Tunneling through triple quantum dots with mirror symmetry

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Indirect exchange interaction between itinerant electrons and nano-structures with non-trivial geometrical configurations manifests a plethora of unexpected results. These configurations can be realized either in quantum dots with several potential valleys or in real complex molecules with strong correlations. Here we demonstrate that the Kondo effect may be suppressed under certain conditions in triple quantum dots with mirror symmetry at odd electron occupation. First, we show that the indirect exchange has ferromagnetic sign in the ground state of triple quantum dot in a two-terminal cross geometry for electron occupation \( N = 3 \). Second, we show that for electron occupation \( N = 1 \) in three-terminal fork geometry the zero-bias anomaly in the tunnel conductance is absent (despite the presence of Kondo screening) due to special symmetry of the dot wave function.

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I. INTRODUCTION

Many-particle effects in quantum tunneling through quantum dots are extensively discussed in the current literature (see, e.g., recent reviews\textsuperscript{14}). Single-electron tunneling under the conditions of strong Coulomb blockade is accompanied by co-tunneling processes with spin-reversal, which involve dynamical screening effects similar to the celebrated Kondo-scattering in magnetically doped metals. The pertinent effect was predicted and observed in single-well quantum dots with odd electron occupation, where the electrons confined in the well are represented by the non-compensated spin 1/2 of an electron on the highest occupied discrete level. This generic pattern may be enriched in many ways, in particular, by studying the tunneling through complex quantum dots containing two or three valleys.

In this paper we are interested in specific physical properties of electron tunneling through complex quantum dots containing several potential valleys with essentially different capacitances. Originally, the idea of coupling several nano-objects having strong and weak Coulomb interactions is formulated in the context of electron and spin structure of complex molecules (e.g., lanthanocenes, containing strongly correlated f-electrons hybridized with weakly correlated molecular orbitals occupied by p-electrons). It is noticed\textsuperscript{5} that the energy difference between the singlet (\( S \)) ground state and triplet (\( T \)) excited state of a molecule with even number of electrons \( N = N_T + N_S \) is anomalously small, so that the triplet excitation affects the magnetic response of the system. The simplest artificial analog of this system is an asymmetric double quantum dot (composed of big and small dots) with even occupation (e.g., \( N = 2 \)) and charging energies \( Q_T \gg Q_S \) for small and big dots. When this double quantum dot is coupled with the metallic leads via the big dot (the T-shaped geometry) then lead-dot electron tunneling may induce an \( S \to T \) crossover\textsuperscript{6,7} the energy \( E_T \) of the triplet state becomes lower than the energy \( E_S \) of the singlet state, and the Kondo-regime may show up. In case of odd occupation \( N = 1 \), the Kondo-Fano regime is relevant, where the Kondo effect induced by an electron localized in the small side dot affects the electron tunneling through the weakly correlated big dot. If the leads are connected via the small dot, the big dot plays the role of additional reservoir for Kondo screening in case of odd \( N \) and the two-channel Kondo effect may be realized under certain conditions\textsuperscript{8,9}.

The more complicated model of asymmetric triple quantum dot (TQD) with a small dot sandwiched between two big dots was considered in Ref\textsuperscript{10} for odd and even occupations \( N = 3, 4 \). It was shown that the Kondo regime is accessible in both cases. Moreover, the TQD with even occupation demonstrates \( SO(n) \) symmetry.

Recently, a mirror symmetric TQD (see figure\textsuperscript{11}) in an "open" regime (near the Coulomb blockade peak) were studied both experimentally\textsuperscript{12} and theoretically\textsuperscript{13}. In this case the big "mesoscopic" dot is connected with two small dots and with metallic reservoirs. As a result, an indirect RKKY exchange interaction between the spins in the couple of small dots occurs, and its sign may be controlled by changing the parameters of the large central dot by applying an external magnetic field.

Here we focus on a mirror symmetric TQD in the "closed" regime, that is, the valley between Coulomb blockade peaks where the total number of electrons in the
FIG. 1: Triple quantum dots in “cross” (a) and “fork” (b) geometry.

TQD is fixed. Our main results are: (i) in the cross geometry (Fig. 1a) with electron occupation $N = 3$, such a dot possesses an unusual property: the indirect exchange tunneling constant between the big dot and the leads is ferromagnetic; the tunneling is therefore absent although the TQD behaves as a local moment; (ii) in a “fork” configuration (Fig. 1b) with electron occupation $N = 1$, TQD exhibits two different tunneling regimes: depending on the gate voltages, the Kondo regime may be observed as a zero bias anomaly or as a finite bias anomaly in the tunnel conductance.

