# Voltage-controlled Kosterlitz–Thouless transitions and various kinds of Kondo behaviors in a triple dot device*

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The transport property and phase transition for a parallel triple dot device are studied by adopting Wilson's numerical renormalization group technique, focusing on the effects of level spacings between neighboring dot sites. By keeping dot 2 at the half-filled level and tuning the level differences, it is demonstrated that the system transits from local spin quadruplet to triplet and doublet sequently, and three kinds of Kondo peaks at the Fermi surface could be found, which are separated by two Kosterlitz–Thouless type quantum phase transitions and correspond to spin-3/2, spin-1, and spin-1/2 Kondo effect, respectively. To obtain a detailed understanding of these problems, the charge occupation, the spin–spin correlation, the transmission coefficient, and the temperature-dependent magnetic moment are shown, and necessary physical arguments are given.

**Keywords:** triple quantum dot, Kosterlitz–Thouless transition, Kondo effect, critical phenomena

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## 1. Introduction

For the last several years, systems of coupled multi-quantum dots have gained significant interests both experimentally[1–6] and theoretically, due to rapid progress in spintronics[7–9] and quantum information.[10,11] An important example of a multi-dot system is the triple quantum dots (TQD). Such structure exhibits many interesting quantum phenomena in the strong correlation limit. For instance, the Aharanov–Bohm (AB) effect and magnetic frustration are studied in systems with triangular geometry,[12–15] and the multi-channel Kondo effect related to a number of Fermi-liquid and non-Fermi-liquid behaviors are investigated in various TQD models.[16–20] Furthermore, TQD systems are also considered as ideal models to show the Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction,[21,22] the quantum interference,[23–26] and various kinds of quantum phase transition (QPT).[13,15,27–32] Basically, these behaviors depend closely on the organizations of the quantum dots and the conduction leads, as well as the coupling/interaction elements which have been taken into account.

Within the above phenomena, the level difference plays an important role as suggested in some double quantum dot (DQD) structures. For instance, a local spin triplet–singlet transition of Kosterlitz–Thouless (KT) type is found as the difference increases.[33] For a parallel DQD system, it is revealed that the triplet–doublet transition could be KT type or first order depends on the breaking of the spin-rotation SU(2) symmetry,[34] and the linear conductance is shown to have an asymmetric line shape of the Fano resonance when the inter-dot tunneling coupling is taken into account.[35] In a spinless two-level dot system, charge oscillation occurs in the presence of level spacing as the gate voltage sweeps.[36] These works are limited in the double dot structures, but less is studied in the TQD system. Compared to the double dot system, TQD structure exhibits more attractive behaviors, owing to its complex geometry and much more Feynman paths for the electron transmission.[25] Furthermore, experimentally speaking, scaling up the number of spin-1/2 qubits is an inevitable step towards the realization of quantum computation, not only for extending the qubit system, but also for performing practical quantum algorithms.[37] Very recently, plenty of experimental works have been carried out on this topic in TQD systems,[5,6,38–41] therefore, to illustrate the electronic transport, phase transition and relevant quantum phenomena in such systems also becomes an emergent task.

In this paper, we consider a parallel TQD system with level spacings between neighboring dot sites. With the help of the numerical renormalization group (NRG) method, and fixing dot 2 at the half-filled level, we demonstrated that the level spacings play important roles in the linear conductance and the QPT. Our main findings include the following: by tuning the level differences, the ground state of the system transits

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from local spin quadruplet to triplet, then doublet sequentially, and three kinds of Kondo peaks at the Fermi surface could be found, corresponding to spin-3/2, spin-1, and spin-1/2 Kondo effect, respectively. Two Kosterlitz–Thouless (KT) type transitions are clarified, resulting from asymmetric Kondo couplings between conduction leads and different dots, as well as the unequal charge occupation of three dots. To handle these problems, some important physical quantities are shown, and necessary physical arguments are given.

