On the Kinetic Energy Driven Superconductivity in the Two-Dimensional Hubbard Model

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Abstract: We investigate the role of kinetic energy for the stability of superconducting state in the two-dimensional Hubbard model on the basis of an optimization variational Monte Carlo method. The wave function is optimized by multiplying by correlation operators of site off-diagonal type. This wave function is written in an exponential-type form given as \( \psi_\lambda = \exp(-\lambda K)\psi_G \) for the Gutzwiller wave function \( \psi_G \) and a kinetic operator \( K \). The kinetic correlation operator \( \exp(-\lambda K) \) plays an important role in the emergence of superconductivity in large-\( U \) region of the two-dimensional Hubbard model, where \( U \) is the on-site Coulomb repulsive interaction. We show that the superconducting condensation energy mainly originates from the kinetic energy in the strongly correlated region. This may indicate a possibility of high-temperature superconductivity due to the kinetic energy effect in correlated electron systems.

Keywords: strongly correlated electrons; mechanism of superconductivity; high-temperature superconductor; two-dimensional Hubbard model; optimization variational Monte Carlo method; Hubbard model

1. Introduction

It is important and challenging to clarify the mechanism of high-temperature superconductivity in cuprates. It has been studied intensively for more than three decades [1]. In the study of cuprate high-temperature superconductivity, it is important to understand the ground state phase diagram. For this purpose, we should investigate electronic models with strong correlation.

It is certain that the CuO\(_2\) plane plays an important role in the emergence of high-temperature superconductivity [2–8]. The CuO\(_2\) plane contains oxygen atoms and copper atoms; thus, the CuO\(_2\) plane can be modeled by the d-p model (or the three-band Hubbard model) [9–25]. The single-band Hubbard model [26–28] is important since it can be regarded as a simplified model of the three-band d-p model and may contain important physics concerning high-temperature superconductivity [29–49]. The Hubbard model was first proposed by Hubbard to describe the metal-insulator transition [50] and has been one of the important fundamental models in condensed matter physics up to now. It may contain important physics concerning high-temperature cuprates, such as antiferromagnetic insulator, superconductivity, stripes [51–58], and inhomogeneous states [59–62].

We employ an optimization variational Monte Carlo method to investigate the ground state of the 2D Hubbard model. In a variational Monte Carlo method, we use variational wave functions with strong correlation between electrons [33,34,36–39]. A variational wave function is improved by introducing correlation operators. The wave function used in this paper is obtained by multiplying the Gutzwiller function by \( \exp(-\lambda K) \) operators, where \( K \) is the kinetic part of the Hamiltonian [47,48,63,64]. We can optimize the wave function further by multiplying by exponential-type operators again [63]. The ground-state energy is lowered greatly with this wave function [47].
The kinetic energy-driven mechanism of superconductivity has been examined in the study of cuprate superconductors for the Hubbard model [42,65–67] and the t-J model [68–70]. This is an interesting subject since there is a possibility that kinetic energy pairing occurs in high-temperature cuprates. In this paper, we discuss the role of kinetic energy based on the improved wave function for the Hubbard model. We evaluate the superconducting condensation energy as a sum of the kinetic and Coulomb energy contributions, and we show that the kinetic energy contribution dominates the condensation energy in the strongly correlated region of large $U$.

2. Hubbard Hamiltonian

We investigate the two-dimensional Hubbard model. The Hamiltonian of the Hubbard model is

$$H = \sum_{ij} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow},$$

(1)

where $t_{ij}$ indicates the transfer integral, and $U$ is the strength of the on-site Coulomb interaction. The transfer integral is $t_{ij} = -t$ when $i$ and $j$ are nearest-neighbor pairs $(ij)$. We put $t' = 0$ in this paper, where $t_{ij} = -t'$ when $i$ and $j$ are next-nearest neighbor pairs. $N$ and $N_e$ denote the number of lattice sites and the number of electrons, respectively. The energy unit is given by $t$. We define the non-interacting part as $K$:

$$K = \sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma}.$$

(2)

When two electrons with spin up and down are at the same site, the energy becomes higher by $U$. This simple interaction may cause many interesting phenomena, such as the metal-insulator transition, antiferromagnetic magnetism, and superconductivity.

