Kosterlitz–Thouless transition, spectral property and magnetic moment for a two-dot structure with level difference*

Yong-Chen Xiong(熊永臣)[1,2,†], Wang-Huai Zhou(周望怀)[1], Jun Zhang(张俊)[1], and Nan Nan(南楠)[1]

[1] School of Science and Advanced Functional Material and Photoelectric Technology Research Institution, Hubei University of Automotive Technology, Shiyan 442002, China

[2] Department of Physics, Faculty of Science, National University of Singapore, Singapore 117551, Republic of Singapore

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By means of the numerical renormalization group method, we study the phase transition, the spectral property, and the temperature-dependent magnetic moment for a parallel double dot system with level difference, where the dot energies are kept symmetric to the half-filled level. A Kosterlitz–Thouless (KT) transition between local spin triplet and singlet is found. In the triplet regime, the local spin is partially screened by the conduction leads and spin−1 Kondo effect is realized. While for the singlet, the Kondo peak is strongly suppressed and the magnetic moment decreases to 0 at a definite low temperature. We attribute this KT transition to the breaking of the reflection symmetry, resulting from the difference of the charge occupations of the two dots. To understand this KT transition and related critical phenomena, detailed scenarios are given in the transmission coefficient and the magnetic moment, and an effective Kondo model refers to the Rayleigh-Schrödinger perturbation theory is used.

Keywords: double dot Structure, Kosterlitz–Thouless transition, numerical renormalization group, strongly correlated effect

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1. Introduction

The spintronics, which includes the charge and spin transports in solid state materials,[1–4] has attracted significant attention for the last several years, due to its potential applications in quantum computation,[5] as well as in quantum information.[3,6] Ever since then, quantum dot system has been considered as an alternative candidate for spintronics device, since its physical parameters could be well manipulated in comparison with bulk solids. After the related properties in single dot have been well elucidated, the research interest has increasingly focused on coupled double quantum dot (DQD) systems, which also provides an important platform to reveal many interesting phenomena in nanoscale structures at low temperature. For instance, for DQD system with parallel geometry, there are always two kinds of spin orderings for the localized electrons in the dots, i.e., the singlet and the triplet. By sweeping the antiferromagnetic spin–spin interaction,[7] the level spacing,[8] the external magnetic field,[9] or the interdot hopping,[10,11] the triplet and singlet could transform to each other through the first-order, the second-order or the Kosterlitz–Thouless (KT)-type quantum phase transitions (QPTs). For DQD system organized in serial configuration, the physic behaviors could be quite different. For example, with increasing hopping between to dots, a crossover between the Kondo singlet of two dots with the channel and the local spin singlet between two dots could be found.[12–14] And if the interdot repulsive capacitive coupling is considered, there exists competition between extended Kondo phases and local singlet phases in spin and charge degrees of freedom.[15] Furthermore, the DQD system is also considered as an important model to reveal the Fermi liquid and non-Fermi liquid behaviors,[16,17] the quantum interference,[18–20] the Fano effect,[21–24] and different kinds of Kondo effect.[9,23,25–28]

Within above quantum behaviors, the KT-type transition is a very important character, and the physical origination is always related to the asymmetric Kondo couplings between conduction leads and different dots. For example, in models of a two-level system, the singlet–triplet QPT is of the first order for symmetric coupling while is of the KT-type one for asymmetric coupling.[29] When the exchange coupling which arises due to Hund's rule is taken into account, the QPT is also a KT-type transition, for the effective couplings are unequal.[8] When two dots are connected to spin-polarized leads, the transition between triplet and doublet could be of the KT-type or the first-order, depending on the spin-rotation SU(2) symmetry.[30] In a triangular system, if the permutation symmetry is broken by a magnetic flux, the QPT changes from a first-order one to a continuous KT-type.[31] In this paper, we consider a double dot structure with level difference. By keeping dot energies symmetric to the half-filled level (which therefore results in equal Kondo couplings between the leads and two dots), and tuning the level difference, we find that although the Kondo couplings are symmetric, it

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†Corresponding author. E-mail: xiongyc_lx@huat.edu.cn

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may also lead to KT transition. We attributed this QPT to the breaking of the reflection symmetry, which is resulted from the difference of the charge occupation on the dots, since in this case the Hamiltonian of the system is not invariant under permutation operation of dots 1 and 2. To gain more information of this model, we also depict the spectral properties and the temperature-dependent magnetic moment with respect to the level difference, and detailed scenarios are given near the critical point. For the purpose of well understanding of these problems, the Wilson's numerical renormalization group technique and an effective Kondo model refers to the Rayleigh–Schrödinger perturbation theory are used.

