Josephson Current in Strongly Correlated Double Quantum Dots

Rok Žitko,[1] Minchul Lee,[2] Rosa López,[3] Ramón Aguado,[4] and Mahn-Soo Choi[5]

[1]*J. Stefan Institute, Jamova 39, SI-1000 Ljubljana, Slovenia*
[2]*Department of Physics, Kyung Hee University, Yongin 446-701, Korea*
[3]*Departament de Física, Universitat de les Illes Balears and Institut de Física Interdisciplinari de Sistemes Complexos IFISC (CSIC-UIB), E-07122 Palma de Mallorca, Spain*
[4]*Teoría y Simulación de Materiales, Instituto de Ciencia de Materiales de Madrid (CSIC) Cantoblanco, 28049 Madrid, Spain*
[5]*Department of Physics, Korea University, Seoul 136-701, Korea*

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We study the Josephson current through a serial double quantum dot and the associated $0-\pi$ transitions which result from the subtle interplay between the superconductivity, the Kondo physics, and the interdot superexchange interaction. The competition between them is examined by tuning the relative strength Δ/T_K of the superconducting gap and the Kondo temperature, for different strengths of the superexchange coupling determined by the interdot tunneling t relative to the level broadening Γ. We find strong renormalization of t, a significant role of the superexchange coupling J, and a rich phase diagram of the 0 and π-junction regimes. In particular, when both the superconductivity and the exchange interaction compete with the Kondo physics ($\Delta \sim J \sim T_K$), there appears an island of π' phase at large values of the superconducting phase difference.

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In a metal containing magnetic impurities the competition between the Kondo physics, which favors screening of the localized spins by the itinerant conduction-band electrons [1], and the antiferromagnetic (AF) exchange interactions between the impurities leads to a quantum phase transition [2]. Even more interesting properties emerge when the metal turns superconducting. For s-wave superconductors, Cooper pairs formed by itinerant electrons [3] are yet another competing singlet state. The intriguing interplay of these phenomena, which might actually coexist in complex materials such as heavy-fermion superconductors, governs the low temperature physics of these systems.

Nanoscale systems allow us to tune the ratio between the relevant parameters (Kondo temperature T_K, AF exchange interaction J, superconducting gap Δ) and enable controlled investigations of such competition. In the simplest case of a single quantum dot (QD) attached to superconducting reservoirs, where only Kondo physics and superconductivity are relevant, a sign change of the Josephson current (from positive 0-junction to negative π-junction behavior) signals a quantum phase transition between a singlet and a doublet ground state as T_K/Δ decreases [4–6]. This 0 to π-junction transition has been experimentally realized, confirming some of these [7] and other physical aspects [8]. A double QD (DQD) coupled to normal metals constitutes a physical realization of the two-impurity Kondo model [9–11], as demonstrated experimentally [12,13]. When the reservoirs become superconducting, this system is then a minimal artificial realization of the competition among the three different spin-singlet ground states. In this Letter we analyze the Josephson current which, as a ground state property, shows signatures of this subtle competition.

Previous studies of this problem were based on the slave-boson mean-field theory (SBMFT) and were not able to fully account for the exchange interaction J. In this work we address the problem with highly reliable numerical renormalization group (NRG). The main results are summarized in Figs. 1 and 2. The interplay between the superconductivity and the Kondo physics is studied by tuning the ratio Δ/T_K. The role of the superexchange coupling is tuned by the interdot tunneling t relative to the dot level broadening Γ. The key finding is a renormalization of t and a significant role of the superexchange coupling J compared with the previous works [9,10,14]. Moreover, we find a rich phase diagram of the 0-π transition. In particular, when all three interactions are in close competition ($\Delta \sim J \sim T_K$), there appears an unexpected island of π' phase at large values of the superconducting phase difference ϕ. We provide clear interpretation by examining the *spin-state-resolved* Andreev bound states inside the superconducting gap.

