Effect of Band Structure on the Symmetry of Superconducting States

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Effects of the band structure on the symmetry of superconducting (SC) states are studied. For a square lattice system with a nearest-neighbor attractive interaction, SC states with various symmetries are found by changing the band structure, or, the shape of the Fermi surface. The spin-triplet ($(p_x + ip_y)$)-wave and spin-singlet ($d$- or $s$-wave) SC states, and states with their coexistence ($d + ip_y$, $s + ip_y$) can be stabilized within the same type of interaction. The stability of interlayer-pairing states with line nodes is also examined, and its relation to the SC state of Sr$_2$RuO$_4$ is discussed.

KEYWORDS: $p$-wave superconductivity, band structure, Ginzburg-Landau theory, Sr$_2$RuO$_4$

The superconducting (SC) state of Sr$_2$RuO$_4$ attracts much attention, since it is likely to have a spin-triplet pairing symmetry. The triplet Cooper pairs in $^3$He are formed due to the ferromagnetic spin fluctuation, so that it may be natural to assume that a SC state in Sr$_2$RuO$_4$ is also realized by the same mechanism. However, recent neutron scattering experiments showed that the peak is located near $\vec{q} = (\pm 2\pi/3, \pm 2\pi/3)$, consistent with band structure calculations [1]. In view of this fact it is proposed that the antiferromagnetic spin fluctuation may lead to the spin-triplet SC state. Similar results have also been obtained in different contexts.

In this article we study the effect of the band structure on the symmetry of SC states. First we treat a tight-binding model on a square lattice system with a nearest-neighbor attractive interaction, SC states with various types of interlayer-pairing states with line nodes are formed due to the ferromagnetic spin fluctuation, and the spin-triplet state may lead to the spin-triplet SC state. First we consider a tight-binding model on a square lattice system with a nearest-neighbor attractive interaction, and the corresponding Hamiltonian is decoupled by a standard mean-field procedure.

$$ H = -\sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} - \mu \sum_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma} - \sum_{i,j} V_{ij} n_{i\uparrow} n_{j\downarrow} $$

where $\mu$ is the chemical potential, and $t_{ij}$ is defined as

$$ t_{ij} = t \sum_{\delta = \pm \hat{x}, \pm \hat{y}} \delta_{i,j+\delta} + t' \sum_{\delta = \pm \hat{x}, \pm \hat{y}} \delta_{i,j+\delta}. $$

Namely, $t$ ($t'$) is the transfer integral for the (next) nearest-neighbor sites and $\hat{x}$ ($\hat{y}$) is the unit vector in the $x$ ($y$) direction (lattice constant is taken to be unity). Similarly the nearest-neighbor attractive interaction $V_{ij}$ is defined as $V_{ij} = V \sum_{\delta = \pm \hat{x}, \pm \hat{y}} \delta_{i,j+\delta} (V > 0)$. This Hamiltonian is decoupled by a standard mean-field procedure.

$$ n_{i\uparrow} n_{j\downarrow} = c_{i\uparrow}^\dagger c_{i\uparrow} c_{j\downarrow} c_{j\downarrow} $$

$$ \rightarrow \Delta_{ij} c_{j\downarrow} c_{i\uparrow}^\dagger + \Delta_{ij}^* c_{i\uparrow} c_{j\downarrow} - |\Delta_{ij}|^2 $$

with $\Delta_{ij} \equiv \langle c_{i\uparrow} c_{j\downarrow} \rangle$ being the SC order parameter (OP). On the square lattice the $d_{x^2-y^2}$- ($\Delta_d$), $p_x$- ($\Delta_p$) and $p_y$-wave ($\Delta_p$) symmetries are possible for the nearest-neighbor interaction, and the corresponding OP’s are defined as

$$ \Delta_d(i) = (\Delta_{i,i+x} + \Delta_{i,i-x} - \Delta_{i,i+y} - \Delta_{i,i-y})/4 $$

$$ \Delta_p(i) = (\Delta_{i,i+x} + \Delta_{i,i-x} - \Delta_{i,i+y} + \Delta_{i,i-y})/4 $$

