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Phonon Assisted Tunneling in Framework of Minimal Model for Molecular Device in Adiabatic and Nonadiabatic Regimes

[1]Rajani Kumari Suman* and [2]Ashok Kumar

Author's Affiliations:
1Research Scholar, University Department of Physics, B.N. Mandal University, Madhepura, North Campus, Singheshwar, 852128, Bihar, India.
E-mail: rajanisuman8719@gmail.com
2University Department of Physics, B.N. Mandal University, Madhepura, North Campus, Singheshwar, 852128, Bihar, India.
E-mail: ashokabnu@yahoo.co.in

***Corresponding author:**
Rajani Kumari Suman, Research Scholar, University Department of Physics, B.N. Mandal University, Madhepura, North Campus, Singheshwar, 852128, Bihar, India.
E-mail: rajanisuman8719@gmail.com

ABSTRACT

Molecular devices are centered on finite bias transport. We have presented the crossover from antiadiabatic to the adiabatic regime of phonon assisted tunneling in the framework of a minimal model for molecular devices. A resonant level coupled by displacement to a single localized vibrational mode was found. It was found that the crossover from the polaronic of the antiadiabatic limit to the perturbative of the adiabatic regime was followed by the polaronic shift rather than the phonon frequency. The perturbative adiabatic limit was made as the bare hopping rate exceeded the polaronic shift leaving an extended window of coupling exceeded the phonon frequency. In extended antiadiabatic regimes the effective low energy Hamiltonian at energies below phonon frequency was purely fermionic and depended at resonance on two parameters tunneling amplitude and effective coulomb repulsion. The effective tunneling amplitude obeyed the empirical scaling for the extended antiadiabatic regime. The resonant phonon assisted tunneling and the relevant measurement of electronic motion was obtained by tunneling rate. The two limits corresponded to the bare electronic tunneling rate either sufficiently small or large in comparison to phonon frequency. It was found that phonon efficiently responded to hopping events by forming a polaron, suppressed the electronic tunneling rate and suppression produced narrow tunneling resonance. The phonon was found slow to respond to the frequent tunneling events having little effect on their rate. In this study framework of the Lang-Firsov transformation was considered by using ordinary perturbation theory of electron-phonon coupling. The obtained results found in good agreement with previously obtained result

KEYWORDS Molecular Device, Finite Bias Transport, Adiabatic Regime, Antiadiabatic Regime, Resonant, Localization, Polaronic Shift, Phonon Frequency, Fermionic, Tunneling, Electron-Phonon Coupling.

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INTRODUCTION

Qiu et al. [1], Sapmaz et al. [2] and Tal et al. [3] studied that phonon assisted tunneling leaded to appearance of inelastic steps and producing differential conductance. Frank-Condon bloackade [4-5] and interplayed was found with Kondo effect [6-8]. Koch et al. [9-10] studied the pair tunneling and nonequilibrium effects on the phonon distribution function. The theoretical activity on molecular devices were presented that the finite bias transport produced thermal equilibrium to the nature of the crossover between two limits of phonon assisted tunneling in adiabatic and antiadiabatic regimes. These were used in electron-phonon coupling to show the limits where the bare electronic motion was either sufficiently fast or sufficiently slow with respect to phonon vibrations. Lang and Firsov [11] studied that extreme limits was controlled in the framework of the Lang-Firsov transformation or using ordinary perturbation theory in the electron-phonon coupling. Hyldgaard et al. [12] showed when the phonon displacement was small in response to zero point motion the classical oscillator period was found independent of the amplitude of oscillations. Wilson [13] and Bulla et al. [14] utilized numerical renormalization group approach for calculating equilibrium properties of quantum impurity system. In the numerical renormalization group the computational efforts grown exponentially with the number of conduction electron. Vichate and Suman [15] studied that the single electron Coulomb blockade structure provided low voltage operation and scaling of transistor to 10nm. The single electron transistor based current mirror was modeled and analysed by simulation and the results showed improved performance of current mirror. Allen et al. [16] and Shruti Suman [17] presented the growth in integrated manufacturing leaded to scaling of transistors to a nanometer range. Nd Jountche [18] studied Gorden Moore the number of transistors per unit area in integrated circuits became double after every eighteen months. Gao etal[19] presented that electron played a very important role in the semiconductor. The flow of electrons was from higher potential to lower potential. The operation of field effect transistor was controlled by threshold voltage. Pandey et al. [20] showed that field effect transistor is called a voltage controlled device and complementary bipolar transistor was current controlled device. Kirton and Armour [21] analysed the response of a nanomechanical to an external drive when it was coupled to single electron transistor. The interaction between the single electron transistor electron and the mechanical resonator depended on the amplitude of the mechanical motion leading to a strongly non linear response to the drive to that of Duffing oscillator. Louis et al. [22] studied the universal properties of quantum transport in graphene nanowires and produced universal conductance fluctuations. It was presented that the three microscopic models produced chiral universal symmetries. Lai et al. [23], Huang et al. [24], Hung and Lai [25] and Jain et al. [26] presented that the transport phenomena in disordered mesoscopic system was strongly affected by the wave behavior of the electron. The wave scattering in nanostructures gave rise to the fundamental phenomena of universal conductance fluctuation, which depended on the dimensionality and the symmetries of the corresponding coherent states [27].

