Superconductor-Quantum Dot-Superconductor Josephson Structures with Attractive Intradot Interaction

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We consider a quantum dot with intradot attractive interaction sandwiched between two superconducting leads. We show that the system possesses quantum phase transitions of fermion parity as long as an external magnetic field is present. Due to the superconducting proximity effects, the possible electronic states for the embedded quantum dot are spin-polarized states with odd occupation and BCS-like states with even occupation. In this work, we adopt a self-consistent theoretical method to extend our considerations beyond the superconducting atomic limit to numerically investigate implications of an attractive interaction in electronic structures. We discuss the difference between results obtained in and away from the atomic limit. We find a reentrant behavior in the energy phase diagram when \( \Delta \) is an order of magnitude larger than the hybridization strength. We also consider the Josephson current phase relations and find a number of examples showing the 0–\( \pi \) phase transitions that may offer important switching effects.

I. INTRODUCTION

Introducing localized magnetic impurities into a host superconductor (SC) leads to the formation of the so-called Yu-Shiba-Rusinov (YSR) states. In such a system, quantum phase transitions (QPTs) associated with fermion parity switch of the YSR states can be achieved via tuning experimental knobs such as gate voltages and external magnetic fields. Recently, there has also been interest on the topological properties of a chain of magnetic impurities in the hope of supporting Majorana bound states in such a solid state system, which is regarded as a candidate of fault-tolerant quantum computers. Therefore, exploring the physics behind the YSR states can help to advance quantum information technology. A similar and closely related setup that allows us to study the physics of QPTs is tunnel junctions involving quantum dots (QDs) coupled to superconducting leads, which is the main focus of this work.

One of the advantages of using QDs in the setup is their high controllability for their electronic structures can be experimentally tuned to achieve desired properties by controlling their sizes, electron densities as well as electrode voltages. Quantum dots alone have also been proved to be useful in many other fields including biomedical applications and quantum information technology. In the latter, qubits, the building blocks of a quantum computer, are implemented by charge or spin degrees of freedom in QDs. Quantum dots can also be used to build a single electron transistor because of the pronounced Coulomb blockade effect in them.

Physics of heterostructures composed of both superconductors and quantum dots have become an important and exciting research topics. When a quantum dot is in contact with superconducting electrodes, the electronic structures of the quantum dot will be drastically modified due to the local formation of Cooper pairs via superconducting proximity effects. The quantum dot thus can possess BCS-like states in contrast to their original discrete states that are under a more direct influence of the Coulomb blockade. Furthermore, one of the most important effects of the SC-QD coupling is the emergence of Andreev bound states (ABS) found in SC-QD heterostructures which carry important information on phase transitions for the dot.

Important physical behavior or physical quantities such as spectral weights and Josephson current can be derived theoretically. In Ref. 12, the effects of the superconductivity on local spectral properties of the dot is investigated. It is found that the low energy spectrum is determined by the superconducting gap. The situation depicted here is similar to a Kondo impurity embedded in superconductors. Consequently, the Kondo effect plays an important role in SC-QD heterostructures and one needs to compare the energy scales of the superconducting gap, \( \Delta \), and the Kondo temperature, \( T_K \). As discussed in Refs. 12, for cases where \( \Delta \ll T_K \), the ground state of the dot is a Kondo/BCS singlet state with the assistance of the Kondo effect. In this regime, the Kondo coupling between the superconducting electrodes and the quantum dot helps the establishment of superconducting correlations in the dot. However, as demonstrated in Ref. 15, the ground state is a BCS singlet with weak and repulsive Coulomb interaction and crosses over to a Kondo singlet when the interaction is strong. For the other extreme limit, \( \Delta \gg T_K \), there is essentially no states around the Fermi level because of the large gap. The Kondo effect is therefore suppressed and the ground state of the dot is a Kramers doublet state as long as the time reversal symmetry is preserved.

