Numerical Renormalization Group Study of Kondo Effect in Unconventional Superconductors

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Orbital degrees of freedom of a Cooper pair play an important role in the unconventional superconductivity. To elucidate the orbital effect in the Kondo problem, we investigated a single magnetic impurity coupled to Cooper pairs with a $p_x + ip_y$ ($d_{x^2-y^2} + id_{xy}$) symmetry using the numerical renormalization group method. It is found that the ground state is always a spin doublet. The analytical solution for the strong coupling limit explicitly shows that the orbital dynamics of the Cooper pair generates the spin 1/2 of the ground state.

KEYWORDS: Kondo effect, unconventional superconductivity, numerical renormalization group

Unconventional superconductivity is characterized by an angular momentum ($p$, $d$, or $f$) of its Cooper pair. It is very sensitive to impurities and surface boundaries, differing from the standard BCS ($s$-wave) superconductivity. As a result, it displays various phenomena associated with breaking of the Cooper pairs. In the last decade, much attention has been paid to the effects of non-magnetic impurities and static boundaries.

At present, the attention shifts to the study of magnetic impurities in the unconventional superconductivity. Recent experimental studies provided evidence of induced effects: (1) breaking time-reversal invariance and (2) dynamical coupling with quasiparticles.

In this letter, we study a single magnetic impurity at the center in two-dimensional superconducting systems. Since we treat short-range scattering here, the impurity couples with only the electrons having no angular momentum ($l = 0$). For the $p_x + ip_y$-wave, the total angular momentum of the Cooper pair is equal to one. The order parameter is expressed by $\Delta e^{i\phi_k}$, where $\phi_k$ is the angle of the Fermi vector measured from the $k_x$ axis. Since the angular momentum is a good quantum number for the $p_x + ip_y$-wave, the $l = 0$ and $l = 1$ orbitals are decoupled, and they are decoupled from the other orbitals. This is the reason why the Kondo effect in the $p_x + ip_y$-wave state can be treated within the two angular momentum spaces. Therefore, we can apply the NRG method to the

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Kondo problem for the $p_x + ip_y$-wave as we do to the two-channel Kondo problem. Let us begin with the following Hamiltonian $H = H_{p_x+ip_y} + H_{\text{imp}}$:

$$
H_{p_x+ip_y} = \sum_{k\sigma} \sum_{\ell=0,1} \epsilon_k a_k^{\dagger \sigma} a_k^{\sigma} + \sum_{k\sigma} \left[ |\Delta|^2 a_k^{\dagger \sigma} a_{k\sigma} + \text{H.c.} \right],
$$

$$
H_{\text{imp}} = \frac{1}{2} \sum_{kk'\sigma\sigma'} \left( -JS \cdot \sigma_{\sigma\sigma'} + V\delta_{\sigma\sigma'} \right) a_k^{\dagger \sigma} a_{k'\sigma'}.
$$

Here, $H_{p_x+ip_y}$ is the Hamiltonian for the $p_x + ip_y$-wave pairing state, and $H_{\text{imp}}$ represents exchange interaction and potential scattering of conduction electrons due to the impurity. $\epsilon_k$ is the kinetic energy of the conduction electron with wave number $k$, and $\Delta$ is the $p_x + ip_y$-wave order parameter. The subscripts $l(=0,1)$ and $\sigma(=\uparrow, \downarrow)$ in $a_k^{\sigma}$ represent the angular momentum and spin of the conduction electron, respectively. $S$ and $\sigma$ are the $S = 1/2$ spin operator and the Pauli matrix for the magnetic impurity and conduction electrons, respectively. $J( < 0)$ and $V$ are the antiferromagnetic and non-magnetic couplings, respectively. Note that the model given by eq. (1) is not a simple two-band Kondo model. Only the $l = 0$ conduction electrons are coupled directly to the local spin. In the normal state, the $l = 1$ electrons are completely decoupled from the local spin. However, in the superconducting state, they are coupled to the $l = 0$ conduction electrons via the $p_x + ip_y$-wave order parameter. We have to take the $l = 1$ electrons into account as well for the $p_x + ip_y$-wave. We can elucidate the orbital effect of the $p_x + ip_y$-wave and compare it with the $s$-wave, since both superconductors are full-gap systems and have the same density of states. We can obtain a similar Hamiltonian for a $d_{x^2−y^2} + id_{xy}$-wave if we replace $\Delta$ by $−\sigma\Delta$ and $l = 1$ by $l = 2$.

