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Phase diagram of cuprate high-temperature superconductors based on the optimization Monte Carlo method

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It is important to understand the phase diagram of electronic states in the CuO_2 plane to clarify the mechanism of high-temperature superconductivity of high-temperature superconductivity. We investigate the ground state of electronic models with strong correlation by employing the optimization variational Monte Carlo method. We consider the two-dimensional Hubbard model as well as the three-band d-p model. We use the improved wave function that takes account of inter-site electron correlation to go beyond the Gutzwiller wave function. The ground state energy is lowered considerably, which now gives the best estimate of the ground state energy for the two-dimensional Hubbard model.

The many-body effect plays an important role as an origin of spin correlation and superconductivity in correlated electron systems. We investigate the competition between the antiferromagnetic state and superconducting state by varying the Coulomb repulsion U, the band parameter t' and the electron density n_e for the Hubbard model. We show phase diagrams that include superconducting and antiferromagnetic phases. We expect that high-temperature superconductivity occurs near the boundary between antiferromagnetic phase and superconducting one. Since the three-band d-p model contains many band parameters, high-temperature superconductivity may be more likely to occur in the d-p model than in single-band models.

Keywords: strongly correlated electrons; optimized wave function: variational Monte Carlo method; antiferromagnetism; superconductivity.

1. Introduction

High-temperature superconductivity has been studied intensively since the discovery of high-temperature cuprates.[1] It is of primary importance to understand the phase diagram of cuprates to clarify the mechanism of high-temperature superconductivity. It has been argued that the electron correlation between electrons plays a significant role in cuprate superconductors because the parent materials without carriers are a Mott insulator. It may be that an interaction with large energy scale is responsible for realization of high temperature superconductivity.[2] We can expect high critical temperature T_c originating from the strong electron correlation. It is clear that an important key is in the CuO_2 plane since the CuO_2 plane is commonly contained in cuprate superconductors. Hence we should clarify the properties of electronic states in the CuO_2 plane.[3–12] The model for the CuO_2 plane is the three-band d-p model. We also often consider the simplified model, by neglecting oxygen sites in the CuO_2 plane, which is called the (single-band) Hubbard model.[13–16]

The Hubbard model is the well-known fundamental model in the solid state physics. This model was first introduced by Hubbard[13] to understand the metal-insulator transition in solids. The Hubbard model has been used to understand the magnetism such as ferromagnetism and antiferromagnetism of various compounds[17,18] since the Heisenberg model is derived from the Hubbard model in some limit.

It has also been examined to understand the inhomogeneous states such as the striped states[19–26] and the checkerboard-like density-wave modulation[27–29] on the basis of the Hubbard model.[30–32] It has been an important subject to clarify whether the 2D Hubbard model has a superconducting (SC) phase or not.[33–38] It was proposed that the two-dimensional (2D) Hubbard model can account for high-temperature superconductivity.[39] Recent numerical results indicate the existence of the d-wave superconducting phase in the 2D Hubbard model.[40,41] For the ladder Hubbard model, which is a variation of the mode, previous studies have indicated positive results on the existence of superconductivity.[42–46]

A variational Monte Carlo method is a useful method to study physical properties of strongly correlated systems.[15,47–52] A simple wave function is given by the Gutzwiller wave function. We have proposed wave functions that are optimized by introducing new variational parameters beyond the Gutzwiller function.[40] We have shown that the ground-state energy is lowered considerably compared to those obtained by previous works.[40] The evaluations obtained by using the optimized wave functions indicates that the superconducting phase exists in the 2D Hubbard model.

2. Model Hamiltonians

The Hamiltonian of the single Hubbard model is given as

$$H = \sum_{ij\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}, \tag{1}$$

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 denoted as $t_{ij} = -t$ and that for next-nearest neighbor pair $\langle\langle ij\rangle\rangle$ is $t_{ij} = -t'$. Otherwise, t_{ij} vanishes. We denote the number of sites as N and the number of electrons as N_e. The energy unit is given by t. $n_{i\sigma}$ is the number operator: $n_{i\sigma} = c^\dagger_{i\sigma}c_{i\sigma}$. The second term in the Hamiltonian represents the on-site repulsive interaction between electrons with opposite spins.

