ORIGINAL PAPER

Phase Diagram and Mechanism of Superconductivity in Strongly Correlated Electrons

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Abstract

We investigate the phase diagram of two-dimensional (2D) Hubbard model by employing the optimization variational Monte Carlo method. The 2D Hubbard model is the most simple electronic model for cuprate high-temperature superconductors. The phase diagram consists of three regions; they are antiferromagnetic insulator region, superconducting region, and the coexistent region of superconductivity and antiferromagnetism. The phase diagram obtained by numerical calculations well agrees with the experimental phase diagram for high-temperature cuprates.

1 Introduction

The mechanism of high-temperature superconductivity has been studied intensively for more than 30 years [1]. It is important to clarify the phase diagram of strongly correlated electron states in the study of high-temperature superconductivity [2–6]. The purpose of this study is to understand the phase diagram of cuprate high-temperature superconductors since the mystery of the phase diagram in cuprates has never been resolved. The electron correlation between electrons plays an important role in cuprate superconductors because the parent materials without carrier doping are Mott insulators and the Cooper pairs have the d-wave symmetry. It is very important to clarify the electronic properties of electrons in the CuO_2 plane [7–14]. The model for the CuO_2 plane has d electron in copper atoms and p electrons in oxygen atoms. We often examine

the simplified model, by neglecting oxygen sites in the CuO_2 plane, which is called the (single-band) Hubbard model [15–19]. It is an important subject whether the two-dimensional (2D) Hubbard model has a superconducting phase or not [20–29]. The variational wave functions have been improved intensively recently [30–35]. Recent results on the 2D Hubbard model are now supporting the existence of superconductivity in the ground state [32–35].

A variational Monte Carlo method is a suitable method to investigate electronic properties of strongly correlated electron systems [17, 36, 37]. A variational wave function is improved and optimized by introducing new variational parameters to control the electron correlation. We have proposed correlated wave functions by multiplying an initial wave function by $\exp(-S)$-type operators [33, 34, 38, 39], where S is a correlation operator. The wave function is further optimized in a systematic way by multiplying by the exponential-type operators repeatedly [33]. The ground-state energy evaluated by our wave function is much lower than that by previous wave functions.

2 Model Hamiltonian

The CuO_2 plane consists of oxygen atoms and copper atoms (shown in Fig. 1). The basic model for this plane is the three-band d-p model which explicitly contains both oxygen p electrons and copper d electrons. When we neglect oxygen atoms in this model, we have the two-dimensional Hubbard
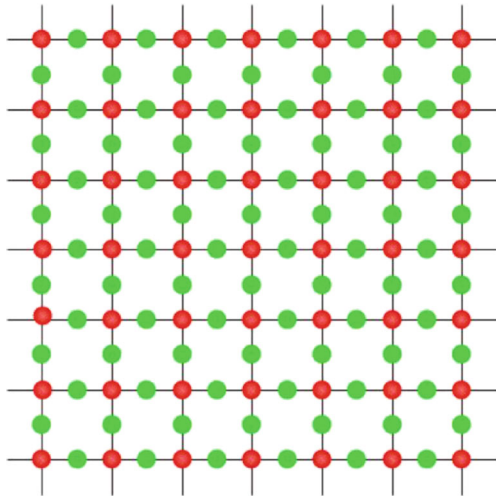
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Fig. 1 Lattice of the CuO$_2$ plane with oxygen and copper atoms

model that consists of only d electrons on a lattice shown in Fig. 2. The Hubbard model is given as

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

where $\{t_{ij}\}$ are transfer integrals and $U(>0)$ 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. $n_{i\sigma}$ refers to 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 with opposite spins.

One may understand the appearance of inhomogeneous states reported for high-temperature cuprates based on the Hubbard model [26, 40–42]. Concerning the existence of
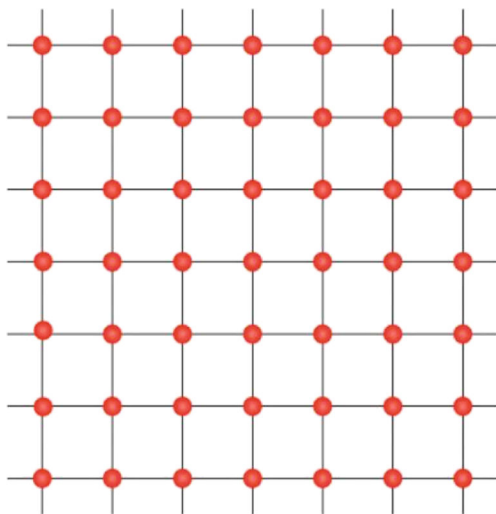

Fig. 2 Lattice of copper atoms in the CuO$_2$ plane

superconducting phase in the 2D Hubbard model, quantum Monte Carlo studies have given negative results and do not support high-temperature superconductivity in the Hubbard model [20–22]. The recent results based on elaborated optimized wave functions, however, have provided a support for superconductivity [33, 34], especially in the strongly correlated region [33]. In our opinion, it seems evident that the 2D Hubbard model has a superconducting phase in the ground state. There is, however, still an issue that should be clarified. This is the competition between superconducting and antiferromagnetic states.

