Spectral properties and quantum phase transitions in parallel triple quantum dots

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The spectral properties and the quantum phase transitions in parallel triple quantum dot systems are investigated using the numerical renormalization-group method. For small interdot hopping t, the Ruderman-Kittel-Kasuya-Yosida (RKKY) exchange interaction between the dots is identified in the spectra and is consistent with that obtained by the perturbation theory. With increasing t, due to the competition between the RKKY exchange and the direct exchange between dots, there exist two first-order quantum phase transitions between the phases with the local spin $S_{dot}=3/2$, $1/2$, and 0 on the dots. At low temperature, the local spin $S_{dot}=3/2$ is partially screened to a residual spin $S=1$, while the local spin $S_{dot}=1/2$ is totally screened. In both local quadruplet and doublet states, the Kondo resonance accompanied with a conductance of the unitary limit $2e^2/h$ is observed, while no Kondo effect is found in the local spin-singlet state.

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I. INTRODUCTION

If a magnetic impurity is embedded in a metallic host, the local magnetic moment is screened at low temperature by the itinerant electron spin, while anomalous resonant scattering of conduction electrons can be observed. This is the Kondo effect,[1] which has also been observed in quantum dot (QD) systems and provides many opportunities for the investigation of strongly correlated electrons. A lot of works on the Kondo effect in single quantum dot systems have been done both theoretically and experimentally.[2–9] Recently, double quantum dots (DQDs)[10–14] and triple quantum dots (TQDs)[15,16] have been fabricated. Due to various interdot coupling and intradot interaction, the coupled DQDs or TQDs have demonstrated quantum phase transition and fascinating physics.[17–33]

In DQD systems serially attached to the metallic leads, as the hopping between dots increases, there exists a crossover between the Kondo singlet state of each dot with its adjacent lead and the local spin-singlet state on the dots.[17–19] If the interdot repulsive interaction is considered, an orbital spin-singlet state with two electrons occupying the bonding orbital is observed.[18] For DQDs with interdot repulsive interaction in the absence of interdot hopping at half-filling, the enhanced Kondo temperature phase was predicted.[34] In models of two spin-$\frac{1}{2}$ magnetic impurities,[21] numerical renormalization-group (NRG) calculations have shown that with increasing exchange coupling between impurities, the singlet-doublet quantum phase transition is either of first order or of the Kosterlitz-Thouless (KT) type, depending on the symmetry of the Kondo coupling. The ferromagnetic Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction mediated by the conduction electrons leads to local magnetic ordering which becomes underscreened by the conduction electrons at low temperature. For large interimpurity exchange, the impurities combine to a singlet. The experiments for DQDs have exhibited the effect of interdot hopping on Kondo physics[20,35] and have demonstrated the competition between the Kondo effect and the RKKY interaction among localized spins.[36]

Recently, the transport properties of DQDs with various configurations have been investigated. In a serial DQD, the slave-boson mean-field theory (SBMFT) shows that the conductance has a two-plateau structure versus the gate voltage and a two or three peak structure versus interdot tunneling.[17] In a system containing one Kondo dot and one noninteracting dot, the NRG calculation exhibits a sizable splitting of the Kondo resonance.[25] In a DQD system with only one of dots coupled to the leads, a two-stage screening of the dot's magnetic moment with decreasing temperature was found using the NRG and SBMFT.[22] In parallel DQDs, the interdot repulsion interaction results in a correlation-induced resonance,[23] while the interdot hopping suppresses the Kondo-assisted transport in the Kondo regime.[37,38]

In this paper, we focus on the effects of magnetic frustration on the spectral properties and quantum phase transition in a coupled triangular quantum dot system shown in Fig. 1. Although the Kondo effects and the tunnel conductance have been investigated for TQD systems with several geometrical configurations,[26,32,33] the frustration in TQDs has not been discussed. In triangular lattices, the interplay between geometrical frustration and strong electron correlation can result in a complicated phase diagram containing many interesting phases.[39] In the present TQDs, the NRG calculation shows that with increasing interdot hopping, the local magnetic moment of the TQD is $S_{dot}=3/2$, $1/2$, and 0 sequentially. At low temperature, the local magnetic moment $S_{dot}=3/2$ and $1/2$ is partially screened to a residual spin $S=1$ and totally screened, respectively, while the Kondo resonance is accompanied with a conductance with unitary limit $(2e^2/h)$. In the local singlet state, no Kondo effect is observed and the conductance nearly vanishes. This is quite different from the

