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Josephson current through double quantum dots

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Abstract

We investigate how the competition between Kondo and antiferromagnetic (AF) correlations influences the Josephson current through double quantum dots (DQDs) and focus our attention on the situation where the superconducting energy gap is smaller than the Kondo temperature. The finite- U slave-boson mean-field method is adopted to treat electronic correlations. With weak AF correlation, two Kondo singlets yield two Andreev bound states below the Fermi level, and the low tunnelling probability through these singlet states leads to small critical Josephson current J_c . Strong AF correlation results in a singlet between the two localized spins, and only in a certain range can one bound state be found. At an intermediate point, the competition between the Kondo and AF correlations leads to a peak in the critical Josephson current, where just one bound state is formed in the gap. The strong parity splitting causes the double occupancy on the bonding orbital of two dots, and no Andreev bound state is found with J_c approaching zero.

1. Introduction

Because of their tunability, quantum dot (QD) systems have attracted a lot of attention. When a dot is connected to normal metallic leads, the coupling between the localized spin on the dot and conduction electrons leads to the Kondo correlation, which is described by an energy scale T_K , the so-called Kondo temperature. When a QD is in the Kondo regime [1–5], the localized spin and conduction electrons forms a spin singlet state, which yields the Abrikosov–Suhl resonance and profoundly affects the electronic transport. If double quantum dots (DQDs) [6–10] are coupled with each other by tunnelling matrix element t_d , the Coulomb interaction U in dots yields an effective antiferromagnetic (AF) coupling $J_M = \sqrt{(2t_d)^2 + (U/2)^2} - U/2$ (or $\sim 4t_d^2/U$ if $t_d \ll U$). This coupling tends to create a singlet state between the localized spins on the two dots. When the two dots are connected to normal leads in a ‘lead–dot–dot–lead’ series, two Kondo spin singlets are formed with $T_K > J_M$, whereas with $J_M > T_K$ one singlet state is created between the two localized spins. This competition between the Kondo and AF correlations results in a resonant conductance peak at $J_M \sim T_K$ in the half-filled case [8–10]. In the limit $J_M \ll T_K$ and $t_d \gg U/4$, the conductance G approaches zero.

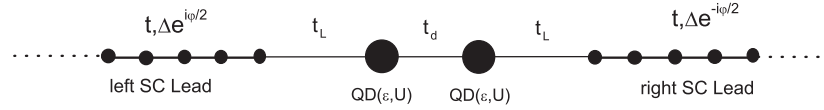


Figure 1. Schematic illustration of the structure.

When a barrier is sandwiched between two identical superconductors (SCs), a Josephson current J is caused by the phase difference φ between the two SCs. When the tunnelling through the barrier is weak and conserves spin, the Josephson current can be expressed as $J = J_c \sin(\varphi)$, where J_c is proportional to the normal conductance through the barrier. But if the barrier is ferromagnetic, negative Josephson coupling is found [11]. Embedding a QD in between two SCs results in competition between the Kondo effect and superconductivity at low temperature [12, 13]. With T_K smaller than the superconducting gap Δ , the Kondo spin singlet is broken, which leads to negative J_c or a π -junction. With $T_K > \Delta$, the Kondo spin singlet is kept. The ordinary 0-junction is obtained and the critical Josephson current J_c is greatly enhanced by the Abrikosov–Suhl resonance [14–21]. Now, it is natural to ask how the competition between Kondo and AF correlations influences the Josephson current if DQDs are embedded in between two SCs.

In the present paper, our focus is put on the situation where Δ is smaller than T_K and the superconductivity is irrelevant with the basic characteristics of the ground state and consequently does not qualitatively change the competitive behaviour between the Kondo and AF correlations. Our purpose is to answer the following questions: (i) how does the competition affect the Andreev bound states, and consequently the Josephson current through the structure, and (ii) is there a fingerprint of the competition in Josephson current, like the resonant peak at $J_M \sim T_K$ in the normal conductance? For this reason, we assume a structure illustrated schematically in figure 1, describe the superconductivity in the BCS scheme and adopt the finite- U slave-boson mean-field theory (f - U SBMFT) of Kotliar and Ruckenstein (KR) [22, 23] to treat the electronic correlations. As we know from the previous studies, the f - U SBMFT of KR can give qualitatively correct results if the localized spins on dots are not ferromagnetic in nature [17–19] and can grasp the basic physics of DQD structures [10, 24]. When $J_M \ll T_K$, the two localized spins on dots and conduction electrons form two Kondo spin singlets, and two Andreev bound states are found below the Fermi level. The low tunnelling probability through the two Kondo singlets results in small J_c . With t_d increased, the bound states gradually move out of the gap. At a specific $J_M \sim T_K$, just one bound state remains in the gap, and a peak appears in the J_c - t_d curve, which characterizes the competition between the Kondo and AF correlations. With $J_M > T_K$, the two localized spins constitute a spin singlet because of the AF correlation, and in a certain range only, an Andreev bound state can be found. When $t_d \gg U/4$, the strong parity splitting leads to the double occupancy on the bonding orbital of two dots, and no Andreev bound state is found with J_c approaching zero.