The effective Hamiltonian is given by the Heisenberg model when $U$ is large in the half-filled case, which leads to the t-J model when holes are doped. Magnetic properties of materials may be described by the Hubbard model by introducing suitable magnetic orders. We discuss superconductivity in the strongly correlated region in this paper. The emergence of superconducting state in this region is closely related to the kinetic energy gain that increases as $U$ increases.

3. Optimized Wave Function

In a variational Monte Carlo method, we calculate the expectation values of physical properties by using a Monte Carlo procedure. We start with the Gutzwiller wave function to take account of electron correlation. The Gutzwiller wave function is

$$\psi_G = P_G \psi_0,$$

(3)

where $P_G$ is the Gutzwiller operator $P_G = \prod_i (1 - (1 - g)n_{i\uparrow} n_{i\downarrow})$, where $g$ is the variational parameter in the range of $0 \leq g \leq 1$. $\psi_0$ indicates a one-particle state, such as the Fermi sea, the BCS state, and the antiferromagnetic state.

We improve the wave function by multiplying by the correlation operator given as [47,63,71–75]

$$\psi_\lambda = \exp(-\lambda K) \psi_G,$$

(4)

where $K$ is the kinetic part of the Hamiltonian, and $\lambda$ is a real variational operator [39,63,72].

There are other methods to improve the Gutzwiller wave function by using Jastrow-type operators [41,76,77]. This operator is written as

$$P_{jdh} = \prod_j \left( 1 - (1 - \eta) \prod_\tau \left[ d_j(1 - e_{j+\tau}) + e_j(1 - d_{j+\tau}) \right] \right),$$

(5)
where $d_j$ is the operator for the doubly-occupied site given as $d_j = n_j^\uparrow n_j^\downarrow$, and $e_j$ is that for the empty site given by $e_j = (1 - n_j^\uparrow)(1 - n_j^\downarrow)$. $\eta$ is the variational parameter that takes the value in the range of $0 \leq \eta \leq 1$. $\tau$ indicates a vector connecting nearest-neighbor sites. The Jastrow-type wave function is written as $\psi_J = P_{Jdh}\psi_G$. An important difference between $\psi_\lambda$ and $\psi_J$ is that $P_{Jdh}$ is the site-diagonal operator, while $\psi_\lambda$ is the site-off diagonal operator.

The one-particle state $\psi_0$ is written in the form

$$\psi_0 = \sum_j a_0^j \phi_j^0, \quad (6)$$

where $\{ \phi_j^0 \}$ is a set of basis functions of the one-particle state in the site representation on a lattice, with $j$ being the label for the electron configuration. $\psi_\lambda$ and $\psi_J$ are given as

$$\psi_\lambda = \sum_j a_\lambda^j e^{-\lambda \tau} P_G \phi_j^0, \quad (7)$$

$$\psi_J = \sum_j a_J^j P_{Jdh} P_G \phi_j^0. \quad (8)$$

Since $P_G$ and $P_{Jdh}$ are diagonal operators, $\psi_J$ is written as

$$\psi_J = \sum_j a_J^j \phi_j^0, \quad (9)$$

where $a_J^j = a_J^j(g, \eta)$ is determined by parameters $g$ and $\eta$. $\psi_J$ is given by a wave function, where the coefficients $\{ a_J^0 \}$ are modified in the one-particle state. Instead, $\psi_\lambda$ is not so simple because $e^{-\lambda \tau}$ generates other basis states from $\phi_j^0$, which means that off-diagonal elements $\langle \phi_i^0 | \tau \phi_j^0 \rangle$ are effectively taken into account. We write $\psi_\lambda$ as

$$\psi_\lambda = \sum_j a_\lambda^j \phi_j, \quad (10)$$

where the set of basis states $\{ \phi_j \}$ may contain basis states which are not included in $\{ \phi_j^0 \}$ since some coefficients $a_\lambda^0$'s may vanish accidentally.