The organization of this paper is arranged as follows. In Section 2, we present the Hamiltonian of the double dot system, the calculate method and the formulas. In Section 3, we show the numerical results and their discussions. Finally, a conclusion is given in Section 4.

2. Model, method, and formulas

The Hamiltonian for the parallel double-dot system reads

$$H=\sum_{k\sigma}\varepsilon_k c^{\dagger}_{k\sigma}c_{k\sigma}+\sum_{i=1,\sigma}^{2}(\varepsilon_i d^{\dagger}_{i\sigma}d_{i\sigma}+U_i n_{i\uparrow}n_{i\downarrow})+\sum_{ki\sigma}(V_k c^{\dagger}_{k\sigma}d_{i\sigma}+\text{H.c.}), \tag{1}$$

where, $c_{k\sigma}$ is annihilation operator for a conduction band electron with spin σ ($\sigma=\uparrow$ or $\sigma=\downarrow$), momentum k, and energy ε_k, while $d_{i\sigma}$ is that for an electron with spin σ and energy level ε_i on dot i ($i=1,2$). $n_{i\sigma}=d^{\dagger}_{i\sigma}d_{i\sigma}$ is the number operator for the spin-σ electrons. U_i is the on-site Coulomb interaction, and V_k is the tunnel matrix element between leads and dots. For the case of simplicity, we choose U_i to be equal on two dots, labeling $U_1=U_2=U$, and V_k to be symmetric with respect to three dots and two leads.

Since the dots are strongly correlated, we use the celebrated numerical renormalization group (NRG) technique[32–35] to solve numerically equation (1), which is a sophisticated theoretical method for quantum impurity problems. To simplify the problem to a more convenient form for numerical study, we first employ a constant density of state for the conduction band of the leads $\rho_0=1/(2D)$, with $2D$ being the band width of the conduction lead. We also approximate a constant hybridization function for the coupling between dots and leads $\Gamma=2\pi\rho_0|V_k|^2$. Following the standard NRG steps, one then defines a series of Hamiltonians H_N as follows:

$$H_N\equiv\Lambda^{(N-1)/2}\left\{\sum_{\sigma,n=0}^{N-1}\Lambda^{-n/2}\xi_n(f^{\dagger}_{n\sigma}f_{n+1,\sigma}+f^{\dagger}_{n+1,\sigma}f_{n,\sigma})+\sum_{i\sigma}\tilde{\varepsilon}_i d^{\dagger}_{i\sigma}d_{i\sigma}+\tilde{U}\sum_i n_{i\uparrow}n_{i\downarrow}+\sum_{i\sigma}\tilde{\Gamma}^{1/2}(f^{\dagger}_{0\sigma}d_{i\sigma}+d^{\dagger}_{i\sigma}f_{0\sigma})\right\}, \tag{2}$$

where, Λ is the discretization parameter, and ξ_n is the Λ-dependent coefficient, which could be replaced by 1 for large n. The remaining parameters are given by

$$\tilde{\varepsilon}_i\equiv\left(\frac{2}{1+\Lambda^{-1}}\right)\frac{\varepsilon_i}{D},\quad \tilde{U}\equiv\left(\frac{2}{1+\Lambda^{-1}}\right)\frac{U}{D},$$
$$\tilde{\Gamma}\equiv\left(\frac{2}{1+\Lambda^{-1}}\right)^2\frac{\Gamma}{\pi D}.$$

In our NRG calculation, Λ is set to be $1.8\sim2.2$, and the number of the low-lying states kept at each iteration is at least 1500.

The local density of states (LDOS) for the dots is written as

$$A(\omega)=\sum_{i\sigma}A_{i\sigma}(\omega)=-\frac{1}{\pi}\sum_{i\sigma}\text{Im}G_{ii\sigma}(\omega), \tag{3}$$

where $G_{ii\sigma}(\omega)$ is the diagonal part of the retarded dot Green's function $G_{ij\sigma}(t)=-\text{i}\theta(t)\langle\{d_{i\sigma}(t),d^{+}_{j\sigma}\}\rangle$. In the calculation of the spectral properties, we adopt a different procedure with respect to the reduced density matrix of the whole system for the purpose of improving the accuracy, as suggested in Refs. [36] and [37] (for related improvement, see Ref. [38]).

