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Thermopower of double quantum dots: Fano effect and competition between Kondo and antiferromagnetic correlations

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Abstract

The thermoelectric properties of double quantum dot (DQD) systems are investigated and our attention is focused on the interplay between the Fano effect and electronic correlations. If the antiferromagnetic (AF) correlation is weak, the derivative of thermopower with the energy level on dots is positive at the particle–hole symmetric point. With the Fano effect introduced, it becomes negative due to the Fano–Kondo effect. The competition between the Kondo and AF correlations yields a zero in the derivative, and with the direct channel open, in the vicinity of that zero, the derivative undergoes an almost discontinuous hopping with its sign reversed. Away from the particle–hole symmetric point, the variation of thermopower is also related to that interplay. Compared with conductance, thermopower can provide more information on the DQD systems. These results are robust to asymmetry and can be verified in experiments with temperature lower than the Kondo temperature.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The interplay between quantum interference effects and electronic correlations plays an important role in mesoscopic physics [1–3]. In this respect, quantum dot (QD) systems have attracted a lot of attention due to their tunability. When a dot is connected to leads, the coupling between the localized spin on the dot and conduction electrons may result in a spin singlet state [4–8], and the correlation energy T_K is termed the Kondo temperature. If double quantum dots (DQDs) [9–13] are connected to leads in a 'lead–dot–dot–lead' series, the interplay between dot–dot tunnelling t_d and Coulomb interaction U yields an effective antiferromagnetic (AF) coupling $J_M = \sqrt{(2t_d)^2 + (U/2)^2} - U/2$, which tends to create a singlet state between the localized spins on the two dots. Competition between the Kondo and AF correlations leads to a resonant conductance peak at $J_M \sim T_K$ in the half-filled case [11–13]. If the two leads are also connected directly, the Fano effect [14] introduces a transmission zero accompanying the resonant peak [15]. In the singly occupied regime, the Fano–Kondo effect [15–19], like the Kondo effect, greatly reduces the conductance if $J_M \ll T_K$, whereas the strong parity splitting blocks the path through the DQDs in the limit $t_d \gg U/4$.

All of these results are obtained from the conductance, which, at low temperature, is mainly determined by the value of the transmission spectrum τ at the Fermi energy ϵ_F. With a temperature difference ΔT across a QD structure, a thermovoltage ΔV should be applied between two leads to nullify the resulting current, and the thermopower [20–28] is defined as $S = -\frac{\Delta V}{\Delta T}$, which is not simply given by $\tau(\epsilon_F)$ but is sensitive to the symmetry of the density of states or the transmission spectrum. In a DQD system, the derivative of thermopower with the energy level ϵ_d on dots at the particle–hole symmetric point can determine whether a peak or dip is formed at the Fermi level in the spectrum. Away from that point, this derivative can still give much useful information if only one peak or one dip is formed in the spectrum. Because the spectrum contains all the physics of the system, the thermopower can provide more information than the conductance and it is a more powerful tool with which to manifest the interplay between the Fano effect and electronic correlations. Here, we extend our previous work on electric properties of DQD systems [15] to their thermoelectric ones. The double motivations of the present paper are: (i) to show how that interplay influences the thermopower and (ii) to clarify what new information can be provided.

For these purposes, the DQD systems are assumed to work in the strong-coupling regime with low temperature. In QD systems, the electron–phonon interaction is weak at low temperature and can be neglected [29–31]. According to our theoretic calculations, when $J_M \ll T_K$, the Kondo correlation prevails, and the derivative of S is positive at the particle–hole symmetric point, whereas with the direct channel open, the derivative becomes negative due to the Fano–Kondo effect. When $J_M \sim T_K$, the competition between the Kondo and AF correlations yields a zero in the derivative, and with the Fano effect introduced, in the vicinity of that zero, the derivative undergoes an almost discontinuous hopping with its sign reversed. Away from the particle–hole symmetric point, the characteristics of S can also be understood from the interplay between the Fano effect and electronic correlations. In this thermoelectric method, the Kondo and Fano–Kondo effects can be distinguished. Compared with conductance [15], thermopower really provides more information on the DQD systems. These results are robust to asymmetry and can be verified in experiments with temperature T lower than T_K.