II. TRIPLE QUANTUM DOT IN A CROSS GEOMETRY

The TQD in the cross geometry (figure 1a) is composed of left $l$, center $c$, and right $r$ dots, with corresponding levels and charging energies $\epsilon_j, Q_j, j = l, c, r$. It is modeled by the Anderson Hamiltonian

$$H = H_d + H_{\text{lead}} + H_t,$$

containing the terms describing the dot, two leads and the dot-lead tunneling, respectively. The first term is

$$H_d = \sum_{j=l,c,r} \sum_{\sigma} \epsilon_j d_j^{\dagger} d_j + \sum_j Q_j n_j^c n_j^r$$

$$+ W \sum_{j=l,r} \sum_{\sigma} (d_j^{\dagger} d_j^c + H.c.).$$

The parameters $Q_j$ are chosen in such a way that for electron occupation $N = 3$, and in the absence of inter-dot tunneling ($W = 0$), each dot is occupied by one electron. In the mirror-symmetric case such configuration is realizable provided

$$\epsilon_l = \epsilon_r \equiv \epsilon_s, \quad \Delta = \epsilon_c - \epsilon_s > 0,$$

$$Q_l = Q_r \equiv Q_s \gg Q_c.$$

At finite $W$ charge transfer from the central dot to the side dots is possible, but the double occupation of the side valleys is still suppressed by strong Coulomb blockade $Q_s \gg W$. In the charge sector $N = 3$ and for the mirror symmetric configuration the lowest energy states are two spin doublets, (even and odd relative to the $l \leftrightarrow r$ permutation), a spin quartet state, and a doubly degenerate charge transfer exciton (with two electrons in the central dot). The corresponding energies are

$$E_{D_+} = 2\epsilon_s + \epsilon_c - 3W^2/\Delta,$$

$$E_{D_-} = 2\epsilon_s + \epsilon_c - W^2/\Delta,$$

$$E_Q = 2\epsilon_s + \epsilon_c,$$

$$E_{E_x} = \epsilon_s + 2\epsilon_c + 2W^2/\Delta.$$  

Here the inequality $W/\Delta \ll 1$ is assumed to be valid. The eigenfunctions of the doublet and quartet states (which predetermine the structure of the effective exchange Hamiltonian, see below) are:

$$|D_+\sigma\rangle = \left[ \cos \theta_u \langle b_{lc}^{\dagger} b_{rs}^{\dagger} b_{cr} b_{ls} \rangle - \sin \theta_u \langle b_{lc}^{\dagger} b_{cr} b_{ls} \rangle \right] |0\rangle,$$

$$|D_-\sigma\rangle = \left[ \cos \theta_u \langle b_{lc}^{\dagger} b_{rs}^{\dagger} b_{cr} b_{ls} \rangle - \sin \theta_u \langle b_{lc}^{\dagger} b_{cr} b_{ls} \rangle \right] |0\rangle,$$

$$|Q, +\frac{3}{2}\rangle = d_{l\uparrow}^{\dagger} d_{r\uparrow}^{\dagger} d_{l\downarrow}^{\dagger} |0\rangle, \quad |Q, -\frac{3}{2}\rangle = d_{l\uparrow}^{\dagger} d_{r\uparrow}^{\dagger} d_{l\uparrow}^{\dagger} |0\rangle,$$

$$|Q, -\frac{3}{2}\rangle = \frac{1}{\sqrt{3}} \sum_{\langle ij \rangle} d_{l\uparrow}^{\dagger} d_{r\uparrow}^{\dagger} d_{k\uparrow}^{\dagger} |0\rangle.$$

Here $b_{ij}^{\dagger} = [d_{i\uparrow}^{\dagger} d_{j\uparrow}^{\dagger} - d_{i\downarrow}^{\dagger} d_{j\uparrow}^{\dagger}(1-\delta_{ij})]/\sqrt{2}$, and rotation angles $\theta_u = \arcsin(\sqrt{3W/\Delta})$, $\theta_q = \arcsin(W/\Delta)$.

The two other terms in Eq. (1) are the band Hamiltonian describing the electrons in the leads

$$H_{\text{lead}} = \sum_{\alpha=s,d} \sum_{\kappa \sigma} E_{\alpha k} c_{\alpha k\sigma}^{\dagger} c_{\alpha k\sigma},$$

and the tunneling Hamiltonian

$$H_t = \sum_{\alpha k \sigma} (V_{\alpha c} c_{\alpha k\sigma}^{\dagger} d_{c\sigma} + H.c.).$$

Following the standard procedure, one derives an indirect exchange interaction between lead and dot electrons, by means of the Schrieffer-Wolff (SW) transformation. For a composite quantum dot, this is accomplished in terms of spin eigenstates of $H_d$ defined in Eqs. (1, 4).

