Reexamination of \textit{d}-wave superconductivity in the two-dimensional Hubbard model

Takao Morinari

Yukawa Institute for Theoretical Physics, Kyoto University Kyoto 606-8502, Japan

(Febuary 7, 2002)

We reexamine the possibility of \textit{d}-wave superconductivity in the hole-doped two-dimensional Hubbard model. In terms of the gauge field description of the spin fluctuations, we show that \textit{d}-wave superconductivity is unstable in the perturbative region with respect to the on-site Coulomb repulsion, \textit{U}. Whereas in the region where \textit{d}-wave superconductivity is possible, there is a strong constraint on the gap of superconductivity. Analysis of the localized spin moments suggests that there is another \textit{d}-wave (\textit{d}_{x^2−y^2}-wave) pairing due to the short-range antiferromagnetic correlation.

74.25.Dw, 74.20.Rp

Over the past few decades a considerable number of studies have been made on the Hubbard model. In spite of its simplicity, we can expect a variety of phenomena: antiferromagnetism, ferromagnetism, and unconventional superconductivity. Among others, the possibility of \textit{d}-wave superconductivity has been considerably investigated since the discovery of the high \textit{T}_c cuprates.\cite{1}

The theory of \textit{d}-wave superconductivity in the Hubbard model is based on the antiferromagnetic spin fluctuations.\cite{1} The mechanism is analogous to the \textit{p}-wave pairing mechanism due to the ferromagnetic spin fluctuations in the \textit{^3}He system.\cite{2} In principle, the theory relies on the perturbative expansion with respect to \textit{U}, the on-site Coulomb repulsion.

However, the theory has some disadvantages. First of all, it is hard to describe the half-filled case in which the on-site Coulomb repulsion. \textit{U} is as large as the carrier hopping amplitude, \textit{t}. Therefore, we must pay particular attention in applying the perturbative expansion in \textit{U}, especially when we deal with the effect of the localized spin moments.

In this paper, we re-examine the possibility of \textit{d}-wave superconductivity in the hole-doped two-dimensional Hubbard model without relying on the perturbative expansion with respect to \textit{U}. Starting from the path-integral form of the partition function, we introduce the Stratonovich-Hubbard field for the value of the localized spin moments. Analysis of it suggests that superconductivity based on the antiferromagnetic spin fluctuations is unstable in the perturbative region. While in the region where \textit{d}-wave superconductivity is possible, we show that there is a strong constraint on the value of the superconducting gap. Instead of the \textit{d}-wave Cooper pairing, there is another \textit{d}-wave (\textit{d}_{x^2−y^2}-wave) pairing due to the antiferromagnetic short-range correlation. This \textit{d}_{x^2−y^2}-wave pairing state is similar to the spinon pairing in the RVB theory.\cite{3,4} However, the crucial difference here is that we do not need the \textit{U}(1) gauge symmetry breaking that is essential for the slave-particle gauge theory.\cite{5}

\textbf{Formulation-} The partition function of the Hubbard model is written as \textit{Z} = \int D\tau Dc \exp(-\textit{S}), where

\begin{equation}
\textit{S} = \int_{0}^{\beta} d\tau \left[ \sum_{j} \tau_{j} (\partial \tau - \mu) c_{j} - t \sum_{(i,j)} (\tau_{i} c_{j} + \tau_{j} c_{i}) + \textit{U} \sum_{j} n_{j\uparrow} n_{j\downarrow} \right].
\end{equation}

Here \textit{\tau} dependence of all fields is implicit and the summation \textit{\sum_{(i,j)}} is taken over the nearest neighbor sites. Carrier fields are represented in spinor representation: \textit{c}_{i} = \textit{\tau} (\textit{c}_{i\uparrow} \textit{c}_{i\downarrow}) and \textit{\tau}_{i} = (\textit{\tau}_{i\uparrow} \textit{\tau}_{i\downarrow}). The on-site Coulomb interaction term can be rewritten as, \textit{U} \sum_{j} n_{j\uparrow} n_{j\downarrow} = \textit{(U}/4) \sum_{j} \left[ (n_{j\uparrow} + n_{j\downarrow})^{2} - (\textit{\tau}_{j} \textit{\sigma} c_{j})^{2} + 2(n_{j\uparrow} + n_{j\downarrow}) \right], where the components of the vector \textit{\sigma} = (\sigma_{x}, \sigma_{y}, \sigma_{z}) are the Pauli spin matrices. Introducing Stratonovich-Hubbard fields for the charge and spin degrees of freedom,\cite{6} we obtain \textit{Z} = \int D\tau Dc D\Omega D\phi D\phi \exp(-\textit{S}), where the action is given by

