

Kosterlitz-Thouless transition induced by Aharonov-Bohm effect in a triple quantum dot

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The three-order superexchange interaction usually neglected in the literature may result in different physics in a triple quantum dot pierced by an external magnetic flux. It is shown that the third-order superexchange interaction survives due to Aharonov-Bohm interference and induces a magnetically tunable Kosterlitz-Thouless quantum phase transition between local singlet and triplet. This transition is demonstrated by a Kondo resonance peak with a width depending exponentially on the distance to the critical point.

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I. INTRODUCTION

Semiconductor quantum dots (QDs) provide many opportunities for studying some fundamental physical phenomena, such as quantum interference,¹ Coulomb blockade, and the Kondo effect.^{2,3} Recent attention has focused on quantum phase transition in coupled double quantum dots (DQDs) and triple quantum dots (TQDs).⁴⁻¹⁵ In these itinerant systems, the exchange interaction generated by superexchange mechanism due to electron hopping plays an important role in determining spin configuration of ground state. For instance, in serial DQD systems, the localized moments on the dots either form Kondo singlet with the conduction electrons in the leads or they form a local spin singlet, depending on the interdot hopping.⁵ In parallel DQDs, the interdot hopping induces the local singlet-triplet transition and suppresses the Kondo-assisted transport.¹⁴⁻¹⁶ In TQD systems, two-channel Kondo effect, non-Fermi-liquid behavior, and local quadruplet-doublet-singlet transitions have been found in various ranges of interdot hopping.^{10,16} When multiple QDs form a ring geometry, electrons traveling in a magnetic flux pick up an Aharonov-Bohm (AB) phase.¹⁷ Therefore, the superexchange process involving transfer of electrons may be affected by the AB interference effect and new physics is to be expected.

Generally, superexchange interaction is considered just in the second-order perturbation theory which involves exchange of electrons between two orbitals each singly occupied with opposite spins.¹⁸ The higher-order superexchange interactions are very small and can be neglected. Especially, the three-order superexchange (TOS) interaction has never been considered because it vanishes in most of itinerant systems due to deletion of contributions from different TOS processes among three orbitals. The simplest ring structure is the triangular QD system, which has been realized experimentally.¹⁹⁻²¹ In the present paper, we show that the TOS interaction survives and induces interesting phenomena in a TQD pierced by an external magnetic field (see Fig. 1). In the absence of magnetic field, the electron hopping between dots 2 and 3 induces a first-order local singlet-triplet transition accompanied with an abrupt disappearance of Kondo peak. When the magnetic flux is turned on, the TOS interaction survives due to AB interference effect and above singlet-triplet transition becomes Kosterlitz-Thouless (KT)

type. A universal scaling form determined by the width of Kondo peak is observed. This device provides a way to detect the TOS processes. It is noticeable that the combination of Kondo and AB effects was also investigated in previous work⁹ for a triangular TQD system with all three dots connected to leads. However, three dots just share one electron in Ref. 9 so that superexchange interaction between different dots was not discussed.

This paper is organized as follows. The model and the calculation algorithms are given in Sec. II. The local density of state, the transmission probability, and the spin correlation are described in Sec. III. Finally the discussion and conclusion are given.

II. MODEL AND CALCULATION METHODS

The TQD system is described by the Hamiltonian

$$H = H_d + H_{\text{lead}} + H_t, \quad (1)$$

$$H_{\text{lead}} = \sum_{jk\sigma} \epsilon_k c_{jk\sigma}^\dagger c_{jk\sigma}, \quad (2)$$

$$H_t = \sum_{jk\sigma} V_k c_{jk\sigma}^\dagger d_{1\sigma}, \quad (3)$$

$$H_d = \epsilon \sum_{i\sigma} d_{i\sigma}^\dagger d_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \sum_{\sigma} [(t_1 d_{1\sigma}^\dagger d_{2\sigma} + t_2 d_{2\sigma}^\dagger d_{3\sigma} + t_1 d_{3\sigma}^\dagger d_{1\sigma}) e^{-i\phi/3} + \text{H.c.}]. \quad (4)$$

Here, H_{lead} is the Hamiltonian for the electrons in the left

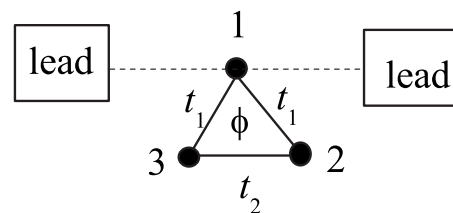


FIG. 1. Triangular quantum dots attached to the leads. t_1 and t_2 denote the interdot hoppings.