The outline of the paper is as follows. In Section 2, we define the model Hamiltonian of the TQD system, and present the calculation algorithms and formulations. In Section 3, we show the quantum phase transitions and transport properties with respect to the increasing level spacings. Finally, a summary is given in Section 4.

## 2. Model and method

We illustrate the second-quantized form of the model Hamiltonian for the triple dot device in Fig. 1,

$$H = H_{\rm d} + H_{\rm l} + H_{\rm dl}, \tag{1}$$

where the first part is for the electrons in the dots,

$$H_{\rm d} = \sum_{i=1,\sigma}^{3} \varepsilon_i d_{i\sigma}^{\dagger} d_{i\sigma} + U \sum_{i=1}^{3} n_{i\uparrow} n_{i\downarrow}. \tag{2}$$

Here, $\varepsilon_i$ is the energy level for the $i$-th dot. For simplicity, we label two level spacings as $\Delta_1 = \varepsilon_2 - \varepsilon_1$ and $\Delta_2 = \varepsilon_3 - \varepsilon_2$, which could be controlled by external gate voltage. $d_{i\sigma}^{\dagger}$ is the creation operator for the electron with spin-$\sigma$ (=$\uparrow$ or $\downarrow$). $U$ is the on-site (intra-dot) Coulomb repulsion, and $n_{i\sigma} = d_{i\sigma}^{\dagger} d_{i\sigma}$, $n_i = n_{i\uparrow} + n_{i\downarrow}$ are the number operators.

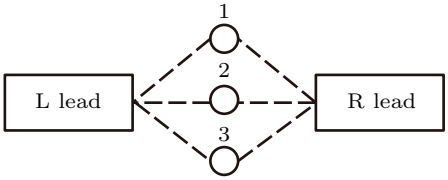



**Fig. 1.** Schematic view of the parallel TQD device connected to the L and R leads.

The second part is for the non-interacting electrons in the conduction lead, $H_{\rm l} = \sum_{\nu k\sigma} \varepsilon_k c_{\nu k\sigma}^{\dagger} c_{\nu k\sigma}$, where $c_{\nu k\sigma}^{\dagger}$ create a spin-$\sigma$ electron of wave vector $k$ and energy $\varepsilon_k$ in lead $\nu$ ($\nu$ = R or L). By contrast, the last term is for the coupling interaction energy between the conduction lead and the dots, $H_{\rm dl} = \sum_{\nu k i\sigma} (V_k c_{\nu k\sigma}^{\dagger} d_{i\sigma} + {\rm H.c.})$, where $V_k$ is the tunnel matrix element, and is assumed to be $\sigma$-independent, identical for three dots, and also symmetric to the right and left leads.

In the following discussion, we concentrate on the quantum behaviors in the strong correlation limit, hence a sophisticated theoretical technique must be adopted. Therefore, we use the celebrated NRG method[42–44] to solve Eq. (1). To simplify the problem into a more convenient form, we first assume the density of state for the conduction lead $\rho_0 = 1/(2D)$ and the hybridization function (dot–lead coupling) $\Gamma = 2\pi\rho_0 |V_k|^2$ are constant. Here, $D$ is the half width of the conduction band, and is chosen for the energy unit throughout this paper. The strong correlation limit is defined as $U \gg \Gamma$, and the number of low-lying states kept at each iteration is about 3000. Furthermore, the discretization parameter $\Lambda$, which characterizes the logarithmic discretization of the conduction band, is set to be 1.8–2.2.

The total charge number $N_{\rm tot}$ and the local spin $S_{\rm dot}^2$ are defined as

$$N_{\rm tot} = \left\langle \sum_i n_i \right\rangle, \quad S_{\rm dot}^2 = \left\langle \left( \sum_i S_i \right)^2 \right\rangle = S_{\rm dot}(S_{\rm dot}+1), \tag{3}$$

where $S_i$ is the local spin operator of dot $i$.