$$ \Delta_{p_x}(i) = \mathbf{i}(\Delta_{i,i+x} - \Delta_{i,i-x})/2. $$

Assuming that these OP’s are uniform (i.e., independent of $i$) we obtain the following self-consistency equations:

$$ \Delta_{d}(i) = \frac{V}{4N} \sum_{k} \omega_{d}(k) \frac{\Delta_k}{E_k} \tanh \left(\frac{E_k}{2T}\right) $$

$$ \Delta_{p_x}(i) = \frac{V}{2N} \sum_{k} \omega_{p_x}(k) \frac{\Delta_k}{E_k} \tanh \left(\frac{E_k}{2T}\right) $$

where $N$ and $T$ are the total number of lattice sites and

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the temperature, respectively, and
\[ E_k = \sqrt{\xi_k^2 + |\Delta_k|^2} \]
\[ \xi_k = -2t'(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - \mu \]
\[ \Delta_k = 2 \sum_{j=d,s,p_x,p_y} \omega_j(k)\Delta_j \] \hspace{1cm} (6)
with
\[ \omega_d(k) = \cos k_x - \cos k_y, \]
\[ \omega_s(k) = \cos k_x + \cos k_y, \]
\[ \omega_{p_x(y)} = \sin k_x(y). \] \hspace{1cm} (7)
In the following we will solve the self-consistency equations to determine the phase diagram in the plane of \( T \) and \( \mu \). These equations are solved by the iteration method, starting from various sets of initial values. When several solutions are obtained for the same set of parameters (\( \mu, T \)), the state with the lowest free energy is adopted as the true one. Here we note that the SC long-range order cannot exist at finite temperature in a purely two dimensional (2D) system. However, \( T_c \) obtained within the MFA in purely 2D systems can give a reasonable estimate of \( T_c \) in the presence of small three dimensionality.

In Fig.1 we show the phase diagram in the plane of \( T \) and \( \mu \) (or, the electron density), for \( t = 1, t' = 0 \) and \( V = 1.5 \). (Due to the particle-hole symmetry, the result for \(-\mu\) is the same as that for \( \mu \), and so it is not shown.) It is seen that a \( d_{x^2-y^2} \)-wave SC state is stabilized near half-filling (\( \mu \sim 0 \)), while an extended \( s \)-wave state occurs at high (and low) densities (\( \mu \sim \pm 4t \)). In the region between \( d \)- and \( s \)-wave states spin-triplet \((p_x \pm ip_y)\)-wave states appear. The \((p_x + ip_y)\) and the \((p_x - ip_y)\)-states are degenerate but different states, and they transform each other under parity \( P \) and time-reversal \( T \) transformation. Then the system breaks \( P \) and \( T \) symmetries spontaneously, and these states are usually denoted as the chiral \( p \)-wave SC states. Near the boundary between triplet \((p_x \pm ip_y)\) and singlet \((d \text{ or } s)\) states we find states where the spin-singlet and the spin-triplet OP’s coexist. These coexisting states, \((d \pm ip_y)\)- and \((s \pm ip_y)\)-states, are degenerate with \((d \pm ip_x)\) and \((s \pm ip_x)\)-states, respectively \( \frac{3}{2} \). The \((d \pm ip_x \pm ip_y)\) and \((s \pm ip_x \pm ip_y)\) states are slightly higher in energy so that they are only local minima of the free energy. There is no reason (regarding symmetry) which precludes the coexistence of spin-triplet and spin-singlet SCOP’s, and it is the energy that decides which state should appear. Actually the coexistence of \( d \)- and \( p \)-wave OP’s has been found in superconductor/(anti)ferromagnet bilayer systems, where the proximity effect induces the imbalance of spin-up and spin-down electron densities \( \frac{2}{3} \).