Model.—The system that we consider is a DQD modeled as a two-impurity Anderson model connected to two superconducting leads: $\mathcal{H} = \mathcal{H}_D + \mathcal{H}_L + \mathcal{H}_{T>}$ where

$$\mathcal{H}_D = \sum_i (\epsilon n_i + U n_{i\uparrow} n_{i\downarrow}) - t \sum_\mu [d^\dagger_{1\mu} d_{2\mu} + (\text{H.c.})] \quad (1)$$

$$\mathcal{H}_L = \sum_{\ell \mathbf{k}} [\epsilon_{\mathbf{k}} n_{\ell \mathbf{k}} - \{\Delta_\ell e^{i\phi_\ell} c^\dagger_{\ell \mathbf{k}\uparrow} c^\dagger_{\ell -\mathbf{k}\downarrow} + (\text{H.c.})\}] \quad (2)$$

$$\mathcal{H}_T = V \sum_{\ell \mathbf{k} \mu} [c^\dagger_{\ell \mathbf{k} \mu} d_{\ell \mu} + (\text{H.c.})]. \quad (3)$$

Here $c_{\ell \mathbf{k} \mu}$ describes an electron with energy $\epsilon_{\mathbf{k}}$, momentum $\mathbf{k}$, and spin μ on the lead $\ell = 1, 2$, and $d_{i\mu}$ an electron in the dot $i = 1, 2$; $n_{\ell\mathbf{k}} \equiv \sum_\mu c^\dagger_{\ell\mathbf{k}\mu} c_{\ell\mathbf{k}\mu}$ and $n_i \equiv \sum_\mu d^\dagger_{i\mu} d_{i\mu}$. ϵ is the single-particle energy on each dot that is tuned by the gate voltages, and U is the on-site Coulomb interaction. The electrons can tunnel between the two dots with the amplitude t. Δ_ℓ is the superconducting gap, and ϕ_ℓ the phase of the order parameter.

The two leads are assumed to be identical except for the superconducting phases. The hybridization between the dots and the leads is $\Gamma = \pi\rho V^2$, where ρ is the density of states in the leads. Since we are interested in the Kondo correlations, we concentrate on the Kondo regime with localized level $-\epsilon \gg \Gamma$ and large charging energy $U \geq 2|\epsilon|$. For the representative results shown below, we choose $\Gamma = 0.014D$ or $\Gamma = 0.02D$, fix $\epsilon = -0.2D$, and take the large $U = \infty$ limit. We examine the results by varying Δ/T_K, t/Γ, and $\phi \equiv \phi_L - \phi_R$.

We solve the Hamiltonian using the NRG [15]. Because of the relatively low symmetry of the problem, the NRG iteration is numerically very demanding and special attention is necessary to obtain reliable results. Using a new discretization scheme the numerical artifacts due to a large discretization parameter Λ are almost completely canceled out [16].

Two crucial effects established in a previous work on the DQD with normal leads [11] remain important in the present case. First, the interdot tunneling t is significantly renormalized compared with the predictions based on the SBMFT [9,10,14]. Second, there are two main contributions to the interdot exchange coupling: (i) J_I generated by virtual tunneling events that involve conduction-band electrons in the reservoirs (dominant in the large-U limit), and (ii) the direct superexchange $J_U \approx 4t^2/U$ (dominant for intermediate U values). Therefore for any U, even in the $U \to \infty$ limit, it is important to take into account the interplay of the superexchange coupling (with a total strength $J = J_I + J_U$) with the superconductivity and the Kondo effect.

Strong coupling limit ($T_K \gg \Delta$).—Figure 1 shows normal-state conductance [(a), (b)] and the critical Josephson current [(c), (d)]. In the strong coupling limit, $\Delta/T_K = 0.1$ (black circles), the critical Josephson current I shows similar features as the normal-state conductance G: it peaks at equal values of t/Γ and, remarkably, when the conductance in the normal state is unitary, the Josephson current reaches the single-mode quantum limit $I^s_c = e\Delta/\hbar$. This is expected since the Kondo effect dominates over the superconductivity; therefore, the transport is determined by the competition between the Kondo physics and the interdot superexchange (for $t/\Gamma < 5$) or interdot molecular orbitals ($t/\Gamma > 5$). As we analyzed in detail in the previous work [11], the peaks in G and I_c at $t/\Gamma \approx 0.4$ (for $\Gamma = 0.014D$) result from the crossover from the "Kondo singlet" to the "superexchange singlet." For $t/\Gamma < 0.4$, $J < T_K$, whereas for $0.4 < t/\Gamma < 5$, $J > T_K$. We stress that the crossover is significantly shifted to smaller $t/\Gamma = 0.4$ compared with the SBMFT results that predict a peak at $t/\Gamma = 1$. As t/Γ increases beyond 5, the DQD starts to form molecular orbitals and effectively behaves as a single QD. The associated Kondo scale rapidly decreases with increasing t. Eventually, $T_K \sim \Delta$ and a 0 to π phase transition is observed, just like in a single-dot system [4–6]. The transition line is plotted in Fig. 2 and it is only weakly dependent on ϕ.