Thus in the SW regime the main contribution to the lead-dot tunneling is given by the components $\sim \cos \theta_{g,a}$. The quartet state has the usual structure prescribed by a standard Young tableau for three electrons, $((ijk))$ indicates the cyclic permutation of three sites $lcr$.

After performing the SW-like canonical transformation, one gets the effective exchange Hamiltonian

$$H_{xx} = J_u S_u \cdot s,$$
where $S_u$ is the spin 1/2 vector operator with components $S_u^+ = |u\uparrow\rangle\langle u\downarrow|$, $S_u^z = (|u\uparrow\rangle\langle u\uparrow| - |u\downarrow\rangle\langle u\downarrow|)/2$, and $s$ is the spin operator of lead electrons defined as $s = \sum_k c_{ek}^\dagger \hat{c}_{ek}\sigma$; $\hat{c}_{ek}$ is the set of Pauli matrices, $c_{ek}$ is the even combination of lead electron annihilation operators (the odd one is excluded from the tunneling Hamiltonian by standard rotation). Remarkably, the exchange constant $J_u$ has ferromagnetic sign,

$$J_u = -\frac{2\cos^2\theta u V^2}{3} \left( \frac{1}{|\epsilon_c|} + \frac{1}{|\epsilon_c + Q_c|} \right)$$

$(|\epsilon_c|$ is the position of the central dot level relative to the Fermi energy of the leads, source and drain contacts are assumed to be equivalent, $V_s = V_d = V$). The reason for an unconventional sign of the exchange interaction is that only one of three electrons in the TQD is involved in exchange interaction with the leads, and the overlap of the two other electrons wave function entering the state $|D_u\sigma\rangle$ gives the factor $-1$. Thus in this geometry we encounter a unique situation, where the Kondo screening is ineffective for a quantum dot with odd occupation.

Yet, a crossover from ferromagnetic to antiferromagnetic scenario is feasible. Indeed, the level spacing in the spin multiplet is governed by the parameter $W/\Delta$. If this spacing is small enough, the renormalization of these levels due to lead-dot co-tunneling becomes relevant in the RG flow equations along with the exchange screening in the framework of Haldane renormalization procedure. Accordingly, the energy levels are renormalized as a result of integrating out the band edges and shrinking the band width from its bare value $D_0$ to a smaller value $D$ comparable with $|\epsilon_c|$. The corresponding RG invariant is,

$$E^*_\Lambda = E_\Lambda(D) - \pi^{-3} \Gamma_\Lambda \ln(\pi D/\Gamma_\Lambda)$$

with tunneling rates $\Gamma_D(u) \approx \pi\rho_0 \cos^2\theta_{(u)G} V^2$ and $\Gamma_Q \approx \pi\rho_0 V^2$. Due to the hierarchy $\Gamma_Q > \Gamma_{Dg} > \Gamma_{Du}$, a level crossing is feasible (see Fig. 2). Physically, it implies a crossover from the non-Kondo (ferromagnetic exchange) regime to the under-screened Kondo regime with a pronounced maximum of the conductance around the degeneracy point. The parameters $W$ and $\Delta$, which determine the initial conditions, can be controlled by gate voltages. Varying these initial conditions, one may tune the region of crossover to the SW regime at the point

$$D \approx E_\Lambda(D).$$

For $D < \bar{D}$ the properties of the system are determined by the SW Hamiltonian. The effective Hamiltonian may be written for $D = D_u$ (marked on the horizontal axis of Fig. 2). If the condition is fulfilled in the vicinity of the crossing point ($D = D_{cr}$), the exchange Hamiltonian (instead of $\mathcal{H}$) acquires the form

$$H_{SW} = J_u S_u \cdot s + J_g S_g \cdot s + J_Q S_Q \cdot s + J_R R \cdot s$$

expressed in terms of operators for localized spin 1/2, $S_u, S_g, S_Q$, and the vector $R$ which induces transitions between the quartet $|Q\rangle$ and the doublet $|D_u\rangle$. There are no transitions between $|Q\rangle$ and $|D_g\rangle$ since these states have different $l - r$ parity.

