Optimized wave function by kinetic renormalization effect in strongly correlated region of the three-band Hubbard model

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Abstract. We investigate the ground state of the two-dimensional single-band Hubbard model and three-band Hubbard model (d-p model) by using a variational Monte Carlo method. We employ an optimization variational Monte Carlo method. In this method the many-body wave function is improved and optimized by introducing variational parameters in the form: \( \psi = \exp(-S)\psi_0 \) where \( \psi_0 \) is a wave function, for example, the Gutzwiller function, and \( S \) is an operator used to include the many-body effect.

The strong magnetic correlation is induced by the on-site Coulomb repulsive interaction \( U \). The magnetic correlation plays a significant role in correlated electron systems as an origin of electron pairing as well as a main competitor of superconductivity. High-temperature superconductivity occurs in the strongly correlated region where \( U \) is greater than the bandwidth. We investigate the stability of antiferromagnetic state in the three-band d-p model.

1. Introduction

It is important to clarify the mechanism of high-temperature superconductivity. The physics of high-temperature superconductivity has been studied intensively since the discovery of cuprate high-temperature superconductors[1]. The electron correlation plays an important role for the appearance of high-temperature superconductivity, because the parent materials without carries are Mott insulators and it has been established that the Cooper pairs of cuprate superconductors have the d-wave symmetry.

The CuO$_2$ plane is commonly contained in high-temperature cuprates, where the CuO$_2$ plane consists of oxygen atoms and copper atoms. The electronic model for this plane is the called d-p model (or three-band Hubbard model)[2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18]. It appears very hard to elucidate the phase diagram of the d-p model because of strong correlation between electrons. We often examine simplified models such as the two-dimensional single-band Hubbard model[19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37] or ladder model[38, 39, 40, 41] to make clear the phase diagram of correlated electron systems.

A variational Monte Carlo method is a useful method to investigate electronic properties of strongly correlated electron systems by calculating the expectation values numerically. A variational wave function can be improved by introducing new variational parameters to control
the electron correlation. We have proposed wave functions that are optimized by multiplying an initial wave function by \( \exp(-S) \)-type operators\[37, 42\], where \( S \) is a suitable correlation operator. The Gutzwiller function is also written in this form. An optimization process is performed in a systematic way by multiplying by the exponential-type operators repeatedly\[42\]. The ground-state energy is lowered considerably by using this type of wave functions\[37\].

2. Hamiltonian

The three-band model that explicitly includes oxygen \( p \) and copper \( d \) orbitals contains the parameters \( U_d, U_p, t_{dp}, t_{pp}, t'_d, \epsilon_d \) and \( \epsilon_p \). Our study is within the hole picture and the Hamiltonian is written as

\[
H_{dp} = \epsilon_d \sum_{i\sigma} d_i^{\dagger} d_i + \epsilon_p \sum_{i\sigma} \left( p_i^{\dagger} p_{i+\hat{x}/2\sigma} + p_i^{\dagger} p_{i+\hat{y}/2\sigma} \right) + t_{dp} \sum_{i\sigma} \left[ d_i^{\dagger} (p_{i+\hat{x}/2\sigma} + p_{i+\hat{y}/2\sigma} - p_{i-\hat{x}/2\sigma} - p_{i-\hat{y}/2\sigma}) \right] + t_{pp} \sum_{i\sigma} \left[ p_i^{\dagger} p_{i+\hat{x}/2\sigma} - p_i^{\dagger} p_{i+\hat{y}/2\sigma} \right] - p_i^{\dagger} p_{i-\hat{x}/2\sigma} + p_i^{\dagger} p_{i-\hat{y}/2\sigma} + \text{h.c.} \right] + t'_d \sum_{\langle\langle ij\rangle\rangle\sigma} \epsilon_{ij} (d_i^{\dagger} d_j + \text{h.c.}) + U_d \sum_{i} d_i^{\dagger} d_i^{\dagger} d_i d_i.
\]  

(1)

