Inelastic Cotunneling and Heat in Quantum Dot

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Abstract— Study and Characterization of thermoelectric properties of quantum dot has found a favorable response through intense practical and theoretical work. Inelastic cotunneling produced heat effect in molecular, granular and nanojunctions is one of the interesting offspring of the former study. Recently a theory and model has been proposed predicting the inelastic cotunneling produced heat in a single grain, we highlight the limitation of this model and propose an extension to the model to overcome the limitation, while doing so we demonstrate the correctness of extension by applying the model to switching of the transport regimes. The model also predicts quantum dots oscillator heat behavior.

Keywords— Quantum dot, Cotunneling, Coulomb blockade, Sequential tunneling.

I. INTRODUCTION

In recent years nanoscience and nanotechnology have proven to be the most active area of research and is sprawling across the domains, starting from nano material science to nano engineering. Nano materials and nano devices involving molecules, single grains and quantum dots are most attractive due to their interesting characteristics [1, 2]. Building any applications involving the nano structure, requires proper characterization and behavioral understanding of these devices which necessitates both the theoretical as well as experimental studies to be conducted. Understanding the quantum transport and its effects is one of the prime thrust area in physics and chemistry. Till date many a flavors of quantum transport has been characterized and reported starting from Coulomb blockade to Negative differential resistance [3, 4]. Recently Glatz and Belborodov reported a model illustrating the heating effect produced by inelastic cotunneling through the single grain [5]. Their model predicts single grain heating of due to inelastic virtual tunneling while relating heat produced to the temperature of the grain, which is found to be in agreement with the basic physical concepts. However the model exhibits divergence of temperature with increasing voltage under steady state limits, so here we bring out a remedial extension to this model while highlighting the possible drawbacks of the former model. We also demonstrate the effectiveness of the extended model by showing its effectiveness in explaining the transition of transport regime.

The paper starts with brief introduction in section I. Section II contains pictorial view of the model under discussion, which is followed by analytical description of the model with sufficient emphasis on driving and control parameters of the heating effect. In section IV we discuss about the numerical simulation results of the model.

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II. MODEL

We consider a quantum dot tunnel coupled to the electrodes as shown in Figure 1. The quantum dot is weakly coupled to the electrodes such that $g_t \ll 1$, where g_t is tunneling conductance and the dot is assumed to be thermally isolated from the environment. The quantum dot is characterized by its energy scales (i) Charging energy and (ii) Average energy level spacing delta.



Fig.1. Quantum dot weakely tunnel coupled to the electrodes: *V* is the driving voltage, arrowas indicate cotunneling mechanism.

III. INELASTIC COTUNNELING AND QUANTUM DOT HEATING

Inelastic cotunneling is the only transport mechanism that contributes to quantum dot heating [6]. It's the creation of electron-hole or exciton (due to the virtual state tunneling) that leads to heating of the quantum dot. As stated by Glatz et al. heat produced by inelastic cotunneling is measurable through the temperature profiling.

The quantum dot heating due to inelastic cotunneling can be described by considering the Joule heating model as

$$C_{\rho} \frac{\partial T_d}{\partial t} = \sigma_{ct} V_d^2 - 2k(T_d - T)$$
(1)

Where $C_{\rho} = \frac{1}{3}T_{d}\rho$ is the heat capacity of the quantum dot with ρ denoting the density of states in the dot, $\frac{\partial T_{d}}{\partial t}$ is the time varying change in temperature of the dot T_{d} , σ_{ct} is the cotunneling conductance, k is the thermal conductivity that is summation of phonon thermal conductivity k_{ph} and electron thermal conductivity k_{e} and V_{d} is the effective dot bias voltage defined as

$$V_d = E_c - eV \tag{2}$$

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Here E_c is the dot electric potential, which may be considered as equivalent of charging energy. The above equation has been derived considering unit area of the dot.

Equation (1) implies that difference in heat produced by the exciton conductance (driven by dots effective potential) and the heat absorbed by thermal conductance results in quantum dot heating by temperature T_d . The thermal conductance removes heat by absorbing it till steady state is reached. The electrodes are taken to be heat sink such that the absorption of heat will not alter their temperature.

