Supercurrent and multiple singlet-doublet phase transitions of a quantum dot Josephson junction inside an Aharonov-Bohm ring

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We study a quantum dot Josephson junction inside an Aharonov-Bohm environment. The geometry is modeled by an Anderson impurity coupled to two directly linked BCS leads. We illustrate that the well-established picture of the low-energy physics being governed by an interplay of two distinct (singlet and doublet) phases is still valid for this interferometric setup. The phase boundary depends, however, nonmonotonically on the coupling strength between the superconductors, causing the system to exhibit re-entrance behavior and multiple phase transitions. We compute the zero-temperature Josephson current and demonstrate that it can become negative in the singlet phase by virtue of the Coulomb interaction U. As a starting point, the limit of large superconducting energy gaps $\Delta = \infty$ is solved analytically. In order to tackle arbitrary $\Delta < \infty$ and $U > 0$, we employ a truncated functional renormalization-group scheme which was previously demonstrated to give quantitatively reliable results for the quantum dot Josephson problem.

I. INTRODUCTION

The low-energy behavior of quantum dot Josephson junctions is governed by an interplay of superconductivity and the Kondo effect. The physics emerging from the competition of these correlation phenomena was discussed decades ago in the context of magnetic impurities inside superconducting metals.[1–3] If the Kondo energy scale T_K is much larger than the superconducting gap Δ, local magnetic moments are screened by virtue of the Kondo effect. This causes Cooper pairs to break, and the ground state of the system becomes a Kondo rather than a BCS singlet. In the opposite limit $T_K \ll \Delta$, Kondo screening is disturbed due to the superconducting gap at the Fermi energy, and the ground state describes free magnetic moments. At temperature $T = 0$, a first-order level-crossing quantum phase transition from a nonmagnetic singlet to a degenerate (so-called magnetic) ground state is observed if Δ/T_K increases.

In recent years, the rise of nanotechnology allowed for sandwiching quantum dots between superconducting electrodes and for measuring the equilibrium Josephson current as a function of well-controllable microscopic parameters.[4–14] This was the motivation to theoretically reinvestigate the interplay between superconductivity and Kondo physics in the context of (Anderson-type) models which feature all parameters (and not only Δ/T_K) necessary to describe the experimental quantum dot Josephson junction.[15–23] Both the phase boundary between the (Kondo) singlet and the (magnetic) doublet phases, and the supercurrent were calculated using reliable many-particle methods to tackle the vital Coulomb interaction U.[18,22,23] In particular, it was demonstrated that the critical supercurrent as a function of the quantum dot energy ϵ can be obtained in good agreement with experimental data.[14]

If a quantum dot is placed in one arm of a nonsuperconducting closed Aharonov-Bohm geometry, signatures of the Fano effect can be experimentally observed in mesoscopic systems.[24–26] In addition, the interferometric setup allows for extracting physical properties which cannot be accessed by measurements on the isolated dot (such as the transmission phase).[27–29] Both situations were investigated theoretically using Anderson-type impurity models as well as appropriate many-body methods in order to obtain a physical understanding consistent with the observed data.[30,31] In contrast, no interferometric experiments on quantum dots within a superconducting environment have been performed so far. However, in consideration of the rapid progress in nanoscience, it is reasonable to assume that experimental (e.g., transport) data on such setups will become available fairly soon.

As mentioned above, both the singlet-doublet phase transition and the supercurrent of the quantum dot Josephson junction were extensively investigated theoretically, most times employing the single impurity Anderson model with BCS source and drain leads.[15–23] In contrast, the Aharonov-Bohm situation where both superconductors are in addition directly linked by a hopping matrix element t_d has only been partly investigated. Zhang[32] used a slave-boson mean-field approach to compute the supercurrent for the (singlet) situation where the Kondo temperature T_K is larger than the energy gap Δ. However, the author failed to obtain correct results in the analytically solvable noninteracting case $U = 0$, rendering his results questionable.[33] The opposite (doublet) situation with $T_K < \Delta$ was studied by Osawa *et al.*[34] They employ, however, a Hartree-Fock framework which cannot account properly for Kondo correlations with the latter being a vital ingredient for the problem at hand. Most surprisingly, both works do not at all address the question whether the general picture of the existence of singlet and doublet low-energy states survives if the superconductors are connected directly and, if so, how the ground state actually depends on the physical parameters (particularly t_d) of the system. It is the first aim of this paper to clarify this issue and to demonstrate that the $T = 0$ "phase boundary" is affected nonmonotonically by a finite coupling $t_d > 0$, causing the system to exhibit re-entrance behavior and multiple singlet-doublet

FIG. 1. (Color online) The interferometric quantum dot Josephson junction considered in this paper.

transitions. Second, we present reliable results for the zero-temperature Josephson current J for arbitrary system parameters [not focusing on a specific regime of Δ/T_K (Ref. 35)] and particularly illustrate that J can become negative in the singlet phase.[37] Our starting point is the so-called atomic limit $\Delta=\infty$ which can be treated analytically even in the presence of finite Coulomb correlations. In order to address arbitrary $\Delta<\infty$ and $U>0$, we employ the functional renormalization group (FRG). By comparison with accurate data obtained from the numerical renormalization-group (NRG) framework, it was illustrated that this (after truncation) approximate method succeeds both qualitatively and quantitatively in producing the phase boundary and supercurrent for the simple quantum dot Josephson junction ($t_d=0$).[23] In addition, we will demonstrate that for $t_d>0$ the FRG scheme benchmarks excellently against the analytic result at $\Delta=\infty$, thereby altogether providing a reliable tool in studying the problem at hand.

This paper is organized as follows. In Sec. II, we introduce the single impurity Anderson model with directly linked BCS superconducting leads and compute the associated noninteracting impurity Green's function. The limit $\Delta=\infty$ is solved analytically in Sec. III A, and Sec. III B is devoted to a short introduction of the FRG framework. The phase boundary of the singlet-doublet level-crossing phase transition as well as the Josephson current are discussed in Secs. IV and V, respectively. We conclude our paper with a short summary (Sec. VI).