2. Model and formulae

In the present paper, the thermoelectric properties of DQD systems are investigated and our interest is focused on the influences of the Fano effect and competition between the Kondo and AF correlations. In order to compare the characteristics of the thermopower with those of the conductance, we take the same DQD structure as in [15], which is schematically illustrated in figure 1. With the electron–phonon interaction neglected [29–31], the Hamiltonian of this mesoscopic system can be described by the following 1D tight-binding form [15]: $H = H_{\rm Lead} + H_{\rm Dot} + H_{\rm T}$, where $H_{\rm Lead} = -t(\sum_{i=-\infty,\sigma}^{-2} + \sum_{i=1,\sigma}^{\infty})(\hat{c}_{i\sigma}^{\dagger}\hat{c}_{i+1\sigma} + {\rm H.c.})$ is for the left and right leads, the DQD are described by $H_{\rm Dot} = \sum_{\alpha}(\epsilon_{\alpha}\sum_{\sigma}\hat{c}_{\alpha\sigma}^{\dagger}\hat{c}_{\alpha\sigma} + U_{\alpha}\hat{n}_{\alpha\uparrow}\hat{n}_{\alpha\downarrow}) - t_d\sum_{\sigma}(\hat{c}_{{\rm L}\sigma}^{\dagger}\hat{c}_{{\rm R}\sigma} + {\rm H.c.})$ and the tunnelling part is $H_{\rm T} = -\sum_{\sigma}(t_{\rm L}^{(\rm L)}\hat{c}_{-1\sigma}^{\dagger}\hat{c}_{{\rm L}\sigma} + t_{\rm L}^{(\rm R)}\hat{c}_{1\sigma}^{\dagger}\hat{c}_{{\rm R}\sigma} + t_{\rm r}\hat{c}_{1\sigma}^{\dagger}\hat{c}_{-1\sigma} + {\rm H.c.})$. Here, $\sigma = \uparrow, \downarrow$ and $\alpha = {\rm L, R}$. As in [15], the time-reversal invariant system is considered, which is realizable in experiments and interesting in theory.

If one dot with energy level ϵ_d and Coulomb repulsion U is connected to leads with a hopping integral t_L, the Kondo temperature is [32] $T_K = \frac{U\sqrt{J_K}}{2\pi}\exp(-\pi/J_K)$, where

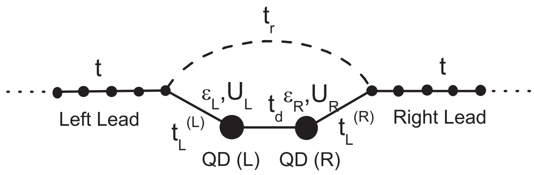

Figure 1. Schematic illustration of a DQD structure. In the main part of this paper, a symmetric structure is considered, where $\epsilon_d = \epsilon_L = \epsilon_R$, $t_L = t_L^{(L)} = t_L^{(R)}$ and $U = U_L = U_R$.

$J_K = \frac{-2U\Gamma}{\epsilon_d(\epsilon_d+U)}$. With the Fermi energy $\epsilon_F = 0$, the hybridization strength $\Gamma = 2t_L^2/t$ in the thermodynamic limit [33]. In order to investigate the competition between the Kondo and AF correlations, the temperature T should be set below T_K. In the DQD system schematically illustrated in figure 1, if $t_L^{(L)} = t_L^{(R)} = 0$, electrons can only tunnel through the direct channel. In this situation, the transmissivity $|T_r|^2 = \frac{4}{(t_r/t+t/t_r)^2}$ and the thermopower is zero.

