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Temperature Gradient and Quantum Transport in Nano Junctions

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Abstract – **In this paper the effect of temperature gradient on quantum transport in nano junctions is presented. The nano junction current density is shown to be proportional to the square of the temperature gradient. The effective delta variation in current density due to the temperature gradient is found to be dependent on the quantum system junction characteristics.**
Keywords: **Seebeck co-efficient, Nano junction, Quantum dot, Landauer-Butticker.**

I. INTRODUCTION

The well-established top down approach of electronics has contributed much to the development of information and technology over the period of decades, with continuous scaling in device dimensions it has contributed tremendously in terms of power and speed. Further scaling will take the current electronics to a platform where the device physics is governed by the ensemble of hundreds or thousands of electrons, which will make the classical drift and diffusion driven transport to be questionable due to the quantum mechanical effects that open up [1, 2]. The future electronics is expected to be shouldered dominated by the nano scale devices with molecular and nano junctions. With the technology shift the devices based on Carbon Nano Tubes (CNT), Graphene Nano Ribbons (GNR), Single Electron Transistors (SET) and Quantum dots are likely to take over and replace the current Silicon based devices [3] due to their advantages in terms of speed of operation, reduced power consumption and device density.

Motivated by their possibilities and scope in future electronics and applications, the charge transport in these nano-scale systems is under prime focus of recent explorations in physics, electrical sciences, chemistry, and materials science. The nano-scale transport can be set up by the applied potential difference or with temperature gradient by thermal conductivity. Thermal conductivity in low dimensional nano structures is interesting and has captivated a considerable attention [4].

Looking at the potential possibilities of this transport in terms of energy conversion, it is worthy and valuable to analyze and investigate the thermally agitated transport in nano-scale junctions.

In 1821 Thomas Johnson Seebeck discovered the conversion of heat into electricity at the junction of different types of materials, the discovery is named after him as Seebeck effect and is described by $\Delta E = -S\Delta T$. Further study of thermal conductivity/heat transfer in solids was conducted by Fourier, who showed that thermal current is proportional to the temperature gradient, J=-$-k\nabla \mathrm{T}$, where k is the thermal conductivity coefficient. The thermal transport properties in nano structures can be different compared to the bulk materials [5], the low dimensions and confinement of fermions renders the bulk material thermal properties to stand invalid. Study and analysis of thermal properties of the nano devices are important looking at their prospective applications in photovoltaic, energy conversion devices and joule heating computation [6].

In this paper we analyze and compute the thermally agitated current density in a nano junction. We begin with the nano junction consisting of a quantum dot with a single energy level coupled to the semi infinite metal electrodes and focus on the strong coupling regime. Physically, this corresponds to a temperature independent tunnel coupling as the energy widening due to the temperate gradient is infinitesimally small. In reference [6] Murphy and co-workers computed and analyzed the Figure of merit while accounting the thermal gradient by absorbing it into Fermi-Dirac distribution at the junctions.

We will begin our discussion with the nano junction structure under consideration, followed by thermal transport and current density modeling.

II. NANO-JUNCTION STRUCTURE

Figure 1 shows the nano-junction structure consisting of a quantum dot or molecule coupled to the quasi two dimensional electrodes. The junction can be a normal (metal electrode-quantum dot-metal electrode) MQM or Hybrid with two different types of electrodes. We consider the two cases (i) MQM and (ii) Hybrid junction: Ferromagnetic electrode-quantum dot-metal electrode. The transport through the quantum dot is of tunneling type and can be elastic or inelastic depending on the electron-electron interaction in the quantum dot. Here we consider a quantum dot with single energy level that makes the tunneling to be a elastic type.

The quantized energy and field inside the quantum dot renders the bulk properties of the material to be in applicable for the quantum dot characterization. The Landauer-Buttiker formulation is applied to calculate and characterize the current density of the nano-junction. The left and right lead edges away from the quantum dot are coupled to the potential source and the energy levels in the dot are controlled by the gate electrode. It is assumed that the left lead is connected to the potential source with a resistive coupling such that the current flowing through the lead will cause heat dissipation in the lead and hence a temperature gradient is setup between the left and the right metal leads. The left lead acts like a virtual thermal bath.

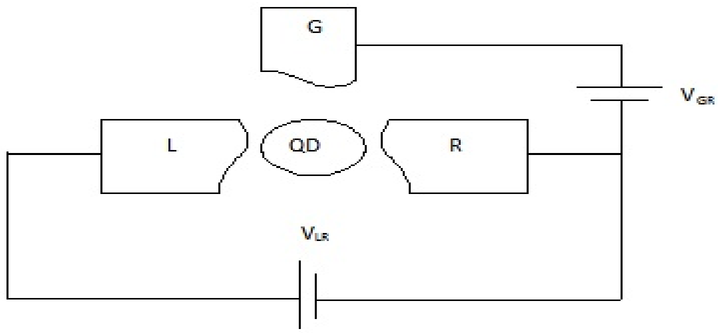

Fig.1 Quantum System with a Quantum dot attached to metal electrodes. L: Left electrode, R: Right electrode and G: Gate.