II. MODEL

In order to describe the geometry depicted in Fig. 1, we introduce the standard BCS and Anderson impurity Hamiltonian

$$H^{\text{dot}} = \sum_\sigma \epsilon d_\sigma^\dagger d_\sigma + U\left(d_\uparrow^\dagger d_\uparrow - \frac{1}{2}\right)\left(d_\downarrow^\dagger d_\downarrow - \frac{1}{2}\right),$$

$$H_{s=L,R}^{\text{lead}} = \sum_{k\sigma} \epsilon_{sk} c_{sk\sigma}^\dagger c_{sk\sigma} - \Delta\sum_k (e^{i\phi_s} c_{sk\uparrow}^\dagger c_{s-k\downarrow}^\dagger + \text{H.c.}),$$

$$\tag{1a}$$

as well as the coupling terms

$$H_{s=L,R}^{\text{coup}} = -\frac{t}{\sqrt{N}}\sum_{k\sigma} c_{sk\sigma}^\dagger d_\sigma + \text{H.c.},$$

$$H^{\text{direct}} = -\frac{t_d}{N}\sum_{k_1 k_2 \sigma} c_{Lk_1\sigma}^\dagger c_{Rk_2\sigma} + \text{H.c.}. \tag{1b}$$

Both $c_{sk\sigma}$ and d_σ denote usual fermionic annihilation operators. The quantum dot is characterized by a gate voltage ϵ

and a local Coulomb repulsion U between spin-up and spin-down electrons. For simplicity, we assume that the left ($s=L$) and right ($s=R$) BCS leads have equal superconducting energy gaps Δ while exhibiting a finite phase difference $\phi=2\phi_L=-2\phi_R$. Both leads are locally coupled to each other and to the quantum dot by (real) hopping amplitudes t_d and t, respectively.

As a first step to solve the quantum many-particle problem associated with Eqs. (1a) and (1b), it is useful to compute the noninteracting Green's function of the quantum dot. This is achieved straightforwardly using the equation-of-motion technique.[34,38] One obtains

$$\mathcal{G}^0(z) = \begin{pmatrix} \langle\langle d_\uparrow d_\uparrow^\dagger \rangle\rangle_z & \langle\langle d_\uparrow d_\downarrow \rangle\rangle_z \\ \langle\langle d_\downarrow^\dagger d_\uparrow^\dagger \rangle\rangle_z & \langle\langle d_\downarrow^\dagger d_\downarrow \rangle\rangle_z \end{pmatrix}_{U=0}$$

$$= \frac{1}{z - \epsilon\tau_3 + t\tau_3 A_L(z) + t\tau_3 A_R(z)}. \tag{2}$$

Here, τ_i denote the Pauli matrices, and A_s determines the lead "self-energy:"

$$A_{s=L,R}(z) = t\frac{t_d g_s(z)\tau_3 g_{\bar{s}}(z)\tau_3 - g_s(z)\tau_3}{1 - t_d^2 g_s(z)\tau_3 g_{\bar{s}}(z)\tau_3}, \tag{3}$$

with the definition $\bar{L}=R$, $\bar{R}=L$ as well as the implicit understanding (here and in the following) that the inverse is multiplied from the left. The local Green's function $g_s(z)$ of the isolated BCS leads is given by

$$g_s(z) = -\frac{\pi\rho}{\sqrt{\Delta^2 - z^2}}\begin{pmatrix} z & -\Delta e^{i\phi_s} \\ -\Delta e^{-i\phi_s} & z \end{pmatrix}. \tag{4}$$

We have assumed the local density of states $\rho=\Sigma_k\delta(\epsilon-\epsilon_{sk})/N$ and thus the hybridization energy

$$\Gamma = 2\pi\rho t^2 \tag{5}$$

to be constant, implementing the so-called wide-band limit.

Following the arguments presented in Ref. 23, one can show that the Josephson current $J_s=i\langle[H,N_s]\rangle$ (with $N_{s=L,R}$ being the particle number operator of the left and right leads, respectively) can be computed from the exact expression (taking $\hbar=1$ and the electron charge $e=1$ in the following)

$$J_s = 2T\sum_{i\omega} \text{Im Tr}[t\mathcal{G}_{sd}(i\omega) - t_d\mathcal{G}_{s\bar{s}}(i\omega)], \tag{6}$$

where T is the temperature of the system, and $\mathcal{G}_{sd}(z)$ and $\mathcal{G}_{s\bar{s}}(z)$ denote the interacting dot-lead and lead-lead Green's function, respectively. The first and second terms of Eq. (6) can naturally be regarded as the impurity and direct contribution to the supercurrent. Employing the equation-of-motion technique and generalizing the resulting relations by virtue of the Dyson equation for $U\neq 0$, both $\mathcal{G}_{sd}(z)$ and $\mathcal{G}_{s\bar{s}}(z)$ can be expressed in terms of the interacting dot Green's function $\mathcal{G}(z)$ as follows:

$$\mathcal{G}_{sd}(z) = A_s(z)\mathcal{G}(z),$$

$$\mathcal{G}_{s\bar{s}}(z) = A_s(z)\mathcal{G}(z)A_{\bar{s}}^{\dagger}(z^*) - \frac{t_d g_s(z)\tau_3 g_{\bar{s}}(z)}{1 - t_d^2 g_s(z)\tau_3 g_{\bar{s}}(z)\tau_3}. \quad (7)$$

At $\Gamma = 0$, the right-hand side of Eq. (6) can be evaluated analytically up to second order in t_d, leading to the sinusoidal law $J \sim \sin(\phi)$ which describes the ordinary Josephson junction.[38]

Employing a gauge transformation, one can show that the supercurrent obtained from Eq. (6) fulfills $J_L = -J_R = J$, provided that $\mathcal{G}(z)$ is given exactly.[23] In the present paper, we focus exclusively on the situation of fully symmetric superconducting leads (featuring equal-energy gaps $\Delta = \Delta_L = \Delta_R$ as well as equal hybridization strengths $\Gamma = 2\Gamma_L = 2\Gamma_R$) and can thus refrain (since $J_L = -J_R$ trivially holds) from addressing the issue of current conservation within the approximate functional renormalization-group approach introduced below.[23]