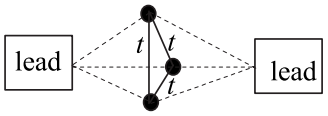

FIG. 1. Parallel triple quantum dots attached to the leads. t denotes the interdot hopping.

previous SBMFT result[37,38] for parallel DQDs, which showed a continuous decrease in conductance as the interdot hopping increases. The above quantum phase transitions are induced by the interplay between the Kondo coupling, the RKKY interaction, and magnetic frustration. A similar origin of the singlet-doublet transition has been found in parallel DQD system.[21,40] However, the RKKY interaction has not been observed directly in the spectral properties in previous works by the SBMFT[37,38] and by the density matrix renormalization group.[40] In this paper, we will show that for both TQD and DQD systems, the peak of RKKY interaction can be identified in the spectra of the density of states (DOS). As the interdot hopping is large enough, the transition occurs and the RKKY peak disappears because the interdot exchange interaction is dominated by the direct exchange interaction induced by the interdot hopping and on-site repulsion on the dots.

This paper is organized as follows. In Sec. II, we give the model and the calculation algorithms. In Sec. III, the local DOS, the transmission probability, and the effective magnetic moment are described. Finally, the discussion and conclusion are given.

II. MODEL AND CALCULATION METHODS

We consider a model of parallel TQDs symmetrically connected to the left and right electrodes, which can be described by the following Hamiltonian:

$$H = \sum_{jk\sigma} \epsilon_k c^\dagger_{jk\sigma} c_{jk\sigma} + \epsilon \sum_i d^\dagger_{i\sigma} d_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - t(d^\dagger_{1\sigma} d_{2\sigma} + d^\dagger_{2\sigma} d_{3\sigma} + d^\dagger_{1\sigma} d_{3\sigma} + \text{H.c.}) + \sum_{jki\sigma} V_k c^\dagger_{jk\sigma} d_{i\sigma}, \quad (1)$$

where $c^\dagger_{jk\sigma}$ creates a spin σ electron of wave vector k and energy ϵ_k in the left ($j=L$) or right ($j=R$) lead, and $d^\dagger_{i\sigma}$ creates a spin σ electron in dot i ($=1,2,3$), $n_{i\sigma}=d^\dagger_{i\sigma}d_{i\sigma}$. t is the hopping between dots and U is the on-site Coulomb repulsion on each dot. V_k is the tunnel matrix element between leads and dots.

We solve this interaction model using the numerical renormalization-group method.[41] We assume a dispersionless conduction band with a half bandwidth D and a constant density of states ρ_0. The hybridization function $\Gamma=\pi\rho_0|V_k|^2$ between the dots and the leads is taken as a constant. In the following discussions, D is taken as the energy unit. In the NRG calculation, the discretization parameter is $\Lambda=1.5-2.5$ and the number of the states kept at each iteration is 1000–2000. In the calculations of spectral properties, a different procedure of evaluating the Green's function with respect to the reduced density matrix of the full system is applied.[42] In order to get continuous curves for spectral densities, appropriate broadening functions and procedure proposed in Ref. 43 are employed. The retarded dot Green's function can be written as

$$G_{ij\sigma}(t) = -i\theta(t)\langle\{d_{i\sigma}(t), d^\dagger_{j\sigma}\}\rangle, \quad (2)$$

and the DOS of the dots is

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

The magnetic moment μ is defined as the contribution of the TQDs to the total magnetic moment of the system

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

where $\chi(T)$ is the magnetic susceptibility of the system, subscript 0 refers to the case without quantum dots, μ_B is the Bohr magneton, g is the g factor, and k_B is Boltzmann's constant. The local spin $\mathbf{S}^2_{dot}$ and the charge Q_{dot} of the dots are defined by

$$\mathbf{S}^2_{dot} = \left\langle \left(\sum_i \mathbf{S}_i\right)^2 \right\rangle = S_{dot}(S_{dot}+1), \quad Q_{dot} = \left\langle \sum_{i\sigma} n_{i\sigma} \right\rangle, \quad (5)$$

where $\mathbf{S}_i$ is the total spin operator of the ith dot. We calculate the spin-resolved conductance through the dots using the Landauer formula[44]

$$G_\sigma = \frac{e^2}{h}\int d\omega \left[\frac{\partial f(\omega)}{\partial \omega}\right] T_\sigma(\omega), \quad (6)$$