METHOD

We have studied the framework of a minimal model for molecular devices considering adiabatic and antiadiabatic regime and cross over between two limits of phonon assisted tunneling. The resonant level coupled by displacement to a localized vibrational model was examined. The effective low energy Hamiltonian and extended antiadiabatic regime to be interacting resonant level model was used with parameters that extracted from numerical renormalization group calculations. The extended antiadiabatic regime was adopted by a crossover region where the polaron got progressed. The charging properties were followed by two mechanisms at the extended antiadiabatic and into crossover region giving rising to characteristic in the low temperature conductance as function of gate voltage single molecule transistors, offered two advantages over their semiconductor counterparts. The phonon assisted tunneling leaded to plethora of

phenomena including the appearance of inelastic steps and peaks in the differential conductance, the Frank-Condon blockade and the interplay with the Kondo effect. We have applied Wilson's numerical renormalization group approach which was a suitable tool for calculating equilibrium properties of quantum impurity systems. The framework of the spinful Anderson Holstein model was used for the study of phonon frequency. The system was used for large values of phonon frequency. The system consisted of a single localized electronic level with energy tunnel coupled to a continuous band of non interacting spineless electron. The level was simultaneously coupled by a displacement to a localized vibrational mode as modeled by the Hamiltonian given by

$$H = \sum_k \in_k c_k^\dagger c_k + \frac{1}{\sqrt{N}} \sum \left\{ d^\dagger c_k + H.c \right\} + \in_d d^\dagger d + \omega_0 b^\dagger b + \lambda \omega_0 \left(d^\dagger d - N_0 \right) \times \left(b^\dagger + b \right)$$

where $d^\dagger$ is electronic level, $\in_d$ is energy, $c_k^\dagger$ spinless electrons, $b^\dagger$ creation of local Einstein phonon that oscillated with frequency ω_0, t is the tunneling matrix element between the level and to the Wannier state closet to the molecule and N is the number lattice sites. λ is the dimensionless coupling measured the relative displacement of the vibrational mode between the configurations, where the level is empty and occupied. Parameter $\left(N_0 \right)$ is the fixing the reference charge of the level. It was eliminated by shifting the bosonic mode according to $\hat{B} = b - \lambda N_0$. Which has the effect of renormalizing the level energy from its bare value $\in_d$ to $\overline{\in}_d$ with $\overline{\in}_d = \in_d + 2N_0 \lambda^2 \omega_0$. The conversion from b to B generated the constant term $-N_0 \lambda^2 \omega_0$ which shifted the spectrum of the Hamiltonian. The zero temperature charge susceptibility was evaluated at $\in_d^*$

$$\Gamma_{eff} = \frac{1}{\pi \chi_c},$$

with

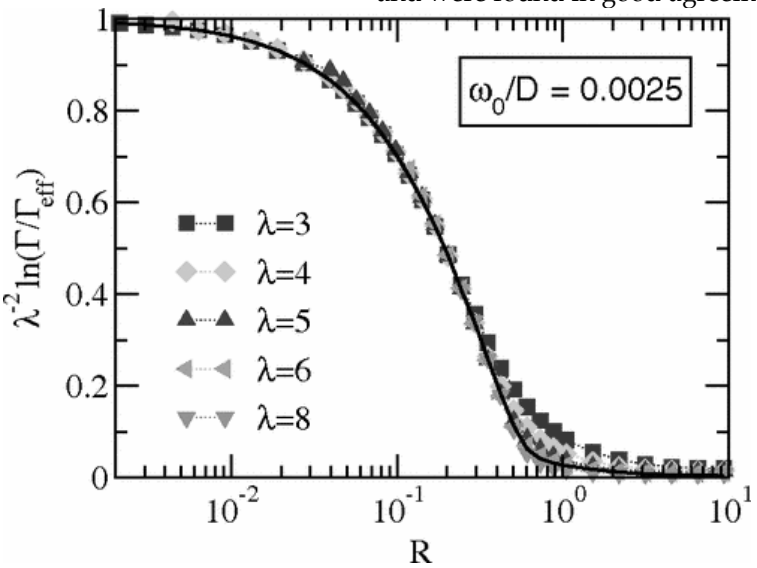
$$\chi_c = -\left. \frac{dn_d}{d \in_d} \right|_{\in_d = \in_d^*}$$

