Magnetsim, Fluctuations and Mechanism of High-Temperature Superconductivity

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Abstract. We investigate the ground state of the two-dimensional d-p model (three-band Hubbard model) by using a variational Monte Carlo method. The superconducting condensation energy is evaluated for the Gutzwiller-BCS wave function. We show that there is a crossover between strongly and weakly correlated regions as the level difference between d and p orbitals increases. The gap function and the condensation energy can be large in the crossover region. This result indicates a possibility of high-temperature superconductivity in the two-dimensional d-p model.

1. Introduction
The research of mechanism of high-temperature superconductivity has attracted much attention since the discovery of cuprate high-temperature superconductors[1, 2]. Because it has been established that the Cooper pairs of cuprate high-temperature superconductors have the d-wave symmetry, the electron correlation plays an important role for the appearance of superconductivity. It is primarily important to clarify the phase diagram of electronic states in the CuO$_2$ plane contained commonly in cuprate high-temperature superconductors. The CuO$_2$ plane consists of oxygen atoms and copper atoms. The electronic model for this plane is the d-p model (or three-band Hubbard model)[3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17]. An interaction with a large energy scale is necessary for the realization of high-temperature superconductivity. It has been argued whether the on-site Coulomb repulsive interaction induces superconductivity for the two-dimensional single-band Hubbard model[18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30] and ladder model[31, 32, 33].

It is also expected that there is a superconducting phase in the two-dimensional d-p model. It is, however, difficult to obtain a clear evidence of superconductivity in the two-dimensional d-p model because the energy gain by introducing the superconducting gap is very small for the Gutzwiller-BCS wave function[8, 13]. Does this mean that there is no superconductivity in the d-p model? The purpose of this paper is to reexamine the stability of the superconducting state in the d-p model by using the variational Monte Carlo method. Numerous works performed so far have focused on the region where the energy difference between d and p levels are located closely each other. This is because there has been a suggestion that the superconducting critical temperature $T_c$ increases as the d-p level difference decreases[34].
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

\[
H_{dp} = \epsilon_d \sum_{i,\sigma} d_{i\sigma}^\dagger d_{i\sigma} + \epsilon_p \sum_{i,\sigma} \left( p_{i+z/2\sigma}^\dagger p_{i+z/2\sigma} + p_{i+y/2\sigma}^\dagger p_{i+y/2\sigma} \right) 
+ t_{dp} \sum_{i,\sigma} \left[ d_{i\sigma}^\dagger \left( p_{i+z/2\sigma} + p_{i+y/2\sigma} - p_{i-z/2\sigma} - p_{i-y/2\sigma} \right) + \text{h.c.} \right] 
+ t_{pp} \sum_{i,\sigma} \left[ \left( p_{i+y/2\sigma}^\dagger p_{i-z/2\sigma} - p_{i+y/2\sigma}^\dagger p_{i-z/2\sigma} \right) \right] 
- p_{i-y/2\sigma}^\dagger p_{i+z/2\sigma} + p_{i-y/2\sigma}^\dagger p_{i+z/2\sigma} + \text{h.c.} ] 
+ t'_d \sum_{\langle i,j \rangle,\sigma} \left( d_{i\sigma}^\dagger d_{j\sigma} + \text{h.c.} \right) + U_d \sum_i d_{i\sigma}^\dagger d_{i\sigma}^\dagger d_{i\sigma} d_{i\sigma}. \tag{1}\]

\( d_{i\sigma} \) and \( d_{i\sigma}^\dagger \) represent the operators for the d hole, \( p_{i+z/2\sigma} \) and \( p_{i+y/2\sigma} \) denote the operators for the p holes at the site \( R_{i+z/2} \), and in a similar way \( p_{i+y/2\sigma} \) and \( p_{i+y/2\sigma}^\dagger \) 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 to reproduce the Fermi surface [35] in several cuprate superconductors such as \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8+\delta [36] \) and \( \text{Tl}_2\text{Ba}_2\text{CuO}_{6+\delta} [37] \). \( U_d \) 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 \( U_d \) [38, 39, 40, 41]. In the low-doping region, \( U_p \) will be of minor importance because \( p \)-hole concentration is small[42]. The parameter values were estimated as, for example, \( U_d = 10.5, U_p = 4.0 \) and \( U_{dp} = 1.2 \) in eV[39] 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 \( t_{dp} \).

3. Superconducting wave function

We examine the superconducting ground state of the two-dimensional d-p model by using the variational Monte Carlo method. The wave function is the Gutzwiller-projected wave function given as

\[
\psi_G = P_G \psi_0, \tag{2}\]

where \( P_G \) is the Gutzwiller operator to control the double occupancy of d holes:

\[
P_G = \prod_i \left[ 1 - (1 - g) n_{d_i\uparrow} n_{d_i\downarrow} \right]. \tag{3}\]

