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## Real two-stage Kondo effect in parallel double quantum dot

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## ABSTRACT

We study the two-stage Kondo effect in asymmetric parallel double quantum dots. In the triplet, the magnetic moment screenings on two dots occur at the same Kondo temperature. In the critical regime of the triplet–singlet quantum phase transition, a two-stage Kondo screening accompanied with two kinds of Kondo resonance with two energy scales is observed. This is contrast to previous works, in which the Kondo peak in the second screening has not been observed. For large asymmetry of the Kondo coupling, the Kondo resonance in the second step is very weak, which indicates that the screening occurs mainly between two dots and is not a real Kondo screening. Therefore, the side-coupled double quantum dots, which have been extensively studied in the literature, are not an ideal candidate to show a real two-stage Kondo screening.

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## 1. Introduction

Double quantum dot (DQD) devices have been the ideal components to study the physics of strongly correlated electrons due to the flexibility to change the geometry and the coupling in a continuous way. In recent years, a flood of works have focused on the Kondo physics and the quantum phase transition (QPT) [1–12]. One of the novel quantum transport phenomena is a two-stage Kondo screening demonstrated experimentally in semiconductor quantum dots [13–15] and carbon nanotube [16,17]. Very recently, the two-stage Kondo effect is observed in nanometer-sized carbon nanotube quantum dots fabricated by electromigration [17]. The experimental signature is a dip within a broad zero-bias conductance peak. The conductance exhibits a nonmonotonic temperature dependence with two characteristic energy scales. The second-stage Kondo temperature increases with increasing the dot–lead coupling. Contrast to this result, in a Kondo box consisting of a large carbon nanotube [16], the second-stage Kondo temperature decreases with increasing the dot–lead coupling. Theoretical works were concentrated on side-coupled double quantum dot systems [18–25], in which only one of the dots (QD1) is coupled to the electrodes and the other dot (QD2) is side-coupled to the QD1. In the case where each of the dots is singly occupied, for small interdot hopping  $t$ , the local spin on the QD1 is screened first by the electrons of the leads at a higher temperature, and then the spin on the QD2 is screened at a lower

temperature. In contrast, for large  $t$ , the two spins form a molecular-type singlet due to the interdot antiferromagnetic interaction  $J_{AF}$  induced by  $t$ .

With increasing  $J_{AF}$ , there is a crossover from the two-stage Kondo screening to a molecular-type singlet. They have a similar consequence: the magnetic moments on the dots are screened totally at zero temperature. The difference is that the former is screened by the leads and the latter is screened by the dots themselves. In the second-stage Kondo screening, the spin on the QD2 can be screened not only by the QD1 but also by the leads. Only the latter is accompanied with the Kondo resonance and is the real Kondo screening. However, in previous works, only the Kondo resonances in the first stage of screening on the QD1 were observed while the Kondo peak in the second step on the QD2 has not been observed [18]. Generally, one should observe two kinds of Kondo resonance in two energy scales of  $T_{K1}$  and  $T_{K2}$  corresponding to two-stage Kondo screening.

In this paper, we investigate the mechanism of the two-stage Kondo screening and the critical phenomena for an asymmetric parallel DQD system in Fig. 1. The Kondo coupling between two dots and leads is  $T_i = 2\pi\rho|V_i|^2$  ( $i = 1, 2$ ), where  $\rho$  is a constant density of states of the conduction electrons in the leads. Without the interdot hopping  $t$ , the ground state is a local spin triplet due to the effective interdot ferromagnetic Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction  $J_{RKKY}$  mediated by the conduction electrons of the leads [7,26]. The competition between  $J_{RKKY}$  and  $J_{AF}$  induces a triplet–singlet Kosterlitz–Thouless (KT) transition at the critical point  $t = t_c$  corresponding to the effective interdot interaction  $J_{eff} = 0$ . For small interdot hopping  $t$ , the spins on two dots

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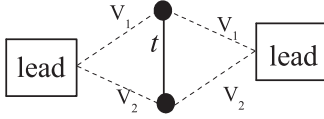


Fig. 1. Parallel double quantum dots attached to the leads.