The three-band d-p model, called the d-p model in this paper, is the model that contains oxygen p orbitals and copper d orbitals. The d-p model is more realistic for high-temperature cuprates than the single-band Hubbard model. The Hamiltonian of the d-p model is written as

$$\begin{aligned} H_{dp} = {} & \epsilon_d \sum_{i\sigma} d^\dagger_{i\sigma} d_{i\sigma} + \epsilon_p \sum_{i\sigma} (p^\dagger_{i+\hat{x}/2\sigma} p_{i+\hat{x}/2\sigma} + p^\dagger_{i+\hat{y}/2\sigma} p_{i+\hat{y}/2\sigma}) \\ & + t_{dp} \sum_{i\sigma} [d^\dagger_{i\sigma}(p_{i+\hat{x}/2\sigma} + p_{i+\hat{y}/2\sigma} - p_{i-\hat{x}/2\sigma} - p_{i-\hat{y}/2\sigma}) + \text{h.c.}] \\ & + t_{pp} \sum_{i\sigma} [p^\dagger_{i+\hat{y}/2\sigma} p_{i+\hat{x}/2\sigma} - p^\dagger_{i+\hat{y}/2\sigma} p_{i-\hat{x}/2\sigma} \\ & - p^\dagger_{i-\hat{y}/2\sigma} p_{i+\hat{x}/2\sigma} + p^\dagger_{i-\hat{y}/2\sigma} p_{i-\hat{x}/2\sigma} + \text{h.c.}] \\ & + t'_d \sum_{\langle\langle ij\rangle\rangle\sigma} \epsilon_{ij} (d^\dagger_{i\sigma} d_{j\sigma} + \text{h.c.}) + U_d \sum_i d^\dagger_{i\uparrow} d_{i\uparrow} d^\dagger_{i\downarrow} d_{i\downarrow}. \end{aligned} \tag{2}$$

$d_{i\sigma}$ and $d^\dagger_{i\sigma}$ represent the operators for the d hole. $d_{i\sigma}$ and $d^\dagger_{i\sigma}$ represent the operators for the d hole. $p_{i\pm\hat{x}/2\sigma}$ and $p^\dagger_{i\pm\hat{x}/2\sigma}$ denote the operators for the p holes at the site $R_{i\pm\hat{x}/2}$, and in a similar way $p_{i\pm\hat{y}/2\sigma}$ and $p^\dagger_{i\pm\hat{y}/2\sigma}$ 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. $\epsilon_{ij} = \pm 1$ indicates the sign of transfer integral that depends on the sign of d orbitals. U_d is the strength of the on-site Coulomb repulsion between d holes. In general U_p is small compared to U_d.[53–57]

The lattice structure of the CuO_2 plane is shown in Fig. 1. We introduced t'_d, which is the transfer integral between next-nearest neighbor d electrons as shown in Fig.2. The one reason to introduce t'_d is to reproduce the deformed Fermi surface in cuprate superconductors such as $Bi_2Sr_2CaCu_2O_{8+\delta}$[58] and $Tl_2Ba_2CuO_{6+\delta}$.[59] When t'_d is finite, the Fermi surface is deformed with large curvature. The other reason is to suppress the antiferromagnetic (AF) correlation because t'_d would play an important role in the competition between superconductivity and antiferromagnetism.

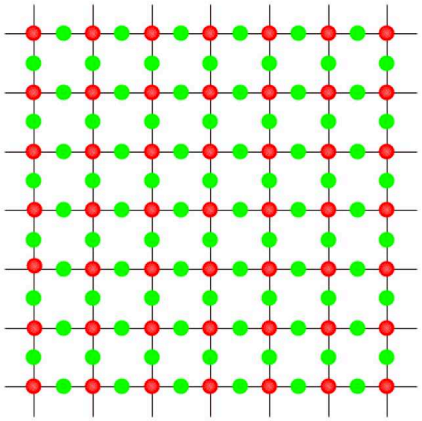

Fig. 1. Lattice structure of the two-dimensional CuO_2 plane.

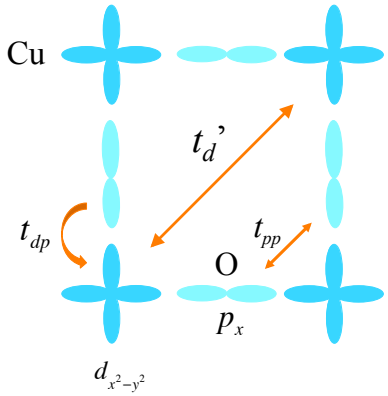

Fig. 2. Transfer integrals in the CuO_2 plane. t'_d is the transfer integral between next-nearest neighbor d electrons. t_{dp} and t_{pp} are conventional transfer parameters.

