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The Effect of the Magnetic Field and Correlation Energy on the Charge Current induced by temperature difference through a Single Quantum Dot System

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Abstract: In this work, a theoretical study has been accomplished to calculate the charge current through a single quantum dot coupled to two normal (non-magnetic) leads. This study is based on Anderson's single-impurity model to model QD with a single level hybridized with two leads. The system is in a thermal non-equilibrium regime due to the difference in the leads temperatures. The equations of quantum dot energy levels and the corresponding occupation numbers are solved self-consistently, then the charge current is calculated as a function of temperature difference in the presence and absence of the magnetic field. The results showed that the rectification and outward rectification with fixed bias voltage, take place by adjusting device parameters such as the correlation interaction and the magnetic field.

Keywords: Anderson model, Quantum dot, Thermoelectric effect, Magnetic field.
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1.Introduction

Currently for small systems, the thermoelectric effect is an important topic. The fundamentals of these systems are still unknown and are being investigated, as these systems provide a better knowledge of physics. Measurements of the thermoelectric properties of these systems provide an alternative method for investigating the charge transport beside additional information about dynamic processes. The modified electronic energy spectrum due to confinement and the QD spin properties have a major influence on the thermoelectric device. A single quantum dot and the molecular junction represent the smallest thermoelectric device [1-12]. Hence, the thermoelectric properties of QD systems contribute to understanding the transport of charge and heat[1,4,9-14]. These systems form an important basis for processing future solid-state quantum information and highly-efficiency thermoelectric nano- devices. The energy spectrum of the QDs can be controlled using voltages applied to the nearby metallic surface of the leads, and magnetic field[15].The temperature of lead is interesting parameter that can be modified the contributions of the charge transport mechanisms to overall electrical and thermoelectric transport[13,14].

In this paper, the theoretical model will be applied [13-15] to study the charge current through a single quantum dot system due to temperature difference with fixed bias voltage [15], in the presence and absence of the magnetic field. The interest is to understand the appearance of the rectification and the outward rectification by changing the system parameters such as intra-dot Coulomb correlation and the magnetic field.

2.The Model Calculation

One of the most relevant models that describing QD systems is Anderson model. It was introduced by P. W. Anderson to define localized magnetic states in metals [16] and later has been adjusted to describe quantum dot systems. In this model, the terms of the Hamiltonian represent the leads and the quantum dot as well as the tunnel hopping (between the dot and the two leads). So the transport through quantum dot embedded between two leads can be described by the single-impurity Anderson model:

$$H = \sum_{\sigma} E_{dot}^{\sigma} n_{dot}^{\sigma} + U n_{dot}^{\uparrow} n_{dot}^{\downarrow} + \sum_{\vec{k}\sigma\alpha} E_{\vec{k}\alpha}^{\sigma} c_{\vec{k}\alpha}^{\sigma\dagger} c_{\vec{k}\alpha}^{\sigma} + \sum_{\alpha} \sum_{\vec{k}\sigma} \left(V_{\vec{k}\alpha}^{\sigma} c_{\vec{k}\alpha}^{\sigma\dagger} d^{\sigma} + V_{\vec{k}\alpha}^{\sigma*} c_{\vec{k}\alpha}^{\sigma} d^{\sigma\dagger} \right) \quad (1)$$

$n_{dot}^{\sigma}(= d^{\sigma\dagger} d^{\sigma})$ is the occupation numbers with spin σ, where $d^{\sigma\dagger}(d^{\sigma})$ is the creation (annihilation) operator of a localized electron on the level. E_{dot}^{σ} is the spin-dependent quantum dot energy level, in the presence of the magnetic field[15,17,18] takes the form:

$$E_{dot}^{\pm\sigma} = E_d + U n_{dot}^{\mp\sigma} \mp \frac{1}{2} E_z, \quad (2)$$

E_d, U and E_z represent the quantum dot effective energy level, the intra-dot Coulomb correlation and Zeeman energy respectively. $E_{\vec{k}\alpha}^{\sigma}$ is the single-electron energy in the leads, and $c_{\vec{k}\alpha}^{\sigma\dagger}(c_{\vec{k}\alpha}^{\sigma})$ is the creation (annihilation) operator with momentum k and spin σ. $V_{\vec{k}\alpha}$ is the hybridization matrix elements.