($j=L$) and right ($j=R$) leads. H_d is the isolated TQD Hamiltonian and H_t is the tunneling Hamiltonian. $d_{i\sigma}^\dagger$ and $c_{jk\sigma}^\dagger$ are dot and lead creation operators, respectively. ϵ and ϵ_k are orbital energy on the dots and leads, respectively. t_1 and t_2 are interdot hoppings, U is the on-site Coulomb repulsion on each dot. V_k is the tunnel matrix element between leads and dots while ϕ is the magnetic flux threaded the TQD ring.

The electronic transport is calculated using the numerical renormalization-group method^{16,22} (NRG). We assume a dispersionless conduction band with a half bandwidth D and a constant density of state ρ_0 . The tunnel coupling between dot 1 and the leads $\Gamma=2\pi\rho_0|V_k|^2$ is taken as a constant. The conductance through the dots is calculated using the Landauer formula²³

$$G = \frac{2e^2}{h} \int d\omega \left[\frac{\partial f(\omega)}{\partial \omega} \right] T(\omega), \quad (5)$$

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

$$T(\omega) = -\frac{1}{2} \Gamma \sum_{\sigma} \text{Im} G_{11\sigma}(\omega). \quad (6)$$

Here the retarded dot Green's function is defined as $G_{ij\sigma}(t) = -i\theta(t)\langle\{d_{i\sigma}(t), d_{j\sigma}^\dagger\}\rangle$. The magnetic moment μ is defined as the contribution of the TQDs to the total magnetic moment of the system,²²

$$\mu^2 = \chi k_B T / (g\mu_B)^2 = (\langle S_z^2 \rangle - \langle S_z \rangle_0^2), \quad (7)$$

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 the Boltzmann constant. S_z is the z component of the total spin of the whole system while $\langle \rangle$ means the thermodynamic expectation values.

III. RESULTS AND DISCUSSION

In the following, the half bandwidth D of the leads is taken as the energy unit. We focus on the strongly correlated regime and take $\Gamma=0.01$, $U=0.1$, $\epsilon=-U/2$, and $t_1=0.01$. For $\epsilon=-U/2$ and half filling, the Hamiltonian $H(\phi+\pi)$ is transformed to $H(-\phi)$ because of particle-hole symmetry. Therefore, we just discuss the cases for $0 \leq \phi \leq \pi/2$. Figure 2(a) shows the transmission coefficient $T(\omega)$ at zero temperature for $\phi=0$ and different t_2 . For small t_2 (e.g., $t_2 \leq 0.008374$), besides two broad Coulomb peaks at $\omega = \pm U/2$, we observe two peaks at about $\omega = \pm 0.005$. Mediated by the antiferromagnetic correlations between dot 1 and dots 2 and 3, a ferromagnetic Ruderman-Kittel-Kasuda-Yosida (RKKY) interaction $J_{\text{RKKY}} \approx 4t_1^2/U$ leads to a local triplet between dots 2 and 3. The peaks at $\omega = J_{\text{RKKY}} \approx \pm 0.005$ result from the process of annihilating (creating) an electron on dot 1 and damaging the RKKY interaction. These peaks are similar to the additional peaks in parallel TQD system,¹⁶ in which the RKKY interaction is mediated by the antiferromagnetic Kondo coupling between conduction and local electrons. When t_2 is larger than critical value $t_{2c}=0.008375$, dots 2 and 3 form a singlet and decouple from dot 1. In this case, the TQD system is just the usual Kondo model with one