In accordance with the Wilson’s NRG procedure, the bare conduction band is discretized logarithmically and the Hamiltonian (1) can be transformed into the following hopping type with staggered potential for both $p_x + ip_y$-wave and $d_{x^2−y^2} + id_{xy}$-wave pairing states:

$$
H_{N+1} = \Lambda^{1/2} H_N + \sum_{\tau\sigma} \left[ \varepsilon_N(c_{N+1,\tau\sigma}^\dagger c_{N\tau\sigma} + \text{H.c.}) + (-1)^N \Lambda^{N/2} \sum_{\tau'\sigma'} \Delta_{\tau'\sigma'}^+ c_{N+1,\tau\sigma}^\dagger c_{N\tau'\sigma'} \right],
$$

$$
H_0 = \Lambda^{-1/2} \left[ \frac{1}{2} \sum_{\tau'\tau\sigma'\sigma} \left( -JS \cdot \sigma_{\sigma'\sigma'} + \hat{V}\delta_{\sigma\sigma'} \right) c_{\tau\sigma'}^\dagger c_{\tau'\sigma} - \sum_{\tau\sigma} \tau'\tau\sigma' \sigma' \right].
$$

The subscript $\tau = \pm$ represents the two channels constructed by the $l = 0$ and $l = 1$ orbitals. Note that the channels are not independent due to the channel-flip ($\sum_{\tau\tau'}$) terms. This means that only one of the paired electrons ($l = 0$) couples with the local spin as in eq. (1), since the operator of the conduction electron at the impurity is written by

$$
\sum_k a_{k,l=0,\sigma} = c_{N=0,\tau=+,\sigma} + c_{N=0,\tau=-,\sigma}.
$$

Here, $c_{N\tau\sigma}$ is the operator of the NRG fermion quasiparticle in the $N$-th shell. In eq. (2), $\varepsilon_N$ is given by

$$
\varepsilon_N = [1 - \Lambda^{-(N+1)}][1 - \Lambda^{-(2N+1)}]^{-1/2}[1 - \Lambda^{-(2N+3)}]^{-1/2},
$$

where $\Lambda$ is the discretization parameter. The values with tilde are normalized by $(1 + \Lambda^{-1})/2$. For simplicity, we used the same values for both the superconducting cutoff energy and the band width, which does not alter the results. Throughout this letter, we keep the lowest-lying 500 states at each renormalization step and take $\Lambda = 3$.

First, we discuss the case of $\hat{J} = 0$ to demonstrate the reliability of our NRG results. Figure 1 shows a finite $\hat{V}$ case in which an excited state (bound state) appears below the gap. The appearance of the bound state is due to the pair breaking effect of the potential scattering (non-magnetic impurity effect). The ratio of the renormalized bound state energy and the renormalized energy gap converges as the renormalization step $N$ increases. The convergence value is represented by $(E_{\text{pot}}/\Delta)^*$. In Fig. 1, $(E_{\text{pot}}/\Delta)^*$ decreases with $\hat{V}$ as expected. The NRG result is in good agreement with the analytic solution given by a function of $\hat{V}$.

$$
E_{\text{pot}} = \Delta \sqrt{1 + (\alpha \hat{V})^2}. \tag{5}
$$

Let us consider the $\hat{J} \neq 0$ case. Since we have confirmed that the potential term $\hat{V}$ does not change the ground state, we restrict ourselves to the $\hat{V} = 0$ case. When $\hat{J} \rightarrow 0$ and $\hat{\Delta} \neq 0$, the impurity spin is decoupled from the quasiparticles and there is no bound state below the superconducting energy gap as expected. In this case, the NRG Hamiltonian has two independent $\tau = \pm$ channels which have the same form as the $s$-wave except for the sign of the order parameter depending on $\tau$. The NRG energy level structure for the $p_x + ip_y$-wave has particle-hole symmetry. In the opposite limit ($\hat{J} \neq 0$), the NRG energy level structure at the fixed point is given by the admixture of a strong coupling type and a free spin type. The former is for the $l = 0$ orbital and the latter is for the $l = 1$. The NRG energy spectra
Fig. 2. $T_K/\Delta$ dependence of the bound state energy $(E_{\text{mag}}/\Delta)^*$ generated by the magnetic impurity. $(E_{\text{mag}}/\Delta)^*$ is measured from the lowest-lying doublet for each $T_K/\Delta$. (a) $p_x + ip_y$-wave case. The ground state is a spin doublet and the first excited state is a particle-hole doublet with no spin (see Table I). The results for fixed $T_K$ are expressed by a circle and a star for $T_K = 9.20 \times 10^{-5}$ and $1.76 \times 10^{-3}$, respectively. Triangle-up and triangle-down are the results for fixed $\Delta = 0.001$ and $0.005$, respectively. (b) s-wave case. In the positive $(E_{\text{mag}}/\Delta)^*$ region, the ground state is a spin doublet and the first excited state is a spin singlet. In the negative $(E_{\text{mag}}/\Delta)^*$ region, the ground and excited states are interchanged. The level crossover takes place at around $T_K/\Delta = 0.3$.