Another important aspect of the QD-SC coupling is the transport property in SC-QD-SC junctions. Specifically, the Josephson effect evaluated in Ref. 14 and 16 is related to the phase transitions of the quantum dot. As illustrated in the above, the BCS-like state of the dot occurs when \( \Delta \ll T_K \) and the transport of a Cooper pair from one of the superconducting electrodes to the other does not require a sign flip of the singlet state.
On the other hand, when $\Delta \gg T_K$, the dot is in the doublet state and acts as a single magnetic impurity. A Cooper pair is then affected by the magnetic impurity and a negative sign is acquired when it is transported from one side to the other. It is clear that for the latter case, the associated Josephson current also gets inverted and the SC-QD-SC is a $\pi$-junction. The doublet-singlet phase transitions can then be experimentally confirmed by measuring the current-phase relations of the junctions.

One simple and elegant model to describe a quantum dot coupled to superconducting leads is the Anderson impurity model. The coupling $t$ between the dot and the conduction electrons of the leads and the Coulomb interaction $U$ between electrons in the dot are important competing energy scales in the Anderson model. However, the Coulomb interaction between electrons involves four operators, and, as a result, the Anderson Hamiltonian can not be simply recast into a bilinear form. Because the Coulomb interaction has important implications in transport properties, it cannot be neglected in the problem. Furthermore, when the dot is singly occupied, it is unlikely to have another electron to flow through the dot when the Coulomb interaction is strong and repulsive. This phenomenon is known as the Coulomb blockade. There, however, exists several ways in the literature to estimate the contribution from the Coulomb interaction including the perturbation expansion in the Coulomb interaction, mean field theory, non-crossing approximation (NCA), numerical renormalization group (NRG), or quantum Monte Carlo and functional methods.

In Ref. 27, the authors carefully discuss physics of SC-QD-SC Josephson junctions with Zeeman effect. In particular, they use both functional renormalization group (fRG) and self-consistent Andreev bound states theory (SCABS) to study the interplay between the Zeeman field, gate voltage, and the flux dependence of Andreev (SCABS) to study the interplay between the Zeeman splitting in the superconducting electrodes, strength of Coulomb interaction and Zeeman field. In Sec. II, we will present a general description of the SCABS method. The results and relevant discussion will be presented in Sec. III. We will summarize the paper in Sec. IV.

### II. THEORETICAL MODEL

#### A. Hamiltonian

We start from the Anderson impurity model Hamiltonian to describe a quantum dot coupled with two superconducting electrodes. The Hamiltonian is given by

$$H = \sum_{i=L,R} H_i + H_d + \sum_{i=L,R} H_{Ti},$$

(1)
where
\[ H_i = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} c_{\mathbf{k}\sigma i}^\dagger c_{\mathbf{k}\sigma i} - \sum_k \left( \Delta_i c_{\mathbf{k}\uparrow i}^\dagger c_{-\mathbf{k}\downarrow i} + \text{H.c.} \right). \] (2a)
\[ H_d = (\varepsilon_d + h) d_i^\dagger d_i + (\varepsilon_d - h) d_i^\dagger d_i - U n_\uparrow n_\downarrow, \] (2b)
\[ H_{T_i} = \sum_{\mathbf{k}\sigma} (t d_i^\dagger c_{\mathbf{k}\sigma i} + \text{H.c.}). \] (2c)

In this total Hamiltonian, \( H_i \) is the Hamiltonian for superconducting leads, and \( i = L, R \) denote the left and right leads, respectively. The kinetic energy of a lead electron with wavevector \( \mathbf{k} \) is \( \varepsilon_{\mathbf{k}} \) and \( c_{\mathbf{k}\sigma i}^\dagger \) is the annihilation (creation) operator of the lead electron with wavevector \( \mathbf{k} \) and spin \( \sigma \) for the left and right leads \((i = L, R)\). \( \Delta_i \) is the superconducting order parameter on the dot and superconducting leads and \( t \) is the corresponding coupling strength.

