Phase coherent transport in hybrid superconducting-semiconducting nanostructures is already extensively investigated. In these devices, quite interesting and surprising features emerge, due to electron-electron interaction. In this letter we study a Quantum Dot (QD) at Coulomb Blockade (CB) with an odd number of electrons $N$, connected to superconducting contacts. Although such a kind of system has not been realized yet, it is very likely that continuous improvement of nanofabrication techniques will soon make it available. In particular, we address the question whether the formation of a Kondo singlet at the dot competes or cooperates with superconductivity spoils Kondo correlations on the dot, characterized by $\pi$-Josephson coupling across the dot. Kondo conductance may be achieved in a QD with $N$ odd within a CB valley by increasing the coupling between dot and leads, provided the temperature $T < T_K$. At $T < T_K$, a strongly correlated state between dot and leads sets in and a resonance in the density of states of the QD opens up at $\mu$. Correspondingly, DC conductance across the dot increases, until it eventually reaches the unitarity limit at $T = 0$. Since charge dynamics is “frozen out” by CB, the QD in this regime is usually modelized as a magnetic impurity with total spin $S = \frac{1}{2}$.

Magnetic impurities embedded in a bulk superconductor are known to strongly influence the superconducting critical temperature. Adding impurity states at energies below the superconducting gap can even give raise to gapless superconductivity.

Tunneling across a magnetic impurity between superconductors with on site Coulomb repulsion has been recently revisited. If $\Delta \geq k_B T_K$, the system is unable to scale toward the strongly-coupled Kondo regime. Sub-gap Cooper pair is strongly suppressed by Coulomb repulsion, unless each co-tunneling step is accompanied by a spin flip at the impurity. It has been proposed that such a mechanism may reverse the sign of the Josephson current through the dot so that the Josephson energy is at a minimum for $\varphi = \pi$, where $\varphi$ is the phase difference between the order parameters of the two superconductors attached to the impurity ($\pi$-junction).

We expect that fine tuning of the parameters of a S-QD-S device (for instance, one may drive the system to a level crossing by tuning an external applied magnetic field which, under appropriate conditions, does not affect Kondo conduction) may allow for the investigation of the full range of physical conditions, from...
\[ \Delta \ll k_B T_K \] when the system can flow toward the strongly coupled Kondo regime prior to the onset of superconductivity in the leads, to \( \Delta \gg k_B T_K \), when perturbation theory holds.

We study the \( T = 0 \) case with \( \Delta \ll k_B T_K \) using a non-perturbative variational technique. This technique has already been applied to the case of a dot with normal contacts, and it has been shown to provide good qualitative results in the perturbative regime as well, where it reproduces the poor man’s scaling equation [15].

To construct the trial state, we start from the state \( |\varphi, s\rangle \), given by the product of the left (L) condensate times the right (R) condensate, with the two order parameters having a phase difference \( \varphi \), times the state of the dot: \( |s\rangle \).

\[ |\varphi, s\rangle = |BCS, L\rangle \times |BCS, R, \varphi\rangle \times |s\rangle. \]  

Here \( s \) is the spin component along the quantization axis of the dot spin \( S_d = \frac{1}{2} \), at CB with odd \( N \).

The minimal model for the Kondo interaction between electrons localized on the QD and electrons from the contacts is \( H_K = J|\varphi, s\rangle \cdot \tilde{S}_d \). The spin density operator of the delocalized electrons, \( \tilde{\sigma}(0) \), at the position of the dot \( x = 0 \) along the vertical axis, is:

\[ \tilde{\sigma}(0) = \frac{1}{2V} \sum_{q,q'}(c_{L,q,\sigma}^\dagger + c_{R,q,\sigma}^\dagger)\tilde{\sigma}_{\sigma,\sigma'}(c_{L,q',\sigma'} + c_{R,q',\sigma'}) \]

We have used the fermion operators \( c_{q,j}(c_{q,j}^\dagger) \) \( j = L, R \) in the plane wave representation to describe the contacts particles and \( V \) is the normalization volume of the leads. We take the symmetric case in which hybridization of the dot with the L and R contacts, \( \Gamma \), is the same. Kondo coupling is antiferromagnetic (AF): \( J > 0 \). The interaction term \( H_K \) can be obtained from a Schrieffer-Wolff transformation as in the case of normal contacts. The superconductivity in the contacts does not affect this derivation, provided \( D \gg \Delta \), where \( D \) is the bandwidth of the itinerant electrons.