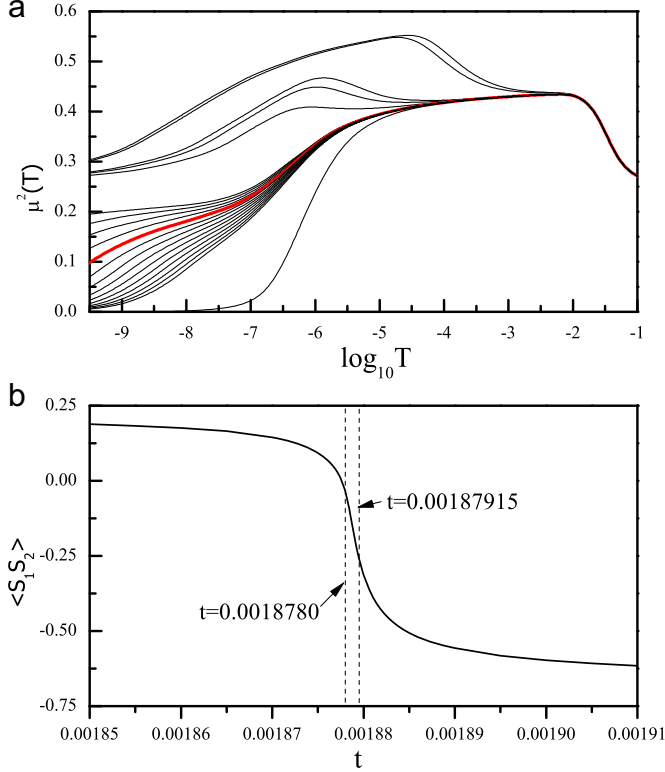


Fig. 2. (a) Temperature-dependent total magnetic moment  $\mu^2(T)$  for different  $t$ , the curves from above to bottom are for  $t=0, 0.001, 0.00185, 0.00186, 0.00187, 0.001878$  to  $0.0018793$  in steps of  $10^{-7}$ , and  $0.001885$ . The thick and red curve corresponds to  $t=0.0018784$ . (b) Spin correlation  $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$  as a function of  $t$  at zero temperature. A two-stage Kondo screening occurs in the regime between the dashed lines. Here,  $U=0.1, \epsilon_i = -U/2, \Gamma_1 = 0.004$ , and  $\Gamma_2 = 0.001$ . (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this paper.)

are screened at the same Kondo temperature. This is contrast to the previous works [27], in which asymmetric Kondo couplings lead to two independent spin-1/2 Kondo screenings in each of the two dots at two different Kondo temperatures. In the regime  $t > t_c$  and close to  $t_c$ , two spins on the two dots nearly decouple with each other due to a very small antiferromagnetic  $J_{\text{eff}}$ , then the two stage Kondo screening occurs. With decreasing temperature, the local spin on the QD1 is screened first by the leads at a higher temperature  $T_{K1}$ , which is accompanied with a Kondo resonance on the QD1. At much lower temperature  $T_{K2}$ , the spin on the QD2 is screened by the leads through the screened QD1. We observe a Kondo peak on the QD2 and a dip on the QD1 with the same width  $\sim T_{K2}$ , which depends exponentially on the distance to the critical point ( $t - t_c$ ). As  $t$  increases continuously, the Kondo peak on the QD2 becomes wider and weaker, and then disappears, which indicates that two-stage Kondo screening vanishes eventually and the singlet between two dots forms. We find that for large asymmetry of the Kondo coupling (e.g.  $\Gamma_1 \gg \Gamma_2$ ), the Kondo resonance in the second step is very weak. Therefore, the side-coupled DQD is not an ideal candidate to show a two-stage Kondo screening since the Kondo resonance peak on the side dot is nearly not observable.