For a more relevant situation in experiments, the leads we consider here are described by a single orbital with energy \( \varepsilon_d \). \( d_i^\dagger \) (\( d_i \)) is the annihilation (creation) operator of a dot electron with spin \( \sigma \). \( U \) is the Coulomb interaction between two electrons on the dot energy level, \( h \) is the Zeeman energy, and \( n_\sigma = d_i^\dagger d_i \) is the number operator of the dot level with spin \( \sigma \). \( U > 0 \) denotes an attractive interaction in our notation. \( H_{T_i} \) is the interaction between the quantum dot and superconducting leads and \( t \) is the corresponding coupling strength.

The Green’s function technique is adopted. Furthermore, they showed that the results obtained from the SCABS behavior of a quantum dot, so we first define the quantum dot Hamiltonian and the QD we consider here is closely the method presented in Refs. 11 and 27, where \( \varepsilon_d \) is the superconducting order parameter of the leads and H.c. is the Hermitian conjugate. \( H_d \) is the QD Hamiltonian and the QD we consider here is described by a single orbital with energy \( \varepsilon_d \). The kinetic energy of a lead electron with wavevector \( \mathbf{k} \) is \( \varepsilon_{\mathbf{k}} \) and \( c_{\mathbf{k}\sigma i}^\dagger \) is the annihilation (creation) operator of the lead electron with wavevector \( \mathbf{k} \) and spin \( \sigma \) for the left and right leads \((i = L, R)\). \( \Delta_i \) is the superconducting order parameter on the dot and superconducting leads and \( t \) is the corresponding coupling strength.

We use Fourier transformation of equations of motions to find the Green’s function in the frequency domain
\[ \hat{G}_{dd}^{-1}(i\omega_n) = i\omega_n + h - \varepsilon_d \sigma_z - t^2 \sum_{i=L,R} \sum_{\mathbf{k}} \sigma_i \hat{G}_{kk\sigma i} \sigma_z, \] (4)
where \( \omega_n \) is the fermionic Matsubara frequency and \( \hat{G}_{kk\sigma i} \) is the bare Green’s function of the BCS Hamiltonian of the lead \( i \)

\[ \hat{G}_{kk\sigma i} = (i\omega_n - H_i)^{-1} = \begin{pmatrix} i\omega_n - \varepsilon_k - \Delta e^{i\phi_i} & -\Delta e^{-i\phi_i} \varepsilon_k \end{pmatrix}^{-1} \]
\[ = \frac{(i\omega_n)^2 - E_k^2}{(i\omega_n)^2 - E_k^2} - \frac{\Delta e^{-i\phi_i}}{(i\omega_n)^2 - E_k^2} \] (5)
and \( E_k = \sqrt{E_k^0 + \Delta^2} \). Note here that we have temporally suppressed the Coulomb interaction.

We then use the assumption that the density of states of leads is a constant \( \rho \) to perform the momentum sum. Next, the relation \( \hat{G}_{dd}^{-1} = i\omega_n - H_{\sigma eff}^0 \) allows us to identify the effective Hamiltonian of the dot. It is given by
\[ H_{\sigma eff}^0 = (\varepsilon_d + h) d_i^\dagger d_i + (\varepsilon_d - h) d_i^\dagger d_i - \Gamma_\sigma \left( d_i^\dagger d_i^\dagger + \text{H.c.} \right), \] (6)
where \( \Gamma = 2\pi t^2 \rho \) and \( \Gamma_\sigma = \Gamma_\sigma \frac{2}{\pi} \arctan \left( \frac{\phi}{2} \right) \). In deriving the effective Hamiltonian, we have used the condition that \( \Delta \gg \omega_n \) in the superconducting atomic limit. Finally, the Coulomb interaction needs to be taken into account and we thus obtain the full local effective Hamiltonian,
\[ H_{\sigma eff} = (\varepsilon_d + h) d_i^\dagger d_i + (\varepsilon_d - h) d_i^\dagger d_i - \Gamma_\sigma \left( d_i^\dagger d_i^\dagger + \text{H.c.} \right) \]
\[ - \frac{U}{2} \sum_\sigma (d_i^\sigma d_i^\sigma - 1)^2. \] (7)

