Impurity Quantum Phase Transition in a Current-Carrying $d$-Wave Superconductor

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We study an Anderson impurity embedded in a $d$-wave superconductor carrying a non-zero momentum of Cooper pairs driven by magnetic flux through the Aharonov-Bohm effect. The zero-temperature impurity behavior is investigated by using the numerical renormalization group method in calculating the energy flows, the impurity spectral functions, and the effective magnetic moments. These results explicitly show that the local impurity state can be changed dramatically from the asymptotically free spin to the completely screened one by tuning the magnetic flux.

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The behavior of a single magnetic impurity in correlated electron systems has attracted intensive interest in condensed matter physics [1]. While the problem is well studied when the host is a simple metal [2], the correlations among the host electrons may lead to much complicated impurity behavior deviating from the Fermi liquid properties [3]. Specifically, the Kondo screened state, i.e., an entanglement state between the impurity spin and a conduction electron, may become unstable at zero temperature upon the depletion of the density of states (DOS) at the Fermi levels, or the change of certain nonthermal parameters. Such kind of impurity quantum phase transition (IQPT) may take place in metallic systems with a pseudo gap [3]. The response of a known impurity behavior upon the change of effective couplings could provide important information of the host itself, and thus can be used to probe the ground state and low-energy physics of the host electrons [3]. On the other hand, within a known host, the different response of a quantum impurity with internal dynamical degrees of freedom versus a static impurity, to an external control parameter, may shed insight on the role played by other parameters [4], of a Cooper pair determines the current flow. Notice that the energy is measured with respect to the Fermi energy. The center-of-mass momentum, $2q$, of a Cooper pair determines the current flow. Other parameters $t_d$, $U$, and $V_k$ are the localized level, the on-site Coulomb interaction, and the impurity coupling, respectively. $N_L$ is the number of lattice sites.

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We can model the above impurity problem by coupling an Anderson impurity to the $d$-wave superconductor carrying a current, using the following Hamiltonian

$$H = H_{BCS} + H_{\text{imp}} + H_{\text{hybrid}},$$

where $H_{BCS} = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}} c_{\mathbf{k}\sigma} ^{\dagger} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}} [\Delta_{\mathbf{k}} c_{\mathbf{k}\uparrow} ^{\dagger} c_{\mathbf{k}\downarrow} + \text{h.c.}], H_{\text{imp}} = \sum_{\mathbf{k},\sigma} \epsilon_d d_{\mathbf{k}\sigma} ^{\dagger} d_{\mathbf{k}\sigma} + U n_{d\uparrow} n_{d\downarrow}$, and $H_{\text{hybrid}} = \frac{\gamma}{2} \sum_{\mathbf{k},\sigma} [V_k c_{\mathbf{k}\sigma} ^{\dagger} d_{\sigma} + \text{h.c.}]$. Here $c_{\mathbf{k}\sigma}$ annihilates one conduction electron of momentum $\mathbf{k}$ and spin projection $\sigma$, while $d_{\sigma}$ annihilates one localized $d$-electron of spin projection $\sigma$. In the tight-binding approximation, the conduction electrons have the normal and $d$-wave superconducting gap dispersions, $\xi_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - \mu$ and $\Delta_{\mathbf{k}} = (\Delta_0/2)(\cos k_x - \cos k_y)$, respectively. Notice that the energy is measured with respect to the Fermi energy. The center-of-mass momentum, $2q$, of a Cooper pair determines the current flow. The obtained results can be tested by scanning tunneling microscopy (STM), which has been used to measure the local electron structure around a doped impurity in conventional [3] and unconventional superconductors [8] in the absence of a current flow.

The $d$-wave superconductor, usually being of quasi two-dimensional layered structure, could be designed with a geometry of hollow cylinder, as shown schematically in Fig. 1. The persistent (super-)current can be generated by piecing a magnetic flux through the axial of the cylinder, due to the Aharonov-Bohm effect [9].

FIG. 1: (Color) An Anderson impurity embedded in a two-dimensional $d$-wave superconductor made in the hollow cylinder geometry. A persistent current $\mathbf{q}$ is generated by the Aharonov-Bohm effect which can be tuned by varying the magnetic flux $\Phi$ passing through the cylinder. The local electron structure around the impurity can be measured by scanning tunneling microscopy.
purity spin being in a strong coupling (SC) limit, or a conventional s-wave superconductor with a hard-gap everywhere on the Fermi surface, where the impurity spin being in the local moment (LM) limit, the existence of nodal zero-energy quasiparticles in a d-wave superconductor [4,10] have a non-trivial implication to the fate of quantum impurity states. Earlier studies by taking the DOS with a soft-gap, \( \rho(E) \sim |E|^r \) \( (r = 1 \) for the d-wave superconductor), have shown the existence of a critical coupling, separating the LM and SC phases [3,11,12,13,14,15]. More intriguingly, we notice that the low-energy excitations in a d-wave superconductor can readily be proliferated by pumping in a supercurrent, which should have a significant control of the impurity state. The purpose of the present work is to demonstrate that the IQPT can be realized by gradually increasing the supercurrent.