\( g \) is a variational parameter in the range from 0 to unity. \( n_{d_{i\sigma}} = d_{i\sigma}^\dagger d_{i\sigma} \) is the number operator for d holes. \( \psi_0 \) is the Fermi sea where the lowest band is occupied up to the Fermi energy \( \mu \). To represent a superconducting state, we take \( \psi_0 \) as the BCS wave function

\[
\psi_{BCS} = \prod_k (u_k + v_k a_k^{\dagger} a_{-k}^{\dagger} ) |0\rangle, \tag{4}\]

where \( a_k^{\dagger} \) 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 \( d_{k\sigma} \) and \( p_{k\sigma} \). The
We calculate the superconducting condensation energy $\Delta$ satisfying the gap $\Delta_{\text{opt}}$ is the ground-state energy with the gap $\Delta$ and $\Delta$ is a variational parameter that is optimized to give the lowest ground energy. The Projected-BCS wave function is written as

$$\psi_S = P_N P_G \psi_{\text{BCS}},$$

where $P_N$ is a projection operator which extracts only the states with a fixed total hole number. In actual evaluations, we can use the method in Ref.[13]. We can also use the wave function obtained by performing the particle-hole transformation for down-spin holes[30, 43]:

$$P_G \psi_{\text{BCS}} = P_G \prod_k (u_k \beta_k^\dagger + v_k \alpha_k^\dagger) |\bar{0}\rangle,$$

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

We use the variational Monte Carlo method in the evaluation of the ground-state energy[8]. We calculate the superconducting condensation energy $\Delta E = E(\Delta \to 0) - E(\Delta_{\text{opt}})$ where $E(\Delta)$ is the ground-state energy with the gap $\Delta$ and $\Delta_{\text{opt}}$ is the value of optimized superconducting gap $\Delta$.

We show the condensation energy as a function of $\Delta$ in Fig.1 where calculations were carried out on an 8 x 8 lattice with 192 atoms. The parameters that we used are $t_{pp} = 0.4$, $u_d = 10$, $U_p = 0$ and $t_d' = 0$ in units of $t_{dp}$. We put 76 holes on the lattice and we set $\Delta_{dp} = \epsilon_p - \epsilon_d = 2, 4$ and 8. As shown in Fig.1, the condensation energy $\Delta E$ becomes extremely large as the level difference $\Delta_{dp}$ increases. When $\Delta_{dp} = 2$, $\Delta E$ is very small and thus it is not easy to determine the condensation energy by numerical calculations. In contrast, surprisingly, $\Delta E$ turns out to be very large when $\Delta_{dp}$ is large. This indicates that the superconducting state is more stabilized in the strongly correlated region in accordance with the phenomenon in the single-band Hubbard model[30]. The existence of high-temperature superconductivity is suggested when the level difference $\Delta_{dp}$ is large.

Let us investigate the behavior of $\Delta E$ when the level difference $\Delta_{dp}$ increases further. We show the optimized gap amplitude $\Delta$ as a function of $\Delta_{dp}$ in Fig.2 where the band parameters are the same as in Fig.1. The figure indicates that there is a maximum in the optimized gap function as a function of $\Delta_{dp}$ in the large-$\Delta_{dp}$ region.

### 4. Discussion

The condensation energy $\Delta E$ exhibits a maximum with a large value, indicating that there occurs a crossover between strongly and weakly correlated regions. This crossover is quite similar to that in the two-dimensional Hubbard model[30]. A large fluctuation presumably exists in the crossover region. This indicates a possibility of high-temperature superconductivity in the d-p model. A crossover from weakly to strongly coupled systems is universal phenomenon that exists ubiquitously in the world. For example, the Kondo effect exhibits a universal logarithmic anomaly that appears as a crossover when the system approaches the strong coupling region (low temperature region) from the weak coupling region (high temperature region)[44, 45, 46, 47, 48, 49]. A two-impurity Kondo problem also shows a crossover[50, 51, 52]. There may be a class of phenomena that shows a crossover between weakly and strongly interacting regions. This class may include, for example, QCD[53], BCS-BEC crossover[54], Hubbard model, sine-Gordon model[55, 56, 57] and the Kosterlitz-Thouless transition.
Figure 1. Superconducting condensation energy as a function of the gap function for \( \Delta_{dp} = 2, 4 \) and 8 in units of \( t_{dp} \). Numerical calculations were carried on \( 8 \times 8 \) lattice with 76 holes. The band parameters are \( t_{pp} = 0.4, t_{dp}' = 0, U_d = 10 \) and \( U_p = 0 \). We used the Gutzwiller-BEC function in eq.(5) where the hole number is fixed to be 76.

Figure 2. Superconducting gap as a function of the level difference \( \Delta_{dp} \equiv \epsilon_p - \epsilon_d \). Numerical calculations were performed on \( 8 \times 8 \) lattice with 76 holes. The band parameters are \( t_{pp} = 0.4, t_{dp}' = 0, U_d = 10 \) and \( U_p = 0 \). The upper curve was calculated by using the Gutzwiller-BEC function in eq.(5) and the lower one is by the wave function in eq.(6).

5. Summary
We investigated the ground state of the two-dimensional Hubbard model on the basis of the variational Monte Carlo method. The superconducting condensation energy was calculated by using the Gutzwiller-projected BCS wave function. Although the condensation energy \( \Delta E \) is very small when the level difference between \( d \) and \( p \) orbitals is small, \( \Delta E \) increases as the level difference increases, suggesting a possibility of high-temperature superconductivity. It would be better to examine the \( d-p \) model by using improved wave functions[30, 35, 58, 59, 60, 61]. The Mott transition based on the \( d-p \) model was investigated with improved wave function[35]. A crossover for the antiferromagnetic correlation can be explored on the basis of improved wave functions.

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