### B. Spectrum of the effective Hamiltonian

In this subsection, we wish to determine the eigenstate and eigenenergies of this effective Hamiltonian, Eq. (7). There are four possible states for the single energy level quantum dot, which we shall call the empty state \( |0\rangle \), spin-up state \( |\uparrow\rangle \), spin-down state \( |\downarrow\rangle \), and the paired state \( |\uparrow\downarrow\rangle \). It is obvious that the empty and paired states themselves alone are not eigenstates of the effective Hamiltonian. However, the superpositions of the empty and paired states are the eigenstates of \( H_{\sigma eff} \). We employ the following Bogoliubov transformation,
\[ |\uparrow\rangle = u |\uparrow\downarrow\rangle + v |0\rangle \] (8a)
\[ |-\rangle = -v |\uparrow\downarrow\rangle + u |0\rangle \] (8b)

\[ G_{dd}(\tau) = -(T_\tau \Psi_d(\tau) \Psi_d^\dagger(0)) = \begin{pmatrix} (T_\tau d_\uparrow(\tau) d_\uparrow(0)) & (T_\tau d_\downarrow(\tau) d_\downarrow(0)) \\ (T_\tau d_\downarrow(\tau) d_\uparrow(0)) & (T_\tau d_\uparrow(\tau) d_\downarrow(0)) \end{pmatrix}. \] (3)
and obtain
\[
\begin{align}
  u &= \frac{1}{\sqrt{2}} \left[ 1 + \frac{\xi_d}{\sqrt{\xi_d^2 + \Gamma_{\phi}^2}} \right] \\
  v &= \frac{1}{\sqrt{2}} \left[ 1 - \frac{\xi_d}{\sqrt{\xi_d^2 + \Gamma_{\phi}^2}} \right]
\end{align}
\] (9a)

For the singly occupied states, \( |\uparrow\rangle \) and \( |\downarrow\rangle \), their eigenenergies are not the same when the time-reversal symmetry is broken by a Zeeman interaction \( h \),
\[
E^0_{\uparrow+} = \xi_d + h.
\] (10)

For the BCS-like states, \( |+\rangle \) and \(-\rangle \), their eigenenergies are
\[
E^0_\pm = -\frac{U}{2} \pm \sqrt{\xi_d^2 + \Gamma_{\phi}^2} + \xi_d,
\] (11)

In Sec. II B, we take the limit that the energy gap \( \Delta \) is infinite whereas in reality the energy gap is usually a few kelvins for most conventional superconducting materials. To incorporate this, we adopt the formalism developed in Ref. 11 to go beyond the superconducting atomic limit. Since the details of the SCABS has already been reported in the literature, we shall not reproduce them here and only write down the results. The energy corrections to these four levels are
\[
\begin{align}
  \delta E_{\uparrow+} &= -t^2 \sum_k \left\{ \frac{1}{E_k + E^0_{\uparrow+} - E^0_{\uparrow\downarrow}} + \frac{1}{E_k + E^0_{\uparrow\downarrow} - E^0_{\uparrow+}} + \frac{2\Delta}{E_k} uv |\cos \phi| \left( \left[ \frac{1}{E_k + E^0_{\uparrow\downarrow} - E^0_{\uparrow\downarrow}} - \frac{1}{E_k + E^0_{\uparrow\downarrow} - E^0_{\uparrow+}} \right] \right) \right\} \\
  \delta E_+ &= -t^2 \sum_k \left\{ \frac{1}{E_k - (E^0_{\uparrow+} - E^0_{\uparrow\downarrow})} + \frac{1}{E_k - (E^0_{\uparrow\downarrow} - E^0_{\uparrow+})} \right\} - \frac{2\Delta}{E_k} uv |\cos \phi| \left( \left[ \frac{1}{E_k - (E^0_{\uparrow\downarrow} - E^0_{\uparrow\downarrow})} + \frac{1}{E_k - (E^0_{\uparrow\downarrow} - E^0_{\uparrow+})} \right] \right) \\
  \delta E_- &= -t^2 \sum_k \left\{ \frac{1}{E_k - (E^0_{\uparrow\downarrow} - E^0_{\uparrow+})} + \frac{1}{E_k - (E^0_{\uparrow+} - E^0_{\uparrow\downarrow})} \right\} + \frac{2\Delta}{E_k} uv |\cos \phi| \left( \left[ \frac{1}{E_k - (E^0_{\uparrow\downarrow} - E^0_{\uparrow\downarrow})} + \frac{1}{E_k - (E^0_{\uparrow\downarrow} - E^0_{\uparrow+})} \right] \right) \\
  \delta E_{\downarrow-} &= 2 |\Gamma_{\phi}| uv,
\end{align}
\] (13a)

where \( E_k = \sqrt{\xi_k^2 + \Delta^2} \).