At the point $D_{cr}$ the degeneracy of spin state of the TQD is maximal, corresponding to the symmetry $SU(2) \times SU(2) \times SU(2)$. Both to the right and to the left of this point some of the states in the spin multiplets are quenched at $T \to T_K$ and $T_K$ depends on the energy gaps $\Delta_{Qg} = E_Q(D) - E_{Dg}(D)$ and $\Delta_{Du} = E_{Dg}(D) - E_{Du}(D)$. To find the function $T_K(\Delta_{Qg}, \Delta_{Du})$, one should solve the scaling equations for the coupling constants in the Hamiltonian $H_{SW}$,

$$\frac{d j_a}{d \ln d} = -[j_a^2 + 2j_R j_b^2], \quad \frac{d j_q}{d \ln d} = -j_q^2, \quad \frac{d j_r}{d \ln d} = -\frac{j_R}{4} (5j_Q - j_a)$$

where $j_a = \rho_0 I_a \ (a = q, u, q, R)$, and $\rho_0$ is the density of states which is assumed to be constant. The procedure is self-consistent because $T_K$ itself determines the characteristic energy interval for states in the spin Hamiltonian involved in its formation. Varying $\bar{D}$ in Fig. 2, from the ferromagnetic non-Kondo regime ($\bar{D} \sim D_u$) to the crossing point $D_{cr}$, one reaches the point $T_K > 0$ which arises due to influence of the excited states $E_Q(D)$ and $E_{Dg}(D)$. Just then, $T_K$ sharply increases, reaching its maximum value in the point of maximum degeneracy $D_{cr}$. Moving further to the left, the level $E_{Du}$ freezes out. This means that the vector $R$ in the Hamiltonian does not contribute anymore to Kondo co-tunneling, and the Kondo effect is determined by the pair of states $E_Q$ and $E_{Dg}$, with the dynamical symmetry of TQD being $SU(2) \times SU(2)$. Further decrease of $\bar{D}$ eventually results in the quenching of $E_{Dg}$. The system then exhibits an under-screened Kondo regime of a localized spin 3/2 moment. Fig. 2 illustrates these crossover effects on $T_K$. 

![Haldane flow diagram](image-url)
The evolution of $T_K$ is reflected in the behavior of tunnel transparency and conductance as a function of energy. Far enough to the left and to the right of the crossing point, this behavior is stepwise. When the dot is in the doublet ground state ($\bar{D} \sim D_u$), the spin multiplet as a whole contributes to the transparency at high energies $\omega \sim \Delta_{Q\bar{g}} + \Delta_{gu}$. With decreasing $\omega$ the quartet $E_Q$ and the even doublet $E_{Dg}$ energies freeze out in this order (they are not renormalized anymore). Eventually, Kondo tunneling is quenched at low energies, so that the zero bias anomaly (ZBA) has a shape of a dip. On the other hand, in the crossover regime, the ZBA follows the conventional Kondo peak. Finally, the structure of the peak at the regime $\bar{D} \sim D_Q$ is even more complicated. Within the framework of our approach we may describe the evolution of transparency for $T > T_K$ where it is approximately described by the simple relation $\mathcal{T}(\omega) \sim \ln^{-2}(T/T_K(\omega))$. The resulting curve is shown in Fig. 3.

![FIG. 3: Evolution of Kondo temperature as determined by scaling equations.](image)

This type of non-universal behavior of $T_K$ is known in the theory of strongly correlated quantum dots with even occupation, where the singlet-triplet level crossing usually occurs. The novelty of the present scenario is that it is manifested in quantum dot with odd occupation where the absence of Kondo effect occurs due to ferromagnetic exchange coupling with the localized spin doublet. The non-universality of $T_K$ occurs as this ferromagnetic exchange competes with two anti-ferromagnetic exchange interactions (with doublet and quartet localized moments), so that, in some sense, one deals with a “three-stage” Kondo effect. Thus, we have completed our discussion pertaining to the cross-shaped TQD of figure 1B.

### III. TRIPLE QUANTUM DOT IN A FORK GEOMETRY

It is then natural to expect peculiar features of Kondo tunneling also in a mirror symmetric TQD in the fork geometry (Fig. 1B) with $Q_{l,r} \gg Q_c$. The dots and leads are labeled $1,2,3$ and each dot is attached to its own lead. In case of $N = 3$, the exchange coupling $J_3$ between the central dot and its adjacent lead is ferromagnetic in accordance with Eq. (9), whereas those for the two other (small) dots $(J_1, J_2)$ are antiferromagnetic. Besides, there are also non-diagonal exchange couplings $J_{ij} = J_{ji}$. All these are coupled within a system of RG flow equations. A question now arises, whether it is possible to find a regime where the Kondo resonance arises only in dots $1,2$, whereas dot $3$ remains Kondo inactive?