The total Hamiltonian is \( H = H_S + H_K \), where \( H_S \), defined in eq. (1) below, is the Hamiltonian for the L and R superconducting contacts in the BCS approximation.

The correlated trial state is constructed by applying a Gutzwiller-like projector \( P_g \) to \( |\varphi, s\rangle \). As \( T \to 0 \), the system scales towards the strongly coupled -large \( J \)-regime. Correspondingly, \( P_g \) gradually projects out the high-energy components of the trial state, so that eventually only a localized spin singlet survives at the QD.

The “projector” \( P_g \) is defined as [15]:

\[ P_g = \left( 1 - \frac{3}{4} g \right) + g(\tilde{\sigma}(0))^2 - 4S_d \cdot \tilde{\sigma}(0) \]

\( g \) is a variational parameter, which ranges between \( g = 0 \) and \( g = 4/3 \). When \( g = 0 \), we have \( P_0 = 1 - 4S_d \cdot \tilde{\sigma}(0) \). \( P_0 \) fully projects out the high energy localized spin triplet at \( x = 0 \). As \( g \) varies from 0 to 4/3, also the localized spin doublet state it increasingly projected out. Eventually, when \( g \) reaches the value \( g = 4/3 \), only the localized spin singlet is left over.

The trial state is defined as:

\[ |g, \varphi\rangle = P_g|\varphi, s\rangle \]  

The value of \( g(J) \) is determined by finding the minimum of the energy functional \( E[g, J, \varphi, \Delta] \), defined as:

\[ E[g, J, \varphi, \Delta] = \langle g, \varphi|H|g, \varphi\rangle \]  

Eq. (3) can be calculated by first expressing the products \( P_g H P_g \) and \( (P_g)^2 \) in terms of the usual fermion quasiparticle operators \( \alpha_{j,q}(\alpha_{j,q}^\dagger), \beta_{j,q}(\beta_{j,q}^\dagger) \) \( j = L, R \) which destroy (create) excitations on the BCS states of the L and R contact and then by normal-ordering the corresponding operator products. The operators are:

\[ \alpha_{j,q} = u_q c_{j,q,\uparrow} - v_q e^{i\delta_q} c_{j,-q,\downarrow} \]

\[ \beta_{j,-q} = u_q c_{j,-q,\downarrow} + v_q e^{i\delta_q} c_{j,q,\uparrow} \]  

\( u_q \) and \( v_q \) are the BCS coherence factors and \( \phi_R = \varphi \) while \( \phi_L = 0 \). The Hamiltonian for the contacts \( H_S \) is conveniently expressed in terms of these operators as:

\[ H_S = E_{BCS} + \sum_{q,j=L,R} E_q(\alpha_{j,q}^\dagger \alpha_{j,q} + \beta_{j,-q}^\dagger \beta_{j,-q}) \]

Here \( E_{BCS} \) is the total ground state energy of the condensates and \( E_q = \sqrt{\xi^2 + \Delta^2} \) are the energies of the quasiparticle excitations with \( \xi_q = q^2/2m - \mu \), (we put \( \hbar = k_B = 1 \) throughout the paper).

The variation of the energy due to the AF coupling at the quantum dot in units of the bandwidth \( D \),

\[ c[\xi, j, \delta, \varphi] = E[g, J, \varphi, \Delta]/D, \]

takes a simple form expressed in terms of the parameters \( \xi = \frac{1}{2}(1 - \frac{4}{3}g) \), \( j = 3J/4D \) and \( \delta = \Delta/D \):

\[ c[\xi, j, \delta, \varphi] = -2j \frac{1 - \frac{1}{3} \delta^2 (1 + \cos(\varphi))/N(0)\lambda^2}{(1 + \xi^2) + (\xi^2 - 1)\delta (1 + \cos(\varphi))/(2N(0)\lambda)} + \frac{2(1 - \xi - \xi^2)\sqrt{1 + \delta^2 - \delta^2 (1 + \cos(\varphi))/N(0)\lambda}}{(1 + \xi^2) + (\xi^2 - 1)\delta (1 + \cos(\varphi))/(2N(0)\lambda)}. \]  

Here \( \lambda \) is the BCS electron-electron interaction strength and \( N(0) \) is the normal phase density of states at the Fermi level for each spin polarization. The first term is the expectation value of \( H_K \), while the second is the raise in the average value of the kinetic energy Hamiltonian, \( H_S \), due to the formation of the singlet between the QD and the environment. The value of \( \xi_{min} \), at which the energy is at a minimum measures how much
higher-energy spin states are projected out: $\xi_{\text{min}} = 0$ corresponds to full projection of states different from a localized spin singlet at the impurity.