III. RESULTS AND DISCUSSION

A. Phase diagram

In this section, we present our theoretical results on phase diagrams and current-phase relations. We first discuss phase diagrams. The phase transition lines are determined by comparing energies for four possible states, \( |+\rangle \), \(-\rangle \), \( |\uparrow\rangle \), and \( |\downarrow\rangle \). The perturbed energies for these states are given by \( E_s = E^0_s + \delta E_s \), where \( s = +, -, \uparrow, \downarrow \). As mentioned in Ref. 11, the singularities in the integrands of Eqs. (13) limit the range of validity. However, one can extend the range as in the Brillouin-Wigner perturbation theory by using renormalized self-energies. We, therefore, replace \( E^0_s \) appeared in the denominators of Eqs. (13) by \( E_s \). As can be seen from the revised expansions, all energy corrections are now coupled with each other and solutions must be determined self-consistently. We find numerically that in the self-consistent scheme \( |\downarrow\rangle \) and \( |\uparrow\rangle \) still being the states with lowest energies and thus are competing with each other. Therefore, the phase transition lines are determined from the condition when \( E_{\downarrow} = E_{\downarrow+} + \delta E_{\downarrow} = E_{\downarrow\uparrow} + \delta E_{\downarrow\uparrow} = E_{\uparrow} \).

In Fig. 1, we present phase diagrams for various situations. Here, the bandwidth \( D \) of the leads is fixed to be \( 5\pi \Gamma \), and the mutual interaction between electrons in the dot is made negative, \(-U < 0\). In the top panel,
we show the phase diagrams for different superconducting gaps with a fixed Zeeman interaction strength $h = U$. The presence of $h$ breaks the time reversal symmetry and a Kramer’s doublet is no longer a good eigenstate. The dot is spin polarized when the spin down state is the ground state of the system which corresponds to regions inside the domes. When $\Gamma_\phi$ is large, the system turns to the BCS-like state due to the large superconducting proximity effects. For $\Delta \to \infty$, or the atomic limit, the radius of the dome is simply determined by Eq. (12). Using the self-consistent approach, we study systems away from the atomic limit ($\Delta$ is finite). It is interesting to note that the radii of the domes are not changed. However, the height of the dome decreases with increasing $\Delta$, which means the BCS-like phase is also decreased.

In the central panel, we show a blow up of $\Delta = 5\pi\Gamma$ case of the top panel. We see an unexpected reentrant structure of the phase boundary. When $\xi_d \gtrsim 0.5U$, as $\Gamma_\phi/U$ increases from 0, the system first enters into the spin polarized state and turns back to the BCS-like state. This phenomenon is also reported in ferromagnet-superconductor heterostructures\cite{36}.

In the bottom panel of Fig. 1, the superconducting gap for the leads is fixed to be $\Delta = \pi\Gamma$ and phase boundaries for three $h/U$ are shown. The phase transitions when $\Gamma_\phi/U \to 0$ occur at the same positions as in the atomic limit [see Eq. (12)]. From this, one can also infer that the applied magnetic field only affects the radii of phase transition lines. The range for the single spin state is increased when the applied magnetic field is increased. This is because a magnetic field tends to break a Cooper pair and the BCS-like state becomes unfavorable.