\( d_{i\sigma} \) and \( d_{i\sigma}^{\dagger} \) represent the operators for the \( d \) hole. \( p_{i+\hat{x}/2\sigma} \) and \( p_{i+\hat{y}/2\sigma} \) denote the operators for the \( p \) holes at the site \( R_{i+\hat{x}/2\sigma} \), and in a similar way \( p_{i+\hat{y}/2\sigma} \) and \( p_{i+\hat{y}/2\sigma} \) are defined. \( t_{dp} \) is the transfer integral between adjacent Cu and O orbitals and \( t_{pp} \) is that between nearest \( p \) orbitals. \( \langle\langle ij\rangle\rangle \) denotes a next nearest-neighbor pair of copper sites. \( t'_d \) was introduced (as shown in Fig.1) to reproduce the Fermi surface\[43\] reported in several cuprate superconductors such as \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta} \)[44] and \( \text{Tl}_2\text{Ba}_2\text{CuO}_{6+\delta} \)[45]. \( \epsilon_{ij} \) takes the values \( \pm 1 \) according to the sign of the transfer integral between next nearest-neighbor \( d \) orbitals. \( U_d \) is the strength of the on-site Coulomb repulsion between \( d \) holes. In this paper we neglect \( U_p \) among \( p \) holes because \( U_p \) is small compared to \( U_d \)[46, 47, 48, 49, 50]. \( U_p \) is not important in the low-doping region where the \( p \)-hole correlation effect is small. The values of band parameters were estimated as, for example, \( U_d = 10.5, U_p = 4.0 \) and \( U_{dp} = 1.2 \) in eV\[47\] where \( U_{dp} \) is the nearest-neighbor Coulomb interaction between holes on adjacent Cu and O orbitals. We neglect \( U_{dp} \) because \( U_{dp} \) is small compared to \( U_d \). We use the notation \( \Delta_{dp} = \epsilon_p - \epsilon_d \). The number of sites is denoted as \( N \), and the total number of atoms is \( N_a = 3N \). The energy unit is given by \( t_{dp} \).

The single-band Hubbard model can be regarded as a simplified version of the three-band \( d-p \) model. This model has been studied more intensively. The Hamiltonian is given by

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

(2)

where \( \{t_{ij}\} \) are transfer integrals and \( U \) is the on-site Coulomb energy. The transfer integral \( t_{ij} \) for nearest-neighbor pairs \( \langle ij \rangle \) is given as \( t_{ij} = -t \) and that for next-nearest neighbor pair \( \langle\langle ij\rangle\rangle \) is \( t_{ij} = -t' \). Otherwise, \( t_{ij} \) vanishes. The number of sites is denoted as \( N \) and the number of electrons is as \( N_e \). The energy unit is given by \( t \). \( n_{i\sigma} \) is the number operator: \( n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma} \). The second term in the Hamiltonian represents the on-site repulsive interaction between electrons.
3. Optimized wave functions

The Gutzwiller-projected wave function is given as $\psi_G = P_G \psi_0$, where $P_G$ is the Gutzwiller operator to control the double occupancy of $d$ holes:

$$ P_G = \prod_i [1 - (1 - g)n_{di\uparrow}n_{di\downarrow}] = \exp \left( -\alpha \sum_i n_{di\uparrow}n_{di\downarrow} \right), $$

where $\alpha = \ln(1/g)$, $g$ is a variational parameter in the range from 0 to unity, $n_{di\sigma} = d_{i\sigma}^\dagger d_{i\sigma}$ is the number operator for $d$ holes. $\psi_0$ is the Fermi sea where the lowest band is occupied up to the Fermi energy $\mu$.

The Gutzwiller wave function is improved in the following way[37, 42, 51, 52, 53, 54, 55]:

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

where $\lambda$ is a variational parameter and $K$ is the kinetic part of the Hamiltonian. The expectation values are evaluated by using the auxiliary field method[42, 56].

