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Thermopower of The Quantum Point Contacts Under the Effects of Boundary Roughness

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Abstract: In this paper we, study the influence of scattering by boundary roughness on electron transport through quantum point contact. It is found that the thermo power of rough quantum point contact shows random and rapid fluctuations and strong with variable the Fermi energy and electrochemical potential. The thermoelectric efficiency as function of electrochemical potential and the oscillations are periodic and even in the electrochemical potential. These results agree with existing experiments and can be used as a guideline for the evaluation of the fabrication process of quantum point contact.

Keywords: Quantum Point Contacts, Boundary Roughness, Fluctuations
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1. Introduction

Recent advances in nanostructure technology have made it possible to define quasi-one-dimensional (Q1D) constructions, which lateral dimensional electron gas (2DEG) formed at semiconductor hetrostructure. Mesoscopic system has been shown to exhibit unusual conductance properties, due to quantum effects [1]. This behavior also affects the thermoelectric effect of such systems [2]. Quantized thermo power in quantum point contact [3-5] and universal thermo power fluctuations [6] have been measured. The definition of thermodynamics transport coefficients for mesoscopic systems presents theoretical challenge.

In this paper we study the thermo power effect in mesoscopic systems with the variable Fermi energy and electrochemical potential at different values of channels length and temperature respectively and thermoelectric efficiency of the quantum point contacts

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as function of electrochemical potential. The thermo power is sensitive to the energy dependence of the conductance.

2. Theory

We model the roughness by dividing a one-dimensional (1D), channel into a large amount of segments in the direction of transport, the segments being thin enough so that one can approximate the potential to be of transverse dependence only. A sample channel of length, L, and average width, W, with random roughness of amplitude δWon each of the two boundaries. We assume a hard wall potential in the transverse direction. We also connect the 1D channel to two semi-infinite reservoirs by smooth entries, in order to avoid the formation of longitudinal resonant states between the entrance and exit [7]. It is interesting to study the influence of scattering by boundary roughness on electron transport through quantum point contact under the variable of the Fermi energy and electrochemical potential. A current between the reservoirs is related to differences in chemical potential or temperature of the reservoirs. Within the linear-response theory, this is generally formulated as

$$J = \hat{L}\,F \tag{1}$$

Where **J** is general current traversing the system and **F** is a generalized affinity. $\hat{L}$ is the transport coefficient matrix. The corresponding net currents are heat and charge fluxes, denoted by Q and G, respectively, and Eq. (1) is written as

$$\begin{pmatrix} I \\ Q \end{pmatrix} = \begin{pmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{pmatrix} \begin{pmatrix} \mu_L/e - \mu_R/e \\ T_L - T_R \end{pmatrix} \tag{2}$$

Where $T_L - T_R = \Delta T$, in order to calculate L_{12}, we use the approximation

$$f_L(\varepsilon, T+\Delta T) - f_R(\varepsilon, T) \approx \left(\frac{-df(\varepsilon-(\mu_F+\alpha\, eV_{sd}))}{d\varepsilon}\right)(\varepsilon-(\mu_F+\alpha\, eV_{sd}))\,\Gamma(\varepsilon)\,\Delta T/T$$

We get

$$L_{12} \equiv \left(\frac{I}{\Delta T}\right) = -\left(\frac{e}{T\,\hbar}\right)\int_{-\infty}^{\infty} d\varepsilon\,(\varepsilon-(\mu_F+\alpha\, eV_{sd}))\,\Gamma(\varepsilon)\left(\frac{df(\varepsilon-(\mu_F+\alpha\, eV_{sd}))}{d\varepsilon}\right) \tag{3}$$

By the same method we calculate L_{21},L_{11}andL_{22}; it is useful to define the following additional quantity, which provides a measure for the efficiency of the thermoelectric effect [4]

$$\Delta \equiv \left(\frac{L_{12}\,L_{21}}{L_{11}\,L_{22}}\right) \tag{4}$$

Where, Δg is a measure of the rate of entropy production in the transport process. The problem of the electron transport through the system is solved by using the scattering–matrix method developed by Xu [8]. The conductance at finite temperature, T, is then given by:-

$$G(\mu_F, T) = \left(\frac{I_{total}}{V}\right) = \left(\frac{2e^2}{h}\right) \int_0^\infty \sum_i \Gamma_i(\varepsilon) \left(-\frac{\partial f(\varepsilon - (\mu_F + \alpha\, eV_{sd})\ , T)}{\partial \varepsilon}\right) d\varepsilon \quad , \tag{5}$$