The organization of this paper is as follows. In section 2, the theoretical model and calculation method are illustrated. In section 3, the numerical results and discussion on them are presented. A brief summary is given in section 4.

2. Model and formulae

In the present paper, we investigate how the competition between the Kondo and AF correlations affects the Josephson current through DQDs. The system is schematically illustrated in the figure 1, where two dots and two SC leads are arranged in a ‘lead–dot–dot–lead’ series. The

two dots are taken as Anderson impurities, each of which has one single-particle energy level ϵ and an on-site Coulomb interaction U . The tunnelling matrix elements of dot–dot and dot–lead are t_d and t_L , respectively. Here, the two SCs are assumed entirely identical except a phase difference φ , and without loss of generality it is assumed that $\varphi_L = -\varphi_R = \varphi/2$. Employing the BCS theory to deal with the SCs, we describe this mesoscopic system by the following 1D tight-binding Hamiltonian:

$$H = H_L + H_R + H_D + H_T, \quad (1)$$

where H_α , ($\alpha = L, R$) H_D and H_T are the Hamiltonians of leads, dot and the coupling between them, respectively. They are

$$H_L = \sum_{i=-\infty}^{-1} \left(-t \sum_{\sigma} c_{i-1\sigma}^{\dagger} c_{i\sigma} + \Delta e^{i\varphi/2} c_{i\uparrow}^{\dagger} c_{i\downarrow}^{\dagger} + \text{H.c.} \right), \quad (2)$$

$$H_R = \sum_{i=1}^{\infty} \left(-t \sum_{\sigma} c_{i\sigma}^{\dagger} c_{i+1\sigma} + \Delta e^{-i\varphi/2} c_{i\uparrow}^{\dagger} c_{i\downarrow}^{\dagger} + \text{H.c.} \right), \quad (3)$$

$$H_D = \sum_{\alpha=L,R} \left(\epsilon \sum_{\sigma} c_{\alpha\sigma}^{\dagger} c_{\alpha\sigma} + U n_{\alpha\uparrow} n_{\alpha\downarrow} \right) - t_d \sum_{\sigma} \left(c_{L\sigma}^{\dagger} c_{R\sigma} + \text{H.c.} \right) \quad (4)$$

and

$$H_T = -t_L \sum_{\sigma} \left(c_{-1\sigma}^{\dagger} c_{L\sigma} + c_{1\sigma}^{\dagger} c_{R\sigma} + \text{H.c.} \right). \quad (5)$$

Here $n_{\alpha\sigma} = c_{\alpha\sigma}^{\dagger} c_{\alpha\sigma}$, with $\sigma = \uparrow$ or \downarrow .

If one dot with energy level ϵ and Coulomb repulsion U is connected to normal leads with the hopping integral t_L , the Kondo temperature can be expressed as [25] $T_K = \frac{U\sqrt{J_K}}{2\pi} \exp(-\pi/J_K)$, where $J_K = \frac{-2U\Gamma}{\epsilon_d(\epsilon_d+U)}$. With the Fermi energy being set as zero, the hybridization strength $\Gamma = 2t_L^2/t$ and the correlation length of spin singlet $\xi_K = \hbar v_F/T_K = 2t/T_K$ at zero temperature [26]. With DQDs embedded in between two SC leads, different electronic correlations compete with each other. In the present paper, we are interested in the situation where Δ is smaller than T_K . If $J_M \ll T_K$, T_K is the largest energy scale and two Kondo spin singlets are formed, whereas if $J_M \gg T_K$, J_M is also much larger than Δ and a singlet is formed between the two localized spins. Here, the superconductivity is irrelevant to the basic characteristics of the ground state and does not change the qualitative behaviour of competition between the Kondo and AF correlations.