The above results show that both triplet and singlet SC states can occur with the same type of interaction. In order to understand this we use the Ginzburg-Landau (GL) theory by expanding the free energy with respect to \( \Delta \) \( \frac{2}{3} \):

\[ F_\Delta = \frac{1}{2} \int d^2r \left( \sum_{j=d,s,p_x,p_y} \left[ \alpha_j \Delta_j^2 + \beta |\Delta_j|^4 \right] + \sum_{i \neq j} \left[ \gamma_{ij}^{(1)} |\Delta_i|^2 |\Delta_j|^2 + \gamma_{ij}^{(2)} (\Delta_i^2 \Delta_j^2 + \text{c.c.}) \right] \right) \] \hspace{1cm} (8)
where the gradient and higher order terms are discarded, and \( S \) is the area of the system. As \( T \) is decreased the OP with the highest (bare) transition temperature \( T_c(0) \) \((\alpha(T_c(0)) = 0)\) appears. The explicit forms of \( \alpha \)'s are given as

\[ \alpha_{d(s)} = 4V \left( 1 - \frac{V}{N} \sum_k \omega_d(s)(k) \frac{\tanh(\xi_k / 2T)}{2 \xi_k} \right) \]
\[ \alpha_{p_x(y)} = 2V \left( 1 - \frac{V}{N} \sum_k \omega_{p_x(y)}(k) \frac{\tanh(\xi_k / 2T)}{\xi_k} \right). \] \hspace{1cm} (9)
The Fermi surface (FS) near the band edge (\( \mu \sim \pm 4t \)) is close to the \( \Gamma \) point or \( k = (\pm \pi, \pm \pi) \), so that \( |\omega_s(k)| \) is large on the FS and thus \( \Delta_s \) is favored. On the other hand the FS at half-filling is the square connecting four points \((\pm \pi, 0), (0, \pm \pi)\), and \( \omega_s(k) \) vanishes there. Then \( \Delta_s \) is suppressed near half-filling and \( \Delta_d \) is favored. For intermediate \( \mu \) \((\mu \sim \pm 2t)\), the FS comes close to the points \( k_x = \pm \pi/2 \) or \( k_y = \pm \pi/2 \) so that \( |\omega_{p_x(y)}(k)| \) can be large. Then the \( p \)-wave states have the highest \( T_c \) in the region between \( d \)- and \( s \)-wave states \((p_x \text{ or } p_y \text{ states are degenerate})\).

When more than one \( \alpha \) become negative there may be a coexistence of several OP’s. In this case \( \gamma \) terms will play important roles. We can explicitly show that \( \beta_i > 0, \gamma_{ij}^{(1)} > 0 \) and \( \gamma_{ij}^{(2)} > 0 \) \((i,j = d, s, p_x, p_y)\). The fact \( \gamma_{ij}^{(2)} > 0 \) indicates that the OP’s would form complex rather than real combinations (if they coexist), and in this case the nodes are removed and the system gains more condensation energy. This is the reason why the chiral \((p_x \pm ip_y)\)-state (rather than \((p_x \pm ip_y)\)-state) appears. The coexisting states also have the complex combinations of OP’s due the same reason. In Fig.1 the region of \((d+ip_y)\)-state is much wider than that of \((s+ip_y)\)-state. This can be understood as follows. The nodes in the \( d \)-wave state can be removed by the introduction of the \( ip_x \) component, while in the \( s \)-state there is already a full gap so that the lowering of the energy due to the second OP is much smaller.

Whether or not the above argument is correct can be tested by considering the case of \( t = 0, t' \neq 1 \), i.e., with only the next-nearest-neighbor hopping terms. The Fermi surface at half-filling consists of the lines \( k_x = \pm \pi/2 \) and \( k_y = \pm \pi/2 \), so that the \((p_x \pm ip_y)\)-state should be most favored near half-filling. This is actually the case as shown in Fig.2. Here the chiral SC state appears at and near half-filling, and \( d \)- or extended \( s \)-wave state occurs away from half-filling.

Next we examine the stability of interlayer-pairing SC states in a tetragonal system with a weak interlayer in-
interaction. The Hamiltonian in this case is

\[ H = H_{2D} + H_{\perp} \]

\[ H_{\perp} = -t_\perp \sum_i \sum_{\delta = \pm \hat{z}, \pm \hat{x} \pm \hat{y}} c_i^\dagger c_{i+\delta} - V_\perp \sum_i \sum_\delta n_i n_{i+\delta, \perp} \]  