In Fig. 2, we fix the bare energy of the quantum dot to be the particle-hole symmetric point, $\xi_d = 0$, and study the superconducting gap versus the Coulomb interaction (we include both attractive and repulsive interaction) phase diagram for several $h$. On the right of each transition line, the Coulomb interaction is more repulsive or less negative depending on the sign of $U$ and the quantum dot prefers to reside in the single-spin state. We note that for a given $\Delta$, the phase transition points move to the left as $\hbar$ is increased. As in the lower panel of Fig. 1, when the magnetic field is stronger, the Cooper pairs become less stable and the region for the single-spin state is enhanced. Therefore, the effect of an applied magnetic field is similar to that of the repulsive Coulomb interaction. As a result, at a given energy gap, a stronger mag-

FIG. 1. Phase diagrams of a single dot coupled to superconducting leads. The system is in the spin-down (BCS) state below (above) each curve. The bandwidth of superconducting leads is $D = 5\pi\Gamma$. For the top panel, we show phase diagrams of three different $\Delta$ with a fixed exchange interaction $h = U$. The central panel is a blow up of $\Delta = 5\pi\Gamma$ of the top panel near the edge of the dome. In the bottom panel, we consider three different ratios of $h/U$. | \( \Delta = 5\pi\Gamma \) | \( \Delta = \pi\Gamma \) | \( \Delta \to \infty \) | \( \Delta = 5\pi\Gamma \) | \( \Delta = \pi\Gamma \) | \( \Delta \to \infty \) |
|---|---|---|---|---|---|
| $\xi_d/U$ | 0.490 | 0.495 | 0.500 | 0.505 | 0.510 |
| $\Gamma_\phi/U$ | 0.00 | 0.05 | 0.10 | 0.15 | 0.20 |

FIG. 2. Phase diagram of a single dot coupled to superconducting leads with fixed energy level of a bare quantum dot, $\xi_d = 0$. The bandwidth of the leads is $D = 10\pi\Gamma$. Several strengths of exchange interaction are considered. The lower left and upper right corners correspond to the BCS-like phase and the spin polarized phase, respectively.
magnetic field shifts the transition point to a less repulsive or more attractive Coulomb interaction. Furthermore, we find that these phase transition curves are smooth when the Coulomb interaction is continuously changed from attractive to repulsive. It can also be seen from the effective unperturbed energies [Eq. 12] that the influence of these two different types of interaction are added together. However, in the atomic limit, the Coulomb interaction only shifts the BCS-like states energy, and it does not affect the single spin states. On the other hand, the magnetic field only shifts the single-spin states, but not the BCS-like state in the unperturbed level. Here, we see that the perturbed energies of the system have the same trend. Furthermore, we note that when a strong magnetic field is applied, the BCS-like state may still be the ground state when the mutual interaction is attractive.

In Fig. 3, the transition lines between the BCS-like state and spin-down states at $\Delta = \pi \Gamma$ for $U$ vs $h$ are plotted in the top panel. Here, we choose $D = 5 \pi \Gamma$. For a fixed $U$ in the top panel, the ground state is the spin-polarized state on the right of the transition line according to the influence of $h$ on the system. For a fixed $h$, the system is in the BCS-like regime below the transition lines where the Coulomb interaction $U$ is small and repulsive or becoming attractive ($U < 0$). It is consistent with the picture of a Cooper pair where a pair of electrons are bound with each other and a smaller repulsive $U$ is less detrimental to the BCS-like state. For an attractive $U$, the system prefers to be in BCS-like states. We consider four different $\xi_d$ and find that when it is decreased the BCS-like region shrinks. It is because the system is away from the particle-hole symmetric point when $\xi_d$ is increased and the BCS-like state of the quantum dot becomes more robust. Again, for a fixed $U$, the system is in the single-spin state on the right of transition lines where $h$ is large. The above discussion shows it is necessary to go beyond the atomic limit in order to quantitatively determine the physics of the SC-QD-SC junctions.

From Eq. (12), we can see that for fixed $\Gamma$ and $\xi_d$, the transition lines are linear in the atomic limit because $-U/2 + h$ is a constant. Although they appear to be linear here when $\Delta$ is finite, we still compute their slopes in the bottom panel of Fig. 3. The results indicate that they deviate from the linear relationship and show that the system behaves quite differently when it is away from the atomic limit. In fact, the slope in the atomic limit is universal regardless of $\Gamma$ and $\xi_d$ and it is equal to $-2$. We clearly see that when $h$ is increased, the system tends to behave like the atomic limit.