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

$$T_\sigma(\omega) = -\frac{1}{2}\Gamma\sum_{ij} \text{Im}\, G_{ij\sigma}(\omega). \quad (7)$$

If the Fermi energy is chosen as $\epsilon_{k_f}=0$, the linear conductance at zero temperature in the limit of zero bias is determined by

$$G_\sigma = T_\sigma(\omega=0)e^2/h. \quad (8)$$

III. RESULTS AND DISCUSSION

We present the numerical solution of the TQD model in Fig. 1 using the NRG method and improve the accuracy in the calculation of the spectral density using the procedure in Refs. 42 and 43. We first discuss the electron-hole symmetric case $\epsilon=-U/2$ and $t=0$. Figures 2(a)–2(d) show the local DOS on the dots at zero temperature for different on-site repulsion U and hybridization Γ. Besides a very narrow central peak at $\omega=0$ and two broad Coulomb peaks at $\omega=\pm U/2$, we observe two additional peaks between them. Comparing with the feature for the single impurity Anderson model (SIAM),[42] one finds that the central peak corresponds to the Kondo peak. The two additional peaks are absent for SIAM. For TQDs and DQDs, there exists interdot ferromagnetic RKKY interaction J_{RKKY} mediated by the antiferromagnetic Kondo coupling between the conduction electrons in the leads and the local electrons on the dots.[21,31] The additional peaks locate at $\omega=\pm J_{RKKY}$. They result from the process of annihilating (creating) an electron in the many-body states with antiferromagnetic spin configuration (e.g., $\uparrow\downarrow\uparrow$), in which the two electrons on two dots have parallel up-spins mediated by the conduction electron with down-spin. In

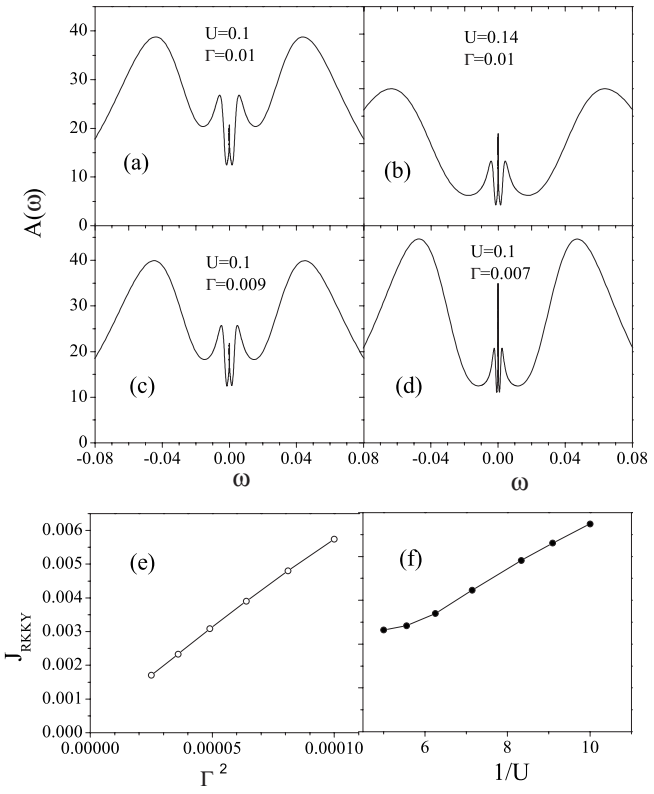

FIG. 2. [(a)–(d)] Local DOS on the dots at zero temperature for $\epsilon=-U/2$, $t=0$, and different U and Γ: two small peaks by the two sides of the central peak are located at $\omega=\pm J_{RKKY}$. [(e) and (f)] Location of the additional peaks J_{RKKY} as functions of Γ^2 and $1/U$, respectively.

Figs. 2(a)–2(d), it is seen that with increasing U or decreasing Γ, the additional peaks move toward the central peak. Figures 2(e) and 2(f) show the location of the additional peaks J_{RKKY} as functions of Γ^2 and $1/U$, respectively. This linear relationship gives $J_{RKKY}\approx 5.4\Gamma^2/U$, which is consistent with the result of the Rayleigh-Schrödinger perturbation theory[31] for the RKKY interaction. Figure 2(f) also indicates that for large U (e.g., $1/U<6$), J_{RKKY} deviates from the above linear relationship because the perturbation theory requires $U/D \ll 1$.