In order to solve the problem, we generalize the NRG method [4,16] to study the impurity properties with an arbitrary form of the DOS, which in the present case is found by diagonalizing \( \mathcal{H}_{\text{BCS}} \) to be 

\[
\rho(E) = \frac{1}{N \nu} \sum_k |u_{k,q}|^2 [\delta(E - E_{k,q}^{(+)}) + \delta(E - E_{k,q}^{(-)})],
\]

where 

\[
E_{k,q}^{(+)} = Z_{k,q} \pm |Q_{k,q} + \Delta_{k,q}^2|^{1/2}, \quad Z_{k,q} = (\xi_{k+q} - \xi_{k-q})/2
\]

and 

\[
Q_{k,q} = (\xi_{k+q} + \xi_{k-q})/2.
\]

The electron- and hole components of the Bogoliubov-de Gennes eigenfunction are given by 

\[
|u(v)_{k,q}|^2 = |1 \pm Q_{k,q}/E_{k,q}^{(0)}|/2.
\]

In the numerical calculations, we take \( t = 1, t' = -0.2, \mu = -0.78, \Delta_0 = 1. \) The energy is measured in units of \( t = 1 \) unless specified otherwise. Without loss of generality, we take \( q_y = 0. \) This choice of \( q = (q_x, q_y) \) corresponds to the circular current perpendicular to the axis as shown in Fig. 4. Its magnitude is then related to the magnetic flux via \( q_x = 2\pi \Phi/(N_L \Phi_0) \) with \( \Phi_0 = h/e. \) In Fig. 2, we show the DOS as a function of energy for various values of \( q_x. \) A small intrinsic lifetime broadening \( 2 \times 10^{-3}, \) and the lattice sites of \( 2^{14} \times 2^{14} \) are chosen. In the absence of the current, the calculated DOS vanishes linearly as expected. However, it increases around the Fermi energy as a response to the non-zero current.

It is sufficient for our purpose to take into account only the coupling between the particle-excitations and the impurity spin. Indeed, it is argued that the local quasi-particle DOS of the superconductor is the only necessary ingredient in a number of cases, in particular the unconventional superconductors [12,13]. For simplicity, we therefore ignore the anomalous part and just study a modified Anderson model with the impurity coupled to the electron-like excitation spectrum. As such, we use the following Hamiltonian to the derivation of the NRG equations [13,19]:

\[
H = \mathcal{H}_{\text{imp}} + D \sum_{\sigma} \int_{-1}^{1} d\epsilon g(\epsilon) a_{\sigma}^\dagger a_{\sigma} + D \sum_{\sigma} \int_{-1}^{1} d\epsilon h(\epsilon) (d_{\sigma}^\dagger a_{\sigma} + a_{\sigma}^\dagger d_{\sigma}), \quad (2)
\]

FIG. 2: (Color) Density of states as a function of energy for various values of drift momentum \( q_x. \)

where we introduced a one-dimensional energy representation for the particle-like excitations \( a_{\sigma}^\dagger a_{\sigma} \), with the scaled energy \( \epsilon \) and the band-cut-offs at \( \pm D. \) The quantities \( g(\epsilon) \) and \( h(\epsilon) \) are the energy dispersion and hybridization, self-consistently defined by \( \rho(E) \) and \( V_k \) respectively as in [19].

To handle the arbitrary \( \rho(\omega) \), we follow the generic scheme of Ref. [19] to discretize the Hamiltonian given by Eq. (2), and then solve it by the NRG for different values of \( U \) and \( \Delta_k \) at the symmetric point \( \epsilon_d = -U/2, \) with the RG parameter \( \Lambda = 2.5. \) At each iteration step we keep \( \approx 200 \sim 1200 \) states, depending on the quantities calculated, and the total number of iterations is \( N_{\text{max}} \approx 100. \) Throughout the work, a value of \( D = 2 \) is chosen. In the following, we briefly discuss the results of the energy flows, the impurity density spectra, as well as the effective impurity moment in various cases.