To study the electric and thermoelectric transport properties of the DQD system, transport coefficients should be calculated, which can be obtained in the linear response regime as [21, 26, 27]

$$L_{ml} = \int_{-\infty}^{\infty} \left(-\frac{\partial f(\epsilon)}{\partial \epsilon}\right) \tau^l(\epsilon)(\epsilon - \epsilon_F)^m \, d\epsilon, \tag{1}$$

where $f(\epsilon)$ is the Fermi–Dirac distribution and $\tau(\epsilon)$ the transmission spectrum function. Then, the conductance and thermopower are given in terms of these coefficients as $G = L_{01}$ and $S = -\frac{1}{T}\frac{L_{11}}{L_{01}}$, respectively. To obtain $\tau(\epsilon)$, the electronic correlations in this DQD system have to be treated. For this purpose, the finite-U slave boson mean-field method of Kotliar and Ruckenstein [13, 34, 35] is adopted, as in [15]. In the strong-coupling regime with low temperature, this method has been applied successfully to the electric transport properties of DQD systems [13, 15] and it can give qualitatively the same results as those obtained from exact numeric methods [11, 12]. In the framework of this approach, auxiliary boson fields are introduced as projection operators, and to eliminate unphysical states, constraint conditions are incorporated via Lagrange multipliers. In this mean-field treatment, the slave boson fields are replaced by their expectation values, and then, the resulting noninteracting Hamiltonian is solved self-consistently by minimization of the free energy with respect to those parameters [34, 35]. In this process, numeric diagonalization is adopted [36, 37], and the symmetry of the system, e.g. the spin degeneracy and the left–right symmetry, can greatly simplify the numeric calculation. The transmission spectrum function $\tau(\epsilon)$ of this essentially noninteracting system is the transmissivity of an incident electron with energy ϵ. The details of this method are given in [15].

3. Results and discussion

In the following calculations, we first study the system with left–right symmetry at temperature $T = 0.001$, and set $t = 1$, $t_L = 0.35$ and $U = 1.4$. The corresponding T_K of a single QD structure at the particle–hole symmetric point $\epsilon_d = -U/2$ is 0.0280, which is larger than T.

Since the thermopower is related to the transmission spectrum, we illustrate τ in figures 2 and 3 for $t_r = 0$ and 0.5, respectively, to understand thermoelectric properties in depth. Consider the situation at the particle–hole symmetric point. Without the Fano effect, when $J_M \ll T_K$, a low peak is formed at $\epsilon = 0$ due to the Abrikosov–Suhl resonance. In fact, if the spectrum of a single QD is $\tau_{SQD}(\epsilon)$, the corresponding one of a DQD [13, 38] $\tau(\epsilon) \approx \tau_{SQD}^2(\epsilon)t_d^2/\Gamma^2$ in the limit of $t_d \to 0$. With J_M increased, the peak height is enhanced

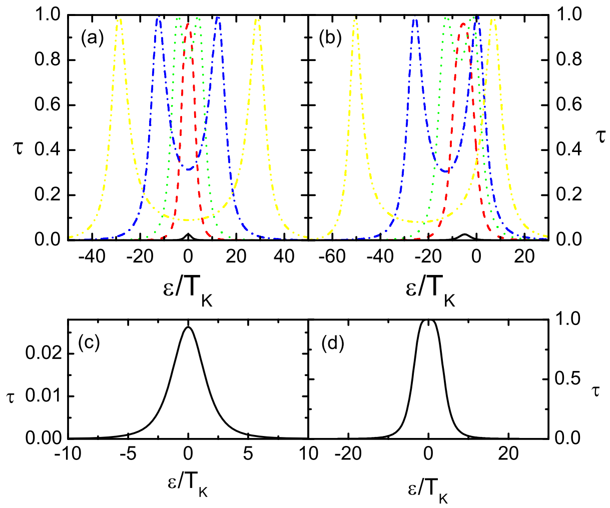

Figure 2. τ–ϵ curves with $t_d = 0.01$ (solid, black), 0.1 (dashed, red), 0.2 (dotted, green), 0.4 (dash–dotted, blue) and 0.8 (dash–dot–dotted, yellow) for $\epsilon_d = -U/2$ (a) and 0 (b). In (c) and (d), $t_d = 0.01$ and 0.12, respectively for $\epsilon_d = -U/2$. The other parameters are $t = 1$, $t_L = 0.35$, $t_r = 0$, $U = 1.4$ and $T = 0.001$.