The linear conductance through the device $G$ is determined by the Landauer formula[45]

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

Here, $f(\omega)$ is the Fermi function and $T(\omega)$ is the transmission probability. The retarded dot Green function is written as $G_{ij\sigma}(t) = -{\rm i}\theta(t)\langle\{d_{i\sigma}(t), d_{j\sigma}^{+}\}\rangle$. Thus

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

If we choose the Fermi energy at $\varepsilon_{k_{\rm f}} = 0$, $G$ at zero temperature in the limit of zero bias is given by

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

Finally, we define the temperature-dependent magnetic moment of the dots $\mu^2(T)$ at temperature $T$ as

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

where $\chi(T)$ is the magnetic susceptibility, $k_{\rm B}$ is the Boltzmann constant, $g$ and $\mu_{\rm B}$ are the electronic $g$ factor and the Bohr magneton, respectively. $\langle \ldots \rangle$ denotes the thermodynamic expectation value, and the subscript 0 labels the case without quantum dots.

## 3. Results and discussion

In this section, we study the phase transition and the electronic transport of the TQD device in the strongly correlated regime, focusing on the phenomena when the level differences sweep upwards. The on-site Coulomb repulsion, the dot-lead coupling, and the charge energy of dot 2 are fixed at $U = 0.1$, $\Gamma = 0.01$, and $\varepsilon_2 = -U/2$, respectively, throughout this paper. For convenience, we choose $\Delta_2 = \Delta_1/2$. However, it is worth noting that our conclusions are robust for general cases, and do not really require $\Delta_1$ and $\Delta_2$ to satisfy the above relation.

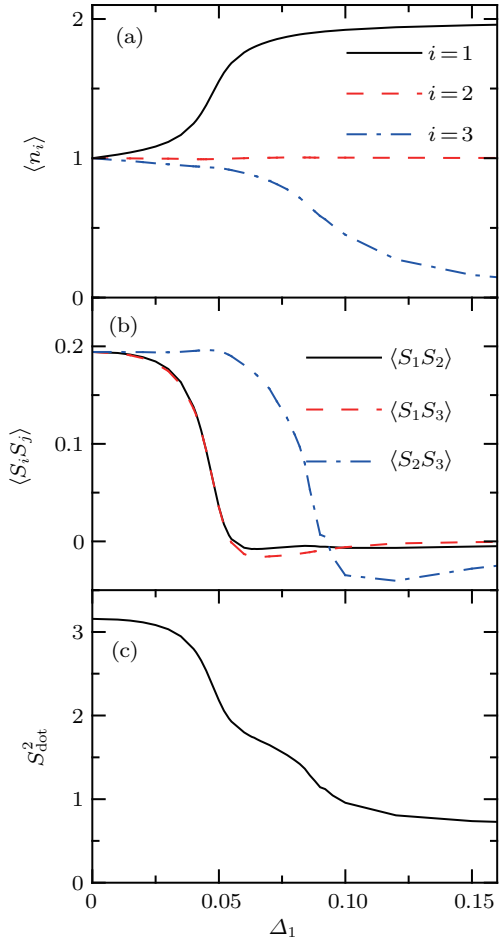



**Fig. 2.** (color online) (a) Charge occupation $\langle n_i\rangle$ on each dot, (b) spin correlation $\langle S_iS_j\rangle$ between dots $i$ and $j$, and (c) local spin $S^2_{\rm dot}$ of the dots at zero temperature as functions of $\Delta_1$. Here, $\Gamma = 0.01$, $U = 0.1$, $\varepsilon_2 = -U/2$ and $\Delta_2 = \Delta_1/2$.