The linear conductance G through the dots is calculated by the Meir–Wingreen's formula[39]

$$G=\frac{\text{e}^2}{h}\int\text{d}\omega\left[\frac{\partial f(\omega)}{\partial\omega}\right]T(\omega), \tag{4}$$

which is known to apply under general conditions. Here, $f(\omega)$ is the Fermi function and the transmission coefficient

$$T(\omega)=-\frac{1}{2}\Gamma\sum_{ij\sigma}\text{Im}\,G_{ij\sigma}(\omega), \tag{5}$$

In this paper, the Fermi level is chosen as $\varepsilon_{k_\text{f}}=0$, thus the linear conductance at zero temperature in the limit of zero bias is given by

$$G=T(\omega=0)\,\text{e}^2/h. \tag{6}$$

Finally, the local temperature-dependent magnetic moment of the dots $\mu^2(T)$ is illustrated as

$$\mu^2(T)=\chi k_\text{B}T/(g\mu_\text{B})^2=\langle S_z^2\rangle-\langle S_z^2\rangle_0, \tag{7}$$

with $\chi(T)$ being the magnetic susceptibility, k_B being the Boltzmann's constant, g being the electronic g factor, and μ_B being the Bohr magneton. $\langle\cdots\rangle$ relates to the thermodynamic expectation value, and the subscript 0 refers to the case without quantum dots.

3. Results and discussion

In this section, we discuss the phase transition and spectrum properties for the 2-dot system in the strongly correlated regime described by $\Gamma\ll U$, focusing on the role of the level difference, which is labeled by $\Delta\equiv\varepsilon_2-\varepsilon_1$. We fix the gate voltage at $V_\text{g}=-U/2$, and the energy levels of two dots

are kept symmetric with respect to the half-filled level, i.e., $\varepsilon_1 = V_g - \Delta/2$ and $\varepsilon_2 = V_g + \Delta/2$. In the following discussion, we choose the half bandwidth of the conduction leads D as the energy unit, and fix $\Gamma = 0.01$, $U = 0.1$.

3.1. Phase transition

We first study the quantum fluctuation for some important physical quantities with respected to an increasing level difference. In Figs. 1(a)–1(c), we show the charge occupation $\langle n_i \rangle$ on each dot, the spin–spin correlation $\langle S_1 S_2 \rangle$ between the two dots, and the local spin $S^2_{\rm dot}$ for the dots at zero temperature as functions of level difference Δ. One finds when $\Delta = 0$, $\langle n_i \rangle = 1.0$, since the strong on-site Coulomb interaction U favors each dot being singly occupied. On the other hand, there exists ferromagnetic RKKY interaction between the two dots mediated by the anti-ferromagnetic Kondo coupling between electrons on the dots and those on the leads, therefore, the local spin on two dots are organized parallelly with $\langle S_1 S_2 \rangle \approx 0.19$, $S^2_{\rm dot} = \langle (\sum_i S_i)^2 \rangle = S_{\rm dot}(S_{\rm dot}+1) \approx 1.7$, and a local spin triplet is generated. Here, $S_{\rm dot} = S_1 + S_2$, with S_i being the spin operator of the ith dot. $\langle S_1 S_2 \rangle$ and $S^2_{\rm dot}$ are little smaller than the ideal values of 0.25 and 2.0, since a finite U/Γ is adopted in the present work. When Δ turns on, the energy level of dot 1 ε_1 decreases, while that for dot 2 ε_2 increases. As a result, $\langle n_1 \rangle$ grows continuously with increasing Δ, $\langle n_2 \rangle$ reduces by contrast. As Δ is large enough, e.g., $\Delta = 0.2$, dot 1 is doubly occupied, while dot 2 becomes empty. In this case, $\langle S_1 S_2 \rangle$ and $S^2_{\rm dot}$ decrease to about 0, thus a spin singlet of the two dots is found.