From Figs. 1 to 3, one can infer that the Coulomb interaction $U$ and Zeeman effect $h$ both similarly affect phase transition lines. A large and repulsive $U$ increases the energy of the BCS-like state while a high $h$ decreases the energy of the single spin state at least at the unperturbed level. As a result, the large (small) and repulsive $U$ requires a small (large) $h$ for the system to stay in the single-spin (BCS-like) state.

### B. Josephson current

Next, we discuss the Josephson current in our system. The Josephson current can be computed by using the formula $J = 2e \frac{\partial F}{\partial \phi}$, where $F = \frac{1}{\beta} \ln(\mathcal{Z}) = \frac{1}{\beta} \ln(\text{Tr}(e^{-\beta H}))$ is the free energy and $\beta = 1/k_B T$. For simplicity, we consider the zero temperature limit where the free energy is reduced to the ground state energy $J = 2e \frac{\partial E_G}{\partial \phi}$. Therefore, we first numerically determine the ground state energy, $E_G$, in the self-consistent scheme as a function of the phase difference $\phi$ between two superconductors. The supercurrent can then be explicitly computed by taking the numerical derivative of $E_G$ with respect to $\phi$.

In the top panel of Fig. 4, we show the Josephson current phase relations for four different Zeeman energies: $h = 0$, $0.5 \Gamma$, $\Gamma$, and $2 \Gamma$. When $\phi \to 0$, $\Gamma_\phi = \Gamma \frac{\pi}{2} \tan^{-1}(\frac{\phi}{\pi})$ is at its maximum and the energy for the $|\rangle$ state, $E_+ = E^0_- + \delta E_-$, is in principle at its minimum. As a result, the ground state energy is usually in the BCS-like regime when $\phi$ is small. Furthermore, the current phase relation in the

![Graph showing phase diagram of a single dot coupled to superconducting electrodes with a fixed gap $\Delta = \pi \Gamma$. Four different energy levels, $\xi$, of the bare dot are shown. The upper right (lower left) of the curves corresponds to the spin-down (BCS-like) states. In the bottom panel, we consider the slopes of the curves in the top panel.](image-url)
small $\phi$ regime is given by $J = J_0 \sin(\phi)$ corresponding to an ordinary 0-junction. On the other hand, when $\phi \to \pi$, $\Gamma_\phi = \Gamma_0 \tan^{-1}(\frac{E_0}{2}) \cos(\frac{\pi}{2})$ is at its minimum and $E_\pi = E_0^0 + \delta E_\pi$ in principle should be higher than that in the small $\phi$ regime. As a result, in a suitable range the ground state energy may be the spin polarized state and the current phase relation becomes $J = J_0 \sin(\phi - \pi)$ corresponding to a so-called $\pi$-junction. However, we find that the supercurrent in the $\pi$-junction is small relative to that in the 0-junction. It is because the spin-polarized state behaves similarly to a magnetic Kondo impurity that prevents other electrons from passing through the quantum dot. In addition, it can also be explained by the superconducting correlations discussed in Ref. 11. Because the spin-polarized state always carries a smaller superconducting correlation, the related Josephson supercurrent is hence smaller.

In the top panel of Fig. 4, we find that the 0-\pi phase transitions are shifted: the region for $\pi$-junction is increased as $h$ increases. We also find that when $\xi_d = 0$, the dot is in the 0 phase for the entire region of $\phi$ when $h = 0$. This is because the 0 phase corresponds to the BCS-like state and without the exchange interaction the dot never turns into a single-spin state for all possible phase difference. We also note when $\phi = \pi$, there is a sudden jump from a large positive current to a large negative current. It suggests that the dot is in the clean limit and that the contribution from the continuum is not considered. This is not surprising because without the inclusion of $h$ the system cannot stay in the single-spin state and the $\pi$-junction is not energetically stable. Note that in the absence of Zeeman field, the junction is in the BCS-like regime corresponding to a 0-junction. When the Zeeman interaction is strong enough, the spin polarized state is favored for all $\phi$, and the junction turns into a complete $\pi$-junction.