3 Optimized Wave Functions

We use an ansatz for the wave function and evaluate the expectation values using the variational Monte Carlo method. A starting wave function to take account of the electron correlation is given by the Gutzwiller ansatz:

$$\psi_G = P_G \psi_0, \qquad (2)$$

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 a trial function of one-particle state. To investigate a stability of the superconducting (SC) state, we use the BCS wave function ψ_{BCS} for ψ_0 with the gap parameter Δ_{SC}. The condensation energy is defined as $E_{cond} = E(\Delta_{SC} = 0) - E(\Delta_{SC} = \Delta_{SC,opt})$ for the optimized gap function $\Delta_{SC,opt}$. The antiferromagnetic (AF) one-particle state ψ_{AF} is given by the eigenstate of the AF trial Hamiltonian given by

$$H_{AF} = \sum_{ij\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} - \Delta_{AF} \sum_{i\sigma} \sigma(-1)^{x_i + y_i} n_{i\sigma}, \qquad (3)$$

where $\mathbf{r}_i = (x_i, y_i)$ are the coordinates of the site i. Δ_{AF} indicates the AF order parameter.

Our wave function is obtained by multiplying ψ_G by an off-diagonal correlation operator to take account of intersite correlation. The wave function is written as [33, 38, 39, 43–47]

$$\psi_\lambda = e^{-\lambda K} \psi_G, \qquad (4)$$

where K indicates the kinetic term of the Hamiltonian $K = \sum_{ij\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma}$ and λ is a real constant which is the variational parameter chosen to lower the ground-state energy [33, 34, 39, 43]. The initial wave function ψ_0 is written by Slater determinants in the real space representation. The basis states are given by Slater determinants. The operator $e^{-\lambda K}$ produces off-diagonal elements between different basis states and lowers the ground-state energy.

This wave function is easily generalized to multi-band models and appears to be a good wave function for the three-band d-p model [34, 48].

4 Phase Diagram and the Effect of t'

We consider the phase diagram as a function of the doping rate (hole density) and examine the effect of the nearest-neighbor transfer t' on it. The common feature of the phase diagram of high-temperature cuprates is that the antiferromagnetic insulator phase exists when the hole density x is small near half-filling and there is the d-wave SC phase when the hole density is larger than the critical value x_c where $x_c \sim 0.05$. The SC phase vanishes when x becomes as large as about 0.25.

We show the phase diagram in Fig. 3 where the condensation energy is shown as a function of the hole density x. The condensation energy is defined as the energy difference given as

$$\Delta E = E(\Delta = 0) - E(\Delta = \Delta_{opt}), \qquad (5)$$

where Δ is the order parameter for SC (Δ_{SC}) and AF (Δ_{AF}) and Δ_{opt} indicates the optimized value of Δ. In Fig. 3, calculations were performed for $U/t = 18$ and $t' = 0$ on a 10×10 lattice and we include the results for the AF state for $U/t = 14$ and 12. There occurs the phase separation when $x < 0.06$, and the AF state in this region is an insulating state [34, 35]. When $x > 0.06$, the ground state becomes d-wave superconducting. In the region near the AF boundary given as $0.06 < x < x_{dSC}$, the AF order and superconductivity coexist where x_{dSC} is approximately
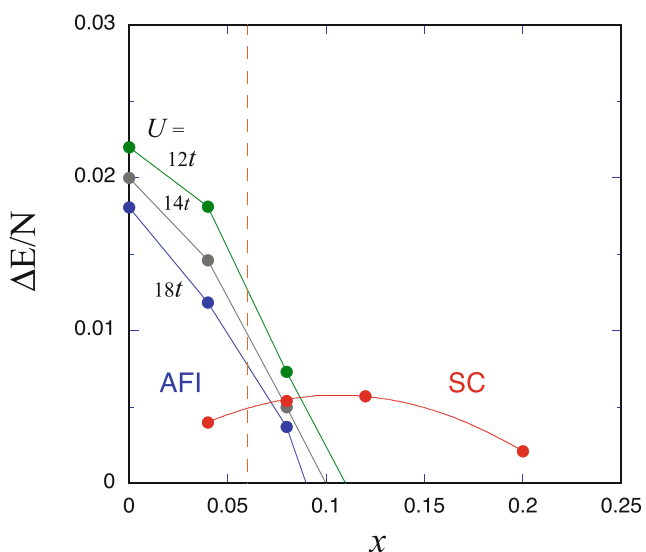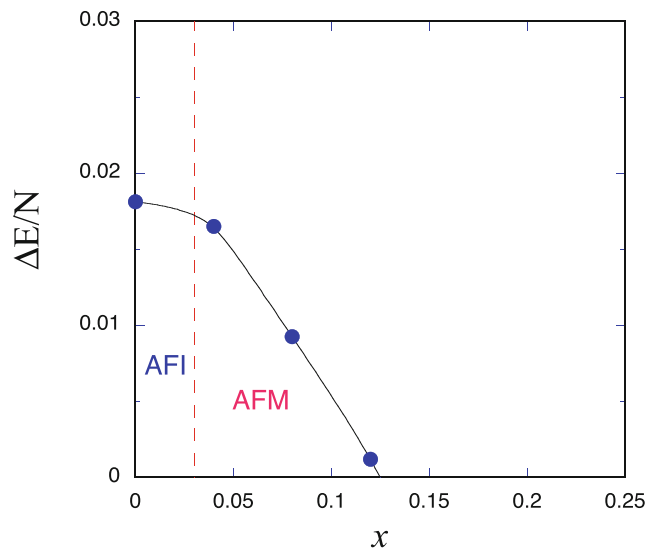