To answer this question, we calculate $T_K$ and $G$ within the same scheme as in the preceding section for a system described by the Hamiltonian (11) with the tunneling term

$$H_t = \sum_{j=1}^{3} \sum_{k\sigma} (V_j c_{j,k\sigma}^\dagger d_{j\sigma} + H.c.)$$

instead of (11). The effective exchange Hamiltonian of this system is obtained in the same way as (12). The mirror $l \rightarrow r$ symmetry entails $V_1 = V_2 \neq V_3$. The ground-state consists of the odd-parity doublet $E_{Dg}$, the corresponding SW Hamiltonian has the form

$$H_{SW} = \sum_{i=1}^{3} J_i S \cdot s_i + J_{12} S \cdot (s_{12} + s_{21}) + J_{13} S \cdot (s_{13} + s_{31}) + J_{23} S \cdot (s_{23} + s_{32}).$$

Here the exchange constant $J_3 < 0$ is the same as $J_u$ (9), whereas $J_{1,2} > 0$. For $\cos \theta_u \approx 1$, these constants are,

$$J_1 = J_2 = 4 \frac{V_2^2}{3 |\epsilon_c|},$$

$$J_3 = -\frac{2}{3} \frac{V_2^2}{|\epsilon_c| + \frac{V_4^2}{|\epsilon_c| + Q_c}},$$

$$J_{12} = 3 \frac{(V_1 W)^2}{2 (\epsilon_c + Q_c - \epsilon_s)^2 |\epsilon_c|},$$

$$J_{13} = J_{23} = -\frac{1}{4} \frac{W V_1 V_3}{\epsilon_c + Q_c - \epsilon_s \left( \frac{1}{|\epsilon_c|} + \frac{1}{|\epsilon_c|} \right)}.$$

The system of RG flow equations for the Hamiltonian
The Kondo temperature is

\[ T_K = D \exp\left(-\frac{2}{j_+ + \sqrt{j_+^2 + 6j_1^2}}\right), \] (18)

where \( j_+ = j_1 + j_2 + j_3, j_- = j_1 + j_2 - j_3, \) so that the Kondo resonance arises in all non-diagonal channels and the TQD looses its ”exotic” properties. The Kondo transparency \( T_q(\omega) \) may be calculated for any pair of electrodes \((ij)\). It is a step-wise function in accordance with multistage Kondo screening process, but no anomalous ”freezing out” of Kondo effect similar to that shown in the left panel of Fig. 4 is expected in this case.

It is appealing, however, to exploit other specific properties of the TQD in the fork configuration. The remarkable feature of the mirror asymmetric TQD is that it can be viewed as a quantum pendulum\[15,16\]. This means that the superposition of two degenerate states \((13)\) and \((23)\) might even lead to level crossing provided the tunneling rate \( \Gamma_b \) is higher than the rate \( \Gamma_n = \rho_1 V^2 \) for the non-bonding state \(|Dn\rangle\) for \( N = 1 \).

So let us assume that the parameters (gate voltages) are tuned so that the TQD is found in a Coulomb blockade valley corresponding to the occupation sector \( N = 1 \). Within the same approximation as \[14\] the lowest eigenstates \(|\Lambda\rangle\) of the Hamiltonian \( H_d \) \[2\] for \( N = 1 \) are the set of spin doublets,

\[ |D\sigma\rangle = \left[ \sin \theta \, d_{3\sigma}^1 + \cos \theta \, \frac{d_{1\sigma}^1 + d_{2\sigma}^2}{\sqrt{2}} \right]|0\rangle, \]
\[ |Dn\sigma\rangle = \left[ \frac{d_{1\sigma}^1 - d_{2\sigma}^2}{\sqrt{2}} \right]|0\rangle, \]
\[ |Dn\sigma\rangle = \left[ -\cos \theta \, d_{3\sigma}^1 + \sin \theta \, \frac{d_{1\sigma}^1 + d_{2\sigma}^2}{\sqrt{2}} \right]|0\rangle \],

with \( \sin \theta = \sqrt{2W/\Delta} \ll 1 \). The corresponding eigenfunctions are

\[ E_{Db} = \epsilon_s - 2W^2/\Delta, \]
\[ E_{Dn} = \epsilon_s, \]
\[ E_{Da} = \epsilon_e + 2W^2/\Delta. \]

Hence, the ground state is a bonding spin doublet \( E_{Db} \), and the eigenstates \(|\Lambda\rangle\) may be interpreted as two even and one odd RVB modes of a ”spin pendulum”.

In the low-energy subspace \( \omega \ll W^2/\Delta \) the effective spin Hamiltonian which describes the Kondo cotunneling has the same form as \[15\] derived above for \( N = 3 \). Here, however, all coupling constants are positive,

\[ J_1 = J_2 = J_{12} = \frac{V_1^2 \cos^2 \theta}{2|\epsilon_s|}, \]
\[ J_3 = \frac{V_3^2 \sin^2 \theta}{|\epsilon_e|}, \]
\[ J_{13} = J_{23} = \frac{V_1 V_3 \sin \theta \cos \theta}{2\sqrt{2}} \left( \frac{1}{|\epsilon_s|} + \frac{1}{|\epsilon_e|} \right), \]

and the Kondo temperature is given by Eq. \[18\].