Let us start our discussion from the quantum phase transition for the TQD system. In Figs. 2(a)–2(c), we depict the charge occupation $\langle n_i\rangle$ of each dot, the spin correlation $\langle S_iS_j\rangle$ between dots $i$ and $j$, and the local spin $S^2_{\rm dot}$ on the dots as functions of $\Delta_1$. We can see when the level differences are absent, three dots are singly occupied with $\langle n_i\rangle = 1.0$, since the intra-dot repulsion $U$ is strong enough. In this case, $\langle S_iS_j\rangle \approx 0.20$ and $S^2_{\rm dot} \approx 3.20$, implying the local spins on three dots are arranged parallelly and a local spin quadruplet is generated, owing to the ferromagnetic RKKY interaction mediated by the Kondo exchange coupling between electrons on the leads and those on the dots. It is noted that $\langle S_iS_j\rangle$ and $S^2_{\rm dot}$ could not reach the ideal values of $1/4$ and $15/4$ for spin quadruplet, as a finite $U/\Gamma$ is adopted. With increasing $\Delta_1$, the level $\varepsilon_1$ decreases, while $\varepsilon_3$ increases but with a lower speed. Therefore, $\langle n_1\rangle$ grows to 2.0 gradually, while $\langle n_2\rangle$ and $\langle n_3\rangle$ retain nearly at 1.0. In this process, $S^2_{\rm dot}$ changes continuously to about 1.75, describing that the ground state is dominated by the spin triplet. In this triplet, dot 1 is almost doubly occupied, hence $\langle S_1S_2\rangle$ and $\langle S_1S_3\rangle$ decrease to about 0, while $\langle S_2S_3\rangle$ has nearly no change. As $\Delta_1$ increases continuously, $\langle n_3\rangle$ decreases to the regime $n_3 \approx 0$. In this case, the system maps to the single impurity case and the ground state is a local spin doublet with $\langle S_iS_j\rangle \approx 0$ and $S^2_{\rm dot} \approx 0.75$.

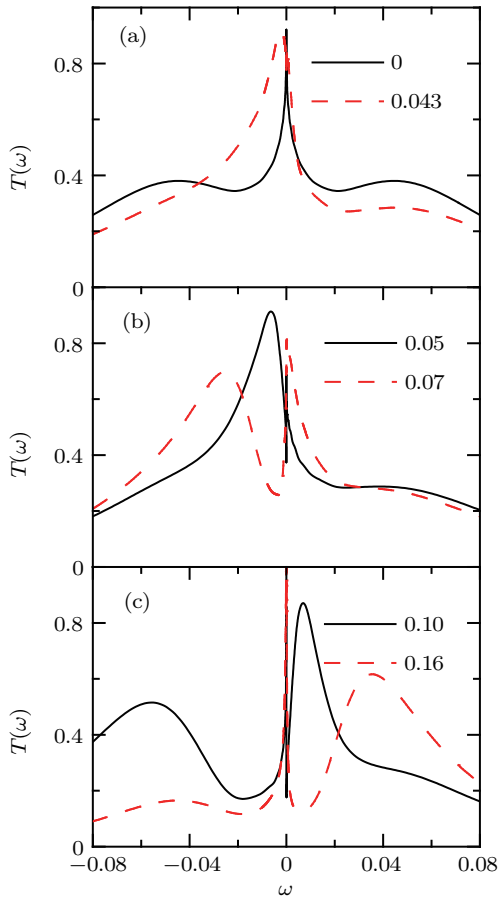



**Fig. 3.** (color online) (a)–(c) Transmission coefficient $T(\omega)$ at zero temperature for various $\Delta_1$. The remaining parameters are the same as in Fig. 2.

Figures 3(a)–3(c) show the transmission coefficient $T(\omega)$ at zero temperature for various $\Delta_1$. It is seen that the spectral weight is symmetric to the Fermi level $\omega = 0$ when $\Delta_1 = 0$, since Eq. (2) satisfies particle–hole (p–h) symmetry. Two Coulomb peaks located at $\omega = \pm U/2$ are found, referring to the process of annihilating (creating) an additional electron (hole) on the bonding orbital $f_{\rm b\sigma} = (d_{1\sigma} + d_{2\sigma} + d_{3\sigma})/\sqrt{3}$. Besides, a Kondo peak could also be seen at the Fermi level, which reaches the unitary limit of $2e^2/h$ corresponding to full conductance. It could be attributed to the process where the itinerant electron screens a local spin-1/2 degree of freedom and results in a partially screened spin-3/2 Kondo effect.[15,21] As $\Delta_1$ increases, the spectral weight moves to the left and is not symmetric to $\omega = 0$, for the p–h symmetry is broken and $N_{\rm tot}$ is away from a triply occupied state. In this process, the amplitude of the Kondo resonance peak decreases, implying that the linear conductance is reduced slightly (see $\Delta_1 = 0.043$ in panel (a)). As $\Delta_1$ exceeds the first critical point $\Delta_1^{\rm c1} = 0.0462$, a sharp Kondo peak appears at $\omega = 0$ (see $\Delta_1 = 0.05$ in Fig. 3(b)), which is related to the partially screened spin-1 Kondo effect, and originates from the screen-