As the interdot hopping is turned on, the electron-hole symmetry is damaged. Figure 3 shows the DOS for $U=0.1$, $\Gamma=0.01$, and various interdot hopping t. For small t (e.g., $t=0.005$), the spectral weight moves toward the direction $\omega<0$. The height of the central Kondo peak is nearly not changed, while the two additional peaks are asymmetric with respect to $\omega=0$. In this case, the interdot exchange interaction includes not only the ferromagnetic RKKY interaction but also the direct exchange (DE) interaction induced by the interdot hopping and the on-site repulsion. The DE interaction will reduce the probability of generating RKKY interaction because these two kinds of interaction need different spin configurations of electrons in the dots. For example, the RKKY interaction favors the parallel spin configuration between dots in the many-body state, while the DE interaction favors the antiparallel spin. Hence, the spectral weight contributed by the RKKY interaction decreases. This feature can

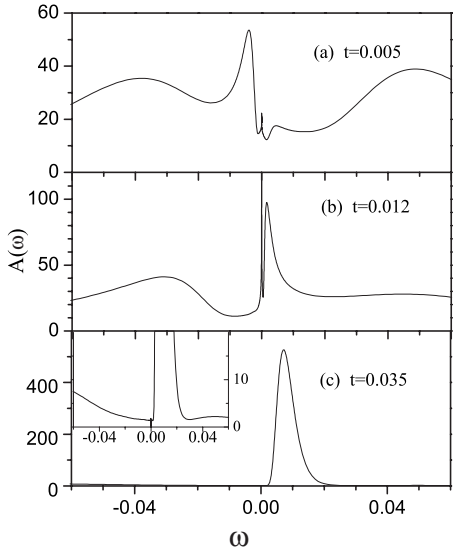

FIG. 3. Local DOS for $U=0.1$, $\Gamma=0.01$, $\epsilon=-U/2$, and various interdot hopping t. Inset in (c): DOS with a different scale shows the finite spectral weight in the regime $\omega<0$.

be seen from the decreasing weight of the additional peak in the part $\omega>0$. On the other hand, with increasing t, the number of electrons in dots increases [see Fig. 4(d)] so that the probability of double occupancy on a dot increases. Therefore, the weight of the additional peak in the part $\omega<0$ increases by the process of annihilating an electron on doubly occupied state. When the interdot hopping t is larger than a critical value $t_{c1}=0.010\,175\,863\,56$ [e.g., $t=0.012$ in Fig. 3(b)], the spectral weight moves to the right. At the Fermi level $\omega=0$, there is a very sharp Kondo peak. The additional peak labeling the RKKY interaction disappears; instead there is a large peak at the right side of the Kondo peak. This feature can be explained by the following picture. As $t>t_{c1}$, due to the magnetic frustration, the interdot exchange interaction is dominated by the DE interaction and the RKKY interaction cannot be realized. On the other hand, when $t>t_{c1}$ the number of electrons in the dots decreases [Fig. 4(c)], and the probability of empty state on the dots increases so that a large peak at the right of central peak forms by the process of adding an electron on an empty state. When t is larger than another critical value $t_{c2}=0.029\,577\,977\,8$ [e.g., $t=0.035$ in Fig. 3(c)], the central peak vanishes and there is no Kondo effect. Most of the spectral weight moves to the part $\omega>0$, which indicates a considerable reduction in the number of electrons in the dots.

In order to explore above quantum phase transition, Fig. 4 shows the temperature dependence of the total magnetic moment μ, the local spin $\mathbf{S}_{dot}^2$, and the charge Q_{dot} of the dots at zero temperature. For $t=0$, the charge $Q_{dot}=3$ and each dot is mainly singly occupied due to Coulomb repulsion U. Due to the interdot ferromagnetic RKKY exchange, for large U the local total spin $\mathbf{S}_{dot}^2$ approaches 3.75 corresponding to quantum number $S_{dot}=3/2$. At low temperature, this local spin is partially screened to a residual spin $S=1$ corresponding to $\mu^2=S(S+1)/3\approx 0.67$. For $t>0$, the magnetic frustration competes with the RKKY interaction so that at $t=t_{c1}$ [thick