III. CURRENT DENSITY AND THERMAL TRANSPORT

The general current density equation describing the quantum transport in a nano junction structure under elastic regime at Zero temperature is given by Landauer-Buttiker formula [7] as

$$J_V = \frac{1}{2\pi\hbar}\int T(\varepsilon)\left(f_L(\varepsilon) - f_R(\varepsilon)\right)d\varepsilon \quad (1)$$

Where $T(\varepsilon)$ is the transmission co-efficient which is probabilistic and is dependent on the tunneling rates at the two junctions through energy junction broadening parameter. $f_L(\varepsilon)$ and $f_R(\varepsilon)$ represents the Fermi levels at the left and right junctions, e is the electron charge and h is the plank constant. The transmission co-efficient is formulated to be of the Lorentzian type distribution.

Equation (1) describes the current density set due to the applied potential difference between the contacts, which brings in a non-equilibrium condition. As we consider the junction to be set in into non-equilibrium by potential as well as temperature gradient, equation (1) is not enough to describe the current density contributed by temperature gradient. In the following discussion we will derive an equation for the current density, considering linear transport regime with the applicability of principal of superposition that enables to take the total current density as sum of the current density due to potential difference and current density due to temperature gradient.

Thermally agitated transport is different in bulk and nano structures. In bulk solid materials thermal transport is observed to be mediated by the acoustic phonons and electrons. In metals the thermal transport is dominated by the electrons due to abundant density of electrons [5].

The temperature gradient developed in the left lead cause's phonon vibrations deep inside the lead far away from the junction, while at the junction electrons accumulate the heat energy which leads to a positive delta variation in the junction potential, the rate of potential variation depends on the temperature gradient that is given by the See beck thermo power equation as

$$S = \frac{\nabla\phi}{\nabla T} \quad (2)$$

Where S is the thermal Seebeck co-efficient. For the nano-junctions with point contacts or quantum dot or molecular junctions, the Seebeck co-efficient is difference between the Seebeck co-efficient of the quantum dot (S_{dot}) and the reference electrode (S_{dot}) or the point contact[Staring], and is given by

$$S = S_{dot} - S_{lead} \quad (3)$$

Temperature gradient introduces a thermal non-equilibrium between the junctions that causes net charge exchange between the junctions, which can be computed through the charge flux density calculations. Maxwell's equation conveys that the net density across a junction is related to the divergence of electric field between the junctions that is given by

$$\nabla \cdot E = \frac{\rho}{\epsilon} \quad (4)$$

Where E is the electric field, ρ is the charge density and ϵ is the permittivity of the nano junction (it depends on the relative permittivity of the quantum dots and the leads). Here the electric field is only due to the scalar potential, as we consider the quantum system environment to be free of any external magnetic field. This makes the vector potential to go null. Net electric field between the junctions, with the scalar potential is

$$E = -\nabla\emptyset \tag{5}$$

Simplification of equation (3) while considering (4)

$$\rho = \epsilon S \nabla \cdot \left(\frac{\nabla T}{\varepsilon}\right) \tag{6}$$

$$\rho = \epsilon S \nabla \cdot (T'_x + T'_y + T'_z) \tag{7}$$

Where T'_x, T'_y, T'_z indicates the temperature gradients along the co-ordinates x, y and z between the junctions. The nano-junction is quasi one dimensional as the degree of freedom is restricted to only one direction (assuming x to represent transverse direction), hence T'_y and T'_z are zero. Therefore the equation (6) reduces to

$$\rho = \epsilon S \nabla \cdot T'_x \tag{8}$$

The divergence is also restricted to the dimension or co-ordinate x due to quasi one dimensional approximation of the junction. This approximation leads to

$$\rho = \epsilon S \frac{\partial}{\partial x} T'_x = \epsilon S T''_x \tag{9}$$

Further considering the temperature variation along the x co-ordinate to be of the type

$$T_x = \Delta T e^{-\Delta x} \tag{10}$$

Evaluation of the equation (7) with equation (8), while $\Delta x \to 0$ (i.e, the nano junctions are very close and the distance is negligibly small, such that the temperature remains constant and charge transport is coherent and elastic) produces a net density to be computed as

$$\rho = \epsilon S \Delta T^2 \tag{11}$$

We will re-write the above equation considering the density to be contributed by temperature gradient, to keep it separate from the voltage driven normal density (ρ_V).

$$\rho_T = \epsilon S \Delta T^2 \tag{12}$$

The current density is related to the charge density through the relation

$$J_T = \rho_T u \tag{13}$$

Where u is the Fermions velocity. The total current density (J) in the quantum system at any point of time is the sum of density due to junction voltage difference and temperature gradient driven density, which is given as

$$J = J_V + J_T \tag{14}$$

Equation (12) and (13) implies that the current density due to the temperature gradient in a nanostructure is proportional to the square of the temperature gradient and depends on the net Seebeck coefficient of the nano junction, permittivity of the nano junction and on the velocity of fermions.

IV. CONCLUSION

We have modeled the effect of temperature gradient on current density in nano junction or a quantum system, it reveals that the temperature gradient driven current density is characterized by the nano junction permittivity, Fermions velocity and junction Seebeck coefficient. The equations hints towards customized nano junction construction depending on the requirement of current density and current, while observing and considering process and fabrication limitations.

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