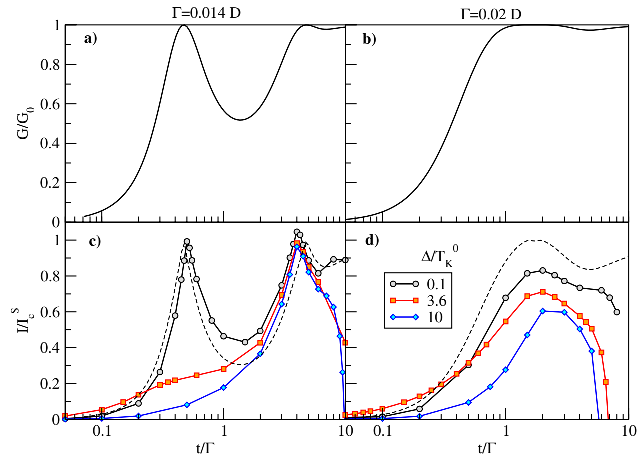

FIG. 1 (color online). Normal-state conductance [(a),(b)] and the critical Josephson current in the superconducting state [(c),(d)] as a function of t/Γ for $\Gamma = 0.014D$ (a),(c) and $\Gamma = 0.02D$ (b),(d). The results are expressed in the units of the conductance quantum $G_0 = 2e^2/h$ and the supercurrent quantum I^s_c. In the superconducting case [(c),(d)], the different curves are for $\Delta/T_K = 0.1$ (black circles), 3.6 (red squares), and 10 (blue diamonds). The dashed line is from an effective noninteracting theory, Eq. (4).

For comparison, we have also calculated the critical Josephson current as $I = \max_\phi I(\phi)$, with [17]

$$\frac{I(\phi)}{I^s_c} = \frac{g}{2}\sin\phi\sqrt{1 - g\sin^2(\phi/2)}, \tag{4}$$

where $g = G/G_0$ is the (dimensionless) normal-state conductance obtained from a NRG calculation. These relations are applicable if the QD state is only weakly affected by the superconductivity. As can be seen in Fig. 1, for $t/\Gamma \lesssim 5$, the result from the effective theory (dashed lines) and the full NRG calculation show a qualitative agreement. For larger t ($t/\Gamma > 5$), we enter the single-dot regime, the Kondo effect is suppressed and the superconductivity becomes dominant, leading to the deviation between the results.

Weak coupling limit ($T_K \ll \Delta$).—The results, shown in Figs. 1 and 2 for $\Delta/T_K = 10$ indicate that the superconducting correlations in the leads suppress the Kondo effect and the Josephson current remains small until the system enters the single-dot regime. It is remarkable that the S-DQD-S system behaves as a 0 junction in the *weak coupling limit* in contrast to the S-QD-S case where the π junction appears in the same regime. In single QDs, the appearance of π junction is due to the reversal of the order