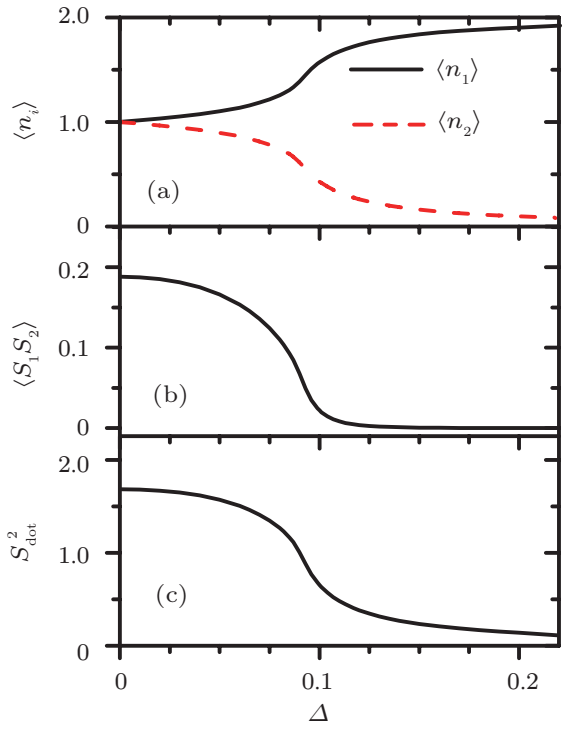


Fig. 1. (color online) (a) Charge occupation $\langle n_i \rangle$ on each dot, (b) spin–spin correlation $\langle S_1 S_2 \rangle$ between two dots, and (c) local spin $S^2_{\rm dot}$ for the dots at zero temperature as functions of level difference Δ. The remaining parameters are given by $\Gamma = 0.01$, $U = 0.1$, $V_g = -U/2$, $\varepsilon_1 = V_g - \Delta/2$, and $\varepsilon_2 = V_g + \Delta/2$.

3.2. Local density of states

Now we focus our attention on the spectral property for the dots. Figures 2(a)–2(b) depict the local density of states (LDOS) for each dot, it is seen that the spectrums for $A_i(\omega)$ are symmetric to the Fermi level $\omega = 0$ when Δ is absent, because in such cases, each dot is half-filled and the system satisfies the particle–hole (ph) symmetry. Several peaks are found which could be identified as the Kondo peak (at $\omega = 0$), the Coulomb peaks (at $\omega = \pm U/2$), and the RKKY peaks (at $\omega = \pm 0.62 \times 64\Gamma^2/\pi^2 U$).[10] With increasing Δ, the spectral weight of $A_1(\omega)$ moves towards the direction $\omega < 0$, and is asymmetric with respect to $\omega = 0$ (see $\Delta = 0.05$ in panel (a)), corresponding to the increase of charge number $\langle n_1 \rangle$. When Δ is large enough (e.g., $\Delta = 0.16$), most of the spectral weight moves to the left part, and the above peaks totally disappear, instead there is a broad peak in the regime of $\omega < 0$. These features could be explained by the following picture. For large Δ, dot 1 is doubly occupied, while dot 2 is empty, therefore, the Kondo screening between electrons on the conduction leads and those in the dots could not occur, thus the Kondo peak could not be realized. Meanwhile, the RKKY interaction, which demands parallel spin ordering between two dots, also vanishes, hence the RKKY peaks are strongly suppressed. The new large peak located at about $\omega = U/2 - \Delta/2$ refers to the the process of annihilating an electron on the full occupied state of dot 1. Since ε_1 and ε_2 are symmetric to the half-filled level, one could understand the evolution of $A_2(\omega)$ in a similar way.

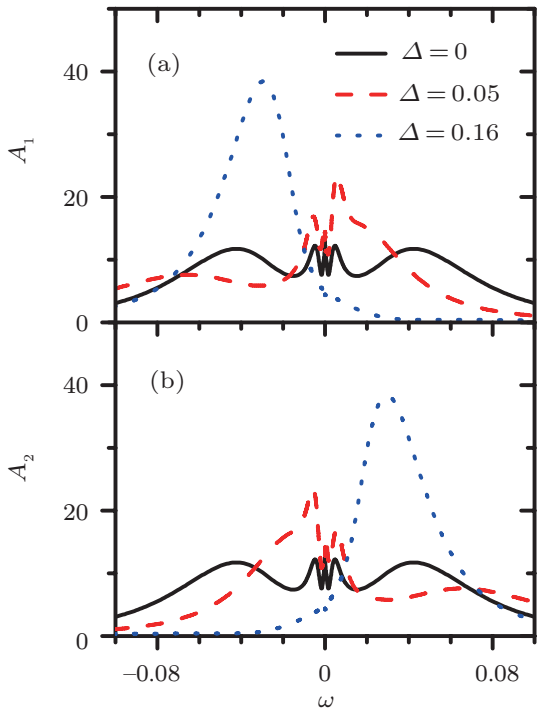


Fig. 2. (color online) (a) and (b) LDOS for dot 1 $A_1(\omega)$ and dot 2 $A_2(\omega)$ respectively for various Δ. Here, the remaining parameters are the same as those given in Fig. 1.