In the central panel of Fig. 4, we consider two slightly larger bare quantum dot energy, $\xi_d$ at fixed $h$ and $U$. We find that as $\xi_d$ increases, the region for the $\pi$ phase is shrinking and the BCS-like state is more stable. The reason behind this is similar to the previous considerations. When $\xi_d$ is away from the particle-hole symmetric point $\xi_d = 0$, $\sqrt{\xi_d^2 + \Gamma_0^2}$ becomes larger and $E_\pi = E_0^0 + \delta E_\pi$ becomes lower. As a result, the BCS-like state (0-phase) is more stable. For $\xi_d = 1.2\Gamma$, there is even no 0-\pi phase transition across the entire $\phi$ range. However, by applying a strong enough magnetic field, the system can still be driven from the 0-phase to the $\pi$ phase (not shown) as clearly demonstrated in the top panel of Fig. 4. In the bottom panel, we consider the particle-hole symmetric point $\xi_d = 0$ and $h = \Gamma$ for several $U$. As can be seen here, the $\phi$ range for the $\pi$ phase, or the spin polarized phase, gets smaller as the attractive interaction gets stronger as we anticipate.

IV. CONCLUSION

In this paper, we use a relatively simple model to include the local effect of an applied magnetic field as well as the phenomenon of attractive Coulomb interaction in superconductor-quantum dot-superconductor Josephson junctions. To go beyond the superconducting atomic limit, we follow a quite successful perturbative scheme based on the path-integral formalism\textsuperscript{11}. In the formalism, all relevant energy scales can be made finite and therefore correspond to more realistic situations.

We first present phase diagrams of superconductor-quantum dot-superconductor junctions under the influence of the interplay between magnetic field and the attractive Coulomb interaction. We use a set of self-consistent equations to calculate Andreev bound state energies and Josephson currents as functions of important experimental knobs including hybridization energy, phase difference between two superconducting electrodes, strengths of Coulomb and exchange interaction, and superconducting energy gap.

We show that in the superconducting atomic limit when an magnetic field is present, its effect is to shift the energy levels of the single spin states of the quantum dot by $\pm h$ depending on the type of spin. On the other hand, the Coulomb interaction shifts the energy levels of BCS-like states (linear combinations of vacuum and paired states) by $-U/2$. As a result, both the magnetic field and Coulomb interaction play important roles in determining the phase transition in the atomic limit ($\frac{\pi}{\hbar} \gg 1$).

When $\frac{\hbar}{\pi} = 5$, we find that the system can exhibit reentrant behavior near the phase boundary. For an attractive Coulomb interaction, the system prefers to stay in the BCS-like state. For this reason, the system tends to exhibit stronger superconducting proximity effects in physical quantities such as superconducting correlation and Josephson current. In order for the dot to transition from the BCS-like state to the single spin state, an external magnetic field must be present. We find that a higher $\xi_d$ will have a lower supercurrent in the 0 phase. In addition, when $U/\Gamma$ is large, the BCS-like regime is enhanced. All the results presented here indicate that superconductor-quantum dot-superconductor provides a platform to study quantum phase transitions as well as switching effects in nanodevices.

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**FIG. 4.** Josephson current of a single dot couple to superconducting leads with a relative phase difference, $\phi$. The bandwidth of conduction electrons in the superconductors is fixed to be $D = 10\pi \Gamma$ and superconducting gaps are the same for both leads and given by $\Delta = \pi \Gamma$. In the top panel, we consider four exchange interactions for fixed mutual interaction $U = \Gamma$ and bare quantum dot energy level $\xi_d = 0$. For the central panel, current phase relations for three different $\xi_d$ at fixed $h = U = \Gamma$. The bottom panel shows cases for three different Coulomb interaction $U/\Gamma$ for a fixed Zeeman interaction $h = \Gamma$ at particle hole symmetric point $\xi_d = 0$. 