3. Optimization variational Monte Carlo method

A starting wave function in the variational Monte Carlo method is given by the Gutzwiller function:

$$\psi_G = P_G \psi_0, \tag{3}$$

where P_G is the Gutzwiller operator $P_G = \prod_j (1-(1-g)n_{j\uparrow}n_{j\downarrow})$ with the parameter g in the range of $0 \leq g \leq 1$. ψ_0 is an initial wave function of one-particle state. We introduce the order parameter in the initial state ψ_0 when we investigate an ordered state with some long-range order. The antiferromagnetic (AF) one-particle state ψ_{AF} is given by the eigenstate of the AF Hamiltonian which is given by

$$H_{AF} = \sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} - \Delta_{AF} \sum_{i\sigma} \sigma (-1)^{x_i + y_i} n_{i\sigma}, \tag{4}$$

for the Hubbard model where $\mathbf{r}_i = (x_i, y_i)$ are the coordinates of the site i. Δ_{AF} indicates the AF order parameter. This is easily generalized to the d-p model. A strongly correlated superconducting state is given by the projected-BCS state by taking $\psi_0 = \psi_{BCS}(\Delta)$ with the order parameter Δ. The expectation values for these wave functions are evaluated numerically by using the Monte Carlo method.

We must improve the Gutzwiller function because we cannot fully take into account electron correlation with it. We multiply the Gutzwiller function by a correlation operator $e^{-\lambda K}$.[40,60–66] The optimized wave function is

$$\psi_\lambda = \exp(-\lambda K)\, \psi_G, \tag{5}$$

where K indicates the kinetic term of the Hamiltonian and λ is a variational parameter (real constant) chosen to lower the ground state energy.[52,61,62] For the Hubbard model, K is given by $K = \sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma}$.

The Jastrow-type wave function has also been proposed to improve the Gutzwiller function.[67] The doublon-holon correlation is included by multiplying by the operator

$$P_{dh} = \prod_j \left(1 - (1-\eta) \prod_\tau \left[d_j(1-e_{j+\tau}) + e_j(1-d_{j+\tau})\right]\right), \tag{6}$$

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 $e_j = (1-n_{j\uparrow})(1-n_{j\downarrow})$. η is the variational parameter in the range $0 \leq \eta \leq 1$. The doublon-holon wave function is written as $\psi_\eta = P_{dh}\psi_G$. This type of wave functions was generalized to a many-parameter wave function.[68] It is not, however, clear whether the Jastrow-type wave function is also relevant for the d-p model.

In this paper, we use the wave function $\psi_\lambda = \exp(-\lambda K)\psi_G$ which we call the off-diagonal type wave function. The ground-state energy obtained by using ψ_λ is lower than that by the Jastrow-type wave functions.[40] An advantage of using the off-diagonal wave function is that it is easy to generalize to the three-band d-p model.[69] The wave function is

$$\psi_{\lambda,dp} = \exp(-\lambda K_{dp})\psi_G, \tag{7}$$

where ψ_G is the Gutzwiller function for the d-p model and K_{dp} indicates the kinetic part of the Hamiltonian H_{dp}. The expectation values for ψ_λ are calculated by adopting the procedure that is used in quantum Monte Carlo simulations.[61]

4. Antiferromagnetism and t'_d in the d-p model

The superconducting phase exists adjacent to the antiferromagnetic phase in high-temperature superconductors; which holds for cuprate superconductors and also iron-based superconductors. It is important to investigate the stability of the antiferromagnetic state in strongly correlated electron systems. We examine this for three-band d-p model. The strength of spin correlation is crucially dependent upon three parameters in the model; they are the strength of the repulsive interaction U_d, the hole density x and transfer integrals t_{pp} and t'_d.

In the d-p model, the antiferromagnetic correlation is strong and is even stronger than that for the 2D Hubbard model. We have introduced the transfer integral t'_d, which is the long-range transfer being analogous to t' in the 2D Hubbard model, to control the antiferromagnetic correlation. We found that the antiferromagnetic correlation is reduced when increasing $|t'_d|$. The inclusion of long-range transfers such as t'_d would increase the possibility of superconductivity in the d-p model.