\begin{equation}
\textit{S} = \int_{0}^{\beta} d\tau \left[ \sum_{j} \tau_{j} (\partial \tau - \mu) c_{j} - t \sum_{(i,j)} (\tau_{i} c_{j} + \tau_{j} c_{i}) + \textit{U} \sum_{j} \sum_{\phi} \phi_{j}^{2} \frac{i}{2} \sum_{j} \phi_{j} \Omega_{j} \cdot \textit{\tau}_{j} \textit{\sigma} c_{j} + \textit{U} \sum_{j} \sum_{\phi} \phi_{j}^{2} \frac{j}{2} \sum_{j} \phi_{j} \tau_{j} c_{j} \right],
\end{equation}

up to constant. Here the vector \textit{\Omega}_{j} is a unit vector, \phi_{j} represents the value of the localized spin moments, and \textit{\sigma}_{0} is the unit matrix in spin space. The scalar \phi_{j} is associated with the charge fluctuations. Note that \phi_{j} = 1 at half-filling. If we consider hole doping, then \phi_{j} takes \phi_{j} \leq 1. For these amplitudes, we do not consider the possibility of inhomogeneous configurations of them because such configurations may compete with superconductivity. In order to focus on the possibility of superconductivity,
we take the uniform values, that is, \( \phi_j = \phi = \text{const.} \) and 
\( i\phi_{c_j} = -(\bar{\tau}_j \sigma_0 c_j) = -(1 - \delta) \), with \( \delta \) the doped hole concentration. As a result, we may write the action in the following form

\[
S = \int_0^\beta d\tau \left[ \sum_j (\partial_\tau - \bar{\mu}) c_j - t \sum_{(i,j)} (\bar{\tau}_i c_j + \bar{\tau}_j c_i) \right] - \frac{\phi U}{2} \sum_j \Omega_j \cdot \bar{\tau}_j \sigma c_j \right] + \frac{\phi^2 U}{4} \beta N, \tag{3}
\]

where \( \bar{\mu} = \mu - U(1 - \delta)/2 \) and \( N \) is the number of the lattice sites. Note that the last term in the square brackets has the form of Hund coupling between the localized spin moments. \([1,8]\) On the other hand, if we expand Eq. (6) with respect to \( \phi \), we may write the action in the second order of the expansion of Eq. (6) with respect to \( \mu_\phi \) and \( \phi \).

The effective action of the boson fields \( \bar{\mu}, \sigma \) yields the antiferromagnetic Heisenberg model. \([7,8]\) The latter relationship is implied from the paramagnon contributions that leads to \( p \)-wave pairing. \([6]\) Apparently, we can trust this interaction only in the perturbative region with respect to \( \phi \). In addition, the interaction exists only when \( \phi \neq 0 \), or coupling to the bosons is lost. Nevertheless we will show later that \( \phi = 0 \) in the perturbative region in \( U \).

For the analysis of the system, we rely on neither the \( \phi U \)-expansion nor the \( t \)-expansion because both of them are reliable only in part of the parameter range of \( U/t \) and \( \delta \). Alternatively, we study the system by taking the continuum limit. Taking such limit is justified when the fluctuations are long-ranged. Since the antiferromagnetic spin fluctuations may be long-ranged near half-filling, we may take the continuum limit. In the continuum limit, the action (3) is reduced to

\[
S = \int d\tau \int d^2 \tau \psi(x,\tau) \left[ (\partial_\tau - \bar{\mu}) \sigma_0 + i A_\tau - \frac{\phi U}{2} \sigma_\tau \right] \left[ -\frac{1}{2m} (-i \sigma_0 \bar{\nabla} + A_\tau)^2 \right] \psi(x,\tau) + \sum_{\alpha x,y,z} \bar{A}_\alpha \cdot \sigma \psi(x,\tau), \tag{7}
\]

where the SU(2) gauge field \( A_\mu \) is defined as \( A_\mu = \sum_{a=x,y,z} A^a_\mu \sigma_a = -i \bar{\nabla}_a U_a \) and \( S_A \) is derived from Eq. (6) in principle.