3.3. Electrical transport

Figure 3(a) illustrates the transmission coefficient $T(\omega)$ at zero temperature for various Δ. When $\Delta = 0$, the Kondo peak turns to reach the unitary limit of 1.0, signals full conductance, which is resulted from the partially screened spin-1 Kondo effect. For small Δ, e.g., $\Delta = 0.05$, the amplitude of the Kondo peak decreases, since in this case the possibilities of dot 1 (2) being doubly (zero) occupied increases, therefore, it is more difficult for the electrons in the leads to form a spin singlet with those in the dots. For large Δ, e.g., $\Delta = 0.16$, dot 1 is fully occupied, and dot 2 is empty, hence the Kondo peak is totally suppressed, instead a large dip at the Fermi level, describing that the electrons could not transmit the dots. In Fig. 3(b), we present $T(\omega)$ at the spin-singlet side near the critical point $\Delta_c = 0.0870$ in an expanded scale. If we define the width of the Kondo dip W as the half-width at half maximum of the dip, one may see W depends exponentially on the distance of a definite Δ to the critical point Δ_c, i.e., $(\Delta - \Delta_c)$, which could be described by an exponential function $\log_{10} W = A \exp[B/(\Delta - 0.0870)^{\nu}]$, and the fitting parameters are given by $A = -0.02261$, $B = 4.66893$, and $\nu = 0.05068$. Figure 3(c) shows that the fitting function agrees very well with our numerical results. This behavior of the characteristic width of the Kondo dip W depicts that the triplet-singlet transition at Δ_c is of the KT type.

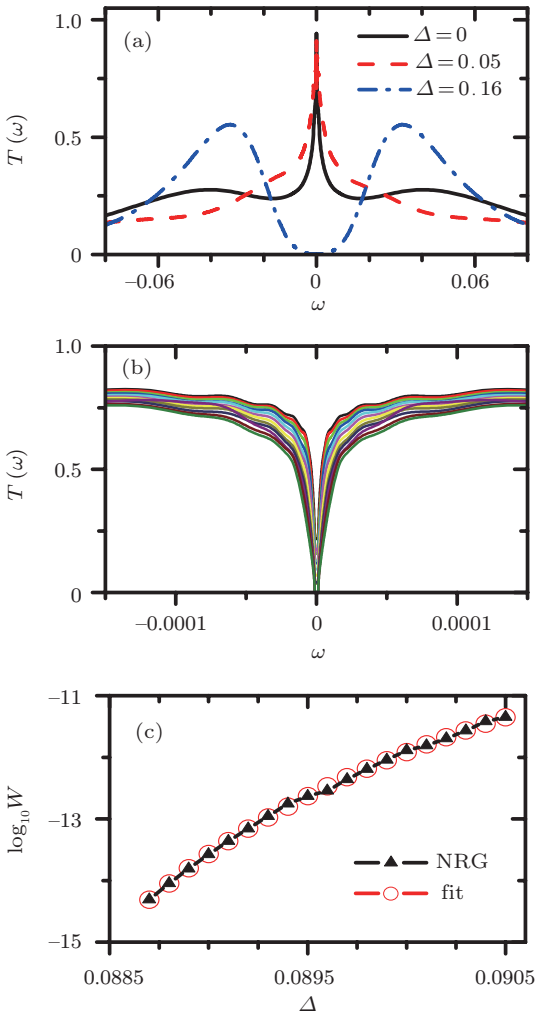


Fig. 3. (color online) (a) Transmission coefficient $T(\omega)$ at zero temperature for various Δ. (b) $T(\omega)$ on the spin singlet side near the critical point in an expanded scale. The curves from top to bottom are for $\Delta = 0.0893$ to 0.0904 in steps of 0.0001. (c) Width of the Kondo dip $\log_{10} W$ (solid line with triangles) extracted from panel (b) and its fitting exponential function (solid line with circles). The remaining parameters are the same as those in Fig. 1.