The Kondo singlet cannot be a ground state in the small $T_K/\Delta$ region. Since this level can be occupied by at most two particles, the ground state has fourfold degeneracy. We note that the local spin is quenched completely for $\Delta = 0$.

When $J$ turns on for a finite $\Delta$, a bound state appears below the energy gap due to the magnetic impurity. Figure 2(a) shows the $T_K/\Delta$ dependence of the bound state energy $(E_{\text{mag}}/\Delta)^*$ for the $p_x + ip_y$-wave. Here, the Kondo temperature is defined by

$$T_K = \sqrt{|J| \exp(-1/|J|)}.$$  

First, we look into the small $T_K/\Delta$ region. As shown in Table I(A), the ground state is a spin doublet. The first excited state is a particle-hole doublet with no spin. In the Kondo effect, it is favorable for the magnetic impurity to form a Kondo singlet. However, the magnetic impurity has to break the Cooper pair to couple with one of the paired electrons. Since this costs considerable energy, the Kondo singlet cannot be a ground state in the small $T_K/\Delta$ region. As $T_K/\Delta$ increases, $(E_{\text{mag}}/\Delta)^*$ decreases monotonically and approaches the ground state energy asymptotically. Thus, the ground state approaches the $\Delta = 0$ result smoothly as $T_K/\Delta$ increases to infinity, and it becomes fourfold degenerate. This result shows that the spin singlet ground state is not realized in all the $T_K/\Delta$ region, which is completely different from the $s$-wave result shown in Fig. 2(b). On the other hand, we find that $(E_{\text{mag}}/\Delta)^*$ for the $p_x + ip_y$-wave is scaled by $T_K/\Delta$ as for the $s$-wave. While the interchange of the ground state does not occur in the $p_x + ip_y$-wave case, almost the same $T_K/\Delta$ dependence of $(E_{\text{mag}}/\Delta)^*$ is obtained in both cases. For the $s$-wave, the energy gap suppresses the Kondo effect in the $(E_{\text{mag}}/\Delta)^* > 0$ region, while the Kondo singlet is stabilized against the energy gap in the $(E_{\text{mag}}/\Delta)^* < 0$ region. This crossover occurs at approximately $T_K/\Delta = 0.3$.

In analogy to the $s$-wave, there is also a crossover at around $(E_{\text{mag}}/\Delta)^* = 0.5$ for the $p_x + ip_y$-wave. Thus, the Kondo effect overcomes the energy gap in the $(E_{\text{mag}}/\Delta)^* < 0.5$ region, although the ground state is still a spin doublet. This implies that the competition between the Kondo effect and the energy gap is characterized by such $T_K/\Delta$ dependence of the bound state energy for all types of superconductivity. We mention here that the NRG energy level structure for the $d_{x^2-y^2} + id_{xy}$-wave is the same as that for the $p_x + ip_y$-wave. Their difference appears only in the wave functions.

Let us discuss the strong coupling limit ($|\tilde{J}| \to \infty$) case where the impurity part $H_0$ is truncated from the conduction electron part. In this limit, the ground state property is given by $H_0$. Converting from the channel $(\tau)$ representation to the angular momentum $(l)$ representation

$$c_{N=0,\tau=\pm,\sigma} = \frac{1}{\sqrt{2}} (f_{l=0,\sigma} \pm f_{l=1,\sigma}),$$  

we can express $H_0 = H_{s-d} + H_\Delta$, where

$$H_{s-d} = -\tilde{J} \sum \mathbf{S} \cdot \sigma \sigma' f_{1,\sigma}^\dagger f_{0,\sigma'},$$  

$$H_\Delta = -\Delta \sum \sigma \sigma' (f_{0,\sigma} f_{1,\sigma'} + f_{1,\sigma} f_{0,\sigma'}).$$  