The system governed by the action (7) is the fermion system with the interaction due to the exchange of the SU(2) gauge field \( A_\mu \). Here the gauge field \( A_\mu \) is associated with the spin fluctuations. The \( z \)-component \( A^z_\mu = -i (\bar{\tau}_0 \partial_\mu z_0 + \bar{\tau}_0 \partial_\mu \bar{z}_0) \) describes the fermionic spin fluctuations. Whereas the \( x \)-component \( A^x_\mu = -i (\bar{z}_0 \partial_0 z_0 + \bar{z}_0 \partial_0 \bar{z}_0) \) describes the antiferromagnetic spin fluctuations. The latter relationship is implied from the analysis of the \( CP^1 \) representation of the antiferromagnetic Heisenberg model. \([6]\)

In order to consider the antiferromagnetic spin fluctuations, we focus on the gauge field \( A^z_\mu \). In terms of the fields \( \tilde{\psi}_\pm = (\psi_\uparrow \pm \psi_\downarrow)/\sqrt{2} \) that diagonalize the gauge charge, the action is rewritten as

\[
S = \int d\tau \int d^2 \tau \left[ \sum_{s=\pm} \tilde{\psi}_s(x,\tau) \left[ (\partial_\tau - \bar{\mu}) + is A^z_\tau \right] \right] \left[ -\frac{1}{2m} (-i \nabla + s A^x_\tau)^2 \right] \tilde{\psi}_s(x,\tau) \right] + \frac{\phi U}{2} \left[ \tilde{\psi}_+(x,\tau) \tilde{\psi}_-(x,\tau) + \tilde{\psi}_-(x,\tau) \tilde{\psi}_+(x,\tau) \right] \right] + S_A, \tag{8}
\]

The action (8) has the form of fermions coupled with the U(1) gauge field.
Analysis of the gap equation. Now we study the possibility of spin singlet superconductivity based on the action \( [8] \). In the following we assume that there exists an attractive interaction induced by the exchange of the gauge field. In the presence of an attractive interaction, the mean field Hamiltonian for the spin singlet pairing state may have the following form

\[
H_{MF} = \frac{1}{2} \sum_{k} \left( \tilde{c}_{k,+}^\dagger \tilde{c}_{k,-} + \tilde{c}_{-k,+} \tilde{c}_{-k,-} \right) \times \begin{pmatrix}
\xi_k & -\phi U/2 & \Delta_k \\
-\phi U/2 & \xi_k & -\Delta_k \\
0 & -\Delta_k^* & \phi U/2 - \xi_k
\end{pmatrix} \begin{pmatrix}
\tilde{c}_{k,+} \\
\tilde{c}_{k,-} \\
\tilde{c}_{-k,+}^\dagger
\end{pmatrix}.
\]

The gap \( \Delta_k \) is evaluated from the gap equation: \( \Delta_k = -\frac{1}{4\Omega} \sum_{k', E_{k'} > \phi U/2} V_{kk'} \Delta_{k'} \), where \( E_{k'} = \sqrt{\xi_{k'}^2 + \Delta_{k'}^2} \). In principle, the interaction \( V_{kk'} \) is derived from Eqs. (1) and (7) by eliminating the gauge field \( A_{\mu}^j \). However, we do not need its explicit form.

At zero temperature, the gap equation is reduced to

\[
\Delta_k = -\frac{1}{2\Omega} \sum_{k', E_{k'} > \phi U/2} V_{kk'} \frac{\Delta_{k'}}{E_{k'}}.
\]

Note that in Eq. (10) the summation in \( k' \)-space is taken over the constraint \( E_{k'} > \phi U/2 \). The presence of the constraint on spin singlet pairing states is understood as follows. One can see that the second term in the braces in Eq. (8) is similar to that of the Zeeman energy term produced by applying an in-plane magnetic field to the system. In fact, such Zeeman energy term is proportional to the applied magnetic field times \( \sum_j (c_{j,1}^\dagger c_{j,1} + c_{j,2}^\dagger c_{j,2}) \). (Here the direction of the in-plane magnetic field is chosen along the \( x \)-axis.) Apparently, in the limit of the large in-plane magnetic field, spin singlet pairing states are unstable. Similarly, in the large \( \phi U \) limit, spin singlet states are not stable. Therefore, if spin singlet superconductivity is stable, then the superconducting gap \( \Delta \) should satisfy

\[
\Delta > \phi U/2 \equiv \Delta_c.
\]

In order to find the doped hole concentration dependence of the constraint, we need to evaluate \( \phi \). For the calculation, we assume the staggered form for \( \Omega_j \) as \( \Omega_j = (-1)^j \frac{\mu}{T_c} \), because we are concerned with the antiferromagnetic spin fluctuations. \[11\] Note that non-zero value of \( \phi \) does not imply the presence of the antiferromagnetic long-range order but it implies the presence of the antiferromagnetic correlation because there is the phase fluctuations, or the effect of the gauge field \( A_{\mu}^j \), as well as the quantum fluctuations.