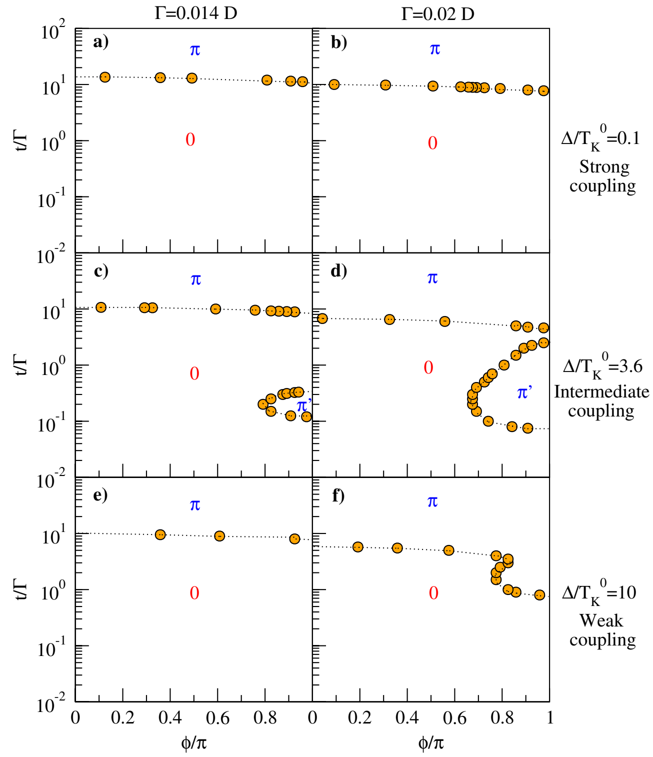

FIG. 2 (color online). Phase boundaries between the 0 and π states for $\Gamma = 0.014D$ (left panels) and $\Gamma = 0.02D$ (right panels). When both the interdot superexchange coupling and the superconductivity are in close competition with the Kondo effect between the superconducting leads and adjacent dots ($t/\Gamma \sim 0.2$, $\Delta \sim T_K$), there appears an island of π' phase at larger phase difference.

of the electrons forming Cooper pairs after tunneling.[4] In the DQD the order is, however, preserved so that no additional phase factor arises from the tunneling; thus, 0 junction is formed even in the Coulomb blockade regime. Specifically, the perturbation theory applied in the weak coupling limit for $U \to \infty$ gives

$$\frac{I}{I_c^s} = \sin\phi \sum_{\mathbf{kq}} \frac{2\Delta t^2 V^4}{E_{\mathbf{k}} E_{\mathbf{q}}[(\epsilon - E_{\mathbf{q}})^2 - t^2][(\epsilon - E_{\mathbf{k}})^2 - t^2]} \times \left(\frac{1}{E_{\mathbf{q}} + E_{\mathbf{q}}} + \frac{1}{2|\epsilon|}\right) \tag{5}$$

with $E_{\mathbf{k}} \equiv \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}$. Our NRG calculations confirm that the ground state is a spin singlet as long as the 0 junction is formed. Hence, in contrast to the single QD system, in a large part of the parameter space there is no phase transition as we move from the weak to the strong coupling limits by varying Δ/T_K.

Subsequent transition into π junction for very large t/Γ in Figs. 2(e) and 2(f) is ascribed to the competition between effective spin-1/2 Kondo correlation and superconductivity as in the strong coupling limit. Since the superconducting gap is now larger than in the strong coupling limit the transition takes place at somewhat smaller values of t/Γ for which the effective Kondo temperature T_K is higher. Moreover, the critical current is relatively large even though the system is in the weak coupling limit, unlike in the single QD where the critical current in this limit is very small ($I/I_c^s < 0.1$) [5]. A very likely explanation is that the one-electron spin-1/2 Kondo state is formed at smaller values of t/Γ and that strong superconductivity is responsible for it. The (one-electron) Kondo assisted tunneling then makes the junction more transparent and enhances the critical current. Hence, the physical origin of the peak in the critical current is different in the weak and strong coupling limits.

Intermediate coupling ($T_K \sim \Delta$).—In this regime, the superconductivity, the superexchange, and the Kondo physics can all be in close competition. This subtle interplay keeps the Josephson critical current finite, somewhere between the current in the weak coupling and strong coupling limits, Figs. 1(a) and 1(d), except for very large t/Γ, where single QD physics again governs the transport.

