Superconducting States in Frustrating $t$-$J$ Model: A Model Connecting High-$T_c$ Cuprates, Organic Conductors and Na$_x$CoO$_2$

Masao OGATA*

Department of Physics, University of Tokyo, 7-3-1, Hongo, Bunkyo-ku, Tokyo 113-0033 Japan

(Received August 31, 2018)

The two-dimensional $t$-$J$ model on a frustrating lattice is studied using mean-field variational theories with Gutzwiller approximation. We find that a superconducting state with broken time-reversal symmetry (d+id state) is realized in the parameter region close to the triangular lattice. The frustration enlarges the region of superconductivity when $t < 0$ for the hole-doped case, which is equivalent to $t > 0$ for electron doping. We also discuss the SU(2) degeneracy at half-filling. The d+id state probably corresponds to the spin gap state at half-filling.

KEYWORDS: Frustration, $t$-$J$ model, time-reversal symmetry breaking, Gutzwiller approximation

---

Fig. 1. Lattice structure of the frustrated two-dimensional $t$-$J$ model. On the bonds forming the square lattice (solid lines), we have $t$ and $J$ terms. $t'$ and $J'$ terms are defined on the diagonal bonds (dashed lines).

---

$\text{t} < 0$, and that a superconducting state with broken time-reversal symmetry (chiral state) is realized in the parameter region close to the triangular lattice. We also discuss the SU(2) degeneracy at half-filling.

The $t$-$J$ model on a lattice in Fig. 1 is written as

$$\mathcal{H} = -t \sum_{\langle i,j \rangle} P_G(c_i^\dagger c_j + \text{H.c.})P_G + J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - t' \sum_{\langle i,j \rangle} P_G(c_i^\dagger c_j + \text{H.c.})P_G + J' \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j,$$

where $P_G = \prod (1 - n_i n_j)$ is the Gutzwiller projection operator which excludes double occupancies. $(i,j)$ represent the summation over nearest-neighbor and one of the next-nearest neighbor pairs as shown in Fig. 1, respectively. The sign of $t$ is crucial since there is no electron-hole symmetry. Hereafter we use $|t|$ as an energy unit and study the parameter range, $t'/t = J'/J = 0.0-1.0$. The model becomes the square lattice $t$-$J$ model when $J'/J = 0$; and the triangular lattice when $J'/J = 1$.

For this Hamiltonian, we consider Gutzwiller-type variational wave function $P_G(\Phi)$ with $|\Phi\rangle$ representing a BCS mean-field wave function. For estimating the variational energy, we use the Gutzwiller approximation in which the effect of the projection is replaced by a statis-

---

* E-mail address: ogata@phys.s.u-tokyo.ac.jp
tical weight as follows\textsuperscript{8,10}
\[
\langle c_i^\dagger c_j \rangle = g_t \langle c_i^\dagger c_j \rangle_0,
\langle S_i \cdot S_j \rangle = g_s \langle S_i \cdot S_j \rangle_0.
\] (2)

Here \(\langle \cdot \cdot \rangle_0\) represents the expectation value in terms of \(|\Phi\rangle\), and \(\langle \cdot \cdot \cdot \rangle\) represents the normalized expectation value in \(P_\Phi\langle \cdot \cdot \cdot \rangle\). In the simplest Gutzwiller approximation we have
\[
g_t = \frac{2\delta}{1 + \delta}, \quad g_s = \frac{4}{(1 + \delta)^2}, \tag{3}
\]
where \(\delta\) is the density of holes, i.e., the electron number is \(n = 1 - \delta\). It has been shown that this approximation gives a fairly reliable estimation for the variational energy for the pure d\(_{x^2-y^2}\)-wave superconducting state when it is compared with the variational Monte Carlo results.\textsuperscript{8,10}

In order to search for the state with the lowest variational energy, we studied large unit cells assuming site dependent order parameters. In this Gutzwiller approximation, we can have order parameters,
\[
\Delta_{ij} = \langle c_i^\dagger c_j \rangle_0, \quad \chi_{ij\sigma} = \langle c_i^\dagger c_j \sigma \rangle_0.
\] (4)