III. SOLUTION STRATEGIES

In order to study the quantum many-particle problem implicated by the Hamiltonian of Eqs. (1a) and (1b), we proceed as follows. First, we demonstrate that in the limit of large BCS gaps $\Delta = \infty$ one can derive an analytic expression for the phase boundary describing the singlet-doublet phase transition (Sec. III A). In order to tackle the Coulomb correlation U at arbitrary $\Delta < \infty$, we introduce a truncated functional renormalization-group scheme (Sec. III B). By comparison with numerical RG data, it was previously shown that the latter provides an accurate tool to calculate the phase boundary as well as the supercurrent for the (noninterferometric) quantum dot Josephson junction.[23]

A. Analytic treatment of the limit $\Delta = \infty$

For $t_d = 0$, it was previously demonstrated (see Refs. 22 and 23) that the limit of large superconducting gaps $\Delta = \infty$ allows for an analytic treatment even in the presence of finite Coulomb correlations U. This is still possible for the Aharonov-Bohm situation. Namely, at $\Delta = \infty$ the noninteracting dot Green's function [Eq. (2)] becomes

$$[\mathcal{G}^0(z)]^{-1} = \begin{pmatrix} z - \tilde{\epsilon} & \tilde{\Delta} \\ \tilde{\Delta} & z + \tilde{\epsilon} \end{pmatrix}, \quad (8)$$

where the effective parameters $\tilde{\epsilon}$ and $\tilde{\Delta}$ are given by

$$\tilde{\epsilon} = \epsilon + \Gamma \frac{\tilde{t}_d \cos(\phi) + \tilde{t}_d^3}{1 + 2\tilde{t}_d^2 \cos(\phi) + \tilde{t}_d^4},$$

$$\tilde{\Delta} = \Gamma \cos(\phi/2) \frac{1 + \tilde{t}_d^2}{1 + 2\tilde{t}_d^2 \cos(\phi) + \tilde{t}_d^4}, \quad (9)$$

and $\tilde{t}_d = \pi\rho t_d$. Including the interacting part, the problem is thus equivalent to diagonalizing the effective two-particle Hamiltonian

$$H_{\text{eff}} = \tilde{\epsilon}d_{\uparrow}^{\dagger}d_{\uparrow} + \tilde{\epsilon}d_{\downarrow}^{\dagger}d_{\downarrow} - \tilde{\Delta}(d_{\uparrow}^{\dagger}d_{\downarrow}^{\dagger} + d_{\downarrow}d_{\uparrow})$$

$$+ U\left(d_{\uparrow}^{\dagger}d_{\uparrow} - \frac{1}{2}\right)\left(d_{\downarrow}^{\dagger}d_{\downarrow} - \frac{1}{2}\right). \quad (10)$$

This can be achieved straightforwardly by virtue of a Bogolyubov transformation.[38] It turns out that the ground state of the system is either nondegenerate (a singlet which at sufficiently large U can be thought of featuring Kondo screening and broken Cooper pairs) or doubly degenerate (a "magnetic" doublet generally associated with a free spin), illustrating that this well-known picture is still valid in the presence of a finite coupling $t_d > 0$. By comparison of the corresponding many-particle energies, one can show that the level crossing and thus the zero-temperature "phase transition" is determined by the implicit equation

$$U^2 = 4\tilde{\epsilon}^2 + 4\tilde{\Delta}^2. \quad (11)$$

Since $\cos(\phi)$ can become negative for $0 \le \phi \le \pi$, the right-hand side of Eq. (11) is not necessarily a monotonic function of the bare parameters ϵ/Γ and t_d/Γ, immediately indicating re-entrance behavior and multiple singlet-doublet phase transitions. This will be discussed in detail in Sec. IV.

B. Functional renormalization-group approach

The functional renormalization group is one implementation of Wilson's general RG idea for interacting many-particle systems.[39] It starts with introducing an energy cutoff Λ into the noninteracting Green's function of the system under consideration. Here, we choose a multiplicative infrared cutoff $\Theta(|\omega| - \Lambda)$ in Matsubara frequency space. By taking the derivative of many-particle vertex functions (such as the self-energy) with respect to the cutoff parameter Λ, one obtains an infinite hierarchy of flow equations, and subsequent integration from $\Lambda = \infty$ down to the cutoff-free system $\Lambda = 0$ leads to an in principle exact solution of the many-particle problem. In practice, however, the infinite hierarchy needs to be truncated, rendering the FRG an approximate method. In this paper, we employ a truncation scheme that keeps the flow equations for the self-energy and the two-particle vertex evaluated at zero external frequencies. The resulting approximation to both quantities is frequency independent, contains at least all terms up to order U, and can be computed numerically with minor effort. It was demonstrated in recent works that this truncated FRG scheme successfully describes correlation effects (e.g., aspects of Kondo physics) in quantum impurity systems.[31,40] In particular, comparison with numerical RG reference data showed that both the singlet-doublet phase transition and the Josephson current of a (noninterferometric) quantum dot Josephson junction can be computed reliably using this framework.[23]

The FRG flow equations for the diagonal and anomalous parts of the self-energy (Σ^{Λ} and $\Sigma_{\Delta}^{\Lambda}$) associated with the Hamiltonian of Eqs. (1a) and (1b) can be obtained by a slight generalization of the derivation presented in Ref. 23. They are given by

$$\dot{\Sigma}^\Lambda = \frac{U^\Lambda}{\pi} \text{Re}[\widetilde{\mathcal{G}}_{22}^\Lambda(i\Lambda)],$$

$$\dot{\Sigma}_\Delta^\Lambda = -\frac{U^\Lambda}{2\pi}[\widetilde{\mathcal{G}}_{12}^\Lambda(i\Lambda) + \widetilde{\mathcal{G}}_{12}^\Lambda(-i\Lambda)], \tag{12}$$

and the flow equation of the effective interaction U^Λ reads

$$\dot{U}^\Lambda = \frac{(U^\Lambda)^2}{\pi} \text{Re}[\widetilde{\mathcal{G}}_{12}^\Lambda(i\Lambda)\widetilde{\mathcal{G}}_{21}^\Lambda(i\Lambda) + \widetilde{\mathcal{G}}_{12}^\Lambda(i\Lambda)\widetilde{\mathcal{G}}_{21}^\Lambda(-i\Lambda)$$

$$- \widetilde{\mathcal{G}}_{11}^\Lambda(i\Lambda)\widetilde{\mathcal{G}}_{22}^\Lambda(i\Lambda) - \widetilde{\mathcal{G}}_{11}^\Lambda(i\Lambda)\widetilde{\mathcal{G}}_{22}^\Lambda(-i\Lambda)]. \tag{13}$$