At $\delta = 0$ the strong coupling fixed point is $j \to \infty$ and $\xi_{\text{min}}(j) \to 0$. In correspondence of the fixed point, there is a large decrease of the Kondo energy:

$$\Omega_K = 2 \frac{1 - \xi_{\text{min}} + (\xi_{\text{min}})^2 - j}{1 + (\xi_{\text{min}})^2}. \quad (7)$$

In Fig. we plot $\xi_{\text{min}}$ vs. $\delta$ for various $j$. As $\delta$ is increased at $j$ large, $\xi_{\text{min}}$ moves from 0 to finite values.

As $\delta$ increases, two regimes can be envisaged:

a) $\Delta \ll T_K$: The Kondo correlated state is firmly established.

The change of $\xi_{\text{min}}$ to first order in $\delta$ is given by:

$$\xi_{\text{min}}(\delta) = \xi_{\text{min}}(\delta = 0) - \frac{\delta(1 + \cos \varphi)}{N(0)\lambda} \left[ \frac{j + 1 - \sqrt{j^2 + 1}}{\sqrt{j^2 + 1}} \right] \quad (8)$$

that shows that, for any value of $\delta$, $\xi_{\text{min}}(\delta) \leq \xi_{\text{min}}(\delta = 0)$. We also see that, as $\varphi$ changes from 0 to $\pi$, $\xi_{\text{min}}$ increases. This clearly shows that the stable configuration for the system is at $\varphi = 0$, what has important consequences for the Josephson conduction, as we are going to show in the following.

In Fig. we plot $\epsilon/j$ vs. $\xi$ for various values of $j$ at $\delta = 0.03$ and $\varphi = 0$. As $j$ increases, $\xi_{\text{min}}$ moves toward $\xi_{\text{min}} = 0$, which corresponds to the strongly coupled fixed point.

From the inset in Fig. we also see that, as $\delta$ increases, the value of the energy at the minimum decreases. In this regime $\epsilon'[j, \delta, \varphi] < \epsilon'[j, 0, \varphi]$, that is, superconductivity favors strong Kondo correlations.

Upon calculating $\epsilon'[\xi, j, \delta, \varphi]$ for $\xi = \xi_{\text{min}}$, we get the best estimate for $\epsilon'[j, \delta, \varphi]$, the energy of the correlated state, to first order in $\delta$:

$$\epsilon'[j, \delta, \varphi] = \Omega_K[1 + B\delta(1 + \cos \varphi)] \quad (9)$$

where $B = [1 - (\xi_{\text{min}})^2]/(N(0)\lambda[1 + (\xi_{\text{min}})^2])$. From Eq. we clearly see that, for large values of $j$, $\epsilon'[j, \delta, \varphi] < \epsilon'[j, \delta = 0, \varphi]$, that is, superconductivity and Kondo effect cooperate.

b) $\Delta \leq T_K$: Superconductivity competes with Kondo ordering.

Expansion in powers of $\delta$ is no longer meaningful. The energy gain due to superconductivity $G_S \sim -\frac{1}{2} N(0)\Delta^2$ becomes dominant with respect to the Kondo energy gain $\Omega_K(\delta = 0)$. Kondo correlations and superconductivity start to compete. The minimum moves from $\varphi = 0$ to $\varphi = \pi$, as shown in Fig. (bottom panel). Indeed, in the bottom panel of Fig. we plot $\epsilon'/j$ vs. $\delta$ for $\varphi = 0$ and $\varphi = \pi$ and $j = 8$. At a critical value of $\delta$, the two curves cross each other, corresponding to crossing of the minimum energy from $\varphi = 0$ to $\varphi = \pi$.

There is a third regime, not covered by our approach:

c) $\Delta > T_K$: Superconducting order is dominant.

Here the Kondo interaction can be treated perturbatively. This regime was studied in Ref. using a NCA perturbative approach. The results in show a change of the sign of the Josephson current that is consistent with our results, as we discuss below.

The Josephson current is given by:

$$I_J = -2e\partial\epsilon^*[j, \delta, \varphi]/\partial\varphi \quad (9)$$

In regime a), $I_J$ is linear in $j\delta$:

$$I_J = -2e\Omega_K B\delta \sin \varphi. \quad (9)$$

Therefore, in this regime Kondo correlations strongly increase the Josephson current. The sign of the current is the conventional one for Josephson systems, that is, the device behaves as a diamagnetic junction. As $\delta$ slightly increases, the dependence of $I_J$ on $\varphi$ develops non sinusoidal terms, in a way similar to the result in Ref. [13].