ing of the local spin triplet between dot 2 and 3 by the conduction electrons. With increasing $\Delta_1$, the spectral weight moves away from $\omega = 0$ and the Kondo peak is broadened, indicating a decrease of the conductance (e.g., $\Delta_1 = 0.07$). When $\Delta_1$ grows larger than the second critical point $\Delta_1^{c2} = 0.0863$, another sharp Kondo peak is observed at the Fermi surface (see $\Delta_1 = 0.10$ in panel (c)), which results from the antiferromagnetic Kondo coupling between the conduction leads and dot 2, since dot 1 is almost doubly occupied and dot 3 is empty. As $\Delta_1$ grows continuously, the Kondo peak keeps at $\omega = 0$, for the TQD is stable in the spin doublet (see $\Delta_1 = 0.16$).

To get more information about the phase transition, we show $T(\omega)$ on the triplet side near $\Delta_1^{c1} = 0.0462$ in Fig. 4(a). One finds that the width of the spin-1 Kondo peak $W_1$ enlarges with increasing $\Delta_1$. Here, the width of the spin-1 Kondo peak is defined as the half width at half maximum of the Kondo peak. Figure 4(b) suggests that $W_1$ depends exponentially on the distance to the critical point $(\Delta_1 - \Delta_1^{c1})$ and can be adequately described using an exponential function $W_1 = P_1 \exp[P_2/(\Delta_1 - \Delta_1^{c1})^{P_3}]$, where the fitting parameters are given by $P_1 = -0.0192$, $P_2 = 3.9409$, and $P_3 = 0.0552$. It is seen that the fitting function (solid line) agrees very well with our NRG results (scatter dots). This behavior describes that the quadruplet–triplet transition at $\Delta_1^{c1}$ is a KT transition. Figure 4(c) gives $T(\omega)$ for various $\Delta_1$ on the doublet side near $\Delta_1^{c2}$. One may also find that the width of the spin-1/2 Kondo peak $W_2$ approaches zero exponentially as $\Delta_1$ is close to $\Delta_1^{c2}$, and can be described by an exponential function $W_2 = P_4 \exp[P_5/(\Delta_1 - \Delta_1^{c2})^{P_6}]$. Here, the fitting parameters are $P_4 = -0.0019$, $P_5 = 6.4015$, $P_6 = 0.0431$. Figure 4(d) indicates that the fitting function (solid line) agrees very well with the NRG results (scatter dots), illustrating the triplet–doublet transition is also of the KT type.