The correlated superconducting (SC) state is represented by the projected-BCS wave function. This is given as

$$ \psi_S = P_{Ne} P_G \psi_{BCS}, $$

where $\psi_{BCS}$ indicates the BCS wave function:

$$ \psi_{BCS} = \prod_k (u_k + v_k \alpha_k^\dagger \alpha_{-k}^\dagger)|0\rangle. $$

$\alpha_{k\sigma}$ indicates the creation operator of the state in the lowest band with the momentum $k$ which is represented by a linear combination of $d$ and $p$ electron operators $d_{k\sigma}^\dagger$ and $p_{k\sigma}^\dagger$. The BCS

\begin{figure}
\centering
\includegraphics[width=0.8\textwidth]{fig1.png}
\caption{The transfer integral $t'_d$ in the CuO$_2$ plane. $t'_d$ is the transfer integral between next nearest-neighbor copper sites. We can also consider the transfer integral $t'_{pp}$ between next nearest-neighbor oxygen atoms.}
\end{figure}

\begin{figure}
\centering
\includegraphics[width=0.8\textwidth]{fig2.png}
\caption{AF and SC order parameters as a function of $U/t$ for the two-dimensional Hubbard model on a $10 \times 10$ lattice[37]. The upper curve AF(G) indicates the result obtained by the Gutzwiller function, and those for AF and SC are obtained using $\psi_\lambda$. We expect a similar phase diagram for the d-p model.}
\end{figure}
parameters $u_k$ and $v_k$ are given by the ratio $v_{fk}/u_k = \Delta_k/(\xi_k + \sqrt{\xi_k^2 + \Delta_k^2})$ where $\xi_k$ is the dispersion relation of the lowest band. We assume the d-wave symmetry $\Delta_k = \Delta (\cos k_x - \cos k_y)$ and we regard $\Delta$ as the superconducting gap. $\Delta$ is a variational parameter that is optimized to give the lowest ground energy. $P_{N_e}$ is a projection operator which extracts only the states with a fixed total hole number.

It is convenient to perform the particle-hole transformation for down-spin holes[37, 52] in multiplying by the operator $\exp(-\lambda K)$:

$$\psi_\lambda = \exp(-\lambda K) P_G \psi_{BCS} = \exp(-\lambda K) P_G \prod_k (u_k \beta_k^\dagger + v_k \alpha_k^\dagger)(\bar{0}),$$

where $\beta_k^\dagger = \alpha_{-k}^\dagger$ and $\alpha_k^\dagger = \alpha_k^\dagger$. $|\bar{0}\rangle$ denotes the vacuum for newly defined $\alpha$ and $\beta$ particles satisfying $\alpha_k |\bar{0}\rangle = \beta_k |\bar{0}\rangle = 0$.

4. Antiferromagnetic state

We show the gap function $\Delta_{AF}$ (antiferromagnetic (AF) state) and $\Delta$ (superconducting state) as a function of $U/t$ for the two-dimensional Hubbard model in Fig.2[37]. In the strongly correlated region where $U$ is larger than the bandwidth, the antiferromagnetic correlation is suppressed and as a result superconducting state can be stable. We would expect a similar phase diagram for the d-p model.

It is important to have control of the antiferromagnetic state in strongly correlated electron systems. It appears however, that the AF state is considerably stable in the three-band d-p model, and is more stable than in the single-band Hubbard model. It is thus necessary to introduce a new parameter $t'_d$. The Fermi surface will have a large curvature as finite $t'_d$ is introduced. This is shown in Fig.3. $t'_d$ also plays a role concerning a stability of the AF state.

We show the ground-state energy $E_g$ and the kinetic energy $E_K$ as a function of $\lambda$ in Fig.4 where $E_K$ is the expectation value of the kinetic part $K$ of the Hamiltonian. The antiferromagnetic state is suppressed by $t'_d$. This is shown in Fig.5 and Fig.6, where the level difference is chosen as $\Delta_{dp} = \epsilon_p - \epsilon_d = 2t_{dp}$ and $4t_{dp}$, respectively. When the level difference is large, we need large $t'_d$ to reduce the antiferromagnetic correlation.