The occupation number n_{dot}^{σ} is given by [19]

$$n_{dot}^{\sigma} = \frac{1}{2} \sum_{\alpha=L,R} \int_{u_{0\alpha}}^{\mu_\alpha} \rho_{dot}^{\sigma}(E) f_\alpha(E, T_\alpha) dE \quad (3)$$

$u_{0\alpha}$ and μ_α are the bottom energy band and chemical potential of the lead $\alpha(= L, R)$, respectively. $\rho_{dot}^{\sigma}(E)$ represents the local density of states for spin σ on the dot,

$$\rho_{dot}^{\sigma}(E) = \frac{1}{\pi} \frac{\Delta^{\sigma}}{(E - E_{dot}^{\sigma})^2 + (\Delta^{\sigma})^2} \quad (4)$$

Where $\Delta^{\sigma} = \Delta_L^{\sigma} + \Delta_R^{\sigma}$, are the broadening in the quantum dot energy levels due to coupling interaction with leads [15] which are energy independent, and $f_\alpha(E, T_\alpha) = \left\{ \exp\left[\frac{(E-\mu_\alpha)}{k_B T_\alpha}\right] + 1 \right\}^{-1}$ is the Fermi distribution function in the lead α. By using Taylor expansion for Fermi function about $\varepsilon = 0$ in the energy interval $(-k_B T_\alpha \le \varepsilon \le k_B T_\alpha)$, with $\varepsilon = E - \mu_\alpha$ and $\varepsilon_{dot}^\sigma = E_{dot}^\sigma - \mu_\alpha$, the analytic solution of Eq.(3) takes the following form[13-15]:

$$n_{dot}^\sigma = \frac{1}{2\pi}\sum_\alpha \sum_{i=1}^{5} C_{i,\alpha}^\sigma I_{i,\alpha}^\sigma \tag{5}$$

where $C_{i,\alpha}^\sigma$ and $I_{i,\alpha}^\sigma$ are listed in table (1) [13-15]. Notably, the functions $C_{i,\alpha}^\sigma$ and $I_{i,\alpha}^\sigma$ are without units.

Table 1 The functions $C_{i,\alpha}^\sigma$ and $I_{i,\alpha}^\sigma$

I	$C_{i,\alpha}^\sigma$	$I_{i,\alpha}^\sigma$
1	-1	$\tan^{-1}\frac{u_{0\alpha} - E_{dot}^\sigma + \mu_\alpha}{\Delta^\sigma}$
2	$1 - \gamma_{1\alpha}^\sigma + (\Delta^\sigma)^2\gamma_{3\alpha}^\sigma$	$\tan^{-1}\frac{-k_B T_\alpha - E_{dot}^\sigma}{\Delta^\sigma}$
3	$\gamma_{1\alpha}^\sigma - (\Delta^\sigma)^2\gamma_{3\alpha}^\sigma$	$\tan^{-1}\frac{k_B T_\alpha - E_{dot}^\sigma}{\Delta^\sigma}$
4	$\frac{\Delta^\sigma}{2}\gamma_{2\alpha}^\sigma - \frac{(\Delta^\sigma)^3}{2}\gamma_{4\alpha}^\sigma$	$\ln\frac{(k_B T_\alpha - E_{dot}^\sigma)^2 + (\Delta^\sigma)^2}{(-k_B T_\alpha - E_{dot}^\sigma)^2 + (\Delta^\sigma)^2}$
5	$2\Delta^\sigma k_B T_\alpha(\gamma_{3\alpha}^\sigma - \gamma_{4\alpha}^\sigma E_{dot}^\sigma)$	1

Where the functions $\gamma_{i\alpha}^\sigma((eV)^{1-i})$ are given [13-15],
$\gamma_{1\alpha}^\sigma = A_{0\alpha} + A_{1\alpha}(E_{dot}^\sigma - \mu_\alpha) + A_{3\alpha}(E_{dot}^\sigma - \mu_\alpha)^3$
$\gamma_{2\alpha}^\sigma = A_{1\alpha} + 3A_{3\alpha}(E_{dot}^\sigma - \mu_\alpha)^2$
$\gamma_{3\alpha}^\sigma = 3A_{3\alpha}(E_{dot}^\sigma - \mu_\alpha)$
$\gamma_{4\alpha}^\sigma = A_{3\alpha}$

and the coefficients $A_{i\alpha}$[13-15],:
$A_{0\alpha} = 0.5$, $A_{1\alpha} = -\frac{0.25}{k_B T_\alpha}$, $A_{3\alpha} = \frac{0.0208333}{(k_B T_\alpha)^3}$
Eq.(2) and Eq.(5) must be solved self-consistently to calculate the occupation numbers $n_{dot}^{\pm\sigma}$ and the corresponding quantum dot energy levels $E_{dot}^{\pm\sigma}$.