One may say that in a coherent Kondo-tunneling regime the system demonstrates perfect entanglement: an electron entering dot 3 from lead 3, splits into two components in accordance with the structure of the state \(|Dn\sigma\rangle\) and this entangled state predicts the total current \( I_1 + I_2 \) through the TQD in the fork geometry. Of course, this statement is valid only at zero temperature, and one may expect that thermal fluctuations are detrimental for a coherent transport, but this effect is suppressed as \((T/T_K)^2\) at \( T \).

The situation becomes even richer, due to the occurrence of soft mode excitations \[20\]: the odd state \(|Dn\sigma\rangle\) may be intermixed with the even state \(|D\sigma\rangle\) due to cotunneling process. This intermixing becomes relevant provided \( T_K \lesssim E_{Dn} - E_{Da} \). This inequality is, of course, invalid for the bare eigenstates \[20\], but the Haldane renormalization of the spectrum similar to that described by Eq. \[10\] may result in softening of this mode. It might even lead to level crossing provided the tunneling rate \( \Gamma_n = \rho_1 V^2 \) for the bonding state \(|D\sigma\rangle\) is higher than the rate \( \Gamma_b = \rho_1 V_1^2 \cos^2 \theta + \rho_2 V_2^2 \sin^2 \theta \) for the bonding state \(|D\sigma\rangle\). If the densities of states are the same in all leads, \( \rho_1 = \rho_2 \), then the condition \( \Gamma_n > \Gamma_b \) means \( V_1 > V_3 \). The RG flow trajectories for this case are presented in Fig. 5. Like in the cross geometry, the TQD acquires an additional degeneracy in the critical region \( d \sim d_{cr} \). However, in this case the sources of degeneracy are the RVB degrees of freedom. As a result,
one encounters the problem of Kondo effect due to an interplay between spin $S$ and pseudospin $\mathbf{T}$, where the latter describes the pendulum degrees of freedom. This problem was discussed in the context of double quantum dots, triple quantum dots, and molecular trimers chemisorbed on metallic surfaces. In this case the actual symmetry of the TQD is $SU(4)$. To show this, we derive below the effective spin Hamiltonian following the method offered in Ref. 14.

It is useful to generalize the notion of localized spin operator $S^i = |\sigma\rangle\langle \sigma'|$ (employing Pauli matrices $\sigma_i$ ($i = x, y, z$) to $S^i_{\Lambda\Lambda'} = |\sigma\rangle\langle \sigma'|\sigma\rangle\langle \sigma'|$, in terms of the eigenvectors $|Db\sigma\rangle, |Dn\sigma\rangle$ from (19)). Similar generalization applies for the spin operators of the lead electrons: $s^i_{\lambda\lambda'} = \sum k|c_{\lambda,k\sigma}^\dagger \tau_i c_{\lambda',k\sigma'}\rangle$. Here the index $\lambda$ denotes conduction electrons in lead 3 ($\lambda = 3$), and in leads 1,2 with $\lambda = e, o$ corresponding to even and odd combinations of conduction electron states in these leads,

$$c_{e,o}^\dagger_{k\sigma} = \frac{1}{\sqrt{2}}(c_{1,k\sigma}^\dagger \pm c_{2,k\sigma}^\dagger). \quad (22)$$

The pseudospin operators $\mathbf{T}$ describing the RVB mode are introduced as follows:

$$\mathbf{T}^+ = \sum_{\sigma} |Db\sigma\rangle\langle Dn\sigma|, \quad \mathbf{T}^- = [\mathbf{T}^+]^\dagger, \quad (23)$$

$$\mathbf{T}^z = \frac{1}{2} \sum_{\sigma} (|Db\sigma\rangle - |Dn\sigma\rangle)\langle Db\sigma| - |Dn\sigma\rangle\langle Dn\sigma|).$$

The five vector operators $\mathbf{S}_{\Lambda\Lambda'}$ and $\mathbf{T}$ constitute the 15 generators of the $SU(4)$ group.