Where

$f(\varepsilon - (\mu_F + \alpha\, eV_{sd})\ , T)$ is the Fermi –Dirac distributions function, the transmission probability is given by

$$\Gamma_i(\varepsilon) = \left[1 + \frac{V_0^2}{4\varepsilon\ (V_0 - \varepsilon)} Sin(K\, L)\right]^{-1} \tag{6}$$

K, is the wave vector

$$K = \left[\frac{2m^*\,(\varepsilon - \alpha\, e\, V_{sd} - E_F)}{\hbar^2}\right]^{\frac{1}{2}} \quad , \tag{7}$$

and

$$\frac{\partial f(\varepsilon - (\mu_F + \alpha\, eV_{sd})\ , T)}{\partial \varepsilon} = (4k_B T)^{-1} \cosh^{-2}\left[\frac{(\varepsilon - (\mu_F + \alpha\, eV_{sd}) - E_F)}{2k_B T}\right] \tag{8}$$

Where T, is the temperature, k_B is the Boltzmann constant, e is the electron charge, $V_{sd}$is source_drain voltage, V_0 is the potential well depth of the semiconductor heterojunction quantum point contact and $\mu_F$is electrochemical potential.

The thermo power, S (μ_F, T), for transport from one equilibrium electron reservoir to another, along a multichannel lead are given by [3, 9]

$$S(\mu_F, T) = \left[\frac{k_B}{e}\right]\ x \left\{ \frac{\sum_i \int_0^\infty d\varepsilon \left[-\frac{df(\varepsilon - (\mu_F + \alpha\, eV_{sd}), T)}{d\varepsilon}\right] \Gamma_i(\varepsilon) \left[\frac{(\varepsilon - (\mu_F + \alpha\, eV_{sd}) - E_F)}{2k_B T}\right]}{\sum_i \int_0^\infty d\varepsilon \left[-\frac{df(\varepsilon - (\mu_F + \alpha\, eV_{sd}), T)}{d\varepsilon}\right] \Gamma_i(\varepsilon)} \right\} \tag{9}$$

Where, ε is the transverse energy associated with the i^{th} channel in the lead, Γ_i is transmission probability from all channels into channels i, and f is the Fermi–Dirac distributions function.

3. Results and Discussion

In the following, we will present our numerical calculations for the thermo power, S (μ_F, T), (Eq.9) for the case GaAlAs/GaAs heterostructure. Our results are characterized as the follows:-

In Fig. (1) Shows that the variation of the thermo power, S(μ_F,T), with the Fermi energy, E_F, with different values of channels length, L. The thermo power is oscillations with the variable Fermi energy, and the fluctuations is random and strong, the values of thermo power at channel length, L = 500 nm is smaller than the values of thermo power at the channels length, L = 100 nm. In Fig. (2) Shows that the variation of the thermo power, S (μ_F, T), with the electrochemical potential μ_F, with different values of the temperatures, T. The thermo power is oscillations with the variable electrochemical potential, and the fluctuations is random and strong, the values of the thermo power at temperature, T= 0.5 K is higher than the values of the thermo power at the temperature, T =0.1 K. In Fig (3) Show that the thermoelectric efficiency of the quantum point contacts as function of electrochemical potential and the oscillations are periodic and even in the electrochemical potential. This result has been confirmed by us [4, 10-12] previously and by many authors [4, 13-14]. The cases in the presence roughness show the strong the thermo power suppression by the roughness.

4. Conclusion

We have studied the generic effects of boundary roughness on the thermopower, S(μ_F,T), of the quantum point contacts. We have shown that in the presence of the boundary roughness, the thermopower of long quantum point contact shows random and rapid fluctuations and strong. These effects are more pronounced on the increasing the Fermi energy, and electrochemical potential, the oscillations is caused by the rough boundaries and oscillations are due to the Coulomb blockade effect and the quantum interference of quasiparticles due to Andreev reflections processes interface. These results agree with existing experiments and can be used as a guideline for the evaluation of the fabrication process of quantum point contact.