The charge current flowing through the system is given by [13,14],

$$I = \sum_\sigma I^\sigma \tag{6}$$

with,

$$I^\sigma = \frac{e}{h}\int_{u_{0\alpha}}^{\mu_\alpha} \pi\Delta^\sigma \rho_{dot}^\sigma(E)(f_L(E-\mu_L, T_L) - f_R(E-\mu_R, T_R))dE \tag{7}$$

by comparing with Eq.(3), Eq.(7) can be written as:

$$I^{\sigma} = \frac{e\Delta^{\sigma}}{\hbar}\left(n^{\sigma}_{dot,L} - n^{\sigma}_{dot,R}\right) \tag{8}$$

It is obvious that the current is determined by the occupation numbers $n^{\sigma}_{dot,L(R)}$ and the broadening of the quantum dot energy levels.

3. Results and Discussion

The quantum dot system is good for studying thermoelectric transport phenomena because it is small, with electrostatically tunable properties and thermoelectric response characteristics that are very sensitive to small thermal bias[13-15]. The current is controlled by the tunneling strength, bias voltage, temperature difference, correlation energy and magnetic field[10,13,14]. Eq.(8) allows us to study the charge current of the system using fixed bias voltage and temperature difference $\Delta T = (T_L - T_R)$. Where the applied bias voltage shifts the bands in the metallic leads without affecting the quantum dot energy spectrum and coupling strength with the two leads.

The results will be presented and discussed to indicate the rectification and outward rectification with two coupling regimes: $\Delta^{\sigma} = \Delta^{-\sigma}$ and $\Delta^{\sigma} \neq \Delta^{-\sigma}$. The charge current is plotted as a function of temperature difference ΔT, where $T_L = 4.5K$ and T_R is varied from $9K$ to $0K$ (i.e. cooling the right lead). In present calculations, the initial conditions are $E^{\sigma}_{dot} = E_d$ and $E^{-\sigma}_{dot} = E_d + U$ and their occupation numbers are $n^{\sigma}_{dot} = 1$ *and* $n^{-\sigma}_{dot} = 0$ while $u_{0R} = u_{0L} = 15.1\, eV$ and $E_d = -0.0222$ eV. All parameters used in calculation are listed in table (2).

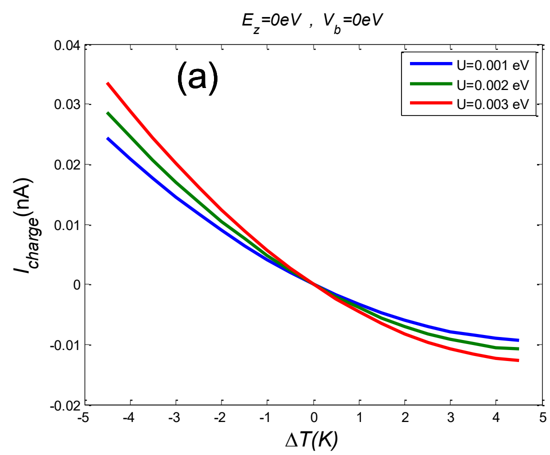
The Coulomb correlation effect can be used to indicate the occurrence of a charge current rectification without applying a magnetic field.
In $\Delta^{\sigma} = \Delta^{-\sigma}$regime, E^{σ}_{dot} and $E^{-\sigma}_{dot}$ are equal and located lower than the chemical potentials. The occupation numbers $n^{\pm\sigma}_{dot}$ have non-magnetic solutions ($n^{\sigma}_{dot} = n^{-\sigma}_{dot}$). When $V_b = 0$, Fig.1a shows the charge current as a function of ΔT for different values of U. The charge current decreases for $T_L > T_R$ and increases for the range $T_L < T_R$. In this case, the device shows rectification effect. For $V_b = 0.001422\, eV$ and for $T_L > T_R$ the charge current increases, while for $T_L < T_R$ it remains very small and the device acts as a rectifier as in Fig.1b. For $U = 0.001\, eV$ with three different values of bias voltage, the device appears outward rectification at $V_b = 0.0012\, eV$ and $0.0016\, eV$, and rectification at $V_b = 0.001422\, eV$ as in Fig.1c. Where E^{σ}_{dot} and $E^{-\sigma}_{dot}$ behave as opened transmitting levels with $I^{\sigma} = I^{-\sigma}$.