Similarly, one may construct the pseudospin operators for the electrons in the leads (1,2):

$$\tau^+ = \sum_{k\sigma} c_{ek\sigma}^\dagger c_{ok\sigma}, \quad \tau^- = [\tau^+]^\dagger, \quad (24)$$

$$\tau_z = \frac{1}{2} \sum_{k\sigma} (c_{ek\sigma}^\dagger c_{ok\sigma} - c_{ok\sigma}^\dagger c_{ek\sigma}).$$

The exchange Hamiltonian for TQD with spin and RVB degrees of freedom is

$$H_{SW} = \sum_{\kappa,\lambda,\mu,\rho} J_{\kappa,\lambda,\mu,\rho} \mathbf{S}_{\kappa,\lambda} \cdot \mathbf{s}_{\mu,\rho} + J_p \mathbf{T} \cdot \tau \quad \text{(25)}$$

with $\kappa, \lambda = b, n$; $\mu, \rho = e, o$, and the coupling constants $J_{\kappa,\lambda,\mu,\rho} = J_{\kappa,\lambda,\mu,\rho} = J_{\kappa,\lambda,\mu,\rho}$ are positive like in (21). The system of scaling equations has the form:

$$\frac{dj_b}{d\ln d} = - \left[ j_b^2 + \frac{2}{j_b} + j_b j_p + j_{13} \right],$$

$$\frac{dj_n}{d\ln d} = - \left[ j_n^2 + \frac{2}{j_n} + j_n j_p \right],$$

$$\frac{dj_{13}}{d\ln d} = - \left( j_{13}^2 + j_{13} \right),$$

$$\frac{dj_{bn}}{d\ln d} = - \left( j_{bn} + j_p \right),$$

$$\frac{dj_p}{d\ln d} = - j_p^2, \quad \text{(27)}$$

where $j_b = j_{bbee}$, $j_n = j_{nnoo}$, $j_{13} = j_{bb33}$, $j_{13} = j_{b33e}$ and $j_{bn} = j_{bnoe}$. From these equations we derive the Kondo temperature

$$T_K = D \exp \left\{ - \frac{2}{j_+ + \sqrt{6j_{13} + (j_{bn} + j_p)^2 + j^2_p}} \right\}, \quad \text{(28)}$$

with $j_+ = j_b + j_n + j_{13}$, $j_+ = j_b - j_n - j_{13}$. Like in the cross geometry, one may manipulate $D$ by changing the gate voltages and scan the dependence $T_K(D)$ similarly to Fig. 14. This curve has a maximum in the critical point $D_{cr}$, and the orbital degrees of freedom are frozen out in the asymptotic regimes $D \gg D_{cr}$ and $D \ll D_{cr}$. We deal in this case with a symmetry crossover $SU(2) \rightarrow SU(4) \rightarrow SU(2)$. However, there is an important difference between the two asymptotic $SU(2)$ symmetries.

![FIG. 6: Evolution of Kondo temperature, $T_K^*$ as determined by Eq. (25).](image)

In the limit $D \gg D_{cr}$ the ground state is $E_{db}$, all three dots are partially occupied in accordance with the structure of the corresponding wave function $|Db\sigma\rangle$ (19). The terms $J_{bbee}$, $J_{bb33}$, $J_{b33e}$ survive in the SW Hamiltonian (25), and Eq. (28) for $T_K$ reduces to Eq. (18). In the limit $D \ll D_{cr}$, the ground state of the TQD is the non-bonding state $E_{Dn}$ with an empty site 3 in accordance with the form of the wave function $|Dn\sigma\rangle$ (19). The SW Hamiltonian (25) contains in this case only the term $\sim J_{nnoo}$ and $T_K = D \exp(-1/j_n)$. The Kondo temperature as a
function of $\bar{D}$ has a maximum in a crossing point $\tilde{D}_{cr}$, but unlike the case of cross geometry (Fig. 3), $T_K(\bar{D})$ is nonzero on both sides of this maximum (Fig. 4).

The change of the ground state wave function from the bonding combination $|D_{bs\alpha}\rangle$ to the non-bonding one $|D_{\sigma}\rangle$, influences the behavior of tunnel conductance. Let us compare the tunnel current between the leads ‘2’ and ‘1’ and between the leads ‘3’ and ‘1’, which is defined by the components $G_{32}$ and $G_{33}$ of the three-terminal conductance matrix $G_{ij} = \partial I_i / \partial V_j$.

When calculating these components as a function of $D$, one immediately sees that the Kondo-type ZBA in $G_{32}$ exists in all three regimes, and the peak of this conductance follows the behavior of $T_K(\bar{D})$. The behavior of $G_{33}$ is more peculiar. The ZBA in this channel exists only until the even components $|D_{bs\sigma}\rangle$ are involved in Kondo tunneling. In the limit $T_K \lesssim E_{Db} - E_{Dn}$ at $\delta \ll \delta_{cr}$ this anomaly disappears, so we encounter a unique situation where the Kondo resonance is absent in conductance in spite of the presence of Kondo screening.