Now we estimate the value of \( \phi \) by solving the saddle point equations derived from the action obtained from Eq. (3) after integrating out \( \tau_j \) and \( c_j \). The variation with respect to \( \phi \) yields

\[
\frac{U}{4\pi^2} \int_{\frac{1}{\sqrt{\gamma+\alpha}}-\alpha}^{\frac{1}{\sqrt{\gamma+\alpha}}} d\gamma K(\sqrt{1-\gamma^2}) = 1, \tag{12}
\]

where \( \alpha = \phi U/(8t) \), \( \nu = \mu/(4t) \), and \( K(\xi) = \int_0^{\pi/2} d\theta (1/\sqrt{1 - \xi^2 \sin^2 \theta}) \) is the complete elliptic integral of the first kind. Meanwhile the variation with respect to \( \mu \) yields

\[
\frac{4}{\pi^2} \int_{\frac{1}{\sqrt{\gamma+\alpha}}-\alpha}^{\frac{1}{\sqrt{\gamma+\alpha}}} d\gamma K(\sqrt{1-\gamma^2}) = 1 - \delta. \tag{13}
\]

In deriving these equations, we have used \( \nu < 0 \) and \( |\nu| > \alpha \), which holds for the hole doped case.

From Eqs. (12) and (13) we find \( U/t \) and \( \delta \) dependence of \( \phi \) and \( \Delta_c \). The boundary between \( \phi \neq 0 \) and \( \phi = 0 \) is shown in Fig. 1 by the solid curve. In the \( \phi = 0 \) regime, there is no attractive interaction due to the absence of the antiferromagnetic spin fluctuations as mentioned above. Note that the \( \phi = 0 \) regime lies in the smaller value of \( U/t \). Apparently, this region contains the parameter range of \( U/t \) and \( \delta \) where perturbation in \( U \) is justified. Therefore, for the states with \( \phi = 0 \), perturbation theory is justified. Although we cannot say whether perturbation theory is reliable in the \( \phi \neq 0 \) regime, states with \( \phi \neq 0 \) are qualitatively different from those with \( \phi = 0 \) because the former is unstable in the \( U/t \rightarrow 0 \) limit. In the language of renormalization group theory, they should belong to different fixed points.) Turning to the conditions of d-wave superconductivity, the boundaries of \( \Delta_c/t = 0.20 \) and \( \Delta_c/t = 0.04 \) in Fig. 1 suggests that the occurrence of d-wave superconductivity is restricted to extremely small parameter region or we need much stronger attractive interaction than the RKKY type interaction.

Another d-wave pairing. So far we discuss the possibility of d-wave superconductivity in the carrier system. Now we discuss that there is another d-wave \( (d_{x^2-y^2} \text{-wave}) \) pairing associated with the localized spin moments.

In the \( \phi \neq 0 \) regime, we may take the form of the antiferromagnetic Heisenberg Hamiltonian for the action of the localized spin moments. In the Hamiltonian formulation, it is written as \( H_{spin} = \frac{J}{4} \sum_{\langle i,j \rangle} \Omega_i \cdot \Omega_j \), with \( J = 4t^2/\nu \). \[12\] Note that the exchange interaction between the localized spins is reduced by factor \( \phi^2 \). Since \( \phi \) is monotonically decreasing function of the doped carrier concentration \( \delta \), this reduction suggests the relation to the Heisenberg antiferromagnet like behavior of spin susceptibility observed in the doped high \( T_c \) cuprates. \[13\]

Now we discuss another d-wave pairing. In order to describe the localized spin moments \( \Omega_j \), we can introduce fermion creation and annihilation operators, \( a^\dagger_j \) and \( a_j \), as \( \Omega_j = a^\dagger_j \sigma a_j \). Due to the constraint \( \Omega_j = 1 \), the fermion operators \( a^\dagger_j \) and \( a_j \) must satisfy.
\[ \sum a^\dagger_{j\sigma} a_{j\sigma} = 1. \]  

(14)

Note that this constraint, the fermion system is half-filled, is independent of the doping concentration \( \delta \). Under the constraint (14), the Hamiltonian \( H_{\text{spin}} \) is reduced to, up to a constant term,

\[ H_{\text{spin}} = -\frac{J\phi^2}{2} \sum_{\langle ij \rangle} D_{ij}^\dagger D_{ij}, \]

(15)

where \( D_{ij} = a^\dagger_{i\uparrow} a_{j\downarrow} - a^\dagger_{i\downarrow} a_{j\uparrow} \) is defined on each bond. Taking the mean fields \( \langle D_{ij} \rangle \) and \( \langle D_{ij}^\dagger \rangle \), we find that the \( d_{x^2-y^2} \)-wave pairing state and the extended \( s \)-wave state are degenerate. If we introduce a slight hopping term for the fermions, then the \( d_{x^2-y^2} \)-wave pairing state is stabilized \[ \] and the gap is of order of \( \phi^2 J \). Although the origin of this \( d_{x^2-y^2} \) pairing is similar to the spinon pairing in the RVB theory, that is, the short-range antiferromagnetic correlation \[ \], the crucial difference is that we do not rely on the \( U(1) \) gauge symmetry breaking that is essential for the slave-particle gauge theory. \[ \]

In addition, it should be stressed that this pairing state does not imply a superconducting state of the fermions because of the constraint (14).