For $\lambda = 0$, the low energy scale Γ_{eff} so defined coincided with the bare hybridization width for various thermodynamic properties associated with the level, e.g. its occupancy and its contribution to the electronic specific heat, reduced in the wide band limit to exclusive functions of $\frac{\in_d}{T}$ and $\frac{T}{\Gamma}$, where T is the temperature. A non-zero λ modified this picture both qualitatively and quantitatively. The occupancy of the level at T=0 was no longer given for large λ by an exclusive function of $\frac{\Delta \in_d}{\Gamma_{eff}}$ but depended on them. With the limit of small λ we have applied ordinary perturbation theory in the electron-phonon coupling λ, postponing for the moment of its range of validity. We have included the adiabatic and non adiabatic limits for the extended antiadiabatic regime where $\omega_0 < \Gamma$ but $\Gamma_{eff} > \omega_0$ and the limit of large detuning $\Gamma = |\in_d|$. The obtained results were compared with previously obtained results.

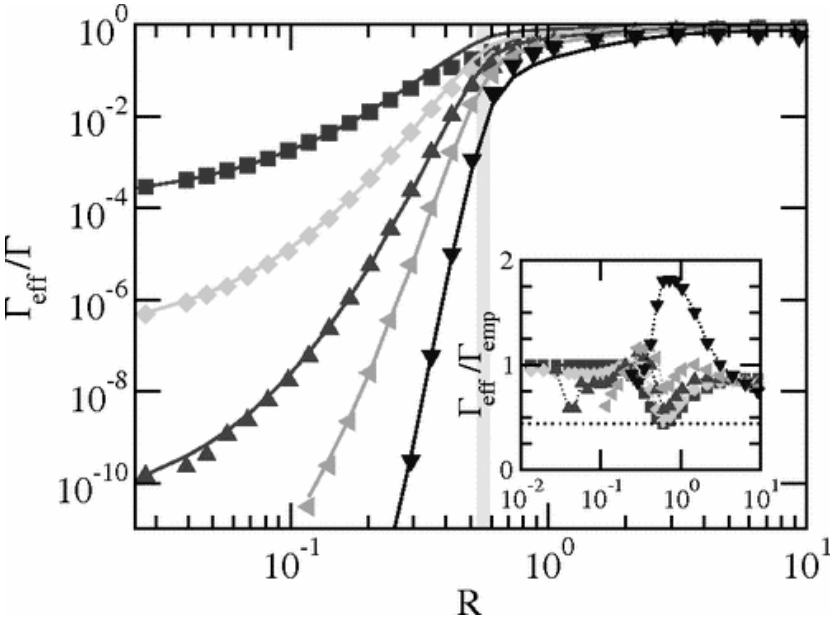
RESULTS AND DISCUSSION

The strong electron-phonon interaction have been presented by considering crossover from the antiadiabatic to adiabatic regime of phonon assisted tunneling in the framework of minimal model for molecular devices, a resonant level coupled by displacement to a single localized vibrational mode. Graph (1) shows the plot of crossover between two limits followed by an approximate scaling form as a function of $R = \frac{\Gamma}{E_p}$ for different values of coupling and was found that all data points approximately collapsed onto a single curve. The collapse was good in the range $R \lesssim 0.2$ and gradually degraded for larger values of R. Graph (2)

