Loss of π-junction behavior in an interacting impurity Josephson junction

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Using a generalization of the noncrossing approximation which incorporates Andreev reflection, we study the properties of an infinite-U Anderson impurity coupled to two superconducting leads. In the regime where Δ and T_K are comparable, we find that the position of the subgap resonance in the impurity spectral function develops a strong anomalous phase dependence—its energy is a minimum when the phase difference between the superconductors is equal to π. Calculating the Josephson current through the impurity, we find that π-junction behavior is lost as the position of the bound state moves above the Fermi energy.

What is the Josephson current through an interacting Anderson impurity? As this phenomenon involves the coherent transport of pairs of electrons through the impurity, one would expect that a strong on-site repulsion would greatly diminish the effect. Though this intuitive expectation is partially correct, there is a variety of nonintuitive behavior also associated with this system.

If the on-site repulsion is large and the impurity is singly occupied, a lowest-order perturbative calculation in the impurity-superconductor coupling reveals that the sign of the Josephson coupling can become negative, meaning that the corresponding ground state of the system has a phase difference of $\delta=\pi$ between the two superconductors.[1,2] An appealing explanation for this behavior was provided by Spivak and Kivelson,[2] who showed that in the limit of single occupancy, it is impossible to transport a pair across the impurity while preserving its spin ordering, leading to an extra factor of (-1). More generally, π junction behavior is expected whenever spin-flip tunneling processes dominate.[3,4] Recent work using a Hartree-Fock type procedure indicates this behavior can survive beyond lowest-order perturbation theory.[5]

Alternatively, in the limit of large impurity-superconductor coupling, the physics of the Kondo effect will also become significant. A resulting enhancement of the Josephson current through the impurity has been predicted in the regime where the superconducting gap Δ is much smaller than the Kondo temperature T_K.[1] Significantly, no π-junction behavior is expected here, as the spin of the impurity is completely screened by the Kondo effect.

Given these prior results, it is natural to ask how large the ratio T_K/Δ must be to see the destruction of π-junction behavior, and what the properties of the junction are in this crossover region; these questions are the motivation for the current paper. We examine the regime where Δ is comparable in magnitude to T_K, a regime in which the effects of both Kondo physics and superconductivity must be treated on an equal footing. Note this parameter range is also of interest as it is more appropriate to mesoscopic quantum dot systems, which would be one possible experimental realization of the model. We find, somewhat surprisingly, that the properties of our system can be understood in terms of another well-studied feature of magnetic impurities coupled to superconductors—the subgap bound state. Typically, the position of this state is a function of the ratio T_K/Δ.[6–9] We find now that this resonance also develops a pronounced dependence on the phase difference—as δ increases from zero, the energy of the bound state *decreases*. This phase dependence is anomalous in the sense that it indicates an energetic preference away from $\delta=0$. Interpreting this subgap state as a current carrying Andreev bound state,[10] we are lead to the conclusion that the system is a π junction if the subgap bound state is located below the Fermi energy E_F. This relation is confirmed by making an explicit calculation of the Josephson current through the impurity.

Formalism. The model we study consists of an infinite-U Anderson impurity coupled to two superconducting leads, each having a different phase. Using a slave-boson representation, we have

$$H=H_0+\varepsilon_d\sum_\sigma f_\sigma^\dagger f_\sigma+W\sum_{\alpha,k,\sigma}(c_{\alpha,k\sigma}^\dagger b^\dagger f_\sigma+\text{H.c.}),\qquad(1)$$

$$H_0=\sum_{\alpha,k,\sigma}\varepsilon_k c_{\alpha,k\sigma}^\dagger c_{\alpha,k\sigma}+\sum_{\alpha,k}(\Delta_\alpha c_{\alpha,k\uparrow}^\dagger c_{\alpha,-k\downarrow}^\dagger+\text{H.c.}).\qquad(2)$$

The $c_{\alpha,k\sigma}^\dagger$ operators here create band electrons, with σ denoting spin and $\alpha=L,R$ labeling the left and right superconducting leads. $\Delta_\alpha=|\Delta|\exp(i\phi_\alpha)$ represents the pair potential in lead α, with the phase difference δ being defined as $\phi_R-\phi_L$. The Anderson impurity has bare energy ε_d, and is represented in the usual manner using auxiliary fermion (f) and boson (b) operators; the $U=\infty$ constraint of single occupancy takes the form $\Sigma_\sigma f_\sigma^\dagger f_\sigma+b^\dagger b=1$.