More interestingly, the phase diagrams in Figs. 2(c) and 2(d) reveal the reentrance behavior as a function of t/Γ for

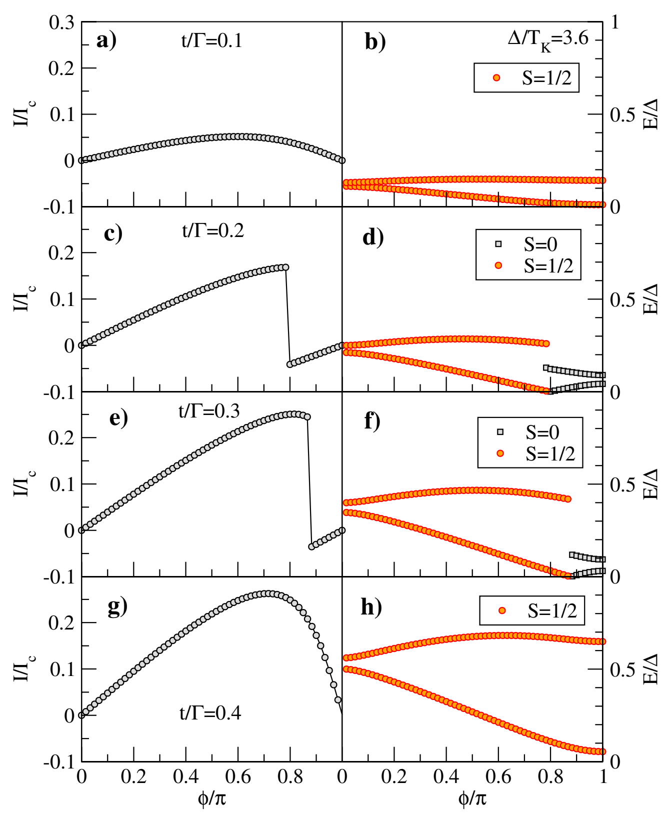

FIG. 3 (color online). Left panels: Josephson current vs phase difference near the π' phase ($\Delta/T_K = 3.6$, $t/\Gamma = 0.1$, 0.2, 0.3, 0.4, and $\Gamma = 0.02D$ from top to bottom). Right panels: Corresponding spin-state-resolved Andreev bound states inside the superconducting gap. Spin doublet states are depicted by (red) circles and singlets by (black) squares. The changes in the spin states are closely related to the island of π' phase in Fig. 2(c) [similar spin-state-resolved Andreev states for corresponding parameters will also explain the island in Fig. 2(d)].

larger superconducting phase difference ϕ. In order to understand this behavior, we closely examine the subgap Andreev bound states, which are Bogoliubov quasiparticle excitations from the ground state [3] and whose derivatives with respect to ϕ give the Josephson current [18]. In Fig. 3 we plot the energy levels of the Andreev states as a function of ϕ. Let us focus on, say, $\phi = 0.9\pi$. For $t/\Gamma < 0.1$, the singlet Kondo clouds are formed between the superconductors and the adjacent dots; thus, the ground state is likewise a spin singlet, while the excitations correspond to doublet states, see Fig. 3(b). As the Josephson current is given approximately by the phase-difference derivative of the Andreev levels, this corresponds to the 0-junction behavior, Fig. 3(a). For $0.4 < t/\Gamma < 5$, the local interdot singlet state is induced on the DQD due to the antiferromagnetic superexchange interaction; thus, the ground state is again a spin singlet, Fig. 3(h), and this results in the 0-junction behavior, Fig. 3(g). In the previous two cases, both Kondo effect and superexchange barely win over the superconductivity, for all values of ϕ. However, for intermediate values $0.1 < t/\Gamma < 0.4$, the Kondo effect is suppressed by the large phase difference [5]. This is indicated by the fact that the ground state is now a doublet, while the excited state is a singlet, as shown in Figs. 3(d) and 3(f). Accordingly, the transport properties are different and, in particular, the π-junction behavior is observed; see Figs. 3(c) and 3(e). This regime is denoted as π' in the phase diagram in Fig. 2. While the π phase for large t corresponds to the single occupancy of the dots, the π' phase occurs for the double occupancy. For large values of Γ ($\Gamma = 0.02D$), the π' island becomes bigger and it merges with the π regime, as visible in Fig. 3(f).

In double quantum dots coupled to two superconducting leads we find a significant role of the superexchange coupling J, and a rich phase diagram featuring different $0 - \pi$ transitions in the Josephson current. For $\Delta \sim J \sim T_K$ there appears an island of π' phase at larger values of the superconducting phase difference. This finding motivates further studies of this regime, which may shed new light on the physics of heavy-fermion superconductors.

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