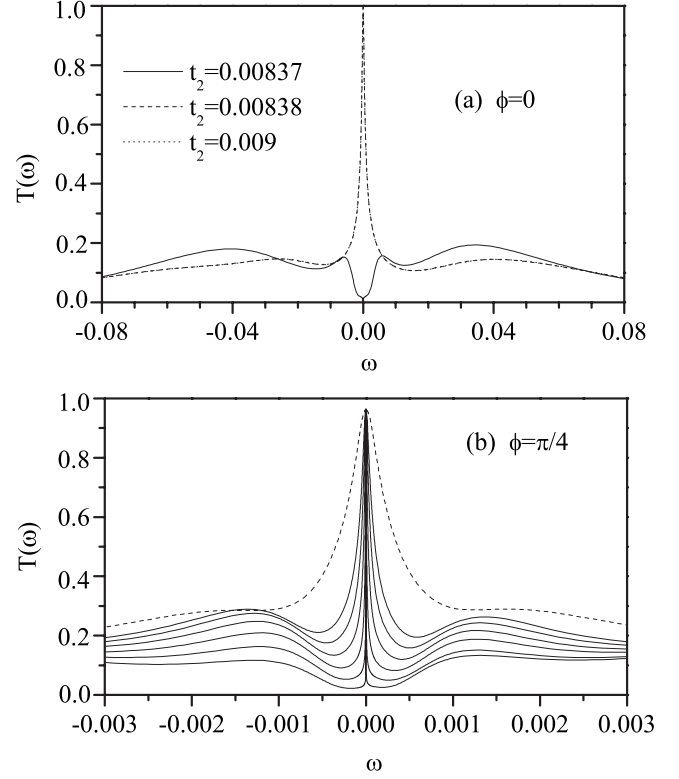


FIG. 2. Transmission coefficient $T(\omega)$ at zero temperature for $\Gamma=0.01$, $U=0.1$, $\epsilon=-U/2$, $t_1=0.01$, and different interdot hoppings t_2 and ϕ . In (a), curves for $t_2=0.00838$ and 0.009 are almost overlapping. In (b), from wide to narrow peaks, $t_2=0.01$ and $t_2=0.009-0.008$ in steps of 0.0002 .

impurity, and the Kondo resonance is observed. In the regime $t_2 > t_{2c}$, the Kondo peak does nearly not change which marks a first-order transition between the local triplet and the singlet.

For nonzero magnetic flux ϕ , the behavior of $T(\omega)$ for small t_2 is similar to that in Fig. 2(a). However, for $t_2 > t_{2c}$, here t_{2c} depends on ϕ while the width of Kondo peak T^* depends exponentially on the distance to the critical point ($t_2 - t_{2c}$). This feature in Fig. 2(b) indicates a KT transition at t_{2c} . In a multilevel dot system²⁴ and in capacitively coupled double quantum dots,²⁵ the similar KT quantum phase transitions with an exponentially small energy scale are also observed.

Figure 3(a) exhibits the characteristic energy scale T^* determined by half-width at half maximum of Kondo peak. The behavior of T^* in the regime $t_2 > t_{2c}$ and close to the critical point t_{2c} can be adequately described using an exponential function $T^* = C \exp[-A/(t_2 - t_{2c})^\alpha]$, where the parameters $C \approx 1$ and $\alpha \approx 0.385$. The parameter A and the critical hopping t_{2c} depend on the magnetic flux ϕ and have the values of 0.423, 0.549, 0.706, and 0.811, and 0.00819, 0.00801, 0.00772, and 0.00747 for $\phi = \pi/16$, $\pi/8$, $\pi/4$, and $\pi/2$, respectively. The energy scale T^* approaches zero more slowly for larger magnetic flux ϕ as t_2 decreases to t_{2c} . This exponentially dependent energy scale T^* is one of the characteristics of KT transition.^{6,24} Figure 3(b) shows the NRG result of the local spin correlation $\langle S_2 \cdot S_3 \rangle$ between dots 2