For $\Delta^{\sigma} \neq \Delta^{-\sigma}$ regime, the solutions of occupation numbers are magnetic. Fig.2a shows the charge current for different values of U. Here Zeeman energy E_z equals to $0eV$ and the constant bias voltage $V_b = 0.001422eV$. The charge current indicates the occurrence of rectification. Where E^{σ}_{dot} and $E^{-\sigma}_{dot}$ are opened transmitting levels ($I^{\sigma} \neq I^{-\sigma}$). For U equals to $0.05\, eV$, $|I^{\sigma}| > |I^{-\sigma}|$ while for $U = 0.1\, eV$ and $U = 0.15\, eV$ $|I^{\sigma}| < |I^{-\sigma}|$ for all values of ΔT. $|I^{\sigma}|$ increases as U increase whereas $|I^{-\sigma}|$ decreases for all values of ΔT. It is thus clear that the physical feature of rectification can depend sensitively on the strength of Coulomb correlation.

In the presence of a magnetic field, the coupling interaction of the quantum dot with the two leads are not equal ($\Delta^{\sigma} \neq \Delta^{-\sigma}$). The occupation numbers $n_{dot}^{\pm\sigma}$ for different E_z are magnetic and $n_{dot}^{\sigma} > n_{dot}^{-\sigma}$ for each value of E_z and ΔT. Fig.2b shows that the system is a rectifier, where E_{dot}^{σ} is blocked ($I^{\sigma} = 0$) and $E_{dot}^{-\sigma}$ is opened transmitting level ($I_{charge} = I^{-\sigma}$). At a specified value of the magnetic field, the $|I^{-\sigma}|$ increases with increasing of the bias voltage and decreases with the increasing of the magnetic field.

Table(2): The set of parameters used in the calculations.

$E_d(eV)$	$U(eV)$	$V_b(eV)$	$E_z(eV)$	$\Delta^{\sigma}(eV)$	$\Delta^{-\sigma}(eV)$	regime
-0.0222	0.001	0	0	0.00308	0.00308	$\Delta^{\sigma} = \Delta^{-\sigma}$ $\Delta_L^{\sigma} = \Delta_L^{-\sigma} = \Delta_R^{\sigma} = \Delta_R^{-\sigma}$
	0.002			0.00312	0.00312	
	0.003			0.00316	0.00316	
	0.001	0.001422		0.00316	0.00316	
	0.002			0.00323	0.00323	
	0.003			0.00329	0.00329	
	0.05			0.00316	0.00495	$\Delta^{\sigma} \neq \Delta^{-\sigma}$ $\Delta_L^{\sigma} = \Delta_R^{\sigma}$, $\Delta_L^{-\sigma} = \Delta_R^{-\sigma}$
	0.1			0.00317	0.00706	
	0.15			0.00318	0.00921	
	0.001		0.2	3.80363×10^{-4}	0.00734	
			0.3	3.76252×10^{-4}	0.00962	
			0.4	3.72141×10^{-4}	0.01175	



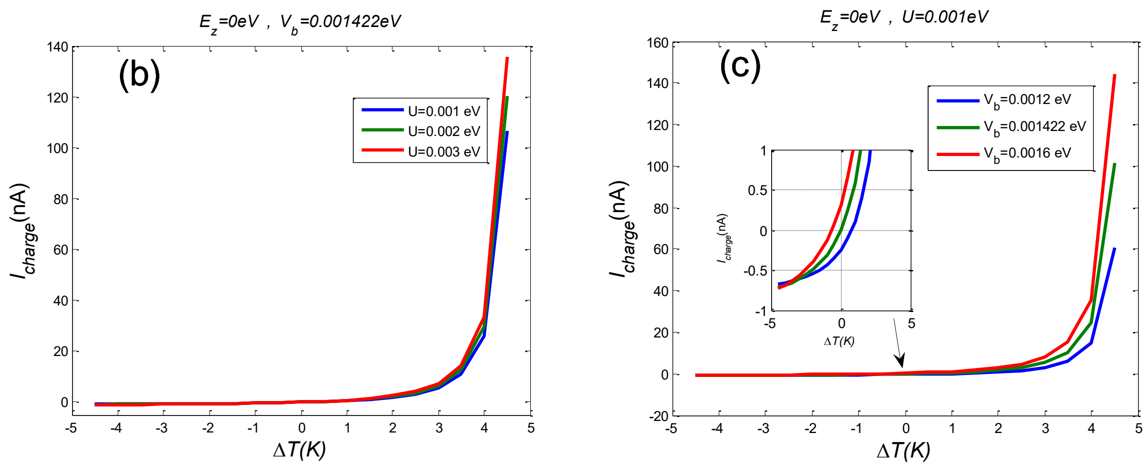


Fig.1.The total charge current I_{charge} as a function of temperature difference ΔT with $\Delta^{\sigma}=\Delta^{-\sigma}$ regime for different values of U(a, b) and different values of V_b(c).