We assume \(\chi_{ij\uparrow} = \chi_{ij\downarrow} = \chi_{ij}\) and that \(\Delta_{ij}\) is a singlet pairing, i.e., \(\Delta_{ij} = \Delta_{ji}\). By minimizing the variational energy we obtain a Bogoliubov-de Gennes equation\textsuperscript{11} and self-consistency equations. We have tried various trial states and found that the uniform state is always stabilized except for some special states realized only very near half-filling. Since these special states may be an artifact of the mean-field-type calculations,\textsuperscript{13} they are not discussed in this paper. The obtained phase diagrams for \(J'/J = 0.3, J'/J' = 0.3\) are shown in Fig. 2 as a function of the ratio \(J'/J\) and the electron density \(n\).

We find that in the region with \(J'/J < 0.675\) the d\(_{x^2-y^2}\)-wave superconducting state is stabilized. This state is the same as in the square lattice case (\(J' = 0\)). When \(J'/J\) exceeds 0.675 a superconducting state with imaginary part of order parameter appears, which we call as d+id state as shown in Fig. 2. Since there is no continuous symmetry in our model, the notation of d+id-wave just represents a discretized version of d\(_{x^2-y^2}\)-id\(_{xy}\)-wave superconductivity. The detailed analysis is shown later. This state has excitation gaps all over the fermi surface and breaks time reversal symmetry. Another interesting feature is that for \(t < 0\) the superconducting region increases as \(J'/J\) becomes large, while its region decreases when \(t > 0\).

Before discussing the superconducting properties, let us here clarify the SU(2) degeneracy realized at half-filling in the present model. By solving the Bogoliubov-de Gennes equations we find various states at half-filling which have exactly the same variational energy with each other. For the uniform state, we have the energy dispersion for quasiparticles as
\[
E_k = \sqrt{\varepsilon_k^2 + |F_k|^2}, \tag{5}
\]
where
\[
\varepsilon_k = -\frac{3}{2}g_s J(\chi_x \cos k_x + \chi_y \cos k_y) - \frac{3}{2}g_s J' \chi_{xy} \cos(k_x + k_y),
\] (6)
\[
F_k = \frac{3}{2}g_s J(\Delta_x e^{-i\theta} \cos k_x + \Delta_y e^{i\theta'} \cos k_y) + \frac{3}{2}g_s J' \Delta_{xy} \cos(k_x + k_y). \tag{7}
\]

Here \(\Delta_x, (\Delta_y)\) is the superconducting order parameter on the bonds in the \(x\)-(\(y\))-direction, and \(\Delta_{xy}\) is in the diagonal direction. We denote \(\theta, (\theta')\) as the phase of the order parameter relative to that on the diagonal bonds. Note that, in this notation, the pure d\(_{x^2-y^2}\)-wave state is represented as \(\Delta_x = \Delta_y = 0\) and \(\theta = \theta' = \pi/2\).

We find that, in each energetically degenerate state, these parameters satisfy the following relations:
\[
\chi_x \chi_y + \Delta_x \Delta_y \cos(\theta + \theta') = 0, \tag{8a}
\chi_x \chi_{xy} + \Delta_x \Delta_{xy} \cos \theta = 0, \tag{8b}
\chi_y \chi_{xy} + \Delta_y \Delta_{xy} \cos \theta' = 0. \tag{8c}
\]

In this case the energy dispersion becomes
\[
E_k = \frac{3}{2}g_s J \sqrt{J'^2(\chi_x^2 + \Delta_x^2) \cos^2 k_x + J''(\chi_y^2 + \Delta_y^2) \cos^2 k_y + J'^2(\chi_{xy}^2 + \Delta_{xy}^2) \cos^2 k_{xy} + J''^2 \Delta_{xy}^2 \cos^2 k_{xy}. \tag{9}
\]
The self-consistency equations are

\[ 1 = \frac{1}{N} \sum_k \frac{\frac{3}{2} g_s J \cos^2 k_x}{E_k}, \]  
\[ 1 = \frac{1}{N} \sum_k \frac{\frac{3}{2} g_s J \cos^2 k_y}{E_k}, \]  
\[ 1 = \frac{1}{N} \sum_k \frac{\frac{3}{2} g_s J' \cos^2 (k_x + k_y)}{E_k}, \]

where \( N \) is the number of sites and the summation over \( k \)
is in the Brillouin zone (in our model \( -\pi \leq k_x, k_y \leq \pi \)).