We have defined the matrix $\widetilde{\mathcal{G}}^\Lambda(i\omega)$ via

$$[\widetilde{\mathcal{G}}^\Lambda(i\omega)]^{-1} = [\mathcal{G}^0(i\omega)]^{-1} - \begin{pmatrix} \Sigma^\Lambda & \Sigma_\Delta^\Lambda \\ (\Sigma_\Delta^\Lambda)^* & -\Sigma^\Lambda \end{pmatrix}. \tag{14}$$

The initial conditions to the coupled differential Eqs. (12) and (13) read $\Sigma^{\Lambda\to\infty}=0$, $\Sigma_\Delta^{\Lambda\to\infty}=0$, and $U^{\Lambda\to\infty}=U$, and one can carry out a numerical integration using standard Runge-Kutta routines in order to obtain the frequency-independent FRG approximations $\Sigma=\Sigma^{\Lambda=0}$ and $\Sigma_\Delta=\Sigma_\Delta^{\Lambda=0}$ to the self-energy. Thereafter, the Josephson current can be computed from Eq. (6) and the approximate impurity Green's function $\mathcal{G}=\widetilde{\mathcal{G}}^{\Lambda=0}$.

IV. PHASE BOUNDARY

A. No direct coupling ($t_d=0$)

For the simple quantum dot Josephson junction ($t_d=0$), it was previously demonstrated that the boundary between the singlet and doublet phases of the system is, even though roughly being governed by the ratio Δ/T_K, an explicit function of all parameters of the system.[15,18,22,23] The latter are the Coulomb interaction U, the quantum dot energy ϵ, the superconducting gap Δ, the dot-lead hybridization Γ, and the phase difference ϕ. According to Eq. (11), the atomic-limit phase boundary for $t_d=0$ is determined by

$$U^2 = 4\epsilon^2 + 4\Gamma^2 \cos^2(\phi/2), \tag{15}$$

illustrating that an increase in either U or ϕ drives the system toward the doublet phase, whereas a nondegenerate ground state is energetically favored the more ϵ is shifted away from particle-hole symmetry.[41] Functional and numerical renormalization-group calculations showed that the overall size of the doublet regime shrinks for $\Delta<\infty$ but all parameter dependencies of the phase boundary can still be understood in analogy to the case of $\Delta=\infty$.[23] We will now demonstrate that the same holds true for the more complicated case of $t_d\neq0$.

B. Aharonov-Bohm situation, $\Delta=\infty$

In order to understand how a direct link between the superconductors affects the boundary of the singlet-doublet phase transition at $\Delta=\infty$, it is instructive to study the parameter dependence of the critical interaction strength U_{crit} for the case of particle-hole symmetry $\epsilon=0$ first. The quantity

U_{crit} can be defined unambiguously, whereas, e.g., a critical coupling strength t_d^{crit} cannot due to the structure of Eq. (11). For $\phi=0$ and $\phi=\pi$, one obtains

$$\frac{U_{\text{crit}}^2}{4} = \begin{cases} \Gamma^2/(1+\widetilde{t}_d^2) & \phi=0, \\ \widetilde{t}_d^2\Gamma^2/(1-\widetilde{t}_d^2)^2 & \phi=\pi, \end{cases} \tag{16}$$

illustrating that there is a fundamental difference between both cases. At small ϕ, the system is driven into the doublet phase if t_d is increased [see, e.g., the curve for $\phi=0.2\pi$ in the inset of Fig. 2(b)]. In contrast, the phase boundary $U_{\text{crit}}(t_d)$ depends nonmonotonically on the direct coupling strength for $\phi=\pi$. At small values of t_d, U_{crit} increases quadratically, acquires a maximal value, and finally falls off quadratically for large t_d [see, e.g., the data for $\phi=0.8\pi$ in the inset of Fig. 2(b)]. Thus, a system which is initially in a doublet state can be driven into the singlet phase by increasing the coupling t_d at fixed U but eventually always re-enters the doublet phase.

Using Eq. (11), one can show that the behavior of the phase boundary $U_{\text{crit}}(t_d)$ for arbitrary ϕ is always qualitatively similar to the case of either $\phi=0$ or $\phi=\pi$. The onset of a nonmonotonic dependence on t_d occurs for $\phi\approx0.29\pi$, implying that one can expect to observe re-entrance behavior even if the phase difference cannot be controlled precisely. If the gate voltage is tuned away from the point of particle-hole degeneracy, the phase boundary exhibits an additional extremum [see Figs. 2(a) and 2(c)]. An additional minimum occurs for either large ϕ and arbitrary $\epsilon\neq0$ or small ϕ and $\epsilon<0$, whereas one observes an additional maximum for small ϕ and $\epsilon>0$. Since the critical value $U_{\text{crit}}(t_d=0)$ is always larger than the asymptote $U_{\text{crit}}(t_d\to\infty)$, the system can exhibit a total of three singlet-doublet phase transitions if the coupling strength t_d is varied at fixed U (and large ϕ).