As we know from the previous studies [10, 17–19, 24], in this situation, the f - U SBMFT of KR [22, 23] can give qualitatively correct results. In the framework of this approach, eight auxiliary boson fields e_α , $p_{\alpha\sigma}$ and d_α are introduced to act as projection operators onto the empty, singly occupied and doubly occupied electronic states at the dot ‘ α ’, respectively. To eliminate the unphysical states, six constraints are imposed: $\sum_{\sigma} p_{\alpha\sigma}^{\dagger} p_{\alpha\sigma} + e_{\alpha}^{\dagger} e_{\alpha} + d_{\alpha}^{\dagger} d_{\alpha} = 1$ and $c_{\alpha\sigma}^{\dagger} c_{\alpha\sigma} = p_{\alpha\sigma}^{\dagger} p_{\alpha\sigma} + d_{\alpha}^{\dagger} d_{\alpha}$. To obtain the exact result in the noninteracting limit, the fermion operator $c_{\alpha\sigma}$ should be replaced by $c_{\alpha\sigma} z_{\alpha\sigma}$, with $z_{\alpha\sigma} = (1 - d_{\alpha}^{\dagger} d_{\alpha} - p_{\alpha\sigma}^{\dagger} p_{\alpha\sigma})^{-1/2} (e_{\alpha}^{\dagger} p_{\alpha\sigma} + p_{\alpha\bar{\sigma}}^{\dagger} d_{\alpha}) (1 - e_{\alpha}^{\dagger} e_{\alpha} - p_{\alpha\bar{\sigma}}^{\dagger} p_{\alpha\bar{\sigma}})^{-1/2}$. Therefore, the Hamiltonian (1) can be replaced by the following effective Hamiltonian:

$$H_{\text{eff}} = H_L + H_R + \tilde{H}_D + \tilde{H}_T + \sum_{\alpha=L,R} \left\{ \lambda_{\alpha}^{(1)} \left(\sum_{\sigma} p_{\alpha\sigma}^{\dagger} p_{\alpha\sigma} + e_{\alpha}^{\dagger} e_{\alpha} + d_{\alpha}^{\dagger} d_{\alpha} - 1 \right) + \sum_{\sigma} \lambda_{\alpha\sigma}^{(2)} \left(c_{\alpha\sigma}^{\dagger} c_{\alpha\sigma} - p_{\alpha\sigma}^{\dagger} p_{\alpha\sigma} - d_{\alpha}^{\dagger} d_{\alpha} \right) \right\}, \quad (6)$$

where the six constraints are incorporated by the six Lagrange multipliers $\lambda_\alpha^{(1)}$ and $\lambda_{\alpha\sigma}^{(2)}$. Here, the original H_D and H_T are replaced by

$$\tilde{H}_D = \sum_{\alpha=L,R} \left(\epsilon \sum_{\sigma} c_{\alpha\sigma}^\dagger c_{\alpha\sigma} + U d_\alpha^\dagger d_\alpha \right) - t_d \sum_{\sigma} (z_{L\sigma}^\dagger c_{L\sigma}^\dagger c_{R\sigma} z_{R\sigma} + \text{H.c.}) \quad (7)$$

and

$$\tilde{H}_T = -t_L \sum_{\sigma} (c_{-1\sigma}^\dagger c_{L\sigma} z_{L\sigma} + c_{1\sigma}^\dagger c_{R\sigma} z_{R\sigma} + \text{H.c.}). \quad (8)$$

To solve the effective Hamiltonian (6) at zero temperature, we first replace the slave boson fields by their expectation values, then obtain the values of e_α , $p_{\alpha\sigma}$, d_α , $\lambda_\alpha^{(1)}$ and $\lambda_{\alpha\sigma}^{(2)}$ by minimization of the ground state energy E_0 of the essentially noninteracting Hamiltonian with respect to these parameters [23]. This is equivalent to the approach using the functional integral method combined with the saddle-point approximation, and leads to a set of self-consistent equations [22, 23]:

$$\sum_{\sigma} p_{\alpha\sigma}^2 + e_\alpha^2 + d_\alpha^2 = 1, \quad (9)$$

$$\langle 0 | n_{\alpha\sigma} | 0 \rangle = p_{\alpha\sigma}^2 + d_\alpha^2, \quad (10)$$