(10)

where the summation on \( \delta \) in the second term is taken over \( \delta = \pm \hat{z} \pm \hat{x}, \pm \hat{z} \pm \hat{y} \) and \( H \) in eq.(1) is redefined as \( H_{2D} \). Here \( \hat{z} \) denotes the unit vector in the \( z \)-direction with a lattice constant \( c \). For the \( t_\perp \)-term we simply take the nearest-neighbor hopping, but we do not consider the nearest-neighbor interaction because of the following reason. The interaction terms with \( \delta = \pm \hat{z} \) (with coupling constant \( V_\perp^{(0)} \)) may lead to the OP of the form \( \Delta_{i, \pm \hat{z}} \). This OP is invariant under the rotation around the \( z \)-axis so that it is decoupled from the in-plane OP (denoted as \( \Delta_{\perp} \)). Since \( \Delta_{\perp} \) has no warping along the \( z \)-axis, it is decoupled from the in-plane OP (denoted as \( \Delta_{\parallel} \)). Between these two states are degenerate when \( t_\perp = 0 \).

Next we consider the case \( t_\perp \neq 0 \). In this case \( \Delta_{\parallel} \) couples to \( \Delta_{\perp}^{(c)} \). Then the latter can be finite once \( V_\perp \) becomes finite. Now the gap function is

\[ \Delta_k = (\sin k_x + i \sin k_y)(\Delta_{\parallel} + \Delta_{\perp}^{(c)} \cos k_z c + i \Delta_{\perp}^{(s)} \sin k_z c). \]

(12)

Since \( \Delta_{\perp}^{(c)} \) is induced by the bilinear coupling to \( \Delta_{\parallel} \), their relative phase is either 0 or \( \pi \), while \( \Delta_{\perp}^{(s)} \) favors a phase \( \pm \pi/2 \) relative to them due to \( \gamma \) terms. In Fig.4 the results are shown for \( t_\perp = 0.4 \). Here \( |\Delta_{\parallel}| > |\Delta_{\perp}| \) and \( \Delta_{\perp}^{(c)} = 0 \) for small \( V_\perp \) and there is a full gap. For large values of \( V_\perp \), \( |\Delta_{\perp}^{(c)}| > |\Delta_{\parallel}| \). However, \( \Delta_{\perp}^{(s)} \) component appears before \( |\Delta_{\perp}^{(c)}| \) exceeds \( |\Delta_{\parallel}| \). Then the state is again fully gapped except an accidental case where \( |\Delta_{\perp}^{(c)}| = |\Delta_{\parallel}| \). We have also examined other values of \( t_\perp \), and the SC state (with \( p_\perp \pm im_\parallel \)-symmetry for the in-plane OP) always has a full gap except an accidental case, unless \( t_\perp \) becomes comparable to \( t \).

In summary we have studied the symmetry of the SC states in a single-band tight-binding model with an attractive interaction between nearest-neighbor sites. It is shown that the spin-triplet and the spin-singlet SC states, and even their coexistence can occur as the band structure is changed. These results can be understood by considering the change of the shape of the Fermi surface.

The present result implies that the band structure is an important factor to determine the symmetry of the SC state. We have also examined the stability of interlayer-pairing states with line nodes. These states are difficult to be stabilized in a model with such a simple band structure (Fermi surface) as that used in the present work. Experimental results of \( Sr_2 RuO_4 \) seem to indicate that the SC state has a spin-triplet symmetry, and that there is a line (or lines) of nodes in the excitation gap. In order to give consistent interpretations of these facts, it would be necessary to consider the model which takes into account the more realistic crystal (and band) structure of \( Sr_2 RuO_4 \). This problem will be examined elsewhere.