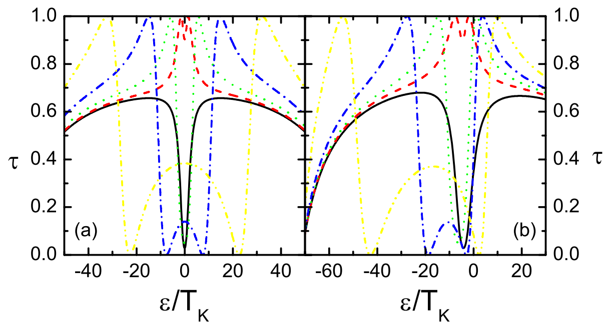

Figure 3. τ–ϵ curves with $t_d = 0.01$ (solid, black), 0.1 (dashed, red), 0.2 (dotted, green), 0.4 (dash–dotted, blue) and 0.8 (dash–dot–dotted, yellow) for $\epsilon_d = -U/2$ (a) and 0 (b). The other parameters are the same as in figure 2 except $t_r = 0.5$.

and its width is expanded until $t_d = 0.12$, where $J_M \sim T_K$ and the peak reaches unity. When the AF correlation prevails, the Kondo spin singlets are broken and the resonant peak is split into double ones. With $t_d \gg U/4$, the doubly occupied bonding state of the two dots is favoured, which further lowers the dip at $\epsilon = 0$. If the direct channel is open, $\tau(0)$ approaches $|T_r|^2$ in the same limit since the path through the dots is blocked. For the same reason, in the region with $|\epsilon|$ larger than the energy splitting between the even and odd states, τ is enhanced from zero to about $|T_r|^2$. (Of course, in the vicinity of band edges, τ decreases to zero.) As a result, when $J_M \ll T_K$, although the Fano–Kondo effect [15, 18] still yields a low $\tau(0)$, a dip, instead of a low peak, is formed. Besides these changes, several others are caused by the Fano effect. In the region $J_M \sim T_K$, the competition between the Kondo and AF correlations still results in a resonant peak. But with J_M further enhanced, this peak is first split and then turned into two symmetric peak–zero pairs because of the destructive interference between the direct path and the path through dots.

Table 1. Table of $J_M = \sqrt{(2t_d)^2 + (U/2)^2} - U/2$ with $U = 1.4$. When $t_L = 0.35$, $T_K = 0.0280$, which is almost identical to the J_M at $t_d = 0.1$.

t_d	0.01	0.1	0.12	0.2	0.4	0.8
J_M	2.86×10^{-4}	0.0280	0.0400	0.106	0.363	1.05

Due to the particle–hole symmetry of the system, $\tau(\epsilon, \epsilon_d) = \tau(-\epsilon, -U - \epsilon_d)$. At $\epsilon_d = -U/2$, the spectrum is symmetric with respect to $\epsilon = 0$. With $\epsilon_d > -U/2$, it moves towards the negative ϵ direction, accompanied by a deformation of its shape, and asymmetry is introduced. But its basic characteristics, such as resonant peaks and transmission zeros, are reserved. These results are also illustrated in figures 2 and 3 as a comparison with the symmetric ones. Here, for the convenience of readers, the same table on the relation between J_M and t_d as in [15] is presented (table 1).

