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CONDUCTANCE OF AN ONE AND DOUBLE-LEVEL QUANTUM DOT

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ABSTRACT. We analytically study the expression of the electric charge current through a two-terminal quantum dot in the linear response approximation. We analyse the one-level and the two-level quantum dot scaled conductance taking into account the relevant parameters. We also present the results for the conductance in the Sommerfeld approximation.

Keywords: *Electrical conductance, Quantum dots, Linear response.*

I. INTRODUCTION

The transport of electric charge through solids has been studied for many decades with the aim of finding new analytical results as well as important experimental applications [1]. The dimensionality effects can strongly affect the properties of the materials, in particular the electrical conduction [2]. These effects also change the thermoelectric properties of the materials [3]. Here the quantum coherence effects are more important than the general properties of a bulk material [4-6]. The main ingredient in the description of transport phenomena in these materials is the transmission function $T(\varepsilon)$[7,8]. It contains microscopic information about the sample and its connections with the leads. In this paper we analyse the charge current response of a quantum dot in contact with two particle reservoirs. First we will analyse the single-level quantum dot case with symmetric coupling (γ_0) to the leads. Then we will study the current conductance of a double-level quantum dot with $t_c$the coupling strength between the two levels of the quantum dot.

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II. MODEL

The transport theory, in the case of thermoelectric phenomena, allows the determination of the electrical conductance through the expression [7]

$$G = e^2 L_0 \tag{1}$$

where e is the electron charge, and L_0 is the quantity

$$L_0 = \frac{1}{h}\int_{-\infty}^{\infty} d\varepsilon T(\varepsilon)\left(\frac{-\partial f_{FD}}{\partial \varepsilon}\right) \tag{2}$$

Here h is the Planck's constant, $T(\varepsilon)$ the transmission function, and f_{FD} is the Fermi-Dirac distribution function defined as ($\mu = 0$, μ is the chemical potential).

$$f_{FD} = \frac{1}{e^{(\varepsilon/k_B T)}+1} \equiv \frac{1}{2} - \frac{1}{2}\tanh\left(\frac{\varepsilon}{2k_B T}\right) \tag{3}$$

where k_B is the Boltzmann's constant, and T the temperature. With the new variable $z = \varepsilon/k_B T$, L_0 becomes

$$L_0 = \frac{-1}{h}\int_{-\infty}^{\infty} dz T\,(k_B T z)\frac{\partial f_{FD}(z)}{\partial z} \tag{4}$$

For accurate analytical calculations we express the Fermi-Dirac function through the series [9]

$$f_{FD}(z) = \frac{1}{2} - \sum_{n=-\infty}^{\infty} \frac{1}{z - 2\pi i(n+\frac{1}{2})} \tag{5}$$

Now we will use equations (4) and (5) in order to calculate first the scaled (G/e^2) conductance of a single level quantum dot [10]. In this case the transmission function is given by

$$T(\varepsilon) = \frac{\gamma_0^2}{(\varepsilon-\varepsilon_0)^2+\gamma_0^2} \tag{6}$$

which, with the z variable, can be rewritten as

$$T(k_B T z) = 2\Re\left[\frac{i\widetilde{\gamma_0}}{2}\frac{1}{z-\widetilde{\varepsilon_0}+i\widetilde{\gamma_0}}\right] \tag{7}$$

where: $\widetilde{\gamma_0} = \gamma_0/k_B T$, and $\widetilde{\varepsilon_0} = \varepsilon_0/k_B T\, v$ are scaled quantities. With these results:

$$L_0 = \frac{-\widetilde{\gamma_0}}{h}\Re\left[i\sum_n \int_{-\infty}^{\infty} dz \frac{1}{z-\widetilde{\varepsilon_0}+i\widetilde{\gamma_0}} \frac{1}{[z-2\pi i(n+\frac{1}{2})]^2}\right] \tag{8}$$

The integral in equation (8) is carried by closing the integration path in the upper complex plane to obtain [11]

$$\frac{-1}{2\pi i(n+\tilde{a})^2};\, n = 0,1,2,\dots \tag{9}$$

where:

$$\tilde{a} = \frac{1}{2} + \frac{i}{2\pi}(\widetilde{\varepsilon_0} - i\widetilde{\gamma_0}) \tag{10}$$

Using the fact that

$$\psi^{(1)}(\tilde{a}) = \sum_{n=0}^{\infty} \frac{1}{(n+\tilde{a})^2} \tag{11}$$

is the trigamma function [12], the scaled conductance will be

$$L_0 = \frac{\widetilde{\gamma_0}}{2\pi h} \Re\psi^{(1)}\left(\frac{1}{2} + \frac{\widetilde{\gamma_0}}{2\pi} + i\frac{\widetilde{\varepsilon_0}}{2\pi}\right) \tag{12}$$

an exact analytical result [11].