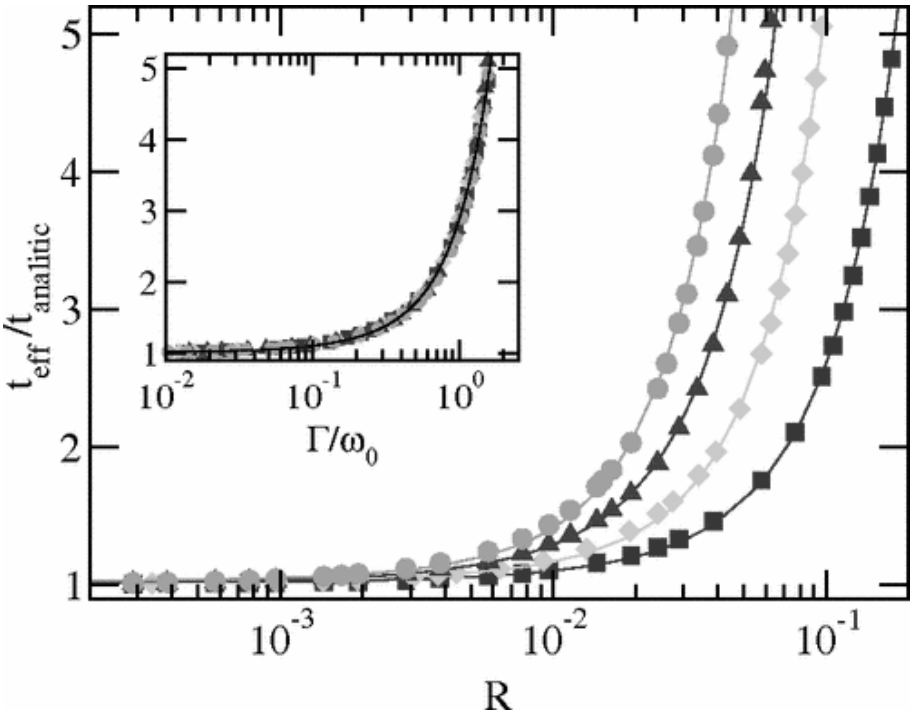
shows he plot of different strengths of electron-phonon coupling λ and the ratio $\frac{\Gamma_{eff}}{\Gamma}$ vs $R = \frac{\Gamma}{E_p}$. The empirical values agreed well with calculated values of Γ_{eff} over many order of magnitude. Deviations were within a factor of 2.3 considering the enormous variation in Γ_{eff} as a function of both λ and Γ. Graph (3) shows the plot of tuning amplitude t_{eff} at energy $\frac{D_{eff}}{\omega_0}$ for several values of $\lambda = 2, 4, 5 \text{ and } 6$. All curves have been normalized by $t_{analytic} = te^{-\frac{\lambda^2}{2}}$ which accounted for the main Gaussian d ependence of t_{eff} on λ. All data points for $\frac{t_{eff}}{t_{analytic}}$ collapsed on to a single curve when plotted versus $\frac{\Gamma}{\omega_0}$ at least for values of Γ upto a few times of ω_0. The effective tunneling amplitude acquired empirical scaling form $t_{eff} = t\exp\left[-\frac{\lambda^2}{2}\right] f\left(\Gamma/\omega_0\right)$ where $f\left(x\right)$ was well fitted by the parabola $f\left(x\right) \approx 1 + 0.9x + x^2$. Graph (3) also shows that t_{eff} developed rapidly with $\frac{\Gamma}{\omega_0}$ increased by a factor of 5 in the limited range covered by the inset of graph (3). The apparent scaling of $\frac{t_{eff}}{t_{analytic}}$ exclusive function of $\frac{\Gamma}{E_p}$ indicated by the scaling plot of Graph (2). The bonding band was no longer complete when a finite bias was applied between he lead electrons rather than their boding and anti bonding with the single bond Hamiltonian for a biased junction. The results found were compared with previous results of theoretical and experimental works and were found in good agreement.



Graph 1: Plot of crossover between two limits versus scaling form for different values of coupling.



Graph 2: Plot of strength of coupling and $\frac{\Gamma_{eff}}{R}$ versus $\frac{\Gamma}{E_p}$.



Graph 3: Plot of tunneling amplitude vs energy.

CONCLUSION

We have studied the phonon assisted tunneling in framework of minimal model for molecular device in adiabatic and nonadiabic regimes. Resonance level coupled by displacement to a localized vibration mode. It was found that the crossover between the two regimes was followed for strong electron phonon interactions by the polaronic shift than the phonon

frequency. The effective low energy Hamiltonian and the extended antiadiabatic was interacting resonant level model with the parameters extracted from numerical renormalization group calculations were made. The extended antiadiabatic regime was governed by a crossover where the polaron got progressed. The phonon configuration strongly deviated from a superposition of two coherent states. The renormalized tunneling rate served as low energy scale settled the width of tunneling resonance and it was found to adopt that the approximate scaling from going from the adiabatic to the antiadiabatic regime. The characteristic feature in the low temperature conductance as function of gate voltage was also found. The obtained results were compared with previously found results of theoretical and experimental research works and were found in good agreement.

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