The NS-NCA. We calculate the impurity spectral function (also called the impurity density of states) for our system using the NS-NCA,[11] an extension of the self-consistent noncrossing approximation (NCA) (Ref. 12) to superconducting systems. The NCA amounts to an infinite order resummation of perturbation theory, and has been shown to be quantitatively reliable down to temperatures below T_K.[12,13] The modification we employ self-consistently includes multiple-Andreev reflection processes in a manner which is formally exact to order $1/N$, where $N=2$ is the spin degeneracy of the impurity. As the success of the normal NCA is attributed to the fact that it too is exact to order $1/N$ (in the absence of superconductivity), the NS-NCA employed here can be

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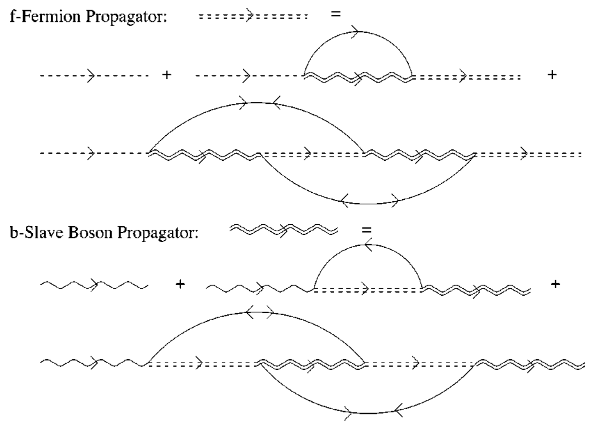

FIG. 1. Diagrammatic representation of the NS-NCA. Dashed lines are *f* fermions, wavy lines are slave bosons, solid lines are lead electrons. Double lines indicate a fully dressed propagator. Anomalous propagators indicate Andreev reflection.

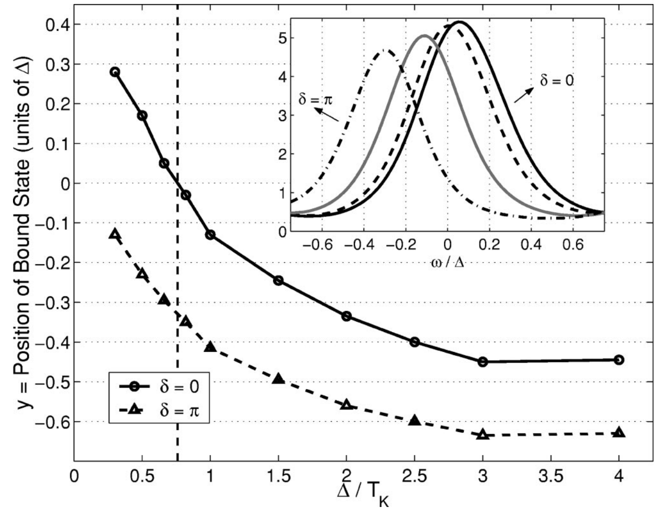

FIG. 2. Position of subgap bound state as a function of Δ/T_K for a fixed $T/\Delta=0.5$, $T_K=0.0005D$. The vertical dashed line indicates the approximate value of Δ for which the bound state resonance crosses the Fermi energy. Inset: plots of the impurity density of states $A_d(\omega)$ for $\Delta/T_K=0.66$ at various phase differences. From right to left, we have $\delta=0$ (solid curve), $\delta=\pi/4$, $\delta=\pi/2$, $\delta=\pi$ (dash-dot curve).

viewed as a natural extension to systems with superconductivity. The graphs determining the *f*-fermion and *b* slave boson propagators are given in Fig. 1.

Note that the anomalous graphs appearing in Fig. 1 always involve *two* Andreev reflections. As these Andreev reflection events pick up the phase of the superconductor in which they occur, and each Andreev reflection is free to occur in either of the two superconductors, the phase difference δ naturally enters the impurity self energies through an interference term. A previous study using the NCA to study the regime $\Delta \gg T_K$ (Ref. 14) neglected these diagrams, and thus omitted the only phase-dependent contribution to the impurity Green function which survives in the limit of a strong on-site repulsion.