The second case we analyse is the two-levels quantum dot case. Here the transmission is given by [10]

$$T(\varepsilon) = \frac{\gamma_0^2}{(\varepsilon - \varepsilon_0 - \frac{t_c^2}{\varepsilon - \varepsilon_1})^2 + \gamma_0^2} \tag{13}$$

Following steps similar to the first case we will have

$$L_0 = \frac{-\widetilde{\gamma_0}}{h} \Re\left[i \sum_n \int_{-\infty}^{\infty} dz \frac{1}{z - \widetilde{\varepsilon_0} - \frac{\widetilde{t_c^2}}{z - \widetilde{\varepsilon_1}} + i\widetilde{\gamma_0}} \frac{1}{[z - 2\pi i(n + \frac{1}{2})]^2}\right] \tag{14}$$

If the tunneling parameter between levels (t_c) is small, L_0 is reduced to

$$L_0 = \frac{-\widetilde{\gamma_0}}{h} \Re\left[i \sum_n \int_{-\infty}^{\infty} dz \frac{z - \widetilde{\varepsilon_1}}{(z - z_1)(z - z_2)} \frac{1}{(z - z_n)^2}\right] \tag{15}$$

where

$$z_1 = \left[\widetilde{\varepsilon_0} + \frac{\widetilde{t_c^2}\Delta\tilde{\varepsilon}}{(\Delta\tilde{\varepsilon})^2 + \widetilde{\gamma_0^2}}\right] - i\widetilde{\gamma_0}\left[1 - \frac{\widetilde{t_c^2}}{(\Delta\tilde{\varepsilon})^2 + \widetilde{\gamma_0^2}}\right] \equiv c - id \tag{16}$$

$$z_2 = \left[\widetilde{\varepsilon_1} - \frac{\widetilde{t_c^2}\Delta\tilde{\varepsilon}}{(\Delta\tilde{\varepsilon})^2 + \widetilde{\gamma_0^2}}\right] - i\frac{\widetilde{\gamma_0}\widetilde{t_c^2}}{(\Delta\tilde{\varepsilon})^2 + \widetilde{\gamma_0^2}} \equiv a - ib \tag{17}$$

$$z_n = 2\pi i\left(n + \frac{1}{2}\right) \tag{18}$$

and $\Delta\tilde{\varepsilon} = \widetilde{\varepsilon_0} - \widetilde{\varepsilon_1}$. After performing the contour integration and the summation we obtain

$$L_0 = \frac{2\pi\widetilde{\gamma_0}}{h} \Re(S_1 - S_2 - S_3) \tag{19}$$

Here,

$$S_1 = \frac{i}{2\pi} \frac{\psi(\frac{\pi + d + ic}{2\pi}) - \psi(\frac{\pi + b + ia}{2\pi})}{c - a + i(b - d)} \tag{20}$$

$$S_2 = \frac{1}{4\pi^2}\frac{1}{[c-a+i(b-d)]^2}$$
$$\{[d^2-c^2+(\widetilde{\varepsilon_1}+a+i(2d-b))c-(b+i(\widetilde{\varepsilon_1}+a))d-(a-ib)\widetilde{\varepsilon_1}]\psi^{(1)}(\tfrac{\pi+d+ic}{2\pi})$$
$$-2\pi(b+i(a-\widetilde{\varepsilon_1}))[\psi(\tfrac{\pi+d+ic}{2\pi})-\psi(\tfrac{\pi+b+ia}{2\pi})]\} \quad (21)$$

and $S_3 = S_2(d \to b; c \to a; a \to c; b \to d)$, and $\psi(z)$ is the digamma function. In Fig.1, we plot the temperature dependence of the scaled conductance for the one-level and for the two-levels quantum dot.

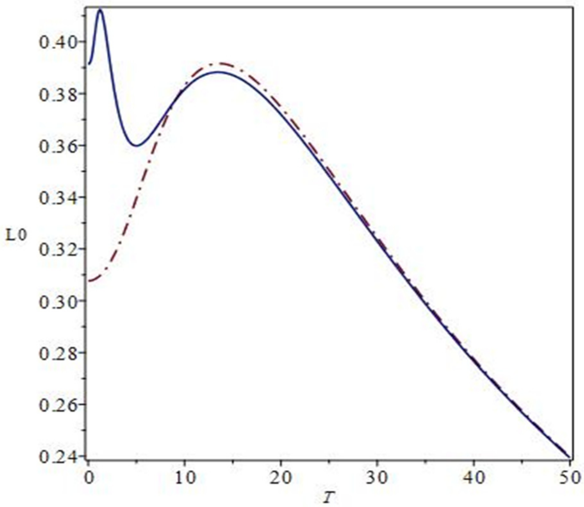

Fig. 1. Scaled conductance as function of temperature. The line correspond to the two-levels quantum dot, and the dashed-dotted line correspond to the one-level quantum dot, for the following parameters: $\widetilde{\gamma_0} = 20\,K/T$, $\widetilde{\varepsilon_0} = 30\,K/T$, $\widetilde{\varepsilon_1} = 5\,K/T$, $\widetilde{t_c} = 5\,K/T$, and for $h = 1$.

In the case when $t_c = 0$ the result (19) reduces to the previous result given by eq. (12).