$$-t_L \sum_{\sigma} \text{Re} \left(\langle 0 | c_{-1(1)\sigma}^\dagger c_{L(R)\sigma} | 0 \rangle \right) \frac{\partial z_{L(R)\sigma}}{\partial e_{L(R)}} + \lambda_{L(R)}^{(1)} e_{L(R)} = 0, \quad (11)$$

$$-t_L \sum_{\sigma'} \text{Re} \left(\langle 0 | c_{-1(1)\sigma'}^\dagger c_{L(R)\sigma'} | 0 \rangle \right) \frac{\partial z_{L(R)\sigma'}}{\partial p_{L(R)\sigma}} + \lambda_{L(R)}^{(1)} p_{L(R)\sigma} - \lambda_{L(R)\sigma}^{(2)} p_{L(R)\sigma} = 0, \quad (12)$$

and

$$\sum_{\sigma} \left\{ -t_L \text{Re} \left(\langle 0 | c_{-1(1)\sigma}^\dagger c_{L(R)\sigma} | 0 \rangle \right) \frac{\partial z_{L(R)\sigma}}{\partial d_{L(R)}} - \lambda_{L(R)\sigma}^{(2)} d_{L(R)} \right\} + \lambda_{L(R)}^{(1)} d_{L(R)} + U d_{L(R)} = 0. \quad (13)$$

To self-consistently solve these equations, we have to calculate the expectation values such as $\langle 0 | c_{j\sigma}^\dagger c_{i\sigma} | 0 \rangle$, with $|0\rangle$ the ground state corresponding to a certain set of variational parameters, then update the variational parameters from the above self-consistent equations, and repeat these two steps until numeric convergence is reached. If a quasiparticle wavefunction is expressed as $\alpha^\dagger |F\rangle = \sum_{i=-\infty, \dots, -1, L, R, 1, \dots, \infty} (u_i c_{i\uparrow}^\dagger - v_i c_{i\downarrow}) |F\rangle$ with $|F\rangle$ the Fermi sea, acting as a background, whose intrinsic structure is irrelevant to our calculation, the corresponding Schrödinger equation can be diagonalized to obtain a series of excited eigenstates $\{\alpha_n^\dagger |F\rangle\}$. $c_{i\uparrow}^\dagger$ and $c_{i\downarrow}$ can be expressed by the quasiparticle operators $\{\alpha_n^\dagger\}$ and $\{\tilde{\alpha}_n\}$. Here, $\tilde{\alpha}_n^\dagger |F\rangle = \sum_i (u_{i,n} c_{i\downarrow}^\dagger + v_{i,n} c_{i\uparrow}) |F\rangle$, the spin degenerate state with $\alpha_n^\dagger |F\rangle$. Because $|0\rangle$ is a state with no quasiparticle excited, the expectation value of $\langle 0 | c_{j\sigma}^\dagger c_{i\sigma} | 0 \rangle$ can be written as $\sum_n v_{j,n}^* v_{i,n}$. Generally, these expectation values can be analytically expressed in terms of variational parameters with the help of the Nambu representation and the Green-function technique [20, 27, 28], but the expressions are complex and tedious when double quantum dots are considered, and we prefer direct diagonalization. In practical calculation, the numeric diagonalization can only be performed in a finite cluster. (Here, the DQDs are located at the centre of the cluster.) If the cluster size is much larger than the longer of the two length scales of the system, ξ_K and the superconducting coherent length ξ_Δ , the results obtained from the cluster calculation are identical with those from the original system [29, 30]. As we can see below the practical capacity of the numeric calculation is small for modern computers.