Due to the fact that the right-hand side of Eq. (11) is a horizontally shifted quadratic function of the impurity energy ϵ (see FRG data for finite $\Delta<\infty$ in Fig. 4), the above-mentioned re-entrance behavior can also be observed by changing the impurity energy ϵ while fixing all other parameters. Tuning ϵ away from particle-hole symmetry can occasionally drive a system which is initially in a singlet state into the doublet and then ultimately back into the singlet phase. In contrast, the dependence of U_{crit} on the phase difference ϕ is always monotonous. At small t_d, a doublet ground state is favored if ϕ is increased, whereas the opposite holds for larger t_d [see Figs. 2(a)–2(c)]. For $\epsilon<0$ and $t_d\to\infty$, the system is again monotonously driven toward the doublet phase if ϕ is increased. One can analytically demonstrate that the crossover between the regimes of $\partial_\phi U_{\text{crit}}\lessgtr0$ is characterized by values of t_d where the phase boundary is completely independent of ϕ.

C. Aharonov-Bohm situation, arbitrary Δ

The truncated FRG scheme introduced in Sec. III B allows for computing (an approximation to) the self-energy but does not yield the many-particle eigenstates of the system under consideration (in contrast, e.g., to the numerical renormalization group). Within this approach, the phase boundary is determined from discontinuities in the supercurrent with the understanding [based on the analytic treatment of the
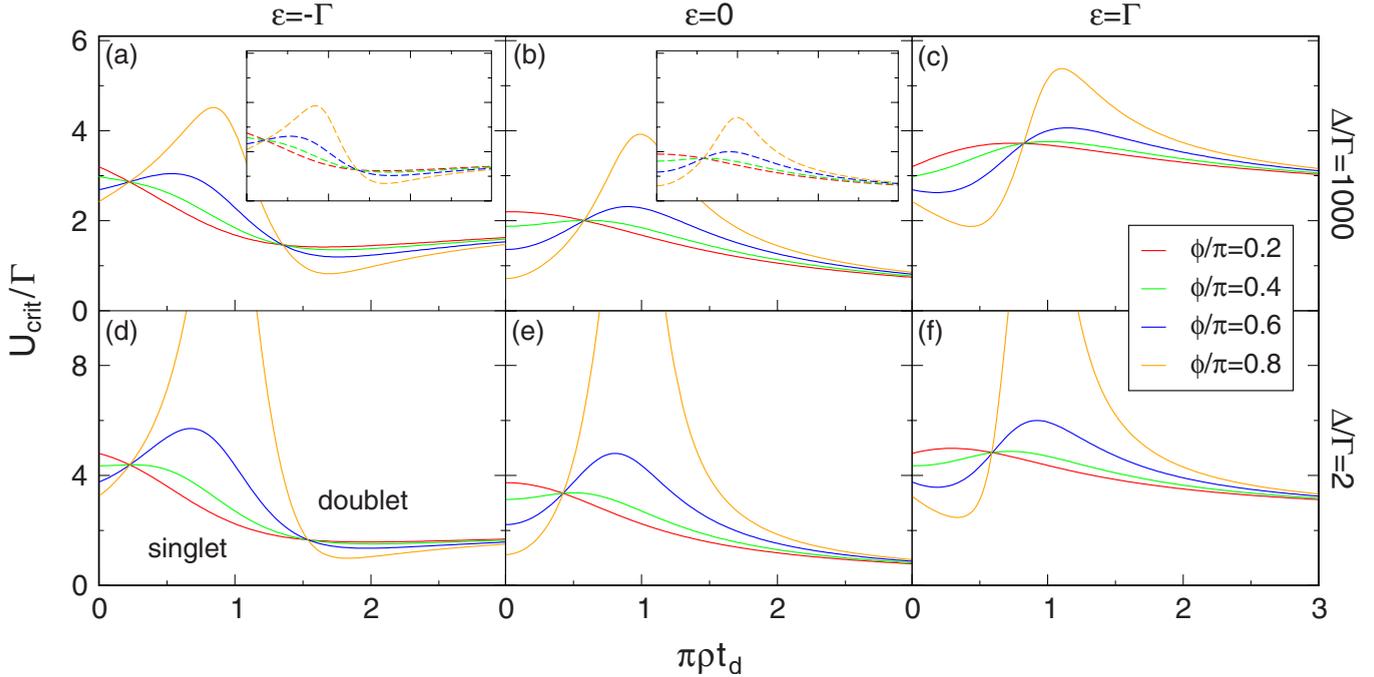
FIG. 2. (Color online) The critical interaction strength U_{crit} as a (nonmonotonic) function of the direct coupling t_d for different BCS gaps Δ and impurity energies ϵ, altogether characterizing the singlet-doublet level-crossing phase transition of the Aharonov-Bohm quantum dot Josephson junction. Solid lines where obtained from the FRG approach introduced in Sec. III B while dashed lines display the analytic result derived in the limit $\Delta=\infty$ [see Eq. (11)]. The phase difference between the left and right superconducting leads is given by $\phi=0.2\pi$, 0.4π, 0.6π, and 0.8π (from top to bottom at $t_d=0$). The axis of the insets are scaled the same as the axis of the corresponding main part.

limit $\Delta=\infty$ as well as on NRG calculations at $t_d=0$ (Ref. 18)] that the ground state is nondegenerate in the limit of small U.

For the simple quantum dot Josephson junction ($t_d=0$), comparison with NRG data illustrated that the approximate FRG scheme describes the phase boundary as well as the supercurrent both qualitatively and quantitatively at small to intermediate Coulomb correlations $U \lesssim 8\Gamma$, whereas at larger U qualitative features of both quantities are still captured correctly.[23] Comparing FRG data for large Δ with the analytic result of Eq. (11) shows that the former is also well suited in tackling the problem at hand. The FRG reproduces all characteristics of the phase boundary at $t_d>0$ correctly [compare the insets of Figs. 2(a) and 2(b) with the main parts]; only the size of the singlet phase is slightly overestimated. The latter tendency was already observed at $t_d=0$.