3.4. Temperature-dependent magnetic moment

In order to gain more information about the low temperature scenario, we give the temperature-dependent magnetic moment $\mu^2(T)$ for different Δ in Fig. 4(a). The upmost curve refers to the case of $\Delta = 0$, one finds the system goes through four different regimes as the temperature T decreases. For high temperatures, e.g., $T > U$, two dots are independent, and each of them contributes $1/8$ to $\mu^2(T)$. As T is reduced to $T \sim 0.01 < U$, the dots are in the local moment regime, where full- and zero-occupied states are suppressed, thus each dot contributes $1/4$ to $\mu^2(T)$ for a total of $1/2$. As T decreases to $T \sim 0.001$, i.e., the order of RKKY interaction, two dots form a local spin triplet and lock into a high spin state. The system contribute $S_{\rm dot}(S_{\rm dot}+1)/3 = 2/3$ to $\mu^2(T)$. Here, $\mu^2(T)$ in the local moment regime ($\mu^2(T) \sim 0.35$) and RKKY regime ($\mu^2(T) \sim 0.42$) are smaller than the ideal values, since the system is not in a pure ground state. At $T \sim 10^{-6}$, an obvious drop takes place due to the Kondo screening of the local spin by the conduction leads, as a result, the local spin is partially screened and $\mu^2(T) \sim 0.25$ at low temperature. This temperature scale could be identified as the so-called Kondo temperature $T_{\rm K}$, and may be expressed by the Haldane's expression $T_{\rm K} \sim U\sqrt{\rho J_{\rm K}} \exp(-1/\rho J_{\rm K})$,[40] where $\rho J_{\rm K} = 8\Gamma/\pi U$ is the effective coupling between the conduction leads and the bonding orbital $f_\sigma = (d_{1\sigma} + d_{2\sigma})/\sqrt{2}$. As Δ increases, the height of $\mu^2(T)$ in the RKKY regime is reduced due to the increasing double (zero) occupancy of dot 1 (2). As $\Delta > \Delta_c$, $\mu^2(T) \to 0$ at low temperature (see $\Delta = 0.0885$ in Fig. 4(a)), since in this regime, the local spin of the dots is 0, and the Kondo screening could not be realized. Figure 4(b) shows the detailed plot of $\mu^2(T)$ on the singlet side near the critical point. If we consider T_0 as the temperature where $\mu^2(T)$ decreases to 0, it is shown that T_0 also depends exponentially on the value of $(\Delta - \Delta_c)$, and could be illustrated by a function $\log_{10} T_0 = A \exp[B/(\Delta - 0.0870)^{\nu}]$, with the fitting parameters read $A = -1.1961$, $B = 1.3559$, and $\nu = 0.0604$. Figure 4(c) shows that the fitting exponential function agrees very well with our NRG results. This behavior also indicates that the transition at Δ_c is a KT-type QPT.