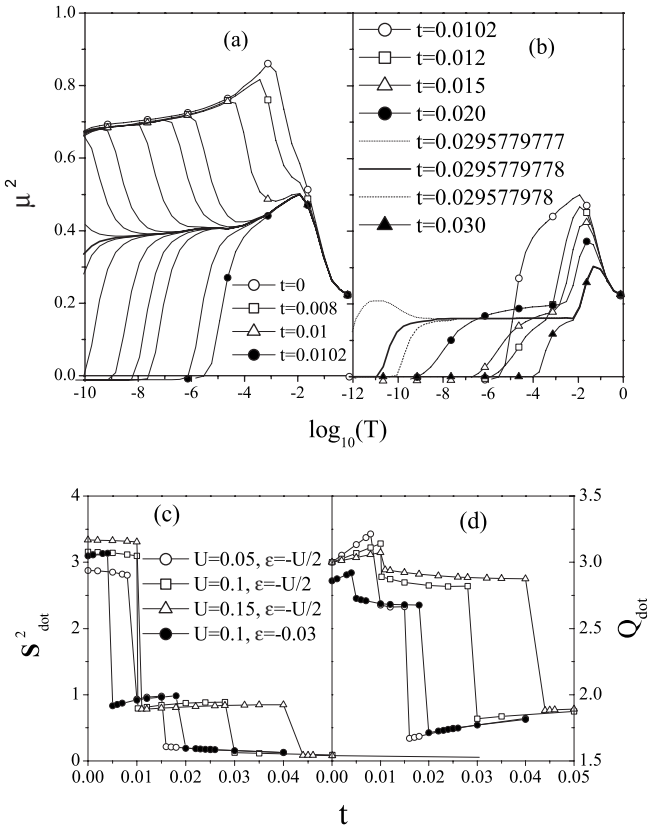

FIG. 4. [(a) and (b)] Total magnetic moment of the TQDs as a function of the temperature for $U=0.1$, $\Gamma=0.01$, $\epsilon=-U/2$, and different t. The thick curves in (a) and (b) correspond to $t=t_{c1}=0.010\,175\,863\,56$ and $t=t_{c2}=0.029\,577\,977\,8$, respectively. The curves in (a) close to t_{c1} are for $2|t-t_{c1}|=10^{-10},10^{-9},\ldots,10^{-5}$. (c) Local spin $\mathbf{S}^2_{dot}$ and (d) the charge Q_{dot} of the dots at zero temperature as function of t for $\Gamma=0.01$ and different U and ϵ.

curve in Fig. 4(a)], there are discontinuous changes of the charge and the local spin. For $t \geqslant t_{c1}$, $\mathbf{S}^2_{dot} \approx 0.75$ corresponding to $S_{dot}=1/2$, which is totally screened at low temperature T^*. Figure 4(a) shows that when t approaches the critical t_{c1}, there is an exponential dependence of the crossover temperature T^*. However, this phase transition is not of KT type and is a first-order transition because there is no mixing between the local doublet $S_{dot}=1/2$ and quadruplet $S_{dot}=3/2$.[21]

For $t>t_{c1}$ in Fig. 4(b), as t increases continuously, the crossover temperature T^* increases first and then decreases exponentially when t approaches another critical point t_{c2}, at which the charge Q_{dot} is close to 2 and the local spin $S_{dot}=0$. This phase transition is also first order because there is no coupling between the local states with different charges. In order to understand this local singlet clearly, we introduce the combinations of the dots orbitals, $a_{1\sigma}=(d_{1\sigma}+d_{2\sigma}+d_{3\sigma})/\sqrt{3}$, $a_{2\sigma}=(d_{1\sigma}-2d_{2\sigma}+d_{3\sigma})/\sqrt{6}$, and $a_{3\sigma}=(d_{1\sigma}-d_{3\sigma})/\sqrt{2}$. Then, the levels of the dots are given by $\epsilon_1=\epsilon-2t$ and $\epsilon_2=\epsilon_3=\epsilon+t$, respectively. For $t>t_{c2}$ (e.g., $t=0.035$), the first orbital ϵ_1 is almost doubly occupied ($\langle n'_{1\sigma}\rangle=0.8910$, here $n'_{i\sigma}=a^\dagger_{i\sigma}a_{i\sigma}$), and other two orbitals are nearly empty ($\langle n'_{2\sigma}\rangle=\langle n'_{3\sigma}\rangle=0.013\,86$). In this case, the Hamiltonian (1) maps to a single impurity Anderson model with impurity