However, the resonance Kondo regime in $G_{33}$ arises as a finite bias anomaly (FBA). To describe this tunneling one has to retain the terms $\sim J_{bs\alpha}$ and $J_p$ in the Hamiltonian (24). These terms describe inelastic tunneling, which acquires a form of Kondo resonance at finite bias in accordance with the mechanism offered in Ref. [21]. In that case the tunneling through the double quantum dot with even occupation in a singlet ground state was considered, and the Kondo regime becomes relevant at finite bias, when the difference in the chemical potentials of source and drain leads compensates the exchange gap between the ground state singlet and excited spin triplet state. In our case the FBA arises at odd occupation when the bias compensates the energy gap $\delta = E_{Db} - E_{Dn}$.

In order to calculate the tunnel conductance in the weak coupling regime, we use the modified Golden Rule formula (22), which reads for the channel ‘3–1’ as $G_{33}(\epsilon V_3, T) / G_0 \sim |\tilde{J}_{13}(\epsilon V_3, T)|^2$, where $G_0 = e^2 / \pi \hbar$, and $\tilde{J}_{13}$ is the solution of the RG flow equations (24) for $D = \max\{\epsilon V_3, T\}$. In case of Kondo-type resonance at finite bias $\epsilon V_3$, the equation for conductance in the vicinity of FBA reads (21)

$$G / G_0 \sim \ln^{-2}(\max\{\epsilon V_3 - \delta, T\}/T_K).$$

Similar equation (with $V_2 \to 0$) describes the ZBA in tunnel conductance in the channel ‘2–1’.

The results of calculation of $G_{22}$ and $G_{33}$ are presented in Fig. 4. One may see from this figure how the ZBA in $G_{22}$ goes through the maximum at the crossing point $D_{cr}$ whereas the ZBA in $G_{33}$ transforms into FBA for small enough $\bar{D}$ when $\delta$ exceeds $T_K$.

Discussion of damping effects, which, to a certain degree, tend to smear the FBA (21,22) is beyond the scope of this work. It should be mentioned, however, that it was shown in Ref. [21] that there exists a wide enough window of parameters, where this damping is not fatal for existence of well shaped FBA. It is worth noting also that the tunnel conductance between the leads ‘1’ and ‘2’ exists in spite of the absence of direct tunneling channel. The tunneling mechanism is connected in this case with the “pendulum” structure of the electron wave function (14) in TQD. In case of ground state $E_{Dn}$ this is the bonding combination $(d_{1\sigma}^1 + d_{2\sigma}^1)|0\rangle$, in case of ground state $E_{Dn}$ this is the resonating valence bond $(d_{1\sigma}^1 \pm d_{2\sigma}^1)|0\rangle$. In the latter case the dot ‘3’ is excluded from cotunneling. It is therefore involved only in the determination of the Kondo temperature.

**IV. CONCLUDING REMARKS**

We have shown in this paper that triple quantum dots in some special geometries demonstrate unusual behavior in the Kondo tunneling regime. This behavior stems from inequivalence of constituents (side valleys and central valley). Asymmetric double quantum dot considered in Ref. [1] was the first example of complex quantum dot with inner and outer "shell". Trimers with inequivalent side and central valleys studied in Refs. [5,10] and in the present paper are more complicated examples of artificial molecules with shell structure. In this case the two side dots form an "inner shell" whereas the big central dot plays the role of an "outer shell". If the outer shell is open, it contributes to the indirect exchange between the electrons in the inner shell.

We considered here the case of closed outer shell and found that such trimer with odd electron occupation $N = 1, 3$ possesses properties, which were observed earlier in dots with even occupation $N = 2$. In particular, the Kondo tunneling may be absent in the ground spin doublet state of TQD due to special symmetry properties of the wave function (odd $l - r$ symmetry in case of $N = 3$ and empty outer shell in case of $N = 1$). Involvement of the low-lying Kondo-active spin doublet results in a two-stage Kondo screening reminiscent of that found in quantum dot with occupation $N = 2$ where the spin excitation spectrum is formed by the singlet-triplet pair (21). Other interesting possibilities now open due to
the resonance valence bond structure of the electron wave function \(^{(19)}\) in case of partially occupied inner shell in a fork geometry with \(N = 1\). In particular the "pendulum effect"\(^{(15,16)}\) perceived in TQD with even occupation \(N = 2, 4\) may be exploited in this type of TQD as well.

The transformation of ZBA into FBA under changing gate voltage is a special manifestation of general phenomenon, known as "critical phase transition", where the symmetry of the ground state changes as a function of a control parameter. Similar effect should be observed in planar and double quantum dots\(^{(21)}\) with even occupation where the singlet-triplet crossover may occur with changing gate voltage or in transition metal molecular complexes\(^{(24)}\). In the latter case local phonons are essentially involved in this transition\(^{(25)}\).

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