In Fig. 3, we show the AF condensation energy as a function of the hole density x where $t'_d = -0.2t_{dp}$ and the level difference $\Delta_{dp} = \epsilon_p - \epsilon_d$ is $\Delta_{dp} = t_{dp}$. The AF region vanishes when x is near 0.1 (10 percent doping). The SC region may exist adjacent to the AF region. The AF order parameter Δ_{AF} is shown as a function of $-t'_d$ in Fig. 4. The decrease of Δ_{AF} with the increase of $-t'_d$ indicates a possibility of pure d-wave SC state. The SC order parameter Δ_{SC} is also shown in Fig. 4.

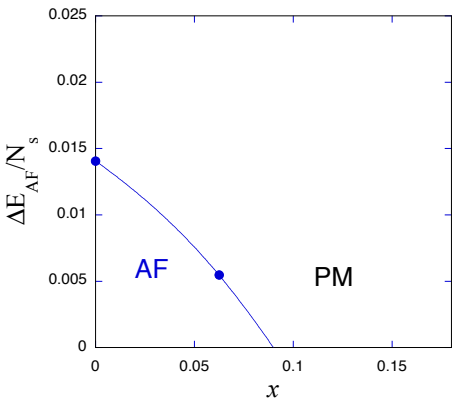

Fig. 3. The condensation energy of the antiferromagnetic state as a function of the hole density x for the two-dimensional d-p model on a 8×8 lattice with 192 atoms. We set $U_d = 10t_{dp}$, $t_{pp} = 0.4t_{dp}$ and $t'_d = -0.2t_{dp}$ and $\Delta_{dp} = \epsilon_p - \epsilon_d = t_{dp}$. The energy unit is given by t_{dp}. We use the periodic boundary condition for the one direction and antiferromagnetic one for the other direction.

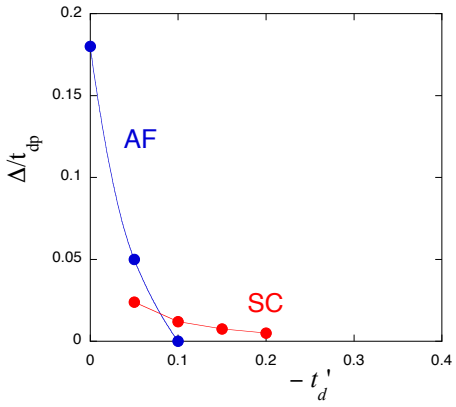

Fig. 4. AF order parameter Δ_{AF} as a function of $-t'_d$ for the two-dimensional d-p model for $U_d = 10t_{dp}$, $t_{pp} = 0.4t_{dp}$ and $\Delta_{dp} = 2t_{dp}$. The hole number is 76 on 8×8 lattice. The boundary conditions are the same as in Fig. 3. The SC order parameter Δ_{SC} is also shown which is obtained by using the BCS-Gutzwiller wave function. Δ_{AF} decreases as $|t'_d|$ increases.

5. Antiferromagnetism and Superconductivity

In the study of superconducting state in strongly correlated electron systems, we use the BCS wave function ψ_{BCS} as an initial one-particle state ψ_0 where

$$\psi_{BCS} = \prod_k (u_k + v_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow})|0\rangle, \tag{8}$$

with coefficients u_k and v_k appearing in the ratio $u_k/v_k = \Delta_k/(\xi_k + \sqrt{\xi_k^2 + \Delta_k^2})$, where Δ_k is the $\mathbf{k}$-dependent gap function and ξ_k is the dispersion relation of conduction electrons.

Inorder to employ the variational Monte Carlo method for the wave function

$$\psi_\lambda = \exp(-\lambda K) P_G \psi_{BCS}, \tag{9}$$

we perform the electron-hole transformation for down-spin electrons:

$$d_k = c^\dagger_{-k\downarrow}, \quad d^\dagger_k = c_{-k\downarrow}. \tag{10}$$

In this notation, the electron pair operator $c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}$ is represented as the hybridization $c^\dagger_k d_k$ where $c_k = c^\dagger_k$. The chemical potential is used to adjust the expectation value of the total electron number. Thus, the chemical potential introduced in ψ_{BCS} is not a variational parameter in this formulation.