The Dyson equations pictured diagrammatically in Fig. 1 lead to a set of coupled integral equations for the *f*-fermion and slave boson propagators. Letting $F(\omega)=[\omega-\varepsilon_d-\Sigma(\omega)]^{-1}$ and $B(\omega)=[\omega-\Pi(\omega)]^{-1}$ represent the *f*-fermion and slave boson retarded propagators, respectively, the equations read

$$\Sigma(\omega)=\frac{\Gamma}{\pi}\int d\varepsilon\Bigg(\rho(\epsilon)B(\omega-\varepsilon)f(-\varepsilon)-\frac{\Gamma}{\pi}\times\int d\varepsilon'\,\tau(\varepsilon)\tau(\varepsilon')B(\omega+\varepsilon)F(w+\varepsilon+\varepsilon')\times B(\omega+\varepsilon')\Bigg), \tag{3}$$

$$\Pi(\omega)=\frac{2\Gamma}{\pi}\int d\varepsilon\Bigg(\rho(\epsilon)F(\omega+\varepsilon)f(\varepsilon)+\frac{\Gamma}{\pi}\times\int d\varepsilon'\,\tau(\varepsilon)\tau(\varepsilon')F(\omega+\varepsilon)B(w+\varepsilon+\varepsilon')\times F(\omega+\varepsilon')\Bigg). \tag{4}$$

In these equations, $\rho(\varepsilon)$ is the electronic density of states, $\Gamma=\pi W^2\rho(0)$ the bare tunneling rate, f the Fermi distribution function, and $\tau(\varepsilon)$ is an effective electron-hole coherence parameter defined by

$$\tau(\omega)=\sum_{k,\alpha} u^*_{k,\alpha}v_{k,\alpha}\delta(|\omega|-\varepsilon_n)f(\omega), \tag{5}$$

where $u_{k,\alpha}$ and $v_{k,\alpha}$ are the usual BCS coherence factors.

Results. We use a Gaussian density states for the band electrons having half width D. For the results shown here, we choose model parameters $\varepsilon_d=-0.67D$ and $\Gamma=0.15D$, which yields an approximate $T_K=0.0005D$.[15] We have solved numerically via iteration the NS-NCA equations in equilibrium for various temperatures, gap sizes and phase differences. Within the NCA, the impurity spectral function $A_d(\omega)$ can be directly related to the *f*-fermion and slave boson spectral functions.

$$A_{d\sigma}(\omega)=\int d\varepsilon[\mathrm{e}^{-\beta\varepsilon}+\mathrm{e}^{-\beta(\varepsilon-\omega)}]A_{f\sigma}(\varepsilon)A_b(\varepsilon-\omega), \tag{6}$$

where the auxiliary particle spectral functions are defined by $A_f=-(1/\pi)\mathrm{Im}\,F$, $A_b=-(1/\pi)\mathrm{Im}\,B$. Note that the equality in Eq. (6) reflects a neglect of vertex corrections which is consistent with the large-*N* nature of the NCA.

The solid curve in Fig. 2 (with points indicated by circles) shows the position y (in units of Δ) of the subgap resonance in the impurity density of states as a function of Δ/T_K at $\delta=0$ and at a constant ratio $T/\Delta=0.5$; this resonance corresponds to the subgap bound state. As has been observed in earlier studies, we find that as Δ/T_K decreases, the position of the bound state increases, with the transition across the Fermi energy occurring when Δ is on the order of T_K. Note that as we are not using a model with particle-hole symmetry, we only have a single subgap state.

A cogent interpretation of this behavior was provided in,[7,8] where the position of the subgap bound state was suggested to result from the competition between two possible ground states. For $T_K>\Delta$, the ground state of the system is the Kondo singlet, and the excited subgap state is a spin doublet. Recall that in the Kondo singlet ground state of the infinite-U Anderson model, there is a small probability of finding the impurity empty, despite the fact that the bare site energy ε_d is well below E_F; this is not true for the doublet state, where the impurity is expected to be singly occupied. Thus, the fact that the bound state is located *above* E_F in this limit (i.e., $y>0$) reflects the fact that one must *add* a particle at the impurity to the singlet ground state to reach the doublet state. The magnitude of y indicates the energy splitting between these two states,

$$y=\frac{E_{\text{excited}}-E_{\text{ground}}}{\Delta}=\frac{E_{\text{doub}}-E_K}{\Delta}>0, \qquad (7)$$

where E_{doub} is the energy of the doublet state and E_K is that of the Kondo singlet state. Similarly, for $\Delta>T_K$, the ground state is the fully-paired doublet favored by the superconductivity; the bound state is located below E_F as one must *remove* a particle from the doublet ground state to reach the excited singlet state. An identical expression holds for y:

$$y=\frac{-(E_{\text{excited}}-E_{\text{ground}})}{\Delta}=\frac{-(E_K-E_{\text{doub}})}{\Delta}<0. \qquad (8)$$

The crossing of E_F by the subgap state is thus seen to indicate a substantial change in the nature of the ground state.