The rest of the paper is organized as follows. In Section 2, we introduce the model Hamiltonian of a DQD connected to conduction leads, and present the numerical renormalization group (NRG) method [28–30], which is a nonperturbative approach to deal with strongly correlated quantum dots and impurity systems. In Section 3, we discuss the two-stage Kondo screening by calculating the total magnetic moment, the local spin correlation and the density of state. We also study the critical phenomena and present the phase diagram in Section 3. A summary is given in Section 4.

## 2. The model and calculation methods

The Hamiltonian of a parallel DQD system connected to two leads in Fig. 1 reads

$$H = \sum_{jk\sigma} \epsilon_k c_{jk\sigma}^\dagger c_{jk\sigma} + \sum_{i=1,2} (\epsilon_i n_i + U n_{i\uparrow} n_{i\downarrow}) - t (d_{1\sigma}^\dagger d_{2\sigma} + d_{2\sigma}^\dagger d_{1\sigma}) + \sum_{ijk\sigma} (V_{ijk} c_{jk\sigma}^\dagger d_{i\sigma} + H. c.) \quad (1)$$

where  $d_{i\sigma}^\dagger$  creates a spin- $\sigma$  electron of energy  $\epsilon_i$  in dot  $i$  ( $=1,2$ ),  $n_{i\sigma} = d_{i\sigma}^\dagger d_{i\sigma}$ ,  $c_{jk\sigma}^\dagger$  creates a spin- $\sigma$  electron of wave vector  $k$  and energy  $\epsilon_k$  in lead  $j$  ( $=L, R$ ).  $U$  is the on-site Coulomb repulsion and  $t$  is the interdot hopping. Here, we assume that the tunnel matrix element  $V_{iLk} = V_{iRk} = V_i$  between leads and dots are symmetric with respect to two leads and is independent of energy band. In our NRG treatment, the discretization parameter  $\Lambda$ , which characterizes the logarithmic discretization of the conduction band, is set to be 1.8–2.5, and the number of the many-body states kept at each iteration is 1000–2000. To achieve the practical form of NRG, we assume a dispersionless conduction band with a half bandwidth  $D$  and a constant density of state  $\rho$  for the conduction band of the leads so that the hybridization function  $\Gamma_{im} = 2\pi\rho V_i V_m^*$  between the dots and the leads also turns to be a constant. The conductance through the dots is calculated using the Landauer formula [31]

$$G = \frac{2e^2}{h} \int d\omega \left[ \frac{\partial f(\omega)}{\partial \omega} \right] T(\omega) \quad (2)$$

with the Fermi function  $f(\omega)$  and the transmission coefficient

$$T(\omega) = -\frac{1}{2} \sum_{ij\sigma} \text{Im} [T_{ij} G_{j\sigma}(\omega)]. \quad (3)$$

The spectral function  $A_{ij\sigma}(\omega) = -(1/\pi) \text{Im} G_{ij\sigma}(\omega)$  and the retarded dot Green function is defined as  $G_{ij\sigma}(t) = -i\theta(t) \langle \{d_{i\sigma}(t), d_{j\sigma}^\dagger(0)\} \rangle$ .

The Kondo screening is described by the magnetic moment  $\mu$ , which is defined as the contribution of the TQDs to the total magnetic moment of the system:

$$\mu^2 = k_B T \chi(T) / (g\mu_B)^2 = (\langle S_z^2 \rangle - \langle S_z \rangle_0^2), \quad (4)$$

where  $\chi(T)$  is the magnetic susceptibility of the system, subscript 0 refers to the case without quantum dots,  $\mu_B$  is the Bohr magneton,  $g$  is the  $g$  factor and  $k_B$  is Boltzmann's constant.

## 3. Results and discussion

In this section, we focus on the effect of the asymmetric Kondo coupling on the two-stage Kondo screening. We are also interested in the QPT and the critical phenomena such as the spectral properties and spin correlation near the critical point. We consider the transport properties of the systems in strongly correlated regime for  $U/\Gamma_{ij} \gg 1$ . In this paper, the half bandwidth  $D$  of the leads is

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