Fig. 4 The condensation energy as a function of the hole density x for $t' = -0.1$

$x_{dSC} \sim 0.08 - 0.09$. The pure d-wave state is realized for $x > x_{dSC}$. When U decreases, the AF order parameter increases.

We investigate the effect of t' here. The AF condensation energy is shown as a function of the hole density x in Fig. 4 for $t'/t = -0.1$ and $U/t = 18$. The AF region becomes large as $-t'$ increases, and thus the $t' = 0$ is most favorable for the pure d-wave SC state. The phase-separation region decreases, that is, the antiferromagnetic insulator (AFI) region decreases due to t'. Figure 5 presents the phase separation (PS) region on the x-t' plane. The PS region disappears when t' is as large as -0.2.

Fig. 3 The condensation energy as a function of the hole density x for $t' = 0$
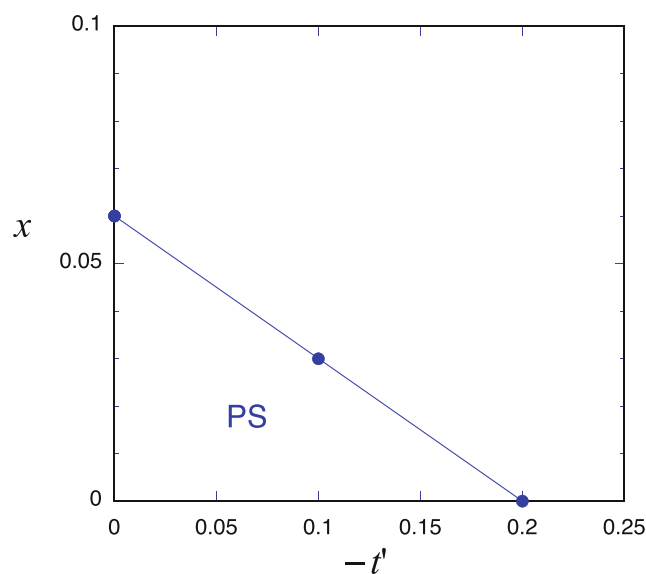

Fig. 5 Phase-separation region in the plane of x and t'

To summarize the results, the t' increases antiferromagnetic correlation and decreases insulator region near half-filling.

5 Summary

We have investigated the ground state of the 2D Hubbard model on the basis of the optimization variational Monte Carlo method. We employ the optimized wave function by introducing new variational parameters to go beyond the Gutzwiller ansatz. The ground-state energy is greatly lowered by our wave function. The metal-insulator transition is also well described by our optimized function [48].

We mainly focused on the effect of t' on the AF correlation and the phase separation. The area of the AF phase increases when we include t' and thus the pure d-wave SC phase decreases. The AFI phase near half-filling decreases as $|t'|$ increases.

The electron pairing interaction is induced due to spin and charge fluctuations in the strongly correlated region. There is a crossover between weakly and strongly correlated region as the strength of the Coulomb interaction U increases. Crossover phenomena have also been investigated in the study of cuprate superconductors [49]. This kind of crossover may be universal which occurs with a singularity in the intermediate region as in the Kondo effect, QCD, and BCS-BEC crossover [50–53]. The kinetic energy induced by the operator $\exp(-\lambda K)$ may drive the electron pairing and helps to bring about high-temperature superconductivity.

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