and 3 for different ϕ . For $\phi=0$, $\langle \mathbf{S}_2 \cdot \mathbf{S}_3 \rangle$ is about 0.25 for $t_2 < t_{2c}$ and -0.75 for $t_2 \geq t_{2c}$. This abrupt change in spin correlation at $t_{2c}=0.008375$ indicates a first-order triplet-singlet transition. For $\phi > 0$, with increasing t_2 , $\langle \mathbf{S}_2 \cdot \mathbf{S}_3 \rangle$ changes exponentially from 0.25 to -0.75 . Obviously, there is mixing between local singlet and triplet. This characteristic of the KT transition is also found in models of two interacting magnetic impurities coupled to a metallic host.⁶ The behavior of $\langle \mathbf{S}_2 \cdot \mathbf{S}_3 \rangle$ also demonstrates that the singlet-triplet transition proceeds most slowly for $\phi=\pi/2$.

In order to explore the origin of the KT transition, we analyze the ground state of the isolated TQD at half filling. The dot Hamiltonian in the second-order perturbation theory is written as

$$H_{2d} = J_1 \mathbf{S}_1 \cdot (\mathbf{S}_2 + \mathbf{S}_3) + J_2 \mathbf{S}_2 \cdot \mathbf{S}_3, \quad (8)$$

with $J_1 = 4t_1^2/U$ and $J_2 = 4t_2^2/U$, where \mathbf{S}_i is the spin operator of dot i . In the subspace with two up-spin electrons, the local singlet $|1\rangle$ and triplet $|2\rangle$ of dots 2 and 3 have the configurations

$$|1\rangle = \frac{1}{\sqrt{2}} d_{1\uparrow}^\dagger (d_{2\downarrow}^\dagger d_{3\uparrow}^\dagger - d_{2\uparrow}^\dagger d_{3\downarrow}^\dagger) |0\rangle, \quad (9)$$

$$|2\rangle = \sqrt{\frac{2}{3}} \left[-d_{1\downarrow}^\dagger d_{2\uparrow}^\dagger d_{3\uparrow}^\dagger + \frac{1}{2} d_{1\uparrow}^\dagger (d_{2\downarrow}^\dagger d_{3\uparrow}^\dagger + d_{2\uparrow}^\dagger d_{3\downarrow}^\dagger) \right] |0\rangle. \quad (10)$$

Their energies are $E_1 = -3U/2 - (4t_2^2 + 2t_1^2)/U$ and $E_2 = -3U/2 - 6t_1^2/U$, respectively. Obviously, as t_2 increases from $t_2 < t_1$ to $t_2 > t_1$, the local triplet transits to the local singlet. When the leads are connected to the TQD, there exists a first-order transition because there is no mixing between local singlet and triplet.⁶ Considering the effect of the coupling between the dots and the leads, the critical point is $t_{2c} = 0.008375$, which is different from that for isolated TQDs. This first-order transition is confirmed by the abrupt appearance and disappearance of the Kondo peak (see Fig. 2) on the two sides of the transition point.

The above result indicates that, in the second-order perturbation theory, the KT transition cannot be observed. We consider the third-order perturbation process. The eigenstate of H_d is $|\Psi\rangle = \sum_i a_i |i\rangle$, where $|i\rangle$ is an eigenstate of

$$H_d^0 = \epsilon \sum_{i\sigma} d_{i\sigma}^\dagger d_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (11)$$

The perturbation of the energy ΔE of local singlet $|1\rangle$ and triplet $|2\rangle$ is obtained by

$$\Delta E a_i = - \frac{1}{U} \sum_{mj} H'_{im} H'_{mj} a_j - \frac{1}{U^2} \sum_{nmj} H'_{in} H'_{nm} H'_{mj} a_j, \quad (12)$$

where $H' = H_d - H_d^0$ and $H'_{ij} = \langle i | H' | j \rangle$. The shift in the energy of local singlet $|1\rangle$ and triplet $|2\rangle$ is determined by

$$\Delta E a_1 = - \frac{4t_2^2 + 2t_1^2}{U} a_1 - \frac{6\sqrt{3}t_1^2 t_2 \sin \phi}{U^2} i a_2, \quad (13)$$