![Figure 1](image-url)

**Figure 1.** Ground-state energy as a function of $U$ on a $10 \times 10$ lattice, where we set $N_e = 88$ and $t' = 0$ with the boundary condition in one direction, and the antiperiodic one in the other direction.
4. Correlated Superconducting State

The correlated superconducting state is obtained by multiplying the BCS wave function by a correlation operator. The BCS wave function is

\[
\psi_{BCS} = \prod_k (u_k + v_k c_{k\uparrow}^c c_{-k\downarrow}^c)(0),
\]

with coefficients \( u_k \) and \( v_k \) that appear in the ratio \( u_k / v_k = \Delta_k / (\xi_k + \sqrt{\xi_k^2 + \Delta_k^2}) \), where \( \Delta_k \) is the gap function with \( k \) dependence, and \( \xi_k = \epsilon_k - \mu \) is the dispersion relation of conduction electrons. We adopt the d-wave symmetry for \( \Delta_k \), and we do not consider other symmetries in this paper since an SC state with other symmetry unlikely becomes stable in the simple single-band Hubbard model. The Gutzwiller BCS state is given by

\[
\psi_{G-BCS} = P_N P_G \psi_{BCS},
\]

where \( P_N \) indicates the operator to extract the state with \( N \) electrons. Here, the total electron number is fixed, and the chemical potential in \( \xi_k \) is regarded as a variational parameter.

The improved superconducting wave function is written as

\[
\psi_{\lambda} = e^{-\lambda K} P_G \psi_{BCS}.
\]

In the formulation of \( \psi_{\lambda} \), we cannot fix the total electron number, and we should use a different Monte Carlo sampling procedure. We perform the electron-hole transformation for down-spin electrons:

\[
d_k = c_{-k\downarrow}^c, \quad d_k^\dagger = c_{-k\uparrow},
\]

and not for up-spin electrons: \( c_k = c_{k\uparrow} \). In the real space, we have \( c_i = c_{i\uparrow} \) and \( d_i = c_{i\downarrow}^c \).

The electron pair operator \( c_{k\uparrow}^c c_{-k\downarrow}^c \) is transformed to the hybridization operator \( c_k^c d_k \). Then, we can use the auxiliary field method after this transformation in a Monte Carlo simulation. This is performed by expressing the Gutzwiller operator in the form [72].

\[
P_G = \prod_i (1 - (1 - g)c_i^c c_i(1 - d_i^\dagger d_i))
= \prod_i \exp(-ac_i^c c_i + ac_i^c d_i^\dagger d_i)
= \left( \frac{1}{2} \right)^N \sum_{s_i = \pm 1} \exp \left[ \sum_i (2as_i - a/2)(c_i^c c_i - d_i^\dagger d_i) \right],
\]

where \( g = e^{-a}, \cosh(2a) = e^{-a/2} \), and \( s_i \) is the auxiliary field that takes the value of \( \pm 1 \). By using this form, the expectation value is calculated as a sum of terms with respect to auxiliary fields, for which we apply the Monte Carlo procedure [63,72].

5. Kinetic Energy in the Superconducting State

In this section, we discuss the role of kinetic energy in the superconducting state in the two-dimensional Hubbard model. We consider the large-\( U \) region, where the kinetic energy of electrons would play an important role. Here, large-\( U \) means that \( U \) is much larger than the band width. The ground-state energy is determined by the balance of the kinetic energy and the Coulomb energy. We show the energy expectation values as a function of \( \lambda \) in Figure 2, where \( E_q / N \) is the ground-state energy per site, \( E_{kin} / N \) is the expectation value of the non-interacting part of the Hamiltonian \( E_{kin} = \langle \psi_{\lambda} K \psi_{\lambda} \rangle / \langle \psi_{\lambda} \psi_{\lambda} \rangle \), and \( E_U \) denotes the Coulomb energy given by \( E_U = U \langle \psi_{\lambda} \sum n_i n_i \psi_{\lambda} \rangle / \langle \psi_{\lambda} \psi_{\lambda} \rangle \). \( E_q \) has a minimum value for a finite value of \( \lambda \).

The kinetic energy part gives a large contribution to \( E_q \) when \( U \) is large. This is shown in Figure 3. When \( U > 10t \), \( E_U \) for \( \psi_{\lambda} \) almost agrees with that for \( \psi_G \). The difference of
$E_{\text{kin}}$ for $\psi_\lambda$ and $\psi_G$ increases for $U > 10t$. The region that may be called the 'kinetic energy phase' exists when $10 < U/t$.