Since there are 8 parameters \((\chi_x, \chi_y, \chi_{xy}, \Delta_x, \Delta_y, \Delta_{xy}, \theta, \theta')\)and 6 equations (8) and (10), we have remaining two degrees of freedom which lead to the various states obtained at half-filling. This is an extension of the SU(2) degeneracy discussed in the square lattice \((J' = 0)\). \(^8,14\) For example, one of the realized states at half-filling has

\[ \chi_x = \chi_y = 0, \quad \chi_{xy} \neq 0, \quad \Delta_x = \Delta_y \neq 0, \quad \Delta_{xy} = 0, \]
\[ \theta = \theta' = \frac{\pi}{4}. \]

(11)

When \( \chi_{xy} \to 0 \), this state is naturally connected to the so-called d+is state realized in the square lattice. Another state with

\[ \chi_x = \chi_y = \Delta_x = \Delta_y \neq 0, \]
\[ \chi_{xy} = 0, \quad \Delta_{xy} \neq 0 \text{ and } \theta = \theta' = \frac{\pi}{2}, \]

is connected to the \( d_{x^2-y^2} \)-wave state for the square lattice.

Since these degenerate states have common values for

\[ D = \sqrt{\chi_x^2 + \Delta_x^2} = \sqrt{\chi_y^2 + \Delta_y^2}, \]
\[ D' = \sqrt{\chi_y^2 + \Delta_y^2}, \]

we plot their \( J'/J \) dependence in Fig. 3(a). As \( J'/J \) approaches to 1, \( D \) becomes equal to \( D' \).

Next let us discuss the doped case. Once some holes are introduced, the above degeneracy is readily lifted, and the lowest non-degenerate state becomes the superconductive state which is shown in Fig. 2. We note that the flux phase proposed before\(^7,15-18\) is not stabilized. Since the order parameters are uniquely determined at finite \( \delta \), we determine the relative phase of the superconducting order parameters, \( \theta \) and \( \theta' \), by taking the limit \( \delta \to 0 \). The obtained phase is shown in Fig. 3(b). When \( \Delta_{xy} \) starts to have a finite value at \( J'/J = 0.675 \), the relative phases are \( \theta = \theta' = \pi/2 \). This means that a small component \( \Delta_{xy} \) appears as an imaginary part \((i\Delta_{xy})\) in addition to the pure \( d_{x^2-y^2} \)-wave state. As \( J'/J \) increases, the relative phase approaches to \( 2\pi/3 \), and when \( J' = J \) (triangular lattice) the three order parameters \( \Delta_x, \Delta_y \) and \( \Delta_{xy} \) become symmetric with each other. This state is consistent with the other works.\(^15,19\) This gradual change of the relative phase gives a natural continuation between the \( d_{x^2-y^2} \)-wave superconductivity in the square lattice and 120-degree phase in the triangular lattice.

In Fig. 4 we show the doping dependences of the order parameters \( \Delta = \Delta_x = \Delta_y = \Delta_{xy} \) and \( \chi = \chi_x = \chi_y = \chi_{xy} \) determined self-consistently at \( t' = t, J' = J \) and \( J/t = 0.3 \) (triangular lattice). Qualitatively similar figure has been obtained recently,\(^19\) but the order parameter \( \chi \) has not been taken into account, which plays an important role in the gauge theories for the \( t-J \) model. As shown in Fig. 4, the superconducting region is large, which is consistent with the high-temperature expansion study for the triangular \( t-J \) model when \( t > 0 \). Surprisingly the superconducting region is even larger for \( t < 0 \), in which case the high-temperature study has shown that the ferromagnetic instability takes place for \( J/t < 0.3 \).\(^20\) In order to clarify the actual ground state in the triangular \( t-J \) model, more careful energy comparisons including ferromagnetism as well as the 120-degrees antiferromagnetism (realized at half-filling) are necessary. In particular, there will be a competition between the ferromagnetic fluctuation and singlet formations for \( J/t > 0.3 \) which leads to a heavy fermion-like behavior appearing in the specific heat.\(^11\) The relation to this competition and the RVB states remains a future problem. In the region with very low electron density, we expect a triplet superconductivity.

