2009-10

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Thermoelectric effects in quantum dots

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ARTICLE INFO

PACS:
72.15.Qm
73.23.Hk
73.50.Lw

Keywords:
Kondo effect
Fano interference
Thermopower
Numerical renormalization-group

ABSTRACT

We report a numerical renormalization-group study of the thermoelectric effect in the single-electron transistor (SET) and side-coupled geometries. As expected, the computed thermal conductance and thermopower curves show signatures of the Kondo effect and of Fano interference. The thermopower curves are also affected by particle–hole asymmetry.

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1. Introduction

The transport properties of mesoscopic devices are markedly affected by electronic correlations. Gate potentials applied to such devices give experimental control over effects once accessible only in special arrangements. In particular, the Kondo effect and Fano anti-resonances have been unequivocally identified in the conductance of single-electron transistors (SET) [1–3]; of Aharonov–Bohm rings [4]; and of quantum wires with side-coupled quantum dots [5]. Another achievement was a recent study of the thermopower, a quantity sensitive to particle–hole asymmetry that monitors the flux of spin entropy [6]. This work presents a numerical renormalization-group study [10–12] of the thermoelectric properties of nanodevices. We consider a quantum dot coupled to conduction electrons in the two most widely studied geometries: the single-electron transistor (SET), in which the quantum dot bridges two-dimensional gases coupled to electrodes; and the \( T \)-shaped device, in which a quantum dot is side-coupled to a quantum wire.

2. Thermoelectric properties

Thermoelectric properties are traditionally studied in two arrangements: the Seebeck (open circuit) and Peltier (closed circuit) setups [13]. In the former, the steady-state electric current vanishes. A temperature gradient drives electrons towards the coldest region, and induces an electric potential difference between the hot and the cold extremes. The expression \( S = - \Delta V / \Delta T \), where \( \Delta V \) is the potential difference induced by the temperature difference \( \Delta T \), then determines the thermopower \( S \). Since the electrons transport heat, the heat current \( Q \) can also be measured, and the thermal conductance \( \kappa \) can be obtained from the relation \( Q = - \kappa \nabla T \).

In the Peltier setup, a current \( J \) is driven through a circuit kept at uniform temperature. The heat flux \( Q = P J \) is then measured and determines the Peltier coefficient \( P \), which is proportional to the thermopower: \( P = ST \).

We prefer the Seebeck setup. The transport coefficients are then computed from the integrals [7]

\[
I_n(T) = -\frac{2}{h} \int_{-D}^{+D} \frac{d\varepsilon}{\varepsilon} \mathcal{F} (\varepsilon, T) \varepsilon \quad (n = 0, 1, 2),
\]

where \( \mathcal{F} (\varepsilon, T) \) is the transmission probability at energy \( \varepsilon \) and temperature \( T \), \( f(\varepsilon) \) is the Fermi distribution and \( D \) is the half width of the conduction band. The electric conductance \( G \), the thermopower \( S \), and the thermal conductance \( \kappa \) are given by [7]

\[
G = \varepsilon I_0(T),
\]

\[
S = -\frac{I_1(T)}{e I_0(T)},
\]

\[
\kappa = \frac{1}{T} \left\{ \frac{I_2(T)}{I_0(T)} - \frac{P(T)}{I_0(T)} \right\}.
\]
respectively. Our problem, therefore, is to compute \( \mathcal{F}(e, T) \) for a correlated quantum dot coupled to a gas of non-interacting electrons.

### 3. Thermal conductance and thermopower of a SET

Recent experiments [3] have detected Fano anti-resonances in coexistence with the Kondo effect in SETs. The interference indicates that the electrons can flow through the dot or tunnel directly from one electrode to the other. The transport properties of the SET can be studied by a modified Anderson model [9,14], which in standard notation is described by the Hamiltonian

\[
H = \sum_{k}\varepsilon_k c_k^\dagger c_k + t \sum_{k \neq k'} (c_{k'}^\dagger c_k + H.c.) + V \sum_{k} (c_k^\dagger c_k + H.c.) + H_d.
\]

Here the quantum-dot Hamiltonian is \( H_d = \varepsilon_d c_d^\dagger c_d + U n_{d,\uparrow} n_{d,\downarrow} \), with a dot energy \( \varepsilon_d \), controlled by a gate potential applied to the dot, that competes with the Coulomb repulsion \( U \). The summation index \( x \) on the right-hand side takes the values \( L \) and \( R \), for the left and right electrodes respectively. The tunneling amplitude \( t \) allows transitions between the electrodes, while \( V \) couples the electrodes to the quantum dot. The Hamiltonian (5) being invariant under inversion, it is convenient to substitute even (+) and odd (−) operators \( c_{k\pm} = (c_k \pm c_{-k})/\sqrt{2} \) for the \( c_k \) and \( c_{-k} \). It results that only the \( c_{k\pm} \) are coupled to the quantum dot. For brevity, we define the shorthand \( \gamma = \pi \rho \), where \( \rho \) is the density of conduction states; and the dot-level width \( \Gamma = \pi \rho V^2 \).