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1) Y. Maeno, H. Hashimoto, K. Yoshiida, S. Nishizaki, T. Fujita, J. G. Bednorz and F. Lichtenberg: Nature 372 (1994) 532.
2) T. M. Rice and M. Sigrist: J. Phys. Condens. Matter 7 (1995) L643.
3) K. Ishida, H. Mukuda, Y. Kitaoaka, K. Asayama, Z. Q. Mao, Y. Mori and Y. Maeno: Nature 396 (1998) 658.
4) G. M. Luke, Y. Fudamoto, K. M. Kojima, M. I. Larkin, J. Merrin, B. Nachumi, Y. J. Uemura, Y. Maeno, Z. Q. Mao, H. Nakamura and M. Sigrist: Nature 394 (1998) 558.
5) A. P. Mackenzie, R. K. W. Haselwimmer, A. w. Tyler, G. G. Lonzarich, Y. Mori, S. Nishizaki and Y. Maeno: Phys. Rev. Lett. 80 (1998) 161.
6) Y. Sidis, M. Braden, P. Bourges, B. Hennion, S. Nishizaki, Y. Maeno and Y. Mori: Phys. Rev. Lett. 83 (1999) 3320.
7) I. I. Mazin and D. J. Singh: Phys. Rev. Lett. 82 (1999) 4324.
8) M. Sato and M. Kohmoto: J. Phys. Soc. Jpn. 69 (2000) 3505.
9) T. Kuwabara and M. Ogata: Phys. Rev. Lett. 85 (2000) 4586.
10) M. Yu. Kagan and T. M. Rice: J. Phys. Condens. Matter 6 (1994) 3771.
11) A. V. Chubukov: Phys. Rev. B48 (1993) 1097.
12) The SC state in a similar model within the spin-singlet symmetry was studied in: H. Tsuchiya, Y. Tanaka and Y. Ushijima: J. Phys. Soc. Jpn. 64 (1995) 922.
13) R. Micnas, J. Ranninger and S. Robaszkiewicz: Rev. Mod. Phys. 62 (1990) 113.
14) S. Nishizaki, Y. Maeno and Z.Q. Mao: J. Phys. Soc. Jpn. 69 (2000) 572.
15) K. Ishida, H. Mukuda, Y. Kitaoka, Z.Q. Mao, Y. Mori and Y. Maeno: Phys. Rev. Lett. 84 (2000) 5387.
16) I. Bonalde, B.D. Yanoff, M.B. Salamon, D.J. van Harlingen, E.M.E. Chia, Z.Q. Mao and Y. Maeno: Phys. Rev. Lett. 85 (2000) 4775.
17) K. Izawa, H. Takahashi, H. Yamaguchi, Y. Matsuda, M. Suzuki, T. Sasaki, T. Fukase, Y. Yoshida, R. Settai and Y. Onuki: cond-mat/0012137.
18) C. Lupien, W.A. MacFarlane, C. Proust, L. Taillefer, Z.Q. Mao and Y. Maeno: cond-mat/0101319.
19) K. Miyake and O. Narikiyo: Phys. Rev. Lett. 83 (1999) 1423.
20) M.J. Graf and A.V. Balatsky: Phys. Rev. B 62 (2000) 9697.
21) T. Dahm, H. Won and K. Maki: cond-mat/0006301.
22) K. Kuboki, M. Ogata, R. Arita and H. Aoki: cond-mat/0101077.
23) Y. Hasegawa, K. Machida and M. Ozaki: J. Phys. Soc. Jpn 69 (2000) 336.
24) A tiny amount of $s$-wave ($d$-wave) component is mixed in the $d + ip_y$ ($s + ip_y$) state. This is because the $x$- and the $y$-directions are not equivalent in this state, and so the absolute values of OP's for both directions are not the same.
25) K. Kuboki: J. Phys. Soc. Jpn. 68 (1999) 3150.
26) For a review see M. Sigrist and K. Ueda, Rev. Mod. Phys., 63, 239 (1991).
27) Y. Hasegawa: private communications.

**Fig. 1** Phase diagram in the plane of $T$ and $\mu$. Parameters used are $t = 1, t' = 0$ and $V = 1.5$.

**Fig. 2** Phase diagram in the plane of $T$ and $\mu$. Parameters used are $t = 0, t' = 1$ and $V = 1.5$. A narrow region between $s$ ($d$) and $px + ip_y$ states is an $s + ip_y$ ($d + ip_y$) state.

**Fig. 3** The $V_{\perp}$ dependence of SC order parameters for $t = 1, t' = 0, V = 1.5, \mu = -2, T = 0$ and $t_{\perp} = 0$. Note that all order parameters are non-dimensional.

**Fig. 4** The $V_{\perp}$ dependence of SC order parameters for $t = 1, t' = 0, V = 1.5, \mu = -2, T = 0$ and $t_{\perp} = 0.4$. Note that all order parameters are non-dimensional.
Fig3
Fig. 4