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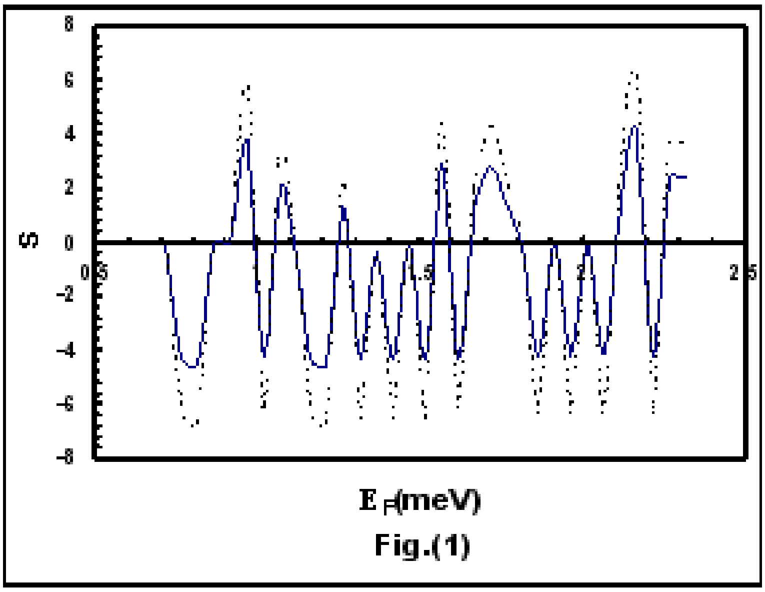

Fig. 1 The thermopower –Fermi energy dependence for different values of channels length L (Solid line L=500 nm, dashed line L=100 nm, $\alpha = 0.5, m^* = 0.047m_e$, W=100 nm).

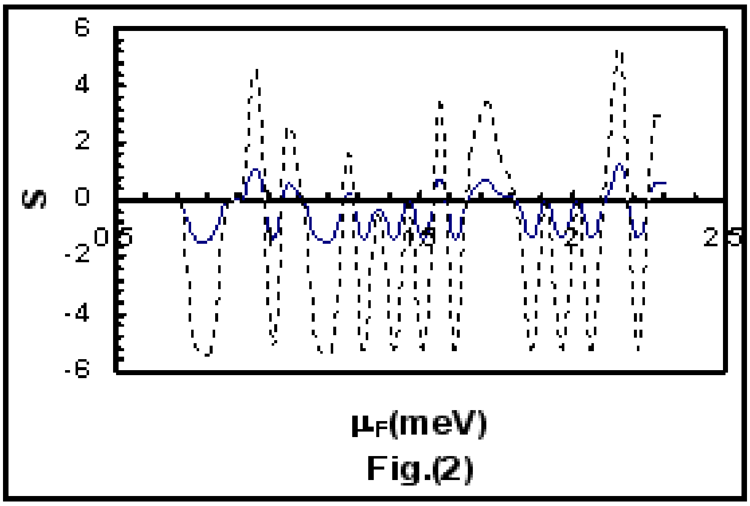

Fig. 2 The thermopower – electrochemical potential dependence for different values of temperatures (Solid line T= 0.1 K, dashed line T= 0.5 K, $\alpha = 0.5$, $m^* = 0.047m_e$, W=100 nm).

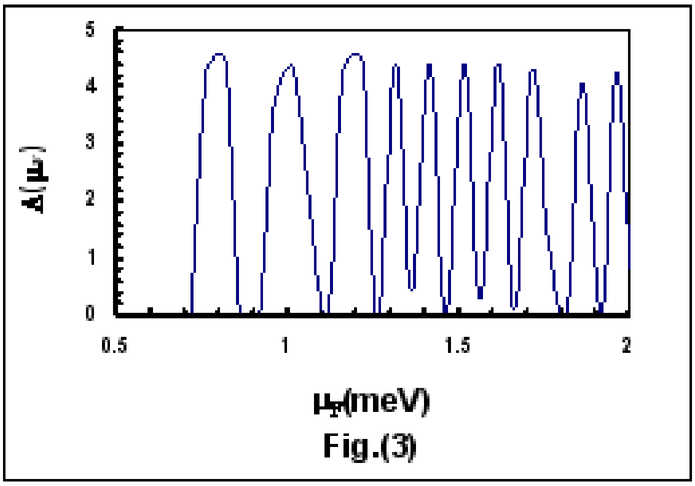

Fig. 3 The thermoelectric efficiency of the quantum point contact as function of electrochemical potential ($\alpha = 0.5$, $m^* = 0.047 m_e$, W = 100 nm).