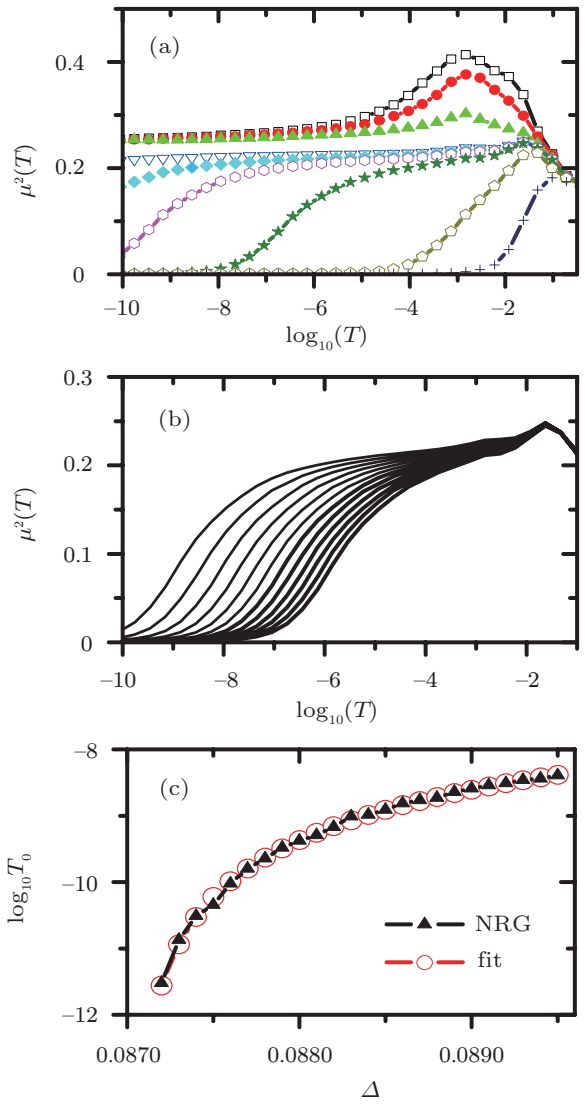


Fig. 4. (color online) (a) Temperature-dependent magnetic moment $\mu^2(T)$ for different Δ. The curves from top to bottom are for $\Delta = 0.0$, 0.05, 0.075, 0.086, 0.0865, 0.087, 0.0885, 0.10, and 0.16 respectively. (b) Detailed $\mu^2(T)$ for different Δ on the singlet side near the critical point $\Delta_c = 0.0870$. The curves from top to bottom are for $\Delta = 0.0872$ to 0.0894 in steps of 0.0002. (c) Screened temperature T_0 (solid line with triangles) extracted from panel (b) and its fitting exponential function (solid line with circles). The remaining parameters are the same as those in Fig. 1.

3.5. Physical origination

In some previous investigations, it is demonstrated that the asymmetric Kondo coupling between the leads and different dots could always result in the KT transition.[8,29,31] However, the origination of the KT transition presented in this work is quite different as discussed in detail in the following. To find out the underlying physical picture, one obtains an effective Hamiltonian by employing the Schrieffer–Wolff transformation,[10,41]

$$H_{\rm eff} = H_{\rm l} + J_{k1}\hat{S}_0 \cdot \hat{S}_1 + J_{k2}\hat{S}_0 \cdot \hat{S}_2, \tag{8}$$

where both Kondo spins are coupled to the same channel, and $\hat{S}_0$ is the conduction electron spin density, $\hat{S}_i$ is the spin operator for the i-th dot. The effective coupling between the leads and two dots J_{ki} are given by

$$J_{k1} = \frac{4\Gamma}{\pi}\left(\frac{1}{|U/2+\Delta/2|} + \frac{1}{|U/2-\Delta/2|}\right),$$
$$J_{k2} = \frac{4\Gamma}{\pi}\left(\frac{1}{|U/2-\Delta/2|} + \frac{1}{|U/2+\Delta/2|}\right). \tag{9}$$

Obviously, here we have $J_{k1} = J_{k2}$, namely, the effective Kondo couplings are symmetric with increasing Δ. Therefore, one could not attribute above KT transition to asymmetric Kondo coupling. On the other hand, it is noted that in our model, one dot turns to be doubly occupied while the remaining one turns to be empty as Δ increases, indicating the reflection symmetry is broken, and the Hamiltonian is not invariant under permutation of dots 1 and 2. We argue this difference induced by symmetry breaking gives rise to the KT transition, which is similar to a DQD model with strong inter-dot Coulomb repulsion.[30] Finally, we stress that the critical point Δ_c could be estimated by the energy level of an isolated DQD model as following. For the local spin triplet, the energy level is $E_{\rm T} = \varepsilon_1 + \varepsilon_2 = -U$, while for the singlet, it reads $E_{\rm S} = 2\varepsilon_1 + U = -\Delta$. When the level difference Δ increases, the energy level of the singlet is pulled down and eventually becomes degenerate with the triplet at $\Delta = U$, as a result, a QPT occurs.

4. Summary

In conclusion, we have studied the phase transition, the spectral property, and the temperature-dependent magnetic moment for a parallel double dot structure with level difference Δ. By means of the numerical renormalization group method, we focus our attention on the strongly correlated regime. A Kosterlitz–Thouless transition between local spin triplet and singlet is found as Δ increases, which could be attributed to the breaking of the reflection symmetry of the two dots, resulted from the difference of the charge number on the two dots. For small Δ, the local spin is partially screened by the conduction leads and the linear conductance turns to reach the unitary limit, corresponding to spin-1 Kondo effect. For large Δ, the magnetic moment is about 0 at low temperature, and the electron could not transmit the dots. To understand this KT transition and related critical phenomena, detailed plots are given in the transmission coefficient and the temperature-dependent magnetic moment, and an effective Kondo model refers to the Rayleigh–Schrödinger perturbation theory is used. These results may be useful for describing the strongly correlated effects in double dots devices, and it may be also of significant importance to understand the Kosterlitz–Thouless-type transition in quantum impurity systems.

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