For the recently discovered superconductor, \( \text{Na}_x\text{CoO}_4 \), the sign of \( t \) is controversial.\(^19,21\) If the sign is negative,
superconductors, the sign of the superconductivity is more favored. For the organic
stuffing, we explain the superconductivity via spin-fluctuation. The Hubbard model has
been used to explain the superconductivity in the phase diagram. However it is
safely survive. Although the detailed study on this issue is necessary, the phase diagram
shown in Figs. 2 and 4 promises that an interesting time-reversal breaking super-
conducting state is one of the strong candidates for the ground state.

In summary we have studied the frustrating t-J model within a Gutzwiller approximation. The frustration induces a superconductivity with broken time-reversal
symmetry in the parameter region close to the triangular lattice. The relative phase between the order parameters gradually changes as a function of $J'/J$ which
connects the $d_{x^2−y^2}$-wave and typical 120-degree phase in the triangular lattice. We also discussed the SU(2) degeneracy at half-filling. We found that there is unexpectedly very large variety of states in strongly correlated frustrating systems.

The author would like to thank very useful discussions and conversations with B. S. Shastry, G. Baskaran, and T. Koretsune.

1) P. W. Anderson, Mat. Res. Bull. 8 (1973) 153.
2) P. Fazekas and P. W. Anderson, Phil. Mag. 30 (1974) 423.
3) P. W. Anderson, Science 235 (1987) 1196.
4) K. Kanoda, private communication.
5) K. Takada et al., Nature 422 (2003) 53.
6) H. Yokoyama and H. Shiba, J. Phys. Soc. Jpn. 57 (1988) 2482.
7) C. Gros, Phys. Rev. B 38 (1988) 931; Ann. Phys. (N.Y.) 189 (1989) 53.
8) F. C. Zhang, C. Gros, T. M. Rice and H. Shiba, Supercond. Sci. Technol. 1 (1988) 36.
9) T. Tanamoto, H. Kohno and H. Fukuyama, J. Phys. Soc. Jpn. 62 (1993) 717 and J. Phys. Soc. Jpn. 63 (1994) 2739.
10) H. Yokoyama and M. Ogata, J. Phys. Soc. Jpn. 65 (1996) 3615.
11) T. Koretsune and M. Ogata, Phys. Rev. Lett. 89 (2002) 116401.
12) A. Himeda and M. Ogata, J. Phys. Soc. Jpn. 66 (1997) 3367.
13) M. Ogata, J. Phys. Soc. Jpn. 66 (1997) 3375.
14) I. Affleck, Z. Zou, T. Hsu and P. W. Anderson, Phys. Rev. B 38 (1988) 745.
15) T. K. Lee and S. Feng, Phys. Rev. B 41 (1990) 11110.
16) X.-G. Wen, F. Wilczek, and A. Zee, Phys. Rev. B 39 (1989) 11413.
17) V. Kalafutar, R. B. Laughlin, Phys. Rev. B 39 (1989) 11879.
18) P. W. Anderson, B. S. Shastry, and D. Hristopulos, Phys. Rev. B 40 (1989) 8939.
19) While preparing this manuscript, we notice a similar work on the triangular lattice, G. Baskaran, cond-mat/0303649 and B. Kumar and B. S. Shastry, cond-mat/0304210.
20) T. Koretsune and M. Ogata, preprint.
21) D. J. Singh, Phys. Rev. B 61 (2000) 13397.
22) H. Kino and K. Kontani, J. Phys. Soc. Jpn. 67 (1998) 3691 and H. Kondo and T. Moriya, J. Phys. Soc. Jpn. 67 (1998) 3695.
23) Z. Weihong, R. H. McKenzie and R. R. P. Singh, Phys. Rev. B 59 (1999) 14367.
24) T. Giamarchi and C. Lhuillier, Phys. Rev. B 43 (1991) 12943.
25) A. Himeda and M. Ogata, Phys. Rev. B 60 (1999) R9935.
26) M. Ogata and A. Himeda, J. Phys. Soc. Jpn. 72 (2003) 374.