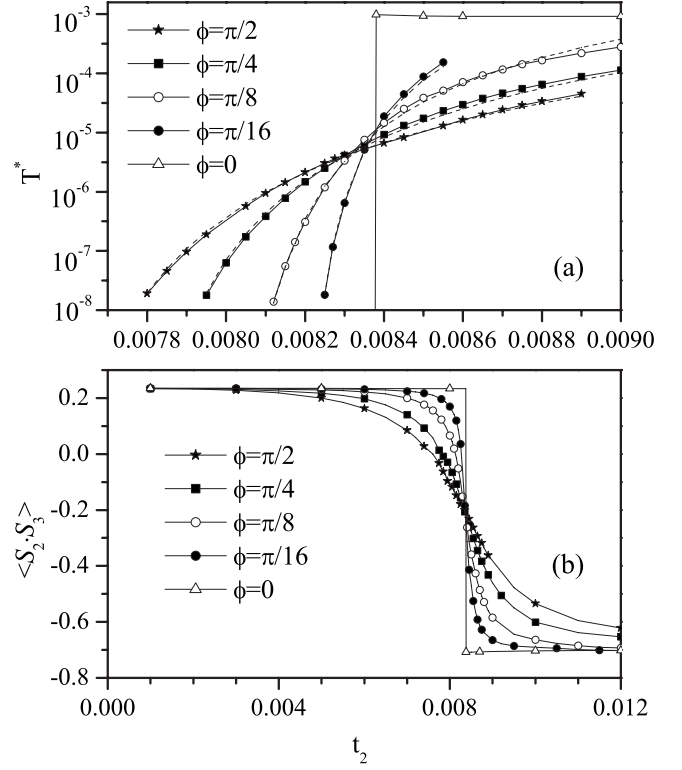


FIG. 3. (a) Characteristic energy scale T^* determined by the width of Kondo peak and (b) local spin correlation $\langle \mathbf{S}_2 \cdot \mathbf{S}_3 \rangle$ as functions of t_2 for different ϕ . Other parameters are the same as in Fig. 2. The dashed lines in (a) correspond to the simulat exponential function in the text.

$$\Delta E a_2 = - \frac{6t_1^2}{U} a_2 + \frac{6\sqrt{3}t_1^2 t_2 \sin \phi}{U^2} i a_1. \quad (14)$$

Obviously, there is mixing between local singlet and triplet in the eigenstate $|\Psi^\pm\rangle = a_1^\pm |1\rangle + a_2^\pm |2\rangle$ with coefficients a_i^\pm determined by Eqs. (13) and (14). Therefore, for $\phi \neq 0$, the transition in the whole system containing leads and TQD is of the KT type.⁶ This KT transition is demonstrated by an exponentially dependent width of Kondo peak T^* in Figs. 2 and 3. The third-order perturbation process involves exchange of electrons among three quantum dots. Figure 4 shows that a configuration in the local triplet transfers to the singlet state. In the intermediate states, three dots are singly occupied, doubly occupied, and empty, respectively. There are 24 ways of doing the similar exchange. For $\phi=0$, these two processes in Figs. 4(a) and 4(b) have reversal contributions to the second term in Eq. (12) so that the TOS interaction vanishes. For $\phi \neq 0$, the TOS interactions survive because of AB interference effect in above processes. According to Eq. (12), the dot Hamiltonian H_d contains by following three-order term H_{3d} besides the second-order term H_{2d}

$$H_{3d} = \frac{12t_1^2 t_2 \sin \phi}{U^2} (S_{1x} S_{2y} S_{3z} + S_{1y} S_{2z} S_{3x} + S_{1z} S_{2x} S_{3y} - S_{1x} S_{2z} S_{3y} - S_{1y} S_{2x} S_{3z} - S_{1z} S_{2y} S_{3x}). \quad (15)$$