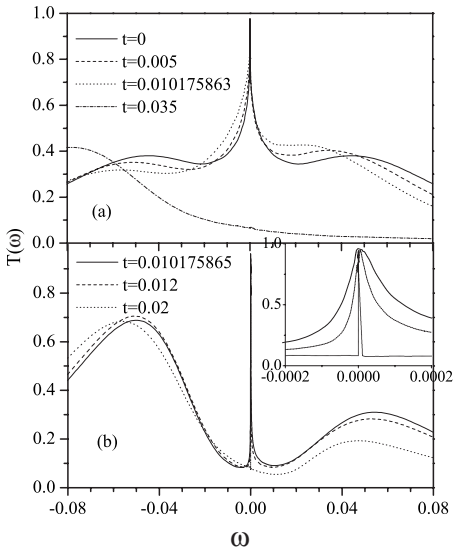

FIG. 5. Transmission $T(\omega)$ at zero temperature for $U=0.1$, $\Gamma=0.01$, $\epsilon=-U/2$, and different t. The inset in (b) is an expanded view around the Fermi level $\omega=0$ and shows that with increasing t, the Kondo resonant peak becomes narrow and sharp.

orbital $a_{1\sigma}$ coupling with the leads. Because the impurity orbital is doubly occupied, the electrons form an orbital spin-singlet state without Kondo effect.

Now, we present the result of electronic transport through the dots. In Fig. 5, we show results for the transmission $T(\omega)=T_\uparrow(\omega)+T_\downarrow(\omega)$ for various interdot hopping. Figure 5(a) shows that for $t=0$, there is a symmetric Kondo resonant peak at $\omega=0$, while with increasing t, the spectra move to the left and the central Kondo resonant peak is still at $\omega=0$ but is not symmetric about $\omega=0$. This means that in the local quadruplet state with $S_{dot}=3/2$, the transmission at the Fermi level reaches the unitary limit at low temperature. If we define the Kondo temperature T_K as the full width at half maximum of the central peak, we find that T_K increases with t. For $t>t_{c1}$, the ground state is in the local doublet state with $S_{dot}=1/2$. Comparing Fig. 5(b) with Fig. 5(a), one finds that the spectra of the transmission for $t>t_{c1}$ are different from those for $t<t_{c1}$. However, in both cases the transmission accompanied with the Kondo resonance reaches the unitary limit. The inset in Fig. 5(b) shows that with increasing t, the Kondo resonant peak becomes narrow and sharp, which means that Kondo resonance is observed at much lower temperature. For $t>t_{c2}$ [e.g., $t=0.035$ in Fig. 5(a)], the problem is similar to the single impurity Anderson model with impurity orbital doubly occupied. The ground state is in the local orbital spin-singlet state. According to the result in Ref. 2, the transmission nearly vanishes at the Fermi level.

It is noticeable that the above feature of the transmission is quite different from the previous SBMFT result[37,38] for parallel DQDs, which showed a continuous decrease in conductance as the interdot hopping increases. To clarify this difference, we also perform the NRG calculation for parallel DQDs with interdot coupling t. The local DOS $A(\omega)$ and the transmission $T(\omega)$ are shown in Fig. 6 for $U=0.15$, $\Gamma=0.01$, and various t. For $t=0$, the DOS shows a central Kondo