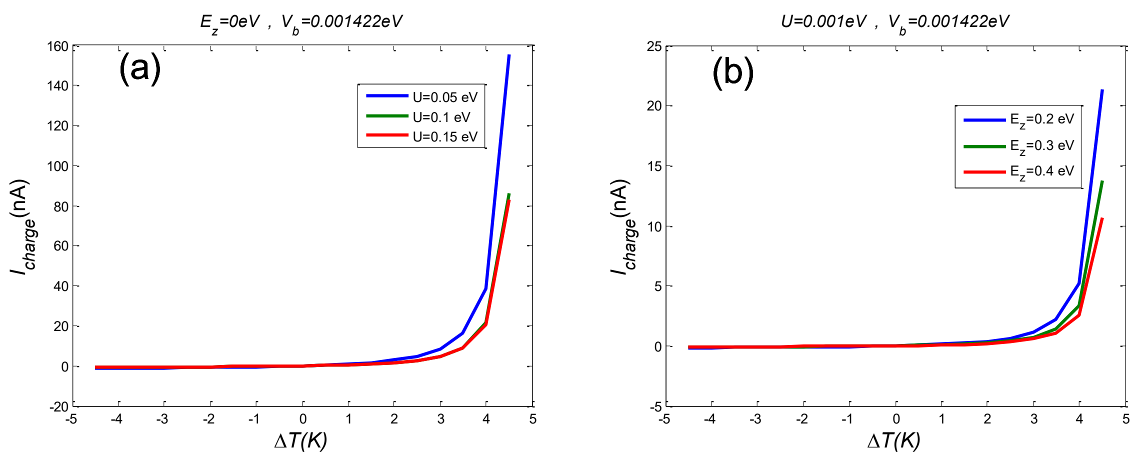


Fig.2. The total charge current I_{charge} as a function of temperature difference ΔT with $\Delta^{\sigma}\neq\Delta^{-\sigma}$ regime and for different values of U(a) and different values of E_z (b).

4. Conclusion

In this work, the charge current rectification mechanism was examined for the simplest quantum dots configuration that consists of a quantum dot embedded between two normal leads under temperature difference. The results indicate that the magnetic field, Coulomb interaction, and the coupling strength are all necessary for the charge current rectification to appear when E_{dot}^{σ} and $E_{dot}^{-\sigma}$ are opened in the absence of the magnetic field while E_{dot}^{σ} is blocked and $E_{dot}^{-\sigma}$ is opened in the presence of magnetic field in $\Delta^{\sigma}=\Delta^{-\sigma}$ and $\Delta^{\sigma}\neq\Delta^{-\sigma}$regimes. It should be noted that the rectification of the charge current is controlled by the strength of coupling interaction, Coulomb interaction and magnetic field [4,10-14].

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تأثير المجال المغناطيسي وطاقة الارتباط على تيار الشحنة الناتج عن اختلاف درجات الحرارة خلال نظام نقطة كمية واحدة

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الملخص: في هذا العمل ، تم انجاز دراسة نظرية لحساب تيار الشحنة خلال نقطة كمية مفردة مقترنة بقطبين اعتياديين (غير مغناطيسيين). تستند هذه الدراسة إلى نموذج الشائبة المفردة لأندرسون لنمذجة نقطة كمية بمستوى طاقة منحل البرم مقترن مع اثنين من الاقطاب. النظام في حالة عدم توازن حراري طبقا لدرجات الحرارة المختلفة عند الاقطاب. يتم حل معادلات مستويات طاقة لنقطة الكمية وأعداد الاشغال حلاً توافقياً، بعد ذلك يتم حساب تيار الشحنة كدالة لاختلاف درجة الحرارة بوجود وغياب المجال. حيث أظهرت النتائج أن تقويم تيار الشحنة وتقويم تيار الشحنة الخارج بوجود فولتية انحياز ثابتة، يتم عن طريق ضبط معاملات الجهاز مثل تفاعل كولوم والمجال المغناطيسي.

الكلمات المفتاحية: نموذج أندرسون ، النقطة الكمية ، التأثير الكهروحراري ، المجال المغناطيسي.