5. Discussion

We discuss how the wave function is improved compared to the Gutzwiller function. We are in a tendency to predict a large AF phase on the basis of the Gutzwiller function. It is necessary to improve and optimize the wave function to examine whether the AF region is indeed so large. The energy gain of the improved wave function $\psi_\lambda$ mainly comes from the kinetic-energy gain as shown in Fig.4. The conduction electrons become rather localized due to the Gutzwiller projection, from which the electronic state favors magnetic correlation. This means that the kinetic-energy gain is relatively reduced compared with that of the Coulomb energy. The exponential kinetic operator $e^{-\lambda K}$ has an effect to move electrons to get the kinetic-energy gain. This will increase the double occupancy, and the variational parameters are determined to lower the ground-state energy by balancing the kinetic energy against the Coulomb repulsive energy. We can lower the ground-state energy further by multiplying the wave function by the Gutzwiller projection again.

The importance of multiplying by $e^{-\lambda K}$ lies in that the AF phase is reduced by suppressing AF correlation. In fact, in the 2D Hubbard model, the AF correlation is considerably suppressed when $U$ is large being greater than the bandwidth where the kinetic-energy gain is dominant over the AF energy lowering. This is also the case for the d-p model. By using the Gutzwiller function, the optimized value of the AF order parameter is very large and is larger than that of
Figure 3. Fermi surface of the three-band d-p model in the non-interacting case. We used $t_{pp} = 0.4t_{dp}$ and $\epsilon_p - \epsilon_d = 2t_{dp}$ for $t_d' = 0$, $-0.2t_{dp}$, and $-0.3t_{dp}$. The hole-doping rate is about 0.13.

Figure 4. Ground-state energy $E_g$ and the kinetic energy $E_K$ as a function of $\lambda$ on $8 \times 8$ lattice with 76 holes. The band parameters are $\epsilon_p - \epsilon_d = 2$, $t_{pp} = 0.4$, $t_d' = -0.2$, $U_d = 10$ and $U_p = 0$ in units of $t_{dp}$.

Figure 5. AF and SC order parameters as a function of $t_d'$ in units of $t_{dp}$ on $8 \times 8$ lattice with 76 holes. The band parameters are $\epsilon_p - \epsilon_d = 2$, $t_{pp} = 0.4$, $U_d = 10$ and $U_p = 0$. We used the Gutzwiller-BCS wave function for SC state.

Figure 6. Antiferromagnetic order parameter as a function of $t_d'$ on $8 \times 8$ lattice with 76 holes. The band parameters are $\epsilon_p - \epsilon_d = 4$, $t_{pp} = 0.4$, $U_d = 10$ and $U_p = 0$. When the level difference $\epsilon_p - \epsilon_d$ becomes large, the AF state is more stabilized.

the superconducting order parameter more than by one order of magnitude in the d-p model. The AF order parameter is reduced to be of the same order as the superconducting one based on our wave function. This would give a possibility of superconductivity.
6. Summary
We investigated the ground state of the two-dimensional three-band Hubbard model on the basis of the optimization variational Monte Carlo method. The antiferromagnetic correlation is very strong and the antiferromagnetic state is very stable in the d-p model. It is thus necessary to introduce long-range transfer integrals such $t'_d$ to conquer the antiferromagnetism in the d-p model. We expect that there also occurs a crossover between strongly correlated and weakly correlated regions by controlling the antiferromagnetic correlation in the d-p model.

There is a crossover in the two-dimensional Hubbard model[37]. A large fluctuation presumably exists in the crossover region. This indicates a possibility of high-temperature superconductivity. A crossover from weakly to strongly coupled systems is universal phenomenon that exists ubiquitously in the world. There may be a class of phenomena that shows a crossover between weakly and strongly interacting regions. This class may include, for example, the Kondo effect[57, 58, 59, 60, 61, 62, 63], QCD[64], BCS-BEC crossover[65], Hubbard model, sine-Gordon model[66, 67, 68] and the Kosterlitz-Thouless transition.

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