![Figure 2](image1.png)

**Figure 2.** Ground-state energy $E_g/N$, kinetic energy $E_{\text{kin}}/N$, and the expectation value of the Coulomb interaction $E_U/N$ as a function of $\lambda$ on a $10 \times 10$ lattice with the periodic boundary condition in one direction, and the antiperiodic one in the other direction. We set $N_e = 88$, $U = 18t$ and $t' = 0$.

![Figure 3](image2.png)

**Figure 3.** Kinetic energy $E_{\text{kin}}/N$ and the Coulomb energy $E_U/N$ as a function of $U$ on a $10 \times 10$ lattice. The boundary conditions are the same as in Figure 2. The electron number is $N_e = 88$, and we put $t' = 0$. Open circles indicate the results for the Gutzwiller function, and solid circles are those for the improved $\psi_\lambda$.

Let us consider the the difference of the kinetic energy defined as

$$\Delta E_{\text{kin}} = E_{\text{kin}}(\psi_G) - E_{\text{kin}}(\psi_\lambda),$$

where $E_{\text{kin}}(\psi_G)$ and $E_{\text{kin}}(\psi_\lambda)$ denote the kinetic energy for $\psi_G$ and $\psi_\lambda$, respectively. Since $\psi_G = \psi_\lambda = 0$ with vanishing $\lambda$, we can write $\Delta E_{\text{kin}} = E_{\text{kin}}(\lambda = 0) - E_{\text{kin}}(\lambda)$ for the optimized value $\lambda$. We show $\Delta E_{\text{kin}}/N$ as a function of $U$ in Figure 4, where the hole doping rate $x$ is $x = 0.12$. $\Delta E_{\text{kin}}$ begins to increase when $U$ is of the order of the band width $U \sim 8t$. $\Delta E_{\text{kin}}$ has a broad peak when $15t < U < 20t$. We define the SC condensation energy $\Delta E_{\text{sc}}$ and the kinetic energy condensation energy $\Delta E_{\text{kin-sc}}$ as

![Figure 4](image4.png)
\[ \Delta E_{sc} = E_g(\Delta = 0) - E_g(\Delta = \Delta_{opt}), \]
\[ \Delta E_{\text{kin-sc}} = E_{\text{kin}}(\Delta = 0) - E_{\text{kin}}(\Delta = \Delta_{opt}), \]

where \( \Delta = \Delta_{sc} \) is the superconducting order parameter, and \( \Delta_{opt} \) is its optimized value. We assumed the \( d \)-wave symmetry for \( \Delta_k = \Delta(\cos k_x - \cos k_y) \). \( \Delta E_{\text{kin-sc}} / N \) is also shown in Figure 4. The figure indicates that \( \Delta E_{\text{kin-sc}} \) increases for large \( U \), showing a similar behavior to \( \Delta E_{\text{kin}} \). \( \Delta E_{\text{kin-sc}} \) can change the sign when \( U \) is small, which is consistent with the analysis for Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ [79].

In Figure 5, we show \( \Delta E_{\text{kin}} / N \) and \( \Delta E_{\text{kin-sc}} / N \) for \( x = 0.20 \). \( \Delta E_{\text{kin}} \) for \( x = 0.20 \) is smaller than that for \( x = 0.12 \). The kinetic energy condensation energy \( \Delta E_{\text{kin}} - \Delta E_{\text{kin-sc}} / N \) is also shown in Figure 4. The figure indicates that \( \Delta E_{\text{kin}} - \Delta E_{\text{kin-sc}} / N \) increases for large \( U \), showing a similar behavior to \( \Delta E_{\text{kin}} \). \( \Delta E_{\text{kin}} - \Delta E_{\text{kin-sc}} / N \) increases for large \( U \), showing a similar behavior to \( \Delta E_{\text{kin}} \). \( \Delta E_{\text{kin}} - \Delta E_{\text{kin-sc}} / N \) changes the sign when \( U \) is small, which is consistent with the analysis for Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ [79].