To exhibit more information about the low-temperature scenario, we present $\mu^2(T)$ for different $\Delta_1$ in Fig. 5. The upmost curve is for the case of $\Delta_1 = 0$. It is seen that TQD goes through four different regimes as $T$ decreases. For example, when $T$ is high enough (e.g., $T > U$), the electrons on three dots are independent, then each dot contributes $1/8$ to $\mu^2(T)$. As $T$ decreases to $T < U$ (e.g., $T \sim 0.01$), the electrons are then in the local moment regime, thus the full- and zero-occupied states are strongly suppressed. Therefore, each of them contributes $1/4$ to $\mu^2(T)$. When $T$ decreases to the order of the RKKY interaction (e.g., $T \sim 0.001$), the electrons on three dots form a spin quadruplet and contribute $S_{\rm dot}(S_{\rm dot}+1)/3 = 5/4$ to $\mu^2(T)$. As a result, $\mu^2(T)$ grows to a higher spin stage. Here, $\mu^2(T)$ in the local moment regime ($\mu^2(T) \sim 0.62$) and the RKKY regime ($\mu^2(T) \sim 0.80$) are smaller than the ideal values, for the TQD is not in a pure ground state in these temperature regimes. When $T$ reduces to the Kondo temperature scale (e.g., $T \sim 10^{-7}$), the itinerant electron screens a local spin-1/2 degree of freedom, thus one finds an obvious drop in $\mu^2(T)$ and $\mu^2(T) \sim 0.67$ at low temperature. As $\Delta_1$ increases, the height of $\mu^2(T)$ in the RKKY regime is reduced, since the possibilities of generating the RKKY interaction decreases due to increasing double occupancy on dot 1. On the other hand, $\mu^2(T)$ at low temperature $\mu^2(\mathrm{T} = 0)$ decreases exponentially. When $\Delta_1$ is large enough (e.g., $\Delta_1 = 0.052$), $\mu^2(\mathrm{T} = 0) \approx 0.25$, since in this case the spin triplet is partially screened by the conduction leads, and the remaining spin-1/2 degree of freedom contribute to $\mu^2(T)$. As $\Delta_1$ grows continuously, $\mu^2(\mathrm{T} = 0)$ reduces exponentially again. When $\Delta > \Delta_1^{c2}$, $\mu^2(T) \to 0$ at low temperature, for in this regime the local spin singlet is totally screened by the conduction electrons.

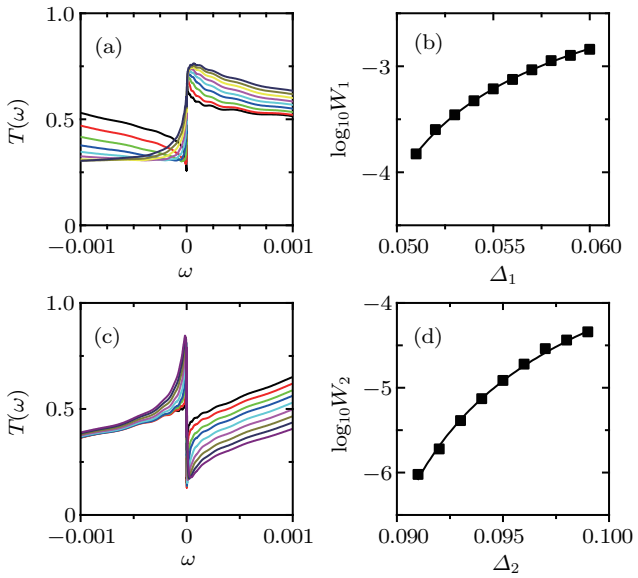



**Fig. 4.** (color online) (a) $T(\omega)$ on the triplet side near the first critical points $\Delta_1^{c1} = 0.0462$. The curves from top to bottom on the left side are for $\Delta_1 = 0.051$ to 0.060 in steps of 0.001. (b) Width of the spin-1 Kondo peak $W_1$ (scatter dots) and its fitting exponential functions (solid lines). (c) $T(\omega)$ on the doublet side near the second critical point $\Delta_1^{c2} = 0.0863$. The curves from top to bottom on the right side are for $\Delta_1 = 0.091$ to 0.099 in steps of 0.001. (d) Width of the spin-1/2 Kondo peak $W_2$ (scatter dots) and its stimulant functions (solid lines). The remaining parameters are the same as in Fig. 2.