As $\delta$ increases, we enter a new regime in which superconductivity competes with Kondo correlations. In this region the Josephson current decreases as $\delta$ increases (see top panel of Fig.3). As $\delta = \delta_p$, the energy minimum moves from $\varphi = 0$ to $\varphi = \pi$. Correspondingly, although the current is now linear in $\delta$, its sign is reversed, that is, the device now behaves as a $\pi$-Josephson junction. These results appear to extend the analysis performed in Ref. [3] in the regime $\Delta > T_K$ to the complementary regime, $\Delta < T_K$.

We now provide the physical interpretation of our results in terms of Andreev bound states in the normal region. In the noninteracting limit, the superconducting gap at the Fermi level $\mu$ in an SNS sandwich generates two localized Andreev states in the normal region with energy within the gap. The one of the two states with positive (negative) energy is mostly particle (hole)-like. In this case, Josephson conduction across the normal region involves both Andreev states.

As interaction is turned on ($J > 0$) and $\Delta \ll T_K$, pair tunneling takes place through the Kondo resonance at $\mu$, whose width ($\sim T_K$) is quite large. At the same time, dot’s spin “disappears”, because of full compensation at the strongly coupled fixed point. Full screening does not allow for extra occupancy of the dot. Accordingly, we expect that the hole-like state will be just above $\mu$ but the particle-like state will be pushed quite high in energy (the higher is the effective coupling, the higher will be the energy of the particle-like state).

When superconductivity starts to weaken Kondo correlations, (regime b) ), the two states are expected to have comparable energy, until, at some point, they cross. Such a crossing, where the particle state energy moves below the hole state energy and the particle state becomes partially occupied, makes the minimum move from $\varphi = 0$ to $\varphi = \pi$. By increasing $\Delta$ even further, we reach the regime discussed in [3], where the particle state has moved below $\mu$ and the minimum of the energy has moved to $\varphi = \pi$. 

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(see bottom panel of Fig.3). This is the perturbative regime, where the Josephson current takes an overall sign and the system behaves as a $\pi$-junction.

FIG. 1. $\xi_{\text{min}}$ vs. $\delta$ for various $j$. For small values of $\delta$, $\xi_{\text{min}}$ is lowered, showing that a small amount of superconductivity favors Kondo correlations. On the other hand, for large $\delta$, $\xi$ abruptly increases, that is a signal of the loss of Kondo regime.

FIG. 2. $\epsilon/\delta$ vs. $\xi$ for different $j$ and for $\varphi = 0$. At the onset of Kondo regime (large $j$), the minimum of the curve moves toward $\xi = 0$. Inset: $\epsilon/\delta$ vs. $\xi$ for two different values of $\delta$. A small superconducting gap appears to lower $\epsilon/\delta$, that is, a small $\delta$ favors Kondo regime.

In conclusion, we have generalized the variational approach introduced in ref. [15] to study Josephson conduction through a quantum dot at Coulomb blockade connected to two superconducting leads. Within such an approach, we analyzed the region of parameters where the dot lays in the strongly coupled Kondo regime and showed that, in this regime, it behaves as a diamagnetic junction, with a corresponding “Kondo enhancement” in the current. Our results appear to be in agreement with earlier predictions on related systems [11]. Moreover, our formalism shows that the transition to $\pi$-junction regime takes place much before antiferromagnetic correlations at the dot can be treated perturbatively, that is, much before Kondo effect has been disrupted by superconductivity. Finally, our results lead us to predict an enhancement in the saturation current in the strongly coupled regime, which should be experimentally detectable as a signature of Kondo effect in the quantum dot between two superconductors.

FIG. 3. Top panel: saturation current $I/(jD)$ vs. $\delta$. For small values of $\delta$, $I/(jD)$ increases linearly with $\delta$. At large enough $\delta$ it decreases and becomes 0 at $\delta = \delta_p$, where the minimum of the energy moves to $\varphi = \pi$. For $\delta > \delta_p$, $I < 0$, that is, the system has crossed over to a $\pi$-junction behavior. Bottom panel: $\epsilon^*/\delta$ vs. $\delta$ for $\varphi = 0, \pi$. At $\delta = \delta_p$ the two curves cross and the minimum moves to $\varphi = \pi$.

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