Due to the spin degeneracy, the number of independent variational parameters is reduced. As soon as these independent variational parameters are determined, the Josephson current

Table 1. Table of $J_M = \sqrt{(2t_d)^2 + (U/2)^2} - U/2$ with $U = 1.4$. When $t_L = 0.4$, $T_K = 0.0541$, which is close to J_M at $t_d = 0.15$, where J_c takes its maximum value in figure 3.

t_d	0.01	0.1	0.15	0.2	0.4	0.8
J_M	2.86×10^{-4}	0.0280	0.0616	0.106	0.363	1.05

can be expressed at zero temperature as

$$J(\varphi) = \frac{2}{\Delta} \frac{\partial E_0(\varphi)}{\partial \varphi} = -2 \operatorname{Im} \left(e^{i\varphi/2} \sum_{i=-\infty}^{-1} \langle 0 | c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger | 0 \rangle - e^{-i\varphi/2} \sum_{i=1}^{\infty} \langle 0 | c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger | 0 \rangle \right). \quad (14)$$

Here the factor of two accounts for the spin degeneracy. Generally, if the barrier structure sandwiched in between SCs is much shorter than ξ_Δ , J can be presented as the sum of currents transferred by individual Andreev bound states [31]. But here, the original definition of J is adopted. The reason can be seen clearly below.

3. Results and discussion

In the following calculation, we always set $t = 1$, $t_L = 0.4$, $U = 1.4$ and $\Delta = 0.04$. Only the results at the particle-hole symmetric point $\epsilon = -U/2$ are considered in this paper. At this point, the Kondo temperature of the normal state $T_K = 0.0541$ and the corresponding Kondo coherent length $\xi_K = 37.0$. Here, Δ is smaller than T_K and $\xi_\Delta = \hbar v_F / \Delta = 2t / \Delta = 50$ since the Fermi energy is set at zero. Generally, the effective Kondo temperature with $t_d \neq 0$ is always larger than Δ in our SBMFT calculation. In numeric diagonalization, the cluster size is set as 300, which can guarantee the numeric convergence even if $t_d = 1$, and the dimension of the matrixes to be exactly diagonalized is small for modern computers.

In figure 2, the eigenenergy variation of the six highest occupied states and the variation of J with φ are presented for different t_d . With t_d increased, the energy positions of these eigenstates are remarkably changed. When $J_M \ll T_K$, two Andreev bound states are formed in the energy gap. With t_d increased, one of the two bound states closer to the gap edge gradually moves out of the energy gap. At $J_M \sim T_K$, that state entirely moves out of the energy gap and only one bound state remains in the gap. With t_d further increased, the remaining bound state also gradually moves out of the superconductor gap, and when $t_d \gg U/4$, no Andreev bound state is kept in the gap. This phenomenon accounts for why the original definition of J is adopted in our calculation. Here, only the eigenstates below the Fermi energy are given, and because they are symmetric with the corresponding $E-\varphi$ curves of eigenstates above the Fermi level they are used as representatives. To obtain figure 2, we take t_d as 0.01, 0.1, 0.2, 0.4 and 0.8, respectively. The corresponding J_M values at different t_d values are given in table 1.

At $\varphi = 0$, these eigenstates are degenerate in pairs. With $\varphi \neq 0$ the Kramers degeneracy is lifted, and at $\varphi = \pi$ the splitting reaches to its maximum value. For a fixed t_d , the state closer to the Fermi energy has the larger amplitude of eigenenergy variation. On the other hand, for $J_M \ll T_K$ and $t_d \gg U/4$, the amplitudes are smaller than those of the corresponding states for $J_M \sim T_K$. As a result, at $J_M \ll T_K$, the $J-\varphi$ curve is sinusoidal in shape, and its amplitude is small. With t_d increased, the amplitude of the $J-\varphi$ curve is enhanced quickly, and its shape deviates from the sinusoidal type. At $J_M \sim T_K$, the amplitude reaches to its maximum. With t_d further increased, the amplitude of the $J-\varphi$ curve is depressed and the sinusoidal line shape is recovered. These results are consistent with the characteristics shown by the variation of the critical Josephson current J_c with t_d , which is plotted in figure 3. With $J_M \ll T_K$ and $t_d \gg U/4$, J_c is small. In the intermediate region, a peak appears. In fact, the