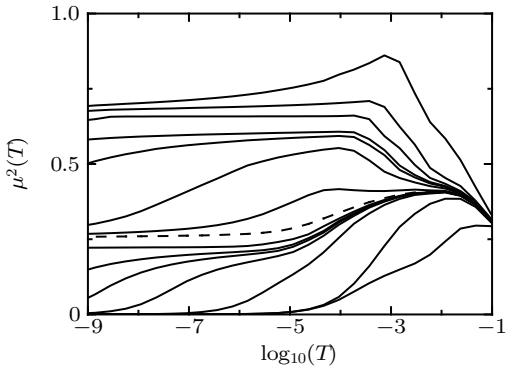



**Fig. 5.** Total magnetic moment of the TQD $\mu^2(T)$ as a function of temperature $T$ according to different $\Delta_1$, the curves from top to bottom are for $\Delta_1 = 0$, 0.04, 0.046 to 0.050 in steps of 0.001, 0.052 (dash line), and $\Delta_1 = 0.08$, 0.087 to 0.09 in steps of 0.001, 0.094, 0.1, respectively. The remaining parameters are the same as in Fig. 2.

To explore the physical origination of the KT transitions, we change Eq. (1) to a three impurities spin-1/2 Kondo model by adopting the Schrieffer–Wolff transformation.[?,21] The effective Hamiltonian then could be written as

$$H_{\rm eff} = H_{\rm l} + \sum_i J_{ki} \hat{S}_0 \cdot \hat{S}_i. \tag{8}$$

Here, $\hat{S}_0$ is the conduction electron spin density, while $\hat{S}_i$ is the spin-1/2 operator for the $i$-th dot. The Kondo coupling between the leads and three impurities $J_{ki}$ are given by

$$\begin{aligned} J_{k1} &= \frac{4\Gamma}{\pi}\left(\frac{1}{|U/2+\Delta_1|}+\frac{1}{|U/2-\Delta_1|}\right), \\ J_{k2} &= \frac{8\Gamma}{\pi U}, \\ J_{k3} &= \frac{4\Gamma}{\pi}\left(\frac{1}{|U/2+\Delta_2|}+\frac{1}{|U/2-\Delta_2|}\right). \end{aligned} \tag{9}$$

With increasing $\Delta_1$, $J_{ki}$ are asymmetric. On the other hand, the charge occupation in three dots also become different. The symmetric broken by these features are the origination of the KT transitions, similar to a two-level dot system with level difference[33] and inter-dot Coulomb repulsion.[34] Furthermore, it is worth noting that one can estimate the critical points by considering the energy levels of an isolated TQD model. For instance, the energy level for the spin quadruplet can be written as $E_{\rm Q} = \varepsilon_1 + \varepsilon_2 + \varepsilon_3 = -3U/2$. While that for the triplet is $E_{\rm T} = 2\varepsilon_1 + \varepsilon_2 + \varepsilon_3 + U = -U - 3\Delta_1/2$, and the level for the doublet is given by $E_{\rm D} = 2\varepsilon_1 + \varepsilon_2 + U = -U/2 - 2\Delta_1$. As $\Delta_1$ increases, the energy levels for the triplet and the singlet are pulled down, and eventually degenerate with the quadruplet at $\Delta_1 = U/3$ and the triplet at $U$ respectively. As a result, two QPTs of the KT type can be found at $\Delta_1^{\rm c1}$ and $\Delta_1^{\rm c2}$.

## 4. Summary

In conclusion, we have studied the phase transition and Kondo behavior in a triple quantum dot device with parallel organization in the strongly correlated regime. We concentrate on the effect of the level differences $\Delta_1 = \varepsilon_2 - \varepsilon_1$ and $\Delta_2 = \varepsilon_3 - \varepsilon_2$. By keeping dot 2 at the half-filled level and tuning the level differences, it is shown that the ground state of the system transits from local spin quadruplet to triplet, then doublet sequentially, three kinds of Kondo peaks at the Fermi surface could be found in the transmission coefficient, which correspond to spin-3/2, spin-1, and spin-1/2 Kondo effect, respectively. Two KT type phase transitions are clarified, resulting from asymmetric Kondo couplings between the conduction leads and different dots, as well as unequal electron occupation of three dots. We believe our work not only clarifies the effect of the level difference on the phase transition and the electronic transport in a triple dot structure, but it may also afford useful guidance for spintronics and molecular electronics devices.

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