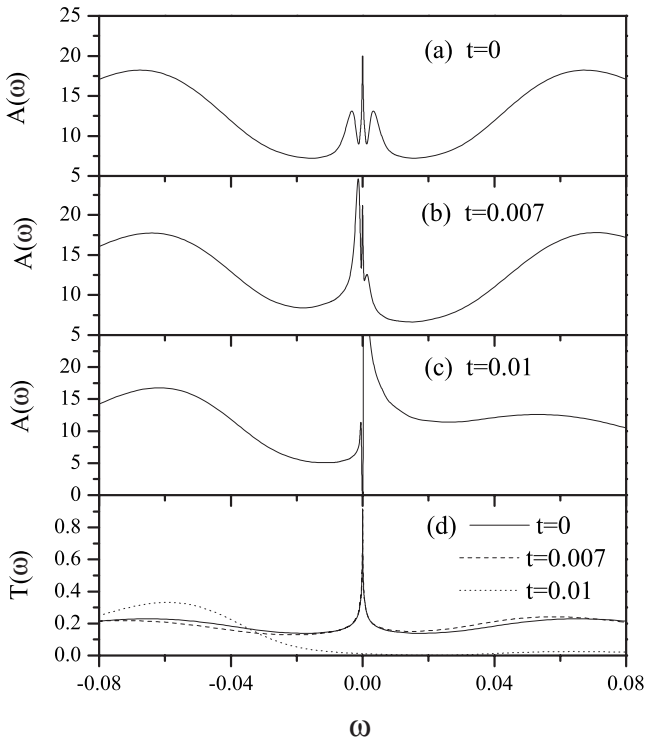

FIG. 6. [(a)–(c)] Local DOS and (d) transmission $T(\omega)$ at zero temperature for $U=0.15$, $\Gamma=0.01$, $\epsilon=-U/2$, and different t for parallel DQDs.

peak, two RKKY peaks, and two Coulomb peaks, which are similar to those for the TQDs. Accompanied with the central Kondo peak, the transmission is saturated with a unitary value. With increasing t, the DOS moves to the left and still exhibits a central peak at $\omega=0$, while the spectral weight contributed by the RKKY interaction decreases. Due to the existence of the central peaks, the conductance with $2e^2/h$ is still observed at the Fermi level. As t increases to a critical $t_c=0.0098$, there is a phase transition from the local triplet $S_{dot}=1$ state to the local singlet $S_{dot}=0$ state.[21,33,40] For $t>t_c$ [e.g., $t=0.01$ in Figs. 6(b) and 6(c)], the DOS shows a dip at $\omega=0$ and no Kondo resonance in the transmission is observed. In previous investigations by SBMFT,[37,38] the quantum phase transition was not observed because the quantum fluctuation is not considered completely. For example, the local charge and local spin in the dots were not shown in Refs. 37 and 38, while our NRG calculations show that abrupt changes in $\mathbf{S}_{dot}^2$ and Q_{dot} are observed at phase transition points. Although the SBMFT result also found the movement of the DOS versus t, the central peak at $\omega=0$ for $t>0$ in Fig. 6(b) has not been observed due to the mean-field approximation. Therefore, their results could not figure out the Kondo resonance with $T(\omega)\approx 1$ for $t>0$. On the other hand, the RKKY interaction has close relationship with many-body states of the system and is also determined by the quantum fluctuation. Hence, the RKKY interaction could not be identified in the spectra of the SBMFT. In our NRG results, the central peak is very sharp and the corresponding crossover energy scale T^* is very small. This means that the Kondo resonance is observed at very low temperature, at which the quantum fluctuation is very important. Therefore, it is not surprising that some features could not be observed by the SBMFT.

The above discussions are focused on the situation $\epsilon=-U/2$. Our NRG calculation shows that for other dot energy ϵ, above quantum phase transitions still exist when the interdot hopping increases. In Figs. 4(c) and 4(d), we also give the local spin $\mathbf{S}_{dot}^2$ and the charge Q_{dot} as functions of t for $\epsilon=-0.03$. One finds that the critical t_{c1} and t_{c2} for $\epsilon>-U/2$ are smaller than those for $\epsilon=-U/2$. This behavior can be understood through the following discussion. When $t>t_{c1}$ or $t>t_{c2}$, the DOS moves to $\omega>0$ and the charge on the dots has a drop. With increasing ϵ, the DOS has a similar behavior. Therefore, the increase of ϵ speeds the phase transitions.

In conclusion, we have investigated the spectral properties and the quantum phase transitions in parallel TQDs. For small interdot hopping t, due to the ferromagnetic RKKY interaction between dots, the TQDs have the local spin $S_{dot}=3/2$, which is partially screened to a residual spin $S=1$ at low temperature. The RKKY interaction identified in the spectra of the DOS is consistent with that obtained by the perturbation theory. With increasing t, the spectral weight contributed by the RKKY interaction decreases due to the competition between the RKKY interaction and the interdot direct exchange. For $t>t_{c1}$, the magnetic frustration reduces the local spin of the dots to $S_{dot}=1/2$, which is totally screened at low temperature. For $t>t_{c2}$, the problem maps to the single impurity Anderson model and the ground state is in the local orbital spin-singlet state $S_{dot}=0$. In both local quadruplet and doublet states, the Kondo resonance accompanied with the central Kondo peak in the DOS is observed and the conductance reaches the unitary limit $2e^2/h$, while no Kondo effect is found in the local spin-singlet state. This transport property is in contrast to the previous SBMFT result, which showed a continuous decrease in conductance as the interdot hopping increases.

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