In models of two interacting magnetic impurities coupled to

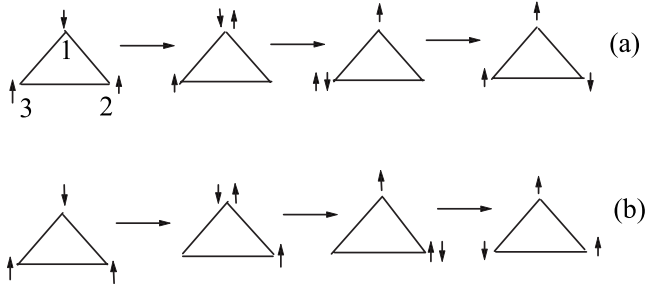


FIG. 4. Two kinds of third-order superexchange processes in triangular dots; up arrow and down arrow denote electrons with up spin and down spin, respectively. In initial and final states, dots 2 and 3 form a triplet and a singlet, respectively. In (a) and (b), electrons travel in the TQD ring anticlockwise and clockwise, respectively.

a metallic host,⁶ if two impurities asymmetrically couple the host, the singlet-doublet transition is of the KT type. In the present model, H_{3d} is transformed to $-H_{3d}$ under permutation of any two dots. This means that dots 2 and 3 asymmetrically couple dot 1. This asymmetric interaction resulting from magnetic flux is the origin of the KT transition. Equations (13)–(15) show that the mixing between local singlet $|1\rangle$ and triplet $|2\rangle$ has the maximum at $\phi = \pi/2$. The NRG results in Fig. 3 for the characteristic energy scale T^* and the local spin correlation $\langle \mathbf{S}_2 \cdot \mathbf{S}_3 \rangle$ also indicates that the singlet-triplet transition proceeds most slowly for $\phi = \pi/2$.

In order to exhibit the low-temperature scenario of the TQD system, Fig. 5 shows temperature dependence of the total magnetic moment μ defined in Eq. (7). For $\phi = 0$, at

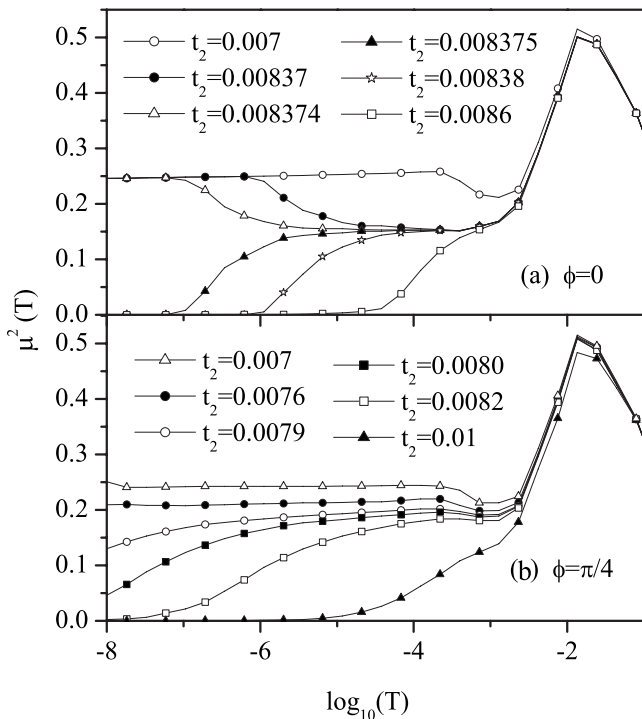


FIG. 5. Total magnetic moment of the TQDs as a function of temperature T for different t_2 and ϕ . Other parameters are the same as in Fig. 2.