To analyze the heating of quantum dot one should solve the differential equation (1), we are interested in the steady state response of the dot hence we will solve it by setting RHS of equation (1) to zero, with this we obtain

$$\sigma_{ct}V_d^2 = 2k(T_d' - T)$$
(3)

In the above equation T'_d is the steady state temperature, the cotunneling conductivity σ_{ct} , thermal conductance of electron k_e and phonon k_{ph} are defined by the following equations [6]:

$$\sigma_{ct} = 2e^2g_t^2 \frac{T_d^2 + (E_c - eV)^2}{E_c^2} \eqno(4)$$

$$k_{e} = \gamma_{e} g_{t}^{2} T_{d} \frac{T_{d}^{2} + (E_{c} - eV)^{2}}{E_{c}^{2}}$$
 (5)

$$k_{\rm ph} = \gamma_{\rm ph} T_{\rm d} \left(\frac{T_{\rm d}}{\theta_{\rm D}}\right)^2 \tag{6}$$

In the equations (4), (5) and (6) $\gamma_{e/ph}$ are the numerical constants ($\gamma_e = \frac{32\pi^3}{15}$ and $\gamma_{ph} = \frac{8\pi^2}{15}$, ref []) and θ_D is the Debye temperature. Substituting the equations (4), (5) and (6) into equation (1) and simplifying, while considering $\frac{T_d}{T} \gg \frac{(E_c - eV)}{T}$ (with normalization by temperature) we obtain

$$\tau'_{\rm d} = \frac{1}{2} \left(1 + \sqrt{1 + \frac{4\upsilon^2}{\gamma}} \right) \tag{7}$$

Where $\tau_d = \frac{T_d}{T}$, $\nu = \frac{(E_C - eV)}{T}$ and

$$\gamma = \gamma_{e} + \gamma_{ph} \left(\frac{E_{C}}{g_{t}\theta_{D}}\right)^{2}$$
(8)

Equation (7) can be simplified considering the case $v^2 \ll \gamma$, we obtain the steady state result as

$$\tau'_d = 1 + \frac{\upsilon^2}{\gamma} \tag{9}$$

In the above equations if we consider $E_C = 0$ then we get the model which was put forth by Glatz et.al.

IV. RESULTS AND DISCUSSION

The earlier quantum dot heat model of Glatz et.al is the special case of the model discussed here that is obtained by setting charging potential $E_c = 0$.

The evaluation of Glatz model with the boundary conditions for the minimum value works fine by approaching the value of unity, but the solution diverges with increasing value of normalized voltage hence the normalized temperature curve diverges to infinity that implies catastrophic phenomena of non stopping inelastic cotunneling events, which mean that Coulomb blockade, will never be lifted or overcome. However with the increasing bias voltage one expects the transport regime to be switched from inelastic cotunneling to the sequential one while overcoming Coulomb blockade. Along with the Coulomb blockade, Coulomb oscillations are predicted with changing quantum dot potential by gate voltage, which necessitates switching of the quantum transport between inelastic cotunneling and sequential tunneling regimes [7].



Fig. 2. Voltage dependence of normalized steady state quantum dot temperature for different values of tunneling conductance.

With this switching of regimes the temperature oscillations are predicted, which is not possible with the earlier model.

With the extended model presented in this paper, one can find that the normalized temperature increases till bias voltage reaches half the way of charge potential and there after starts reducing as shown in Figure 2. This behavior holds good as inelastic cotunneling must reduce and cease to act when bias voltage approximately reaches and exceeds the coulomb charging energy. The extended model presented here overcomes the problem of divergence and it also explains the switching of transport regime properly. The model also exhibits quantum dot oscillatory temperature response as shown in Figure 3, for different values of dot potential set by elevated blockade due set by the gate.



Fig. 3. Quantum dot temperature oscillatory response for different values of tunnel junction conductance.

From Figure 2 and 3, it can be noted that the maximum value attained by the dot temperature depends on the junction conductance and the quantum dot potential that is controlled by the gate voltage.

V. CONCLUSIONS

We have presented an extended quantum dot heating model, predicting the thermal behavior of the quantum dot with respect to the bias voltage. The model successfully explains the potential induced heating of quantum dot while predicting and characterizing the thermal oscillations of the quantum dot. The results are expected to help in design and development of quantum dot thermal applications.

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