FRG calculations at finite $\Delta<\infty$ demonstrate that all parameter dependencies of the phase boundary are similar to the case of $\Delta=\infty$; only the size of the doublet regime shrinks [see Figs. 2, 3, and 4(a) for detailed comparisons of $U_{crit}(t_d)$ and $U_{crit}(\epsilon)$, respectively]. This is again consistent with results for the simple quantum dot Josephson junction ($t_d=0$).[23] Since the FRG scheme, however, is approximative in U but the critical interaction strength U_{crit} becomes large for small Δ, it is reasonable to additionally study the phase boundary in terms of a different quantity. It turns out that a critical phase difference ϕ_{crit} can always be defined unambiguously, and that the behavior of $\phi_{crit}(t_d, U)$ for arbitrary Δ is similar to the atomic-limit solution [see Fig. 4(b)]. One can thus conclude that all parameter dependencies of the phase boundary can be understood from Eq. (11), only the

size of the doublet regime shrinks monotonously for finite $\Delta<\infty$.[42]

V. JOSEPHSON CURRENT

In this section, we present zero-temperature FRG results for the equilibrium supercurrent J flowing through the Josephson junction in the presence of a finite phase difference ϕ between the superconducting leads. According to Eq. (6),
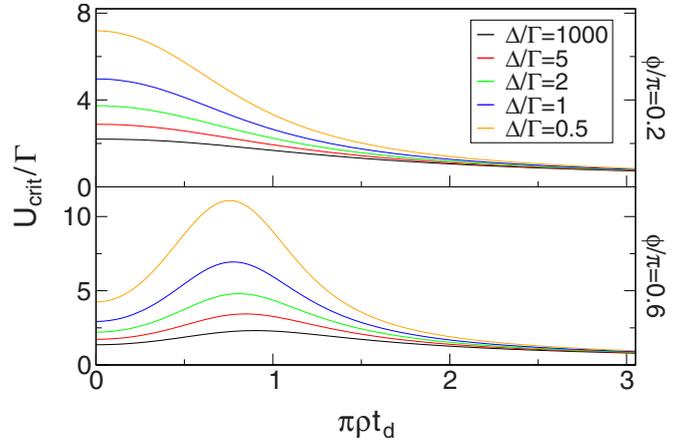

FIG. 3. (Color online) The same as Fig. 2, but for fixed $\epsilon=0$ and different $\Delta/\Gamma=1000$, 5, 2, 1, and 0.5 (from bottom to top). The phase boundary always resembles the analytic form derived in the limit $\Delta=\infty$ [Eq. (11)]; only the size of the doublet phase shrinks monotonously with the BCS energy gap.

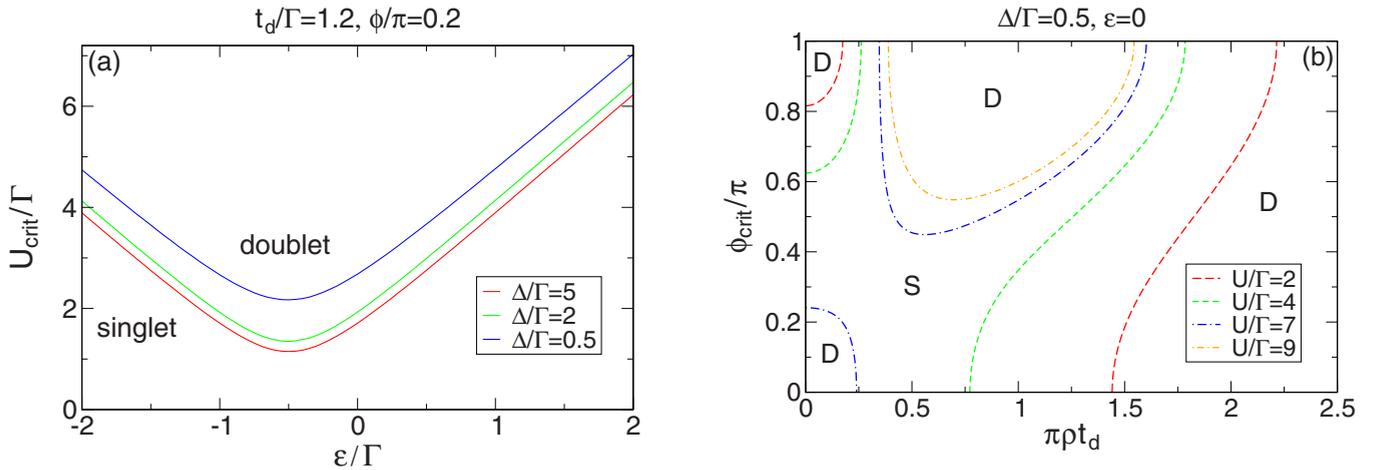FIG. 4. (Color online) (a) FRG results for the critical interaction U_{crit} as an (almost quadratic) function of the impurity energy ϵ for $\Delta/\Gamma=5$, 2, and 0.5 (from bottom to top). (b) Critical phase difference ϕ_{crit} separating the singlet (S) from the doublet (D) phase as a function of the direct coupling t_d. The displayed behavior is similar to analytic result derived at $\Delta=\infty$.

this current can be interpreted to comprise of a "direct" and an "impurity" contribution. In contrast to the phase boundary, it is not determined solely by the dot Green's function, rendering it impossible to derive an analytic result for J in the limit $\Delta=\infty$. Thus, we focus exclusively on discussing FRG data for the Josephson current, again recalling that this framework was successfully benchmarked against numerical RG reference data for $t_d=0$.[23]