Actually even in the absence of the current, there should be an IQPT from the SC state to the LM state upon increasing repulsive \( U \) at the finite impurity coupling. Fig. 3 shows the low lying energy levels as a function of odd number of iteration \( N \) for various values of \( U \) in increasing order and for fixed (and \( k \)-independent) \( V = 0.01. \) For small values of \( U \) (see, e.g., Panel (a)), for small \( N, \) the levels start and remain close to the free orbital fixed point. For larger \( N, \) they make a rapid crossover to the LM fixed point. Due to the marginal nature of the d-wave superconducting host, they remain near the LM fixed point for a finite number of iterations as manifested by a plateau, and then gradually crossover to the SC limit. This length of the plateau increases with increasing \( U \) (see Panels (c), (d)). For the large values \( U, \) the low lying energy levels always flow to a LM fixed point (see Panels (c), (d)), suggesting the impurity state is in the localized regime. Correspondingly, we show in Fig. 4 the impurity spectral function and the effective magnetic moment for fixed \( V = 0.01. \) As can be seen in Fig. 4 the
spectral density exhibits a narrow Kondo resonance peak at the Fermi energy in the SC state while shows only a gap-like behavior in the LM state. Also from the inset of Fig. 4 one can see that the screened moment, which is essentially zero in the SC state, saturates at the maximal value 0.25 as $U$ approaches to a larger value. These results provide a base to study the effect of non-zero $q$ starting from the LM phase.

We then calculate the similar quantities for fixed $U = 0.1$, and $V = 0.01$ with $q_y = 0$ and various $q_x$. As shown in Fig. 5 the length of plateau in the energy flow becomes shortened with the increasing $q_x$ (i.e., the supercurrent flow). This evolution of energy flows from the LM line-shape to the SC one is similar to the soft-gap Anderson impurity model. It indicates that the impurity state originally staying in the LM regime can be driven into the SC state. In the present case, the transition takes place around $q_x \approx 0.003$, though it is not so sharp as compared with the soft-gap model. The impurity spectral function begins to show a central peak at zero energy as we increase $q_x$ across this critical value (see Fig. 6). This feature is similar to the soft-gap Anderson model where the impurity spectral function diverges at zero energy for the SC and quantum critical phases. Remarkably, the sum rule is within 95% accuracy in our case, which is better than that in the soft-gap model. The IQPT is also indicated in the effective moment, plotted in the inset of Fig. 6. It shows that the effective moment approaches to the free moment value 0.25 for $q_x < 0.003$, and approaches to zero for $q_x > 0.003$. The latter case indicates a SC phase where the impurity spin is completely screened. Our numerics also shows that the increase in the number of states, kept in the iterations, improves the proxy of the saturated values of the effective moment to 0.25 (0) in the LM (SC) limit.

Our NRG results demonstrate the existence of finite critical point around $q_{x,c} \approx 0.003$ when $q_y = 0$, $U = 0.1$, and $V = 0.01$. The impurity is in the LM and SC phases for $q_x < q_{x,c}$ and $q_x > q_{x,c}$, respectively. We find that this conclusion is robust if, for $q_x = q_y = 0$, $V$ varies in the LM phase. In general, $q_{x,c}$ will increase with $U$ for fixed $V$. The precise value of $q_{x,c}$ requires extremely high precision of the DOS of the low-energy excitations, which could be achieved within $10^{-16} \sim 10^{-12}$ for the soft-gap Anderson model. However, for the present model, such
high accuracy of the DOS needs sufficiently small intrinsic lifetime broadening and sufficiently large system size $N_L$, so that a detailed analysis on the scaling behavior in the critical phase is challenging. Nevertheless, it is sufficient for our purpose to predict a critical point separating the SC and LM phases by tuning the current or the magnetic flux.

Our findings have several implications: (i) In a $d$-wave superconductor, quasiparticle resonances can be induced around a doped static impurity in the strong scattering limit. Upon the flowing of a supercurrent, the resonance peak is suppressed in amplitude and broadened in width [20]. In contrast, for the quantum impurity, a Kondo resonance emerges when it is driven into the SC phase by the supercurrent. This distinction of the response to the supercurrent can help us to decipher whether a doped atom plays the role of a static or quantum impurity in a $d$-wave superconductor. (ii) In high-$T_c$ cuprates like Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$, the nanoscale inhomogeneity with the existence of small- and large-gap domains [21, 22] has been ubiquitously observed by the STM. When a magnetic impurity is doped into the system, it is in the LM phase in the absence of a supercurrent. In this case, the impurity plays the role of a weak potential scatter [23], and the resonance as due to the quasiparticle scattering is located far away from the Fermi energy. This resonance should be observed in both types of domains. When a supercurrent flows in the sample, the impurities in the small-gap domains should be first driven into the SC phase and a Kondo resonance will emerge very close to the Fermi energy while those in the large-gap domains are still in the LM with no Kondo resonance. These interesting phenomena, which can be observed by STM, should serve as a direct test of our prediction.

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