B T = 0.4$; (b) $k_B T = 0.6$; (c) $k_B T = 0.8$.

Fig. 20 Map of G in the V_b - V_m -space for $\lambda = 0.6$ and $U = 3$ for (a) $k_B T = 0.4$; (b) $k_B T = 0.6$; (c) $k_B T = 0.8$.

Figs. 19 and 20 show the three-dimensional contour maps of the current density and the differential conductance respectively as a function of eV_b and eV_m in the presence of el-ph and el-el interactions and quantum dissipation for different values of temperature. One may note from Figs.19 (a-c) that J decreases with increasing temperature and also the boundary regions of the map shrink with increasing temperature. Similarly, Figs. 20 (a, b, c) show that G decreases with increasing temperature. However, the boundary regions in G -curves seem to broaden with temperature.

5. Conclusion

We have investigated, in this work, the quantum dissipative effect on the electronic transport properties of a single molecular transistor at finite temperature in the presence of el-el and el-ph interactions. The dissipative effect arises from the interaction of the QD phonon with the phonons of the substrate that plays the role of a heat reservoir. It has been assumed that the QD phonon interacts with the phonons of the substrate according to the Caldeira-Leggett model. This interaction gives rise to quantum dissipation and has been treated exactly by a canonical transformation which leads to the renormalization of the frequency of the QD phonon. The el-ph interaction term has been decoupled by applying the standard Lang-Firsov transformation followed by an averaging with respect the zero-phonon state. Finally the transport parameters are determined by employing the Keldysh technique and the equation of motion method and the effect of temperature, damping rate and el-ph interaction on the spectral function, current density and differential conductance are investigated. Also the quantum dissipative effects on the spectral weight are studied at finite temperature. It is observed that the spectral weight increases with increasing damping rate. It is also found that the damping enhances the current density at finite temperature but not as significantly as at zero temperature. As expected, the current density decreases with increasing el-ph interaction and temperature and the differential

conductance also behaves in the similar way. This device has potential application as a spin filter in the presence of an external magnetic field or spin-orbit interactions.

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Acknowledgements

M.K. gratefully acknowledges the financial support from CSIR, India for SRF (09/414(1100)/2015-EMR-I) fellowship.

N.R.C gratefully acknowledges the financial support from DST, India through ISPIRE faculty fellowship.

Author contributions

A.C. gave the idea. M.K. and C.N.R. carried out the analytical calculation. M.K. performed the numerical computation. M.K. wrote the manuscript. A.C. reviewed the manuscript.

Competing interests

The authors declare no competing interests.

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Figures

Figure 1

Schematic diagram of an SMT device showing a QD placed on a substrate and connected to source S and drain D. V_B is the bias voltage and V_G is the gate voltage.

Figure 2

$A(\omega)/A(0)$ as a function of ω for different values of $k_B T$ at $\lambda=0.6$, $\gamma=0.02$, $eV_b=2.5$, $eV_m=0.5$.

Figure 3

$A(\omega)/A(0)$ vs ω for different values of γ at $\lambda=0.6, k_B T=0.6, eV_b=2.5, eV_m=0.5$.

Figure 4

L_n vs λ for different $k_B T$ at $\gamma = 0.02$.

Figure 5

L_n vs $k_B T$ for different γ at $\lambda=0.6$.

Figure 6

J/J_0 vs eV_b for different values of $k_B T$ at $\lambda = 0.6$, $eV_m = 0.5$, $\gamma = 0.02$.

Figure 7

J/J_0 vs eV_b for different values of λ at, $eV_m=0.5$, $\gamma=0.02$, $k_B T=0.6$

Figure 8

J/J_0 vs eV_b for different values of γ at $\lambda=0.6$, $eV_m=0.5$, $k_B T=0.6$

Figure 9

J/J_0 vs λ for different values of $k_B T$ at $eV_b = 2.5$, $eV_m = 0.5$, $\gamma = 0.02$

Figure 10

J/J_0 as $k_B T$ for different values of λ with $eV_b=3.6$, $\gamma=0.02$, $U=3$.

Figure 11

G/G_0 vs eV_b for different values of $k_B T$ at $\lambda=0.6, eV_m=0.5, \gamma=0.02$

Figure 12

G/G_0 vs λ for different values of $k_B T$ at $\lambda=0.6$, $eV m=0.5$, $\gamma=0.02$.

Figure 13

G/G_0 vs eV_b for different values of $k_B T$ with $\lambda=0.6$, $eV_m=0.5$, $\gamma=0.02$.

Figure 14

G/G_0 as a function of eV_b for different values of λ with $eV_m=0.5$, $\gamma=0.02$ at $k_B T=0$

Figure 15

G/G_0 as a function of eV_b for different values of λ with $eV_m=0.5$, $\gamma=0.02$ at $k_B T=0.6$

Figure 16

G/G_0 vs eV_m for different values of $k_B T$ at $eV_b=3.6, \gamma=0.02, U=3$ and $\lambda=1$.

Figure 17

G/G_0 vs $k_B T$ for different values of λ at $eV_m=0.5$, $\gamma=0.02$.

Figure 18

Three-dimensional plots for: (a) J/J_0 as a function of $k_B T$ and λ ; (b) G/G_0 as a function of $k_B T$ and λ (at $eV_b=2.5$).

Figure 19

Map of J in the $V_b - V_m$ – space for $\lambda=0.6$ and $U=3$ for (a) $k_B T=0.4$; (b) $k_B T=0.6$; (c) $k_B T=0.8$. Note: The designations employed and the presentation of the material on this map do not imply the expression of any opinion whatsoever on the part of Research Square concerning the legal status of any country, territory, city or area or of its authorities, or concerning the delimitation of its frontiers or boundaries. This map has been provided by the authors.

Figure 20

Map of G in the $V_b - V_m$ – space for $\lambda=0.6$ and $U=3$ for (a) $k_B T=0.4$; (b) $k_B T=0.6$; (c) $k_B T=0.8$. Note: The designations employed and the presentation of the material on this map do not imply the expression of any opinion whatsoever on the part of Research Square concerning the legal status of any country, territory, city or area or of its authorities, or concerning the delimitation of its frontiers or boundaries. This map has been provided by the authors.