Competition between Singlet and Triplet Superconductivity in the Extended Hubbard Model with Exchange Interaction on a Square Lattice

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Abstract. Phase boundary between spin singlet and triplet superconductivity in the extended Hubbard model with exchange interaction on a square lattice is calculated within meanfield approximation. Basically, antiferromagnetic exchange interaction $J$ is advantageous for the singlet pairing, while ferromagnetic $J$ prefers the triplet pairing. When off-site interaction $V$ is repulsive, the singlet phase and the triplet phase are separated by normal state in the phase diagram against $V$ and $J$. If $V$ is effectively attractive, however, the singlet and triplet states can compete against each other. We calculate the phase boundary between singlet and triplet phase for various band filling. It is shown that the triplet phase penetrates rather deeply into antiferromagnetic exchange regime for lower band filling, whereas the penetration of the singlet phase is confined in a narrow range of ferromagnetic exchange regime.

Many unconventional superconductors are considered to have magnetic interaction as their origin. In the superconductivity (SC) of high-$T_c$, heavy fermion, Sr$_2$RuO$_4$, (TMTSF)$_2$PF$_6$, and iron pnictides, spin fluctuation mediated interaction is thought to play an essential role. Basically, antiferromagnetic (AF) exchange interaction is advantageous for singlet pairing and ferromagnetic (FM) exchange favors triplet pairing. However, the triplet SC mediated by FM exchange is difficult to realize[1], because the contribution of FM exchange to triplet pairing is three times smaller than that of AF exchange to singlet pairing. To overcome the difficulty, the effects of anisotropic exchange interaction[2, 3, 4], contribution from charge fluctuation[5, 6], phonon mediated interaction[7], refinement of electronic structure[1] have been investigated.

We study the extended Hubbard model with exchange interaction on a square lattice

\[ H = \sum_{i,j} (t_{ij} - \mu \delta_{ij}) c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_{<i,j>} V_{ij} n_i n_j + \sum_{<i,j>} J_{ij} S_i \cdot S_j, \]  

where $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma} (\sigma = \uparrow, \downarrow)$, $n_i = \sum_{\sigma} n_{i\sigma}$, $S_i^\lambda = \sum_{\alpha \beta} \epsilon_{\alpha\beta}^\lambda c_{i\alpha}^\dagger \sigma_{\alpha\beta}^\lambda c_{i\beta}$, $S_i = (S_i^x, S_i^y, S_i^z)$, and $\sigma^\lambda (\lambda = x, y, z)$ are Pauli matrices. Only the nearest neighbor interactions are considered for $V_{ij} = V$ and $J_{ij} = J$. We consider the interactions as phenomenological parameters without addressing the origin of the interaction, and treat the problem within meanfield approximation to obtain a basic picture of relation between SC and exchange interaction, which would serve to understand the importance of more elaborated model and approximation. Although Micnas et al. studied the details of models including this Hamiltonian in the same sort of manner[8], we
focus on the role of exchange interaction in competition of singlet and triplet SC. In $k$ space, the Hamiltonian is written as

$$\mathcal{H} = \sum_{k\alpha} \varepsilon(k) c_{k\alpha}^\dagger c_{k\alpha} + \frac{1}{2} \sum_{kk'q\alpha\beta\delta} V_{\alpha\beta\gamma\delta}(k, k', q)c_{-k+q\alpha}^\dagger c_{k\beta} c_{k'\gamma} c_{-k'+q\delta}, \quad (2)$$

where $\mathcal{H}$ is the Hamiltonian written as of singlet (extended) $s$-wave or $d$-wave SC.