high temperature $T \sim 0.02$ (e.g., $4t_1^2/U < T < U$), each dot has a free local spin of $1/2$ and contributes $1/4$ to μ^2 . Because there is some possibility of double occupation in this regime, μ^2 is about 0.5 which is smaller than the maximum $3/4$. With decreasing T (e.g., $T \sim 0.001 < 4t_1^2/U$) the interdot superexchange interactions drive the triple dots to a singlet with $\mu^2 \approx 1/4$. In lower temperature $T \rightarrow 0$, for $t_2 < t_{2c}$, dots 2 and 3 form a local triplet which couples to dot 1 antiferromagnetically and leads to a doublet ground state of the whole TQD system. For $t_2 \geq t_{2c}$, dots 2 and 3 form a local singlet and decouple from dot 1 while dot 1 is totally screened by Kondo coupling, and a Kondo resonance is observed. For $\phi \neq 0$ (e.g., $\phi = \pi/4$), the local triplet-singlet transition is continuous. For $t_2 > t_{2c}$ and far from t_{2c} , dots 2 and 3 form a perfect singlet and dot 1 is totally screened by conduction electrons. For $t_2 > t_{2c}$ and near t_{2c} , there is a mixing between local triplet and singlet of dots 2 and 3. The total spin of dots 2 and 3 is not zero for a singlet so that there exists weak coupling between dots 2 and 3 and dot 1. With decreasing T , this coupling partially screens the spin of dot 1 and results in a residual moment of about 0.2 . In lower temperature $T \rightarrow 0$ dot 1 is screened by Kondo coupling with the leads. For $t_2 < t_{2c}$ and near t_{2c} , the coupling between dots 2 and 3 and dot 1 is strong enough, and completely screens the spin of dot 1 so that Kondo screening cannot occur. Therefore the Kondo effect originates from the competition between Kondo coupling and above interdot coupling.

To summarize, we have investigated electronic transport in triangular QDs pierced by an external magnetic flux. The NRG results show that, in the absence of magnetic flux, there is a first-order quantum phase transition between the local triplet and the singlet as the interdot hopping t_2 increases to a critical point t_{2c} . This transition is demonstrated by the abrupt appearance and disappearance of the Kondo peak on the two sides of the transition point, and is also confirmed by the abrupt change in the local spin correlation $\langle \mathbf{S}_2 \cdot \mathbf{S}_3 \rangle$ at t_{2c} . If the magnetic flux is turned on in the singlet side of the transition, the width of the Kondo resonance peak exponentially approaches zero as t_2 is close to t_{2c} . This behavior indicates that the triplet-singlet transition is of the KT type. Another characteristic of the KT transition is that, with increasing t_2 , $\langle \mathbf{S}_2 \cdot \mathbf{S}_3 \rangle$ changes exponentially from 0.25 of the triplet to -0.75 of the singlet. This means that there is mixing between local singlet and triplet. Above characteristic with an exponentially small energy scale, and that with mixing between singlet and triplet are also found in other KT transitions in other quantum dots or two impurity systems but their origins are quite different.^{6,24,25} Based on the perturbation theory for the isolated TQD, we find that the TOS interaction survives due to AB effect and results in the mixing between the local singlet and triplet. The TOS interaction has never been considered in the literature because it vanishes in most itinerant electron systems. The KT quantum phase transition induced by the TOS interaction can be continuously tuned by magnetic flux. For small magnetic flux, the transition proceeds faster as t_2 approaches t_{2c} while for $\phi = \pi/2$, it proceeds most slowly.

It is noticeable that the calculations are performed in strongly correlated regime $U \gg t_1, t_2, \Gamma$ and in half-filling case, the qualitative results do not depend on the precise

parameters. Recently, a triangular trimer of Cr ions on a gold surface has been realized experimentally and Kondo effect with a Kondo temperature $T_K \approx 50$ K has been observed.¹⁸ This fact provides a possibility in demonstrating our findings. In experiment, the tunnel coupling Γ , t_1 , and t_2 can be tuned by varying the distance between Cr adatoms. The Kondo temperature can be estimated by Haldane's expression $T_K = 0.182U\sqrt{\rho_0 J_K} \exp(-1/\rho_0 J_K)$ with $\rho_0 J_K = 8\Gamma/\pi U$. The parameters $U=0.1$ and $\Gamma=0.01$ in this paper and a band-

width $D=10^5$ K (Ref. 26) lead to $T_K \approx 18$ K which can be easily realized experimentally.

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