In order to discuss how a direct link between the superconducting leads affects the supercurrent J, it is instructive to recall the simple quantum dot Josephson junction ($t_d=0$) first. For small Δ/T_K, the system is in the singlet phase for all impurity energies ϵ, and the current $J(\epsilon)$ exhibits a line shape which resembles the linear-response conductance of the ordinary single impurity Anderson model (see the $t_d=0$–curves of Fig. 5). In the opposite limit, $J(\epsilon)$ changes discontinuously at some critical value $\pm\epsilon_{\mathrm{crit}}$ as the system enters the doublet phase. The current becomes negative and almost independent of the impurity energy.[43] In both cases, the evolution of $J(\epsilon)$ in the presence of a finite link $t_d>0$ is
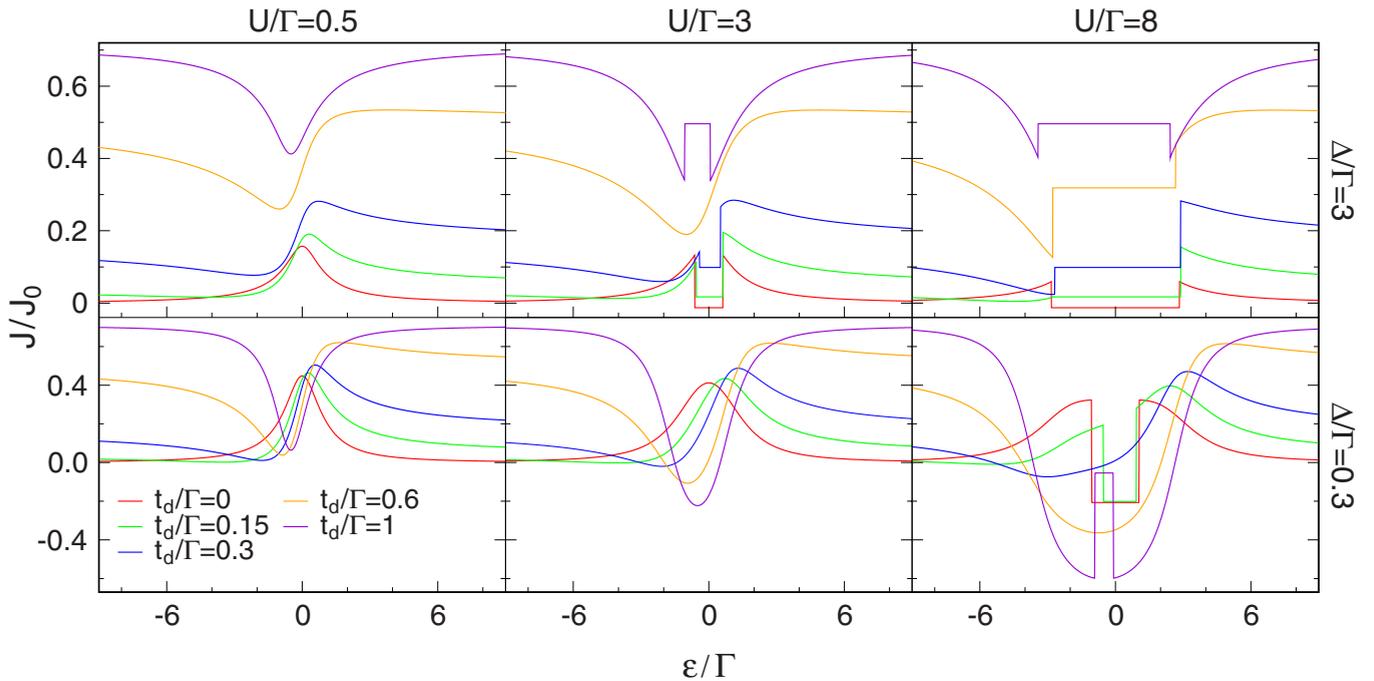

FIG. 5. (Color online) Josephson current J (in units of $J_0=e\Delta/\hbar$) as a function of the impurity energy ϵ for constant $\phi=0.5\pi$, and $t_d/\Gamma=0$, 0.15, 0.3, 0.6, and 1.0 (from bottom to top at large ϵ). The results were obtained from the FRG framework. In presence of a finite coupling t_d, $J(\epsilon)$ acquires a Fano-type line shape analogous to the linear-response conductance of the ordinary Anderson model, and the nonmonotonic phase boundary manifests as repeatedly appearing and disappearing discontinuities. In addition, one observes that the Josephson current can become negative in the singlet phase (see, e.g., the lower right panel which describes a singlet situation at intermediate and large ϵ). The displayed behavior is generic for arbitrary phase differences ϕ.
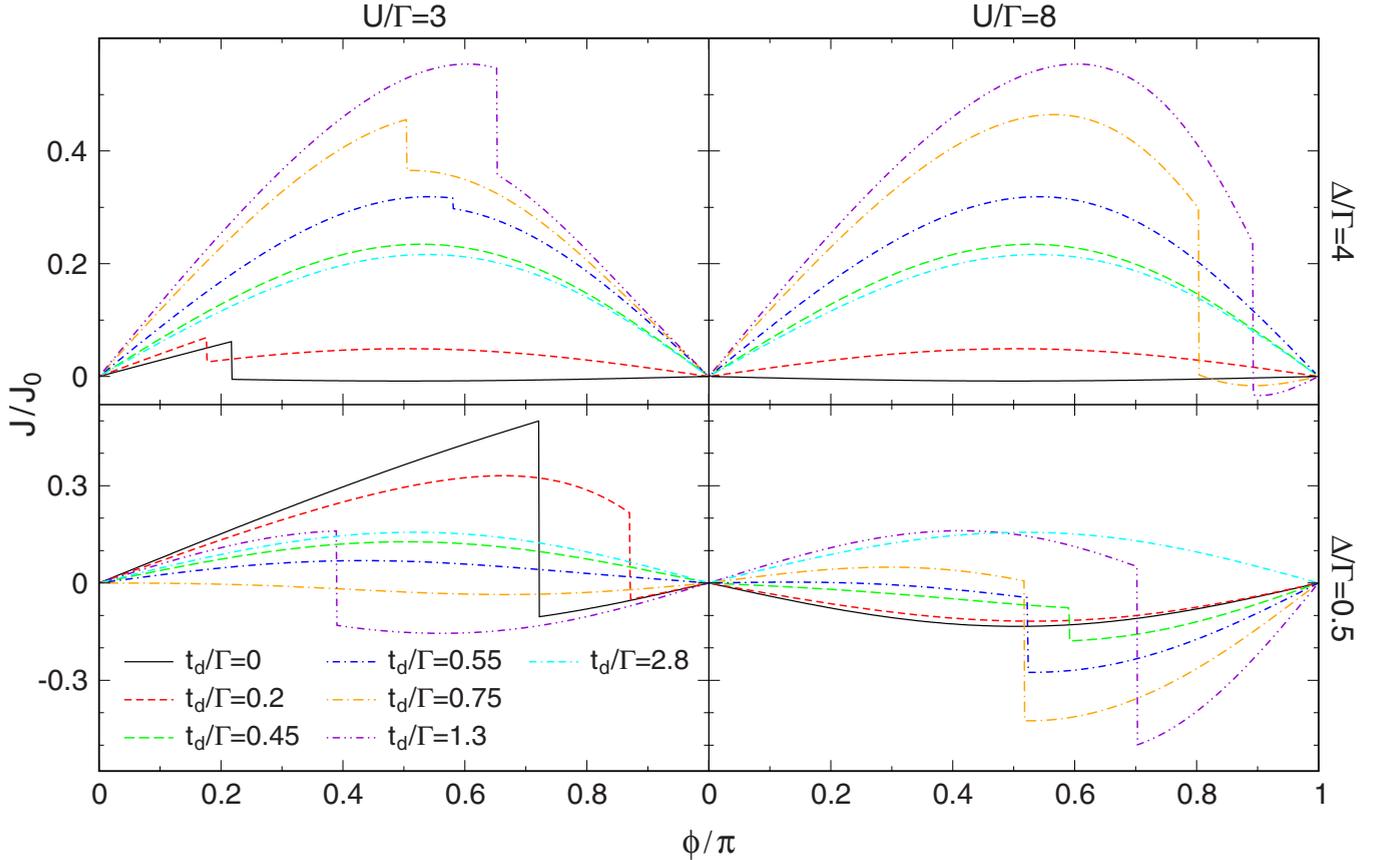
FIG. 6. (Color online) Josephson current J (in units of $J_0=e\Delta/\hbar$) as a function of the phase difference ϕ for particle-hole symmetry $\epsilon=0$. Note that in the lower right panel the system is in a singlet state for $t_d \approx \Gamma$ and large ϕ, illustrating that the current can become negative in this regime by virtue of the Coulomb interaction.