As is illustrated in figures 2 and 3, the appearance of one peak, one dip, double peaks or peak–zero pairs in the spectrum is related to the interplay between the Fano effect and electronic correlations. At low temperature, G is mainly determined by $\tau(0)$, and the characteristics of that interplay can only be partly shown in the G–t_d curve [15] with $\epsilon_d = -U/2$. For example, although the Kondo and Fano–Kondo effects lead to one peak and one dip, respectively, in the spectrum, G cannot distinguish between these two different effects because $\tau(0)$ is low in both of them. On the other hand, at $\epsilon_d = -U/2$, $S = 0$, but with ϵ_d deviating from $-U/2$, the spectrum asymmetry leads to a nonzero S. If a peak is formed at $\epsilon = 0$, with ϵ_d a little enhanced from $-U/2$, the transmissivity in the range from $\epsilon = 0$ to T is smaller than that in $[-T, 0]$ and S is increased from zero. Whereas, if a dip is formed, S is turned into negative. In other words, $\mathrm{d}S/\mathrm{d}\epsilon_d$ can signal whether a peak or dip is formed at $\epsilon = 0$. In the Kondo regime, the introduction of Fano effect turns one peak into one dip, and these two different effects can be distinguished by the $\mathrm{d}S/\mathrm{d}\epsilon_d$–$t_d$ curve. This demonstrates the statement that thermoelectric properties can provide more information on the DQD system than electric ones.

The $\mathrm{d}S/\mathrm{d}\epsilon_d$–$t_d$ curves for $t_r = 0$ and 0.5 are plotted in figures 4(a) and (b), respectively. In the regime $J_M \sim T_K$, the transitions of spectrum structure—from one peak to double peaks and double peaks to peak–zero pairs—yield zero $\mathrm{d}S/\mathrm{d}\epsilon_d$ at two different points, where G reaches its extremum. Around the minimum of G, related to the latter transition, which can happen only in the situation with $t_r \neq 0$, $\mathrm{d}S/\mathrm{d}\epsilon_d$ undergoes an almost discontinuous hopping with its sign reversed. The $\mathrm{d}S/\mathrm{d}\epsilon_d$–$t_d$ curves give the thermoelectric properties around the particle–hole symmetric point. Away from this point, they can still give much useful information if only one peak or one dip is formed in the spectrum. But if double peaks or peak–zero pairs are formed, S itself has to be studied.

In the situation with double peaks, $\mathrm{d}S/\mathrm{d}\epsilon_d$ is negative at $\epsilon_d = -U/2$. As ϵ_d increases, the right peak passes through $\epsilon = 0$ and S changes from negative to positive. A similar phenomenon can be found in the situation with peak–zero pairs, where the S sign reverses twice—from positive to negative and then negative to positive—due to the successive passage of the right zero and peak. Here, the former reversal is almost discontinuous and a large hopping is formed. Because $S \sim \frac{1}{L_{01}} = \frac{1}{G}$, the 'discontinuity' is associated with the conductance 'zero'. This 'discontinuity' in S leads to that in $\mathrm{d}S/\mathrm{d}\epsilon_d$–$t_d$ curves. All of these explain the basic characteristics of the S–ϵ_d curves, which are also related to the interplay between the Fano effect and electronic correlations since the spectrum is determined by that interplay. These results are presented in figure 5, where $S(\epsilon_d) = -S(-U - \epsilon_d)$ due to the particle–hole symmetry.

In the above calculations, left–right symmetry is assumed. This symmetry can be destroyed in two different ways. In the first one, fixed differences are introduced in between the structural

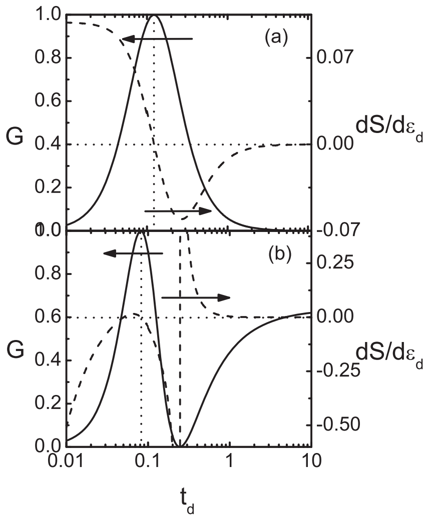

Figure 4. G–t_d (solid) and $dS/d\epsilon_d$–t_d (dashed) curves at $\epsilon_d = -U/2$ for $t_r = 0$ (a) and 0.5 (b). The dotted lines are used to guide the eyes.