In the absence of magnetic fields, the transmission probability through the SET is [8,9]

\[
\mathcal{T}(e, T) = T_0 + \frac{4\Gamma^2 \sqrt{T_0 R_0}}{1 + \gamma^2} \Im[\mathcal{G}_{ddd}](e, T) + \frac{2\Gamma (T_0 - R_0)}{1 + \gamma^2} \Im[\mathcal{G}_{ddd}](e, T),
\]

where \( \mathcal{G}_{ddd}(e, T) \) is the retarded Green’s function for the dot orbital, and we have defined \( T_0 = 4\gamma^2 / (1 + \gamma^2)^2 \) and \( R_0 = 1 - T_0 \).

To compute \( \mathcal{F} \), we rely on the numerical-renormalization group (NRG) diagonalization of the model Hamiltonian [10]. Although the resulting eigenvectors and eigenvalues yield essentially exact results for \( \Im[\mathcal{G}_{dd}](e, T) \), the direct computation of \( \Im[\mathcal{G}_{dd}](e, T) \) is unwieldy. We have found it more convenient to define the Fermi operator

\[
b = \left( \frac{4\Gamma^2}{1 + \gamma^2} \right)^{1/2} c_d + \left( \frac{4\gamma^2}{1 + \gamma^2} \right)^{1/2} \frac{1}{\sqrt{\pi} \rho} \sum_k \frac{c_{k\pm}}{k},
\]

because the imaginary part of its retarded Green’s function \( \mathcal{G}_{dd}(e, T) \) is directly related to the transmission probability: aided by the two equations of motion relating \( \mathcal{G}_{dk} \) to \( \mathcal{G}_{dd} \), and \( \mathcal{G}_{dd} \) to \( \mathcal{G}_{dd} \), straightforward manipulation of Eq. (6) show that \( \mathcal{F}(e, T) = -\Im[\mathcal{G}_{dd}](e, T) \). In practice, we (i) diagonalize \( H \) iteratively [10]; (ii) for each pair of resulting eigenstates \( \langle m | n \rangle \), compute the matrix elements \( \langle m | b_d | n \rangle \); (iii) thermal average the results [15,16] to obtain \( \Im[\mathcal{G}_{dd}](e, T) \); (iv) substitute the result for \( \mathcal{F}(e, T) \) in Eq. (1); and (v) evaluate the integral for \( n = 0, 1, 2 \) to obtain \( I_n(T) \) (\( n = 0, 1, 2 \)).

![Fig. 1](image.png)

**Fig. 1.** Thermal conductance \( \kappa \), normalized by the temperature \( T \), as a function of the dot energy for \( U = 0.3 \)D and four \( t \) s, at the indicated temperatures. The top panel, with \( t = 0 \), shows no sign of interference. The second (third) panel, with \( t = 0.16D \) (\( t = -0.16D \)) displays a Fano antiresonance. In the bottom panel, \( t = 0.32D \), the conductance vanishes in the Kondo valley as \( T \to 0 \).

The top panel shows the standard SET, with no direct tunneling channel. At the lowest temperature \( \varepsilon_d T = 10^{-9}D \), the model Hamiltonian close to the strong-coupling fixed point, the Kondo screening makes the quantum dot transparent to electrons, so that in the Kondo regime \( F = \min [2\varepsilon_d, 2\varepsilon_d + U] \) the Wiedemann–Franz law pushes the ratio \( 3k_b T \theta \) to the unitary limit \( 2e^2 / h \). At higher temperatures, the Kondo cloud evaporates and the thermal conductance drops steeply. The maxima near \( \varepsilon_d = 0 \) and \( \varepsilon_d = -U \) reflect the two resonances associated with the transitions \( c_d^\dagger c_d^\dagger \) and \( c_d \).