Fano type.[32,34] In addition, the nonmonotonic dependence of the phase boundary on the coupling strength t_d results in multiple singlet-doublet phase transitions manifesting as the appearance and disappearance of discontinuities of $J(\epsilon)$ (see Fig. 5). One should particularly note that no matter how small U or Δ, the system will always enter the doublet phase in the limit of large hoppings t_d, provided that the impurity energy is not too large.

For the simple quantum dot Josephson junction ($t_d=0$), the supercurrent is always positive (negative) in the singlet (doublet) phase. Both no longer necessarily hold in the presence of a finite coupling t_d. Whereas it is rather intuitive that J can become positive in the doublet regime due to the additional direct link (having in mind the ordinary Josephson junction where two superconductors are coupled by a hopping t_d and $J>0$ holds for $0<\phi<\pi$), one can most notably also observe a negative current in the singlet phase,[44] particularly at small BCS energy gaps Δ (see Fig. 5). It is, however, imperative to point out that this is solely caused by the Coulomb interaction, and the supercurrent at $U=0$ (where the FRG becomes exact) always remains positive in the singlet phase. In contrast, Zhang (Ref. 32) obtains a negative singlet current yet in the noninteracting limit, rendering these results *a priori* highly questionable.

The Josephson current as a function of the phase difference ϕ displays the same characteristics as $J(\epsilon)$. Multiple phase transitions manifest as appearing and disappearing dis-

continuities of $J(\phi)$ (see Fig. 6), and can be ultimately understood from the functional form of the atomic-limit phase boundary [Eq. (11)]. In addition, the current can become negative in the singlet phase in presence of both a direct coupling t_d and finite Coulomb correlations. The actual form of $J(\phi)$ is rather complicated. It is displayed for various parameter sets in Fig. 6.

VI. CONCLUSIONS AND OUTLOOK

In this paper, we have investigated a quantum dot Josephson junction embedded within an Aharonov-Bohm environment. By analytically solving the atomic limit of large BCS gaps $\Delta=\infty$, we have shown that the low-energy physics of this system is governed by an interplay of two distinct (singlet and doublet) phases in complete analogy with the noninterferometric case where both superconductors are not coupled directly. The phase boundary, however, depends nonmonotonically both on the coupling strength t_d and the quantum dot energy ϵ. By carrying out functional renormalization-group calculations (which benchmark excellently against the atomic-limit result) at arbitrary Δ, we have demonstrated that the overall size of the doublet regime shrinks monotonously with the gap size but the functional

form of the phase boundary always remains similar to the analytic expression derived at $\Delta = \infty$. Thus, even if all system parameters cannot be adjusted experimentally in a precisely controlled way, one can quite generally expect to observe re-entrance behavior within an interferometric quantum dot Josephson junction. At finite couplings t_d, the supercurrent $J(\epsilon)$ acquires a Fano-type line shape analogous to the linear-response conductance of the ordinary Anderson model. Most importantly, we have shown that Coulomb correlations can cause J to become negative in the singlet phase.

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[42] Since our FRG scheme turns out to be quantitatively reliable only up to some intermediate Coulomb interaction $U/\Gamma \approx 8$ (where Kondo correlations start to become important), we cannot describe the singlet-doublet phase transition in the extreme limit of $\Delta/\Gamma \ll 1$ (as this would require $T_K/\Gamma \ll 1$), no matter which quantity is used to describe the phase boundary. However, for the simple quantum dot Josephson junction ($t_d=0$), it was demonstrated that generic physics shows up for small values of T_K/Δ (but not necessarily extremely small T_K itself).[18,22] Since we do not observe any qualitative changes apart from an overall increase in the size of the singlet phase in going from $\Delta=\infty$ to $\Delta/\Gamma \approx 0.2$, it is reasonable to assume that the same holds for the problem at hand.

[43] For the simple quantum dot Josephson junction ($t_d=0$), it was previously observed that in the doublet phase the supercurrent obtained from the FRG is completely independent of both the two-particle interaction strength U and the impurity energy ϵ (Ref. 23). Even though this is an artifact of the approximative approach, numerical RG calculations showed that physical properties only vary slightly in this regime (Ref. 22).

[44] Some generalized perturbative approach (Ref. 15) could be employed in order to get some intuitive understanding why J can become negative in the singlet phase. This is, however, out of the scope of this paper.