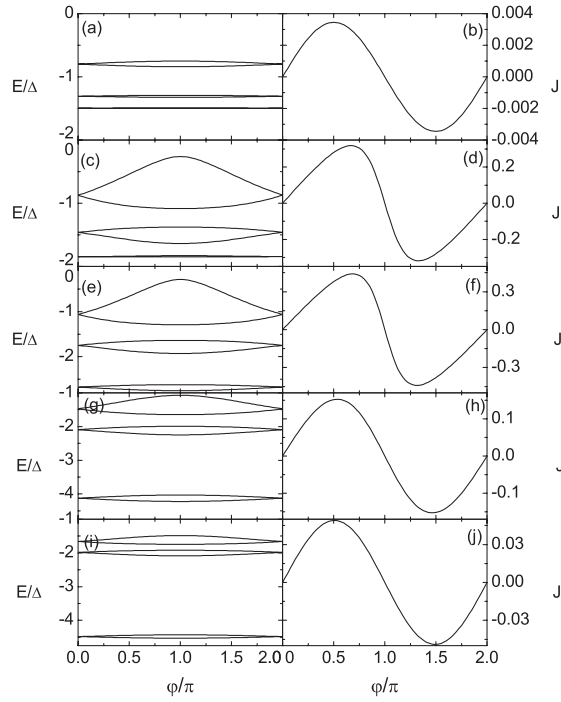


Figure 2. E - φ and J - φ curves for $t_d = 0.01$ ((a) and (b)), 0.1 ((c) and (d)), 0.2 ((e) and (f)), 0.4 ((g) and (h)) and 0.8 ((i) and (j)). The other parameters are $t = 1$, $t_L = 0.4$, $U = 1.4$, $\epsilon = -0.7$ and $\Delta = 0.04$.

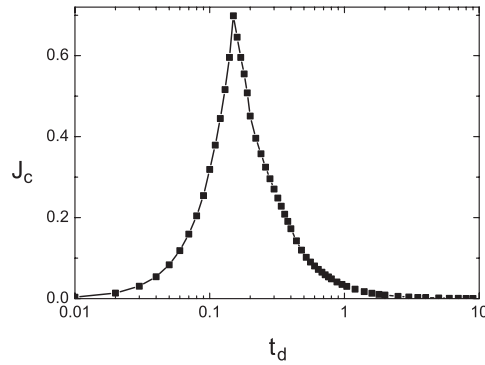


Figure 3. J_c - t_d curve with the same other parameters as in figure 2. The filled squares correspond to calculated results and the solid line is used to guide eyes.

bound state closer to the gap edge entirely moving out of the gap, the maximum amplitude of E - φ curves and the peak value of J_c are realized simultaneously with the same $t_d = 0.15$, which corresponds to $J_M = 0.0616 \sim T_K$. The J_c peak plays the same role as the resonant peak in the normal conductance and characterizes the competition between Kondo and AF correlations.

How do we interpret the variation of Andreev bound states and critical Josephson current with the direct coupling between the two dots? When $J_M \ll T_K$, two Kondo spin singlets are

formed on the two dots, respectively, by the localized spin on dots and conduction electrons on adjacent leads. As a result, two Andreev bound states are formed. Because of the small tunnelling probability through the two Kondo singlets in this regime, J_c is also small. With the AF correlation strengthened, the bound state closer to the gap edge gradually moves out of the gap, and at $J_M \sim T_K$ there is one very bound state in the gap, which yields the peak in the J_c-t_d curve. With $J_M > T_K$, the two localized spins on dots form a spin singlet because of the AF correlation. In this situation, an Andreev bound state can only be found in a certain φ range. With $t_d \gg U/4$, the parity splitting leads to double occupancy on the bonding orbital of the two dots, which tends to block the electronic transport. The critical Josephson current approaches zero and no Andreev bound state is formed. This scenario further explains how the competition between Kondo and AF correlations affects the Josephson current through a DQD system.

4. Summary

In summary, we investigate the influence of competition between the Kondo and AF correlations on the Josephson current through DQDs in the situation where Δ is smaller than the Kondo temperature T_K . In this situation, the superconductivity does not qualitatively change the competitive behaviour between the Kondo and AF correlations, and we can deal with electronic correlations by the f - U SBMFT. When $J_M \ll T_K$, the two localized spins on dots and conduction electrons form two Kondo spin singlets, and correspondingly two Andreev bound states are found. The low tunnelling probability through the two Kondo singlets leads to small J_c . With t_d increased, the Andreev bound states gradually move out of the energy gap. At $J_M \sim T_K$, only one bound state is formed in the gap and a peak appears in the J_c-t_d curve, which characterizes the competition between the Kondo and AF correlations. The strong AF correlation results in a singlet composed of the two localized spins, and one bound state can only be found in a certain range of φ . When $t_d \gg U/4$, the strong parity splitting leads to double occupancy on the bonding orbital of the two dots, and no Andreev bound state is formed with J_c approaching zero.

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