In the next two panels, the direct tunneling amplitude substantially increased, the current through the dot tends to interfere with the current bypassing the dot. To show that a particle–hole transformation is equivalent to changing the sign of the amplitude \( t \), we compare the curves with \( t = 0.16D \) (second panel) with \( t = -0.16D \) (third panel). At low temperatures, in the former (latter) case, the interference between the \( c_d^\dagger c_d^\dagger \) and \( c_d \) transitions is constructive near \( \varepsilon_d = 0 \) (\( \varepsilon_d = -U \)) and destructive near \( \varepsilon_d = U \) (\( \varepsilon_d = 0 \)). At intermediate dot energies, \( \varepsilon_d \simeq -U/2 \), the amplitudes for direct transition and for transition through the dot have orthogonal phases and fail to interfere, so that the resulting current is the sum of the two individual currents.

In the bottom panel, the direct tunneling amplitude \( t \) is dominant. For gate potentials favoring the formation of a dot...
moment, heat flows from one electrode to the other. In the Kondo regime, however, at low temperatures, the Kondo cloud coupling the dot to the electrode orbitals closest to it blocks transport between the electrodes. As the Kondo cloud evaporates, the thermal conductance in the $t_d \approx -U/2$ rises with temperature, so that the resulting profile is symmetric to the one in the top panel. The two resonances near $\epsilon_d = 0$ and $-U$ which are independent of Kondo screening, keep the thermal conductance low even at relatively high temperatures.

Fig. 2 shows thermopower profiles for the same amplitudes $t$ discussed in Fig. 1. In contrast with the thermal conductance, the thermopower is sensitive to particle–hole asymmetry: heat currents due to holes (electrons) make it positive (negative). For the standard SET ($t = 0$, top panel), the thermopower is negligible at low temperatures and vanishes at the particle–hole symmetric parametrical point $\epsilon_d = -U/2$.

With $|t| = 0.16D$, particle–hole symmetry is broken at $\epsilon_d = -U/2$, and temperatures comparable to $T_K$. For $t = 0.16D$, the sensitivity to particle–hole asymmetry makes the interference between electron (hole) currents constructive (destructive) for both $\epsilon_d = 0$ and for $\epsilon_d = U$, while for $t = -0.16D$ it is destructive (constructive).

For $t = 0.32D$, direct tunneling again dominant, in the Kondo regime ($\epsilon_d \approx -U/2$) the thermopower becomes sensitive to the Kondo effect, which is chiefly due to electrons (holes) above (below) the Fermi level. The thermopower therefore emerges as a probe of direct-tunneling leaks in SETs, one that may help identify the source of interference in this and other nanodevices.

**4. Side-coupled quantum dot**

We have also studied the T-shaped device, in which the dot is side-coupled to the wire [5]. Again, we considered the Seebeck setup. The quantum wire now shunting the two electrodes, we drop the coupling proportional to $t$ on the right-hand side of Eq. (5) and employ the standard Anderson Hamiltonian

$$H_d = \sum_k \epsilon_d c_k^\dagger c_k + V \sum_k (c_k^\dagger c_k + H.c.) + H_d, \quad (8)$$

where $H_d = \epsilon_d c_d^\dagger c_d + U n_d^\dagger n_d$ is the dot Hamiltonian. The transmission probability is now given by $\bar{T}(\epsilon, T) = 1 + \pi \rho V^2 \Im \langle G_{dd}(\epsilon, T) \rangle$ where $G_{dd}(\epsilon, T)$. Following the procedure outlined above, we have diagonalized the Hamiltonian $H_t$ iteratively and computed the electrical conductance, the thermal conductance and the thermopower as functions of the gate potential $\epsilon_d$.

Fig. 3 displays results for $U = 0.3D$, and $\Gamma = 0.01D$.

Not surprisingly—the wire is equivalent to a large tunneling amplitude, i.e., to $t \sim D$—the transport coefficients mimic those of the $t = 0.32D$ SET. At low temperatures ($T \ll T_K$) in the Kondo regime, for instance, the Kondo cloud blocks transport through the wire segment closest to the dot. The thermal and electrical conductances thus vanish for $\epsilon_d \approx -U/2$. As the temperature rises, the evaporation of the Kondo cloud allows transport and both conductances rise near the particle–hole symmetric point. At low temperatures, the sensitivity to particle–hole asymmetry enhances the thermopower in the Kondo regime, a behavior analogous to the bottom panel in Fig. 2.
5. Conclusions

We have calculated the transport coefficients for the SET and the side-coupled geometries. In both cases, the thermal dependence and the gate-voltage profiles show signatures of the Kondo effect and of quantum interference. Our essentially exact NRG results identify trends that can aid the interpretation of experimental results. In the side-coupled geometry, in particular, the Kondo cloud has marked effects upon the thermopower.

Acknowledgments

This work has been funded by BZG. Financial support by the FAPESP and the CNPq is acknowledged.

References