While the behavior of the bound state at $\delta=0$ has received much attention, the effects of having a phase difference has not, to our knowledge, been previously studied. The triangles in Fig. 2 indicate the bound state positions y for the same values of T_K/Δ as the solid curve, but now with a phase difference of $\delta=\pi$ between the superconductors. We find that for all values tested, *y decreases* as we increase δ to π—the subgap bound state has an anomalous phase dependence. This behavior is seen more explicitly in the inset of Fig. 2, where we plot the subgap resonance for various values of δ.

The phase dependence of the subgap state can also be interpreted in terms of a competition between the Kondo singlet and the fully paired doublet states. The Kondo state is again expected to be the ground state for $T_K>\Delta$, while the the doublet state will be the ground state in the opposite regime. Significant now, however, is the fact that the phase dependence of these two states is quite different. In the doublet state, the impurity can be viewed as a local moment and we thus expect a negative Josephson coupling and that E_{doub} will be a *minimum* at $\delta=\pi$. In the Kondo singlet state, the impurity spin has been screened and thus we do not expect any anomalous Josephson coupling—E_K will be a *maximum* at $\delta=\pi$. With these associations, it follows from Eqs. (7) and (8) that *y is minimized at* $\delta=\pi$, meaning that the subgap state has an anomalous phase dependence. Note that for small values of Δ/T_K, it is possible to make the subgap state cross E_F and thus change markedly the nature of the system ground state by only changing δ.

At this point, it is natural to attempt to make a connection to the Josephson effect. Recall that for a noninteracting system, it is possible to discuss the Josephson current as being at least partially carried by Andreev bound states existing in the weak link between the two superconductors.[10] These states have a phase-dependent energy, and thus contribute to the current through the relation $I=(2e/\hbar)dF/d\delta$, where F is the free energy of the junction. For the simple case where a noninteracting impurity couples the two superconductors, there are always two Andreev bound states with energies $\pm|\varepsilon(\delta)|$; as the lower-energy state $-|\varepsilon(\delta)|$ has a "normal" phase dependence $(dE/d\delta>0)$, the Josephson current is always positive.

In the present case, matters are quite different due to the strong on-site interaction. We have only one apparent Andreev bound state, and its phase dependence is anomalous $(dE/d\delta<0)$. We would thus naively expect that the Josephson current would both become negative and enhanced in magnitude as the bound state crosses below E_F and becomes "occupied." Of course, this picture is oversimplified, as there are other possible contributions to the Josephson current—due to interactions, the impurity contribution to the free energy F is not just a simple function of the impurity density of states.

The conjecture made above can be tested by making an explicit calculation of the dc Josephson current through the impurity. Using a technique similar to that used in Ref. 16 to calculate the normal current through an interacting impurity, we arrive at the following exact expression for the Josephson current:[17]

$$I_J=\frac{4e}{\hbar}\Gamma\sin\left(\frac{\delta}{2}\right)\sum_k\frac{W^2}{\Gamma}\times\int d\omega f(\omega)\frac{-\text{Im}}{\pi}[g_k^{R,12}(\omega)G_d^{R,21}(\omega,\delta)]. \qquad (9)$$

Here, $g_k^{R,12}(\omega)$ indicates an anomalous BCS propagator and $G_d^{R,21}(\omega,\delta)$ is the anomalous impurity propagator; without loss of generality, we have chosen $\phi_L+\phi_R=0$.

We calculate the anomalous impurity propagator within the NCA using the lowest-order contributing graph,[11,12] without making any further approximation. To calculate an approximate value of the 0 temperature Josephson current, we use Eq. (9) with the Fermi function taken at $T=0$, but with all spectral functions calculated at $T=0.5\Delta$ [the NCA is unreliable at $T=0$ (Ref. 13)]. This is a reasonable procedure, as we expect no qualitative changes in the spectral functions as the temperature is further lowered; the subgap resonances will only be sharpened. Retaining a finite T Fermi function would smear the contribution of the subgap resonances, and thus obscure the behavior we are interested in.