A. SOMMERFELD EXPANSION

In this section, we will give approximate results of the conductance valid in the low temperatures region. For the one-level quantum dot we will approximate the trigamma function (for large z), according to the relation:

$$\psi^{(1)}\left(\frac{1}{2}+z\right)=\frac{1}{z}-\frac{1}{12z^3}\dots \quad (22)$$

Using (22) with $z=(\gamma_0+i\varepsilon_0)/2\,\pi k_B T$, L_0given by eq.(12) will be

$$L_0\simeq\frac{1}{h}\frac{\gamma_0^2}{\gamma_0^2+\varepsilon_0^2}[1-\frac{(\pi k_B T)^2}{3}\frac{\gamma_0^2-3\varepsilon_0^2}{(\gamma_0^2+\varepsilon_0^2)^2}] \quad (23)$$

In a similar way, for the two-levels quantum dot, the Sommerfeld expansion is:

$$L_0=\frac{1}{h}\frac{\gamma_0^2}{(\varepsilon_0-\frac{t_c^2}{\varepsilon_1})^2+\gamma_0^2}[1+\frac{(\pi k_B T)^2}{3}\cdot R] \quad (24)$$

with

$$R=\frac{4(\varepsilon_0-\frac{t_c^2}{\varepsilon_1})^2(1+\frac{t_c^2}{\varepsilon_1^2})^2}{[(\varepsilon_0-\frac{t_c^2}{\varepsilon_1})^2+\gamma_0^2]^2}-\frac{1+\frac{2t_c^2}{\varepsilon_1^2}+\frac{3t_c^4}{\varepsilon_1^4}-\frac{2t_c^2\varepsilon_0}{\varepsilon_1^3}}{(\varepsilon_0-\frac{t_c^2}{\varepsilon_1})^2+\gamma_0^2} \quad (25).$$

Higher values of t_c(up to a limit of it) lead to increased values of the conductance (in the low temperatures limit), as one can see in Fig.2.

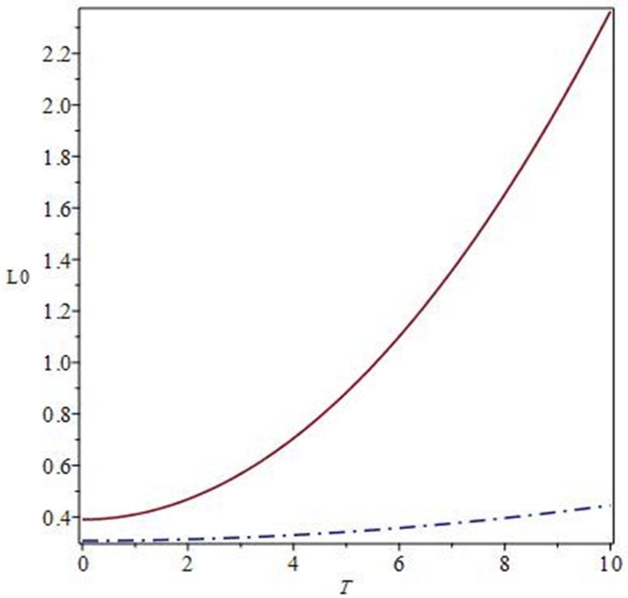

Fig. 2. Scaled conductance as function of temperature in the Sommerfeld approximation for the two-levels quantum dot. The line correspond to $t_c=5$, and the dashed-dotted line correspond to $t_c=0$**.** The parameters are: $\varepsilon_0=30, \gamma_0=20, \varepsilon_1=5$, and $h=k_B=1$.

B. HIGH-TEMPERATURES EXPANSION

Here we will analyse only the one-level quantum dot case. In the high temperatures limit the trigamma function (for small z) is approximated as

$$\psi^{(1)}\left(\frac{1}{2}+z\right)=\frac{\pi^2}{2}-14\zeta(3)z+\frac{\pi^4 z^2}{2}\dots \qquad (26)$$

Using eq.(12) the main contribution to the conductance, in this case, will be

$$L_0 \simeq \frac{\pi\gamma_0}{4hk_BT} \qquad (27)$$

in agreement with the plot from Fig. 1.

III. CONCLUSIONS

We analytically calculate the electrical conductance of an one-level and double-level quantum dot. These obtained results are useful for the study of thermoelectric effects in mesoscopic structures. The differences in the temperature dependence of the conductance for one-level and for two-levels quantum dot are highlighted. The difference are substantial at low temperatures, while at high temperatures they are insignificant. At low temperatures, the tunneling effects between the levels in the dot (for the two-levels quantum dot) and the quantum interference effects leave a significant mark on the conductance. At high temperatures, the quantum effects are erased by the thermal effects, and the conductance is similar in both cases. We also obtained Sommerfeld expansion results for the quantum dot conductance. These results are valid in the low temperatures limit. As one see from Fig. 1 and Fig. 2, the results of the Sommerfeld approximation deviate significantly from the exact results, as the temperature increases and, for the parameters used, the results of the approximation are valid only at extremely low temperatures.

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