The Coulomb energy gain in the presence of the SC order parameter \( \Delta E_{U-sc} / N \) is also evaluated, where
\[ \Delta E_{U-sc} = E_U(\Delta = 0) - E_U(\Delta = \Delta_{opt}). \]
\( \Delta E_{U-sc} \) is the Coulomb energy contribution to the SC condensation energy; namely, we have
\[ \Delta E_{sc} = \Delta E_{\text{kin-sc}} + \Delta E_{U-sc}. \]

Our result shows that
\[ \Delta E_{\text{kin-sc}} > 0, \quad \Delta E_{U-sc} < 0, \]
for the improved state \( \psi_{\lambda-BCS} \). We show the SC condensation energy \( \Delta E_{sc} (\Delta_{sc}) \) and the Coulomb energy part \( \Delta E_{U-sc} (\Delta_{sc}) \) as a function of \( \Delta_{sc} \) in Figure 6 where \( \Delta E_{sc} (\Delta) = E_g(\Delta = 0) - E_g(\Delta) \) and \( \Delta E_{U-sc} (\Delta) = E_U(\Delta = 0) - E_U(\Delta) \). The positive \( \Delta E_{\text{kin-sc}} > 0 \) indicates that the SC state \( \psi_{\lambda-BCS} \) becomes stable due to the kinetic energy effect.

![Figure 4. Kinetic-energy difference \( \Delta E_{\text{kin}} / N \) and the kinetic energy difference in the SC state \( \Delta E_{\text{kin-sc}} / N \) (×25) as a function of \( U \) on a 10 × 10 lattice. Since \( \Delta E_{\text{kin-sc}} / N \) is small compared to \( \Delta E_{\text{kin}} / N \), we multiplied \( \Delta E_{\text{kin-sc}} / N \) by 25. The boundary conditions are the same as in Figure 1. The electron number is \( N_e = 88 \) (\( n = 0.88 \) and we put \( t' = 0 \).)](image-url)
Figure 5. Kinetic-energy difference $\Delta E_{\text{kin}}/N$ and the kinetic energy difference in the SC state $\Delta E_{\text{kin-sc}}/N$ ($\times 25$) as a function of $U$ on a $10 \times 10$ lattice for $N_e = 80$ ($n = 0.80$) and $t' = 0$. The boundary conditions are the same as in Figure 1.

Figure 6. SC condensation energy $\Delta E_{\text{sc}}(\Delta_{\text{sc}})/N$ and its Coulomb energy part $|\Delta E_{\text{U-sc}}(\Delta_{\text{sc}})/N|$ as a function of $\Delta_{\text{sc}}$ on a $10 \times 10$ lattice for $N_e = 88$ ($n = 0.88$) and $U = 18$. We set $t' = 0$. $\Delta E_{\text{U-sc}}$ is negative for this set of parameters. The boundary conditions are the same as in Figure 1.

6. Summary

We investigated the ground state of the two-dimensional Hubbard model by using the optimization variational Monte Carlo method with focus on the strongly correlated large-$U$ region. The ground-state energy is greatly lowered due to $\exp(-\lambda K)$ correlation operator. The optimization variational Monte Carlo method is effective even in strongly correlated regions where $U$ is much larger than the bandwidth.

In the large-$U$ region, the kinetic energy term becomes dominant in the ground state, and the kinetic energy effect dominates the antiferromagnetic correlation. The kinetic energy difference $\Delta E_{\text{kin}} = E_{\text{kin}}(\psi_G) - E_{\text{kin}}(\psi_A)$ increases when $U > 10t$ and has a broad peak. The kinetic condensation energy $\Delta E_{\text{kin-sc}}$ behaves like the kinetic energy difference $\Delta E_{\text{kin}}$ for $U > 10t$. There is a correlation between $\Delta E_{\text{kin-sc}}$ and $\Delta E_{\text{kin}}$. The condensation energy $\Delta E_{\text{sc}}$ mainly comes from the kinetic energy part $\Delta E_{\text{kin-sc}}$ and there is a competition between the kinetic energy and the Coulomb energy. Hence there are two competitions...
in the Hubbard model; one is that between superconductivity and antiferromagnetism and the other is that between kinetic energy effect and Coulomb repulsive interaction. As a result of competitions, superconducting transition occurs. The result shows that superconductivity in the strongly correlated region is induced by kinetic energy effect. We expect that high-temperature superconductivity would be realized in the strongly correlated region of the two-dimensional Hubbard model.

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**Abbreviations**

The following abbreviations are used in this manuscript:

- VMC variational Monte Carlo method
- AF antiferromagnetic
- SC superconductivity or superconducting
- 2D two-dimensional
- AFI antiferromagnetic insulator
- PI paramagnetic insulator

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