Plotted in Fig. 3 is the approximate 0 temperature phase derivative of the Josephson current $(dI_J/d\delta)$ thus obtained as a function of Δ/T_K, taken at $\delta=0$. Comparison to Fig. 2 indicates that π-junction behavior is indeed lost when the bound state crosses above the Fermi energy, as expected from a noninteracting picture. Similar results hold at other values of δ–$(dI_J/d\delta)$ changes sign at roughly the same value of Δ/T_K at which the bound state crosses the Fermi energy. It would thus appear that the subgap bound state is the entity responsible for carrying the reversed-sign Josephson current associated with π-junction behavior.

Note that in some respects, our conclusion here resembles what was found in a study of the Josephson current through a *noninteracting* magnetic insulating layer;[18] there also, the transition to π-junction behavior is accompanied by an anomalous Andreev bound state crossing below the Fermi

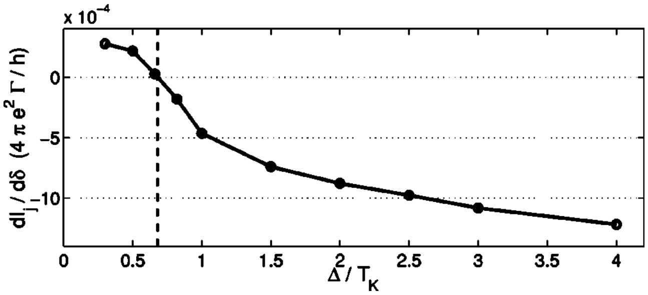

FIG. 3. Approximate $T=0$ phase derivative of the Josephson current ($dI_J/d\delta$) at $\delta=0$ for various values of Δ/T_K. Note the transition from negative to positive current (indicated by the vertical dashed line) coincides with the subgap bound state crossing the Fermi energy (see Fig. 2).

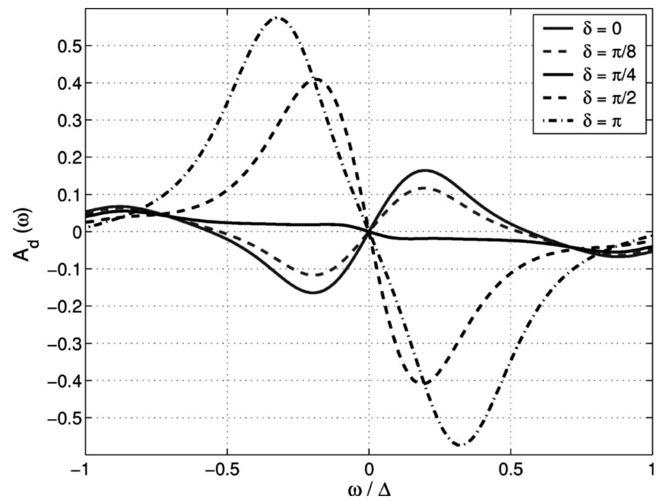

FIG. 4. Anomalous impurity spectral function $\mathrm{Im}\, G_d^{R,21}$ for various values of the phase difference δ with fixed $\phi_L+\phi_R=0$, $\Delta=0.66T_K$, $T=0.5\Delta$. Note that as δ increases, the spectral function changes sign; this coincides with the bound state crossing below the Fermi energy (see inset of Fig. 2).

energy. We stress again that the present situation is quite different due to the strong on-site repulsion—there is no *a priori* reason guaranteeing that the general noninteracting theory relating I_J to Andreev bound states should be applicable to the interacting system studied here. We find only a single subgap state in the impurity density of states, whereas in the noninteracting case bound states always occur in pairs, with one member of each having $dE/d\phi<0$.

Also of interest in the present system is the behavior of the superconducting phase of the impurity itself. We find that this phase undergoes a shift by π as the bound state passes through the Fermi energy. When the bound state is above E_F, the impurity simply has the average phase of the two superconducting leads—at low energies, the signs of both the real and imaginary parts of the anomalous impurity Green function ($G_d^{R,21}$) are the same as those of the average anomalous Green functions of the superconductors. However, when the bound state moves below E_F, we find that the anomalous impurity green function changes sign. We interpret this to mean that the impurity has acquired an additional phase of π. This behavior is shown Fig. 4. It is clear from Eq. (9) that this additional factor of (-1) will cause a sign change in the Josephson current. A similar phase shift was found in earlier work involving a single superconductor,[9] though a transition was not observed.

Conclusions. Using an extension of the NCA, we have studied the properties of an infinite-U Anderson impurity coupled to two superconductors. We find that the subgap bound state develops an anomalous phase dependence, and that π-junction behavior is lost when the bound state crosses above E_F.

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