Substituting these expressions to the gap equation, we obtain linear systems of equations for $\Delta$ and $\tau^\alpha$. In meanfield approximation, the gap equation for uniform SC is given by

$$\Delta_{\alpha\beta}(k) = -\sum_{k'\gamma\delta} V_{\alpha\beta\gamma\delta}(k, k', 0) F_{\gamma\delta}(k'), \quad (5)$$

where $\Delta(k) = d_0(k)\tau^0 + d_\alpha(k)\tau^\alpha$, $E_{k\pm} = \sqrt{[\varepsilon(k)]^2 + |d_0|^2 + |d_\alpha|^2 \pm |p|}$, $p = i(d \times d') + d_0 d^* + d_\alpha d'$, and $\beta = 1/k_B T$. In the limit of $T \rightarrow T_c$, the gap equation is linearized and separated into singlet and triplet component:

$$d_0(k) = -\frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} dk' W(k') \left\{ \frac{U}{2} + 2K_0 (\cos k_x \cos k'_x + \cos k_y \cos k'_y) \right\} d_0(k'), \quad (6)$$

$$d_\lambda(k) = -\frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} dk' W(k') \cdot 2K (\sin k_x \sin k'_x + \sin k_y \sin k'_y) d_\lambda(k') \quad (\lambda = x, y, z), \quad (7)$$

where $W(k) = \text{tanh}(\beta |\varepsilon(k)|/2)/|\varepsilon(k)|$. From the linearized gap equation, the order parameters $d_\lambda(k)$ can be written as

$$d_0(k) = \Delta_0 + \Delta_\alpha (\cos k_x + \cos k_y) + \Delta_d (\cos k_x - \cos k_y), \quad \Delta_\alpha (\cos k_x + \cos k_y) + \Delta_d (\cos k_x - \cos k_y), \quad (8)$$

$$d_\lambda(k) = \Delta_{\lambda px} \sin k_x + \Delta_{\lambda py} \sin k_y \quad (\lambda = x, y, z). \quad (9)$$

Substituting these expressions to the gap equation, we obtain linear systems of equations for $\Delta_0$, $\Delta_\alpha$, $\Delta_d$, and $\Delta_{\lambda px}$, $\Delta_{\lambda py}$. The critical temperature $T_c$ of each state is determined by the condition that the linear system of equations has nontrivial solutions. The conditions for $T_c$ of singlet (extended) $s$-wave ($\Delta_0$ or $\Delta_\alpha \neq 0$) and $d$-wave ($\Delta_d \neq 0$) are,

$$-K_0 I_U = 1, \quad (10)$$

$$-K_0 I_d = 1, \quad (11)$$

respectively, and the condition for $T_c$ of triplet $p$-wave pair ($\Delta_{\lambda px}$, $\Delta_{\lambda py} \neq 0$) is

$$-K I_p = 1, \quad (12)$$
where

\[ I_0 = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} dkW(k), \quad I_s = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} dkW(k)(\cos k_x + \cos k_y), \]

\[ I_{ss} = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} dkW(k)(\cos k_x + \cos k_y)^2, \quad I_d = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} dkW(k)(\cos k_x - \cos k_y)^2, \]

\[ I_p = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} dkW(k)(\sin^2 k_x + \sin^2 k_y), \quad I_U = I_{ss} - \frac{1}{2} \frac{U}{I_d} \frac{I_P^2}{I_U + 1}. \]

In this simple approximation, \( T_c \) is determined only by \( U, V, J \), and the affinity of the gap function and the band structure, especially Fermi surface determined by band filling for low temperature. The conditions for \( d \)- and \( p \)-wave are not so complicated. As is seen from the coupling constants \( K_0 = \frac{1}{2}(V - 3J), K = \frac{1}{2}(V + J) \) and the conditions eq. (11), (12), the necessary condition that \( d \)-wave or \( p \)-wave has a finite \( T_c \) is \( J > V/3 \) or \( J < -V \) respectively. Antiferromagnetic exchange interaction \((J > 0)\) contributes to \( d \)-wave pair and ferromagnetic interaction \((J < 0)\) contributes to triplet \( p \)-wave pair. The contribution of AF exchange to \( d \)-wave is three times larger than that of FM exchange to \( p \)-wave. Apparently, this factor three always works advantageously for \( d \)-wave. Indeed, if the off-site interaction \( V \) is repulsive \((V > 0)\), \( d \)-wave and \( p \)-wave phase are separated each other by normal phase and the \( d \)-wave phase occupies three times larger region in the phase diagram against \( V \) and \( J \). If \( V \) is attractive \((V < 0)\), however, \( d \)- and \( p \)-wave can compete against each other. For negative \( V \), the necessary condition for \( d \)-wave, \( J > V/3 \), confines the \( d \)-wave phase three times smaller region than that of \( p \)-wave phase, \( J < -V \).