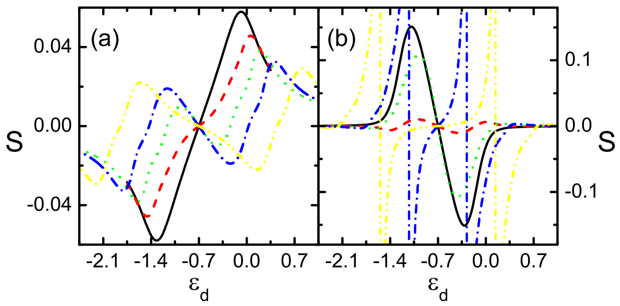

Figure 5. S–ϵ_d curves for $t_r = 0$ (a) and 0.5 (b). The curve features have the same meanings as in figure 3.

parameters of the left and right dots. Here, the particle–hole symmetry is still reserved. If we define $\epsilon_d \equiv (\epsilon_L + \epsilon_R)/2$, the symmetric point is located at $\epsilon_d = -(U_L/2 + U_R/2)/2$. In this situation, a remarkable change can only be found for strong differences. In the other way, a fixed ratio is introduced in between the energy levels of the two dots. Although the particle–hole symmetry is broken, the spectrum is symmetric at $\epsilon_d = -(U_L/2+U_R/2)/2$, where $S = 0$, and $dS/d\epsilon_d$ shows the same variation trend with t_d as in the particle–hole symmetric system if that ratio is not too large. In our calculations, T is set as 0.001. In the range $T < T_K$, with T increased, the G–ϵ_d curve is nearly independent of T since even T_K is a low value, whereas the S–ϵ_d curve increases as a whole with its shape almost unchanged. But because more states participate in electronic transport, the conductance dip is enhanced from zero. As a result, the 'discontinuous' sign reversal related to the dip is smoothed, but the corresponding hopping is still large. Although our main results are obtained from the system with left–right symmetry at a certain temperature, the basic characteristics of the thermoelectric effect are robust to asymmetry and temperature only if $T < T_K$.

In experiments, the thermovoltage ΔV is measured at a small fixed ΔT, and consequently, the characteristics of S can be obtained with structural parameters such as ϵ_d, t_d and t_r varied.

Because $S = 0$ at the particle–hole symmetric point (in the generalized sense), $dS/d\epsilon_d$ can be determined in a similar method, but here ϵ_d should be fixed, with its value a little enhanced from the symmetric point. In particular, when $J_M \ll T_K$, with the Fano effect introduced, ΔV measured in the latter method is turned from negative to positive. This is a clear phenomenon and cannot be confused with others. In these ways, the interplay between quantum interference effects and electronic correlations can be studied from the thermoelectric properties.

4. Summary

In summary, we investigate the thermoelectric properties of DQD structures and focus our attention on the influences of the Fano effect and competition between the Kondo and AF correlations. When $J_M \ll T_K$, $dS/d\epsilon_d$ is positive at the particle–hole symmetric point if the Fano effect is not introduced. With the direct channel open, $dS/d\epsilon_d$ becomes negative due to the Fano–Kondo effect. At $J_M \sim T_K$, the competition between the Kondo and AF correlations yields a zero in the $dS/d\epsilon_d$–t_d curve, and with the Fano effect introduced, in the vicinity of that zero, the derivative undergoes an almost discontinuous hopping with its sign reversed. Away from the particle–hole symmetric point, the characteristics of S can also be understood from the interplay between the Fano effect and electronic correlations. In this thermoelectric method, the Kondo and Fano–Kondo effects can be distinguished, and compared with conductance, thermopower really provides more information on the DQD systems. These results are robust to asymmetry and can be verified in experiments with T lower than T_K.

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