Note that the order parameter corresponds to the hopping parameter between the $l = 0$ and $l = 1$ local orbital sites, since the $p_x + ip_y$-wave Cooper pair is formed by the $l = 0$ and $l = 1$ particles. When $|\tilde{J}| \to \infty$, the $l = 0$ particle couples with the local spin strongly to form a spin singlet $|s\rangle = f_{0,\uparrow}^\dagger |\downarrow\rangle - f_{0,\downarrow}^\dagger |\uparrow\rangle$. Here, $|\sigma\rangle (\sigma = \uparrow, \downarrow)$
is the wavefunction of the local spin. The spin doublet \( \langle f_1 \downarrow | s \rangle \) and spin singlet \( \langle f_1 \uparrow f_1 \downarrow | s \rangle \) are degenerate since the hopping between \( l = 0 \) and \( l = 1 \) is forbidden. At a finite \( |J|, \Delta \) in eq. (8) lifts the degeneracy. The wavefunctions for the spin doublet \( \psi_{S=1/2} \) and spin singlet \( \psi_{S=0} \) are given by the linear combination of the following terms:

\[
\psi_{S=1/2} = c_1 \left( f_{1\downarrow} | s \rangle + c_2 \left( f_{0\uparrow} f_{1\downarrow} | \sigma \rangle + c_3 \left( f_{1\uparrow} f_{1\downarrow} | \sigma \rangle \right) + c_4 \left( f_{1\uparrow} f_{1\downarrow} | \sigma \rangle \right) \right),
\]

\[
\psi_{S=0} = c_6 | s \rangle + c_7 \left( f_{1\uparrow} \downarrow - f_{1\downarrow} \uparrow \right) \]  

Here, \( c \) is a coefficient. The perturbation theory shows that \( \psi_{S=1/2} \) is the ground state, whose energy is lower than that of \( \psi_{S=0} = -\frac{2}{3} |J| (|\Delta|/J)^2 \). When \( |J| \) is very large, coefficient \( c_1 \) of the first term in \( \psi_{S=1/2} \) is the largest. In the strong coupling limit, the local spin is almost quenched by the \( l = 0 \) particle forming the Kondo singlet \( |s\rangle \). However, the \( l = 1 \) particle is connected weakly to the quenched local spin \( |s\rangle \). This does not mean that the \( l = 1 \) electrons destroy the Kondo singlet. They gain the superconducting condensation energy and then generate the spin \( 1/2 \) of the ground state in the strong coupling limit. As \( |\Delta| \) decreases, coefficients \( c_2 \) and \( c_3 \) of the second and third terms, respectively, in \( \psi_{S=1/2} \) increase. This indicates that the weight of the local spin becomes larger in the spin of the ground state. Thus, the ground state always has a spin \( 1/2 \) for the \( p_x + ip_y \)-wave. The \( T_K/\Delta \) dependence of the bound state energy shown in Fig. 2(a) reflects the continuous change of the wavefunction of the spin doublet ground state.

Contrary to the \( p_x + ip_y \)-wave, the wavefunctions for the \( s \)-wave are given by \( \varphi_{S=0} = |s\rangle \) and \( \varphi_{S=1/2} = f_{0\uparrow} f_{1\downarrow} |\sigma \rangle \) in the strong coupling limit. In this case, the hopping between the \( l = 0 \) and \( l = 1 \) orbital sites is replaced by the potential at the \( l = 0 \) site:

\[
H_\Delta = -\Delta \left( f_{0\uparrow} f_{0\downarrow} + f_{1\uparrow} f_{1\downarrow} - 1 \right). \]  

This is because the \( s \)-wave Cooper pair is formed by only the \( l = 0 \) particles. The ground state is characterized by \( \varphi_{S=0} \) (\( \varphi_{S=1/2} \)) in a large (small) \( T_K/\Delta \) region. For the \( s \)-wave, the \( l \neq 0 \) conduction electrons are completely decoupled from the local spin.

In conclusion, we have studied the Kondo effect unique to the \( p_x + ip_y \)-wave superconductor, where the orbital dynamics of the Cooper pair produce the spin of the ground state. For large \( T_K \), the \( l = 0 \) electrons couple with a local spin strongly to form a Kondo singlet, while the other electrons with \( l = 1 \) are coupled to the Kondo singlet weakly via the superconducting order parameter. The NRG study has shown that the ground state is a spin doublet in all the \( T_K/\Delta \) region, which is different from the results for the \( s \)-wave and \( d_{x^2-y^2} \)-wave cases. It is interesting to search for a new type of Kondo effect due to the orbital effect of the Cooper pair in unconventional superconductors.

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