The parametric representation of the phase boundary between \( d \)- and \( p \)-wave with parameter \( T_c \) is obtained by rewriting the eq. (11) and (12)

\[
\begin{align*}
V &= -\frac{1}{2}(3I_p^{-1} + I_d^{-1}), \\
J &= -\frac{1}{2}(I_p^{-1} - I_d^{-1}).
\end{align*}
\]

The phase boundary between \( s \)- and \( p \)-wave is given by

\[
\begin{align*}
V &= -\frac{1}{2}(3I_p^{-1} + I_U^{-1}), \\
J &= -\frac{1}{2}(I_p^{-1} - I_U^{-1}).
\end{align*}
\]

The phase boundary between \( s \)- and \( d \)-wave is given by

\[
J = \frac{1}{3} V + \frac{2}{3} I_d^{-1}, \quad I_d = I_U.
\]

We numerically calculated \( T_c \) and the phase boundary between the states with different symmetries for various band-filling \( n \). The on-site repulsion is fixed at \( U = 8.0 \) in this calculation, which has little effect on the results. Fig. 1 shows \( T_c \) as a function of \( V \) and \( J \) for \( n = 0.20, 0.28, \) and \( 0.60 \). Fig. 2 shows the phase boundary between the states with different symmetries for several \( n \) at \( T = 0.001 \). For the lowest band filling \( n < 0.20 \), \( s \)-wave penetrates into the FM regime, and for \( 0.14 \leq n \leq 0.60 \), \( p \)-wave penetrates into AF regime. For \( 0.38 \leq n \leq 1.00 \), \( d \)-wave penetrates into FM regime if we neglect other ordered phases around half-filling \( (n = 1) \).

Seeing the phase boundary between SC and normal state in Fig. 2 around \( J = 0 \), we note the penetration of singlet SC into FM regime is small compared to that of \( p \)-wave into AF regime, because the penetration of singlet SC is restricted by the conditions \( J \geq \frac{1}{3} V + \frac{2}{3} I_U^{-1} \) and \( J \geq \frac{1}{3} V + \frac{2}{3} I_d^{-1} \), whereas the restriction for the penetration of triplet, \( J \leq -V - 2I_p^{-1} \), is not so severe. As a result, \( p \)-wave can penetrate into AF regime to \( J \approx 0.33 \), whereas the \( d \)-wave
Figure 1. $T_c$ of $s$(red)-, $d$(blue)-, and $p$(green)-wave as a function of $V$ and $J$ for (a) $n = 0.20$, (b) 0.28, (c) 0.60, where $U = 8.0$.

Figure 2. Phase diagram against $V$ and $J$ for several $n$. (a) $n = 0.06$, (b) 0.20, (c) 0.28, (d) 0.30, (e) 0.60, (f) 1.0, where $T = 0.001$, and $U = 8.0$.

penetrates only to $J \approx -0.18$. Though the penetration of $s$-wave is rather deep ($J \approx -0.69$), that is restricted to the lowest filling range, and fairly large $|V|$ is required.

In summary, if off-site interaction $V$ is attractive, we can consider the destructive role of exchange interaction $J$, which destroys singlet superconductivity more effectively than triplet superconductivity not depending on the origin of $V$ and $J$. The contribution of ferromagnetic exchange to triplet is certainly small, but triplet superconductivity is robust for the changes in magnetic interaction.

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