This pairing state provides another \( d_{x^2-y^2} \) pairing which is independent of \( d_{x^2-y^2} \)-wave superconductivity. The fact that this pairing state originates from the antiferromagnetic correlation between the localized spin moments suggests that it can be associated with the pseudogap phenomenon observed in the high \( T_c \) cuprates. If we apply the theory to the \( Cu \) site degrees of freedom in the \( CuO_2 \) plane in the cuprates, then the \( d_{x^2-y^2} \) pairing can be identified with that observed by angle-resolved photoemission spectroscopy. \[ \]

Furthermore, there is the experiment that indicates the existence of the pseudogap of \( d_{x^2-y^2} \) symmetry also in the insulating phase. \[ \]

Since our \( d_{x^2-y^2} \) pairing exists also in the insulating phase, the experiment supports the relationship between experimentally observed pseudogap with \( d_{x^2-y^2} \) symmetry and the \( d_{x^2-y^2} \) pairing due to the antiferromagnetic correlation.

Summary: To summarize, we have reexamined the possibility of \( d \)-wave superconductivity in the hole-doped Hubbard model. We have shown that \( d \)-wave superconductivity is unstable in the perturbative region in \( U \). Whereas in the region where \( d \)-wave superconductivity is possible, there is a strong constraint on the superconducting gap. Instead, there is another \( d_{x^2-y^2} \)-wave pairing due to the antiferromagnetic spin correlation.

Acknowledgement- I would like to thank M. Sigrist, Y. Morita, and M. Tsuchiizu for helpful discussions. This work was supported in part by a Grant-in-Aid from the Ministry of Education, Culture, Sports, Science and Technology.

[1] See, for example, D. J. Scalapino, Phys. Rep. 250, 329 (1995); T. Moriya and K. Ueda, Adv. Phys. 49, 555 (2000).
[2] P. W. Anderson and W. F. Brinkman, in The Helium Liquids, ed. by J. G. M. Armitage and I. E. Farquhar (New York, Academic Press).
[3] P. W. Anderson, G. Baskaran, Z. Zou, and T. Hsu, Phys. Rev. Lett. 58, 2790 (1987).
[4] G. Kotliar and J. Liu, Phys. Rev. B 38, 5142 (1988).
[5] C. Nayak, Phys. Rev. Lett. 85, 178 (2000).
[6] J. Hubbard, Phys. Rev. B 19, 2626 (1979).
[7] H. J. Schulz, Phys. Rev. Lett. 65, 2462 (1990).
[8] P. Lacour-Gayet and M. Cyrot, J. Phys. C 7, 400 (1974).
[9] N. Read and S. Sachdev, Phys. Rev. B 42, 4568 (1990).
[10] As shown in Ref. [5], spiral phase is expected away from half-filling because the kinetic energy of carriers enhances ferromagnetic interaction between the localized spins. In order to concentrate on \( d \)-wave superconductivity based on antiferromagnetic correlations, the staggered component is taken here.
[11] D. C. Johnston, Phys. Rev. Lett. 62, 957 (1989).
[12] A. G. Loeser, Z.-X. Shen, D. S. Dessau, D. S. Marshall, C. H. Park, P. Fournier, and A. Kapitulnik, Science 273, 325 (1996); H. Ding, T. Yokoya, J. C. Campuzano, T. Takahashi, M. Randeria, M. R. Norman, T. Mochiku, K. Kadowaki, and J. Giapintzakis, Nature 382, 51 (1996).
[13] F. Ronning, C. Kim, L. Feng, D. S. Marshall, A. G. Loeser, L. L. Miller, J. N. Eckstein, I. Bozovic, Z.-X. Shen, Science 282, 2067 (1998).
FIG. 1. The boundary between $\phi \neq 0$ and $\phi = 0$ in the $U/t - \delta$ plane. The boundary is given by the solid curve. The dashed curve represents $\Delta_c/t = 0.20$ and the dotted curve $\Delta_c/t = 0.04$. 