In this section we examine the AF and SC states as a function of the level difference Δ_{dp}. When U_d is fixed, Δ_{AF} increases as Δ_{dp} increases from zero and has a peak when $\Delta_{dp} \sim U_d/2$. This is shown in Fig. 5 where we consider the case

$\Delta_{dp} \geq 0$. This means that the AF correlation becomes maximum in the symmetric case where $\Delta_{dp} = U_d/2$. The pure d-wave SC state may exist for negative t'_d. In Fig. 6 we show the SC order parameter as well as the AF one for $t'_d = -0.2t_{dp}$. Δ_{SC} obtained by the Gutzwiller wave function is also shown in Fig. 6. It is not clear whether the coexistent state of AF and SC orders in the AF region when Δ_{dp} becomes large. The SC phase exists when the level difference Δ_{dp} is small.

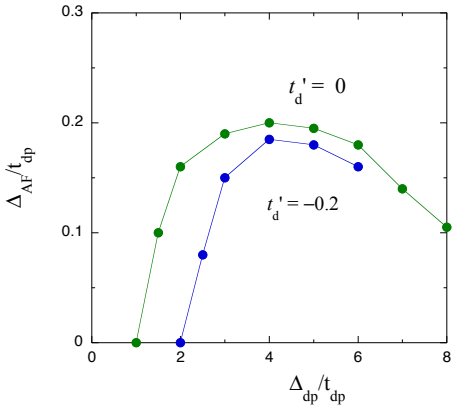

Fig. 5. Antiferromagnetic order parameter Δ_{AF} as a function of the level difference $\Delta_{dp} = \epsilon_p - \epsilon_d$ for the three-band d-p model with 76 holes on 8×8 lattice where $x = 0.1875$. We used $U_d = 10$, $U_p = 0$ and $t_{pp} = 0.4$ in units of t_{dp}. Δ_{AF} has a peak when $\Delta_{dp} \sim U_d/2$ for fixed U_d for $t'_d = 0$ and $r'_d = -0.2$.

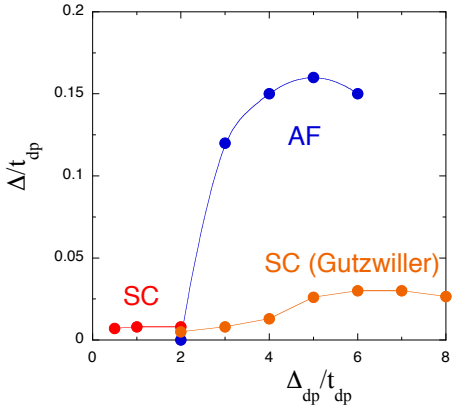

Fig. 6. Antiferromagnetic and superconducting order parameters as a function of the level difference Δ_{dp}. The system is a 8×8 lattice with 76 holes where we use the periodic boundary condition in one direction and antiperiodic one in the other direction. We set $U_d = 10$, $U_p = 0$, $t_{pp} = 0.4$ and $t'_d = -0.2$ for AF state. The superconducting region exists when the level difference is small. The SC order parameter for the Gutzwiller function shows the result for $t'_d = 0$.

6. Summary

We examined the ground-state properties of the 2D d-p model by using the optimization variational Monte Carlo method. The optimized wave function is formulated by multiplying by $\exp(-S)$ operators. The ground-state energy ls lowered greatly compared to those of the Gutzwiller wave function and also several proposed wave functions with many variational parameters. We have the lower ground-state energy because of the kinetic-energy gain due to the variational parameter λ. The wave function is straightforwardly generalized to multi-band models such as the three-band d-p model.

The antiferromagnetic state is very stable near the half-filled case in the d-p model. In general, according to variational Monte Carlo calculations, the AF correlation in the d-p model is extremely stronger than that in the Hubbard model.

The antiferromagnetic correlation is reduced as the hole density increases. The AF order parameter Δ_{AF} takes the maximum value at near the symmetric case where $\Delta_{dp} = \epsilon_p - \epsilon_d = U_d/2$ for fixed U_d. The d-wave superconducting phase exists in the region where $\epsilon_p - \epsilon_d$ is small.

There may be a crossover as Δ_{dp} decreases from strongly correlated region to the weakly correlated one. In the weakly correlated region where Δ_{dp}/t_{dp} is small, the AF correlation is reduced, which indicates that spin and charge fluctuations are large and will cause superconductivity. High-temperature superconductivity would occur in the crossover region. The crossover behavior may be a universal phenomenon. The Kondo effect shows a crossover from weakly coupling to strongly coupling regions as the temperature decreases.[70,71] An anomaly that occurs in the crossover plays an essential role.[72–77] This anomaly is closely related to the asymptotic freedom.

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