

Research Article

Superconductivity, Antiferromagnetism, and Kinetic Correlation in Strongly Correlated Electron Systems

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We investigate the ground state of two-dimensional Hubbard model on the basis of the variational Monte Carlo method. We use wave functions that include kinetic correlation and doublon-holon correlation beyond the Gutzwiller ansatz. It is still not clear whether the Hubbard model accounts for high-temperature superconductivity. The antiferromagnetic correlation plays a key role in the study of pairing mechanism because the superconductive phase exists usually close to the antiferromagnetic phase. We investigate the stability of the antiferromagnetic state when holes are doped as a function of the Coulomb repulsion U . We show that the antiferromagnetic correlation is suppressed as U is increased exceeding the bandwidth. High-temperature superconductivity is possible in this region with enhanced antiferromagnetic spin fluctuation and pairing interaction.

1. Introduction

The study of high-temperature superconductivity has attracted much attention since the discovery of cuprate high-temperature superconductors [1]. It is very important to clarify the properties of electronic states in the CuO_2 plane [2–9]. The model for the CuO_2 plane is called the d-p model (or is called the three-band Hubbard model). We often consider the simplified model, by neglecting oxygen sites in the CuO_2 plane, called the (single-band) Hubbard model [10–15].

It remains unresolved as to whether the two-dimensional Hubbard model has a superconducting phase or not [16, 17]. It is believed that the electron correlation between electrons plays a significant role in cuprate superconductors. It is obvious that interaction with large energy scale is responsible for realization of high-temperature superconductivity. This subject has been investigated for more than two decades by using electronic models such as the two-dimensional Hubbard model, the d-p model, and the ladder Hubbard model [18–21].

The antiferromagnetic (AF) correlation plays a primarily important role in correlated electron systems. For example, the existence of striped states [22–29] can be understood on the basis of the two-dimensional Hubbard model [9, 30, 31].

The checkerboard-like density-wave modulation, observed by scanning tunneling microscopy (STM) [32–34], is also possible in some region of the parameter space in the Hubbard model [31]. The possibility of the coexistent state of antiferromagnetism and superconductivity has been reported [35, 36], and we can show the coexistence using the Hubbard model [9]. Thus the two-dimensional Hubbard model can describe some of anomalous properties reported for cuprate superconductors. The spin fluctuation, which is one of candidates of attractive interaction for high-temperature superconductivity, comes from the antiferromagnetic spin correlation. It is thus important to examine the stability of the antiferromagnetic state.

In the mean-field theory the antiferromagnetic correlation is enhanced as U is increased. This is also the case for the wave function of simple Gutzwiller ansatz. When we consider electron correlation beyond the Gutzwiller ansatz (mean-field wave function), the nature of the antiferromagnetism changes in the strongly correlated region where U is larger than the bandwidth. The AF correlation is increased as U is increased from zero and is maximally enhanced when U is about the bandwidth. The AF correlation shows a tendency to be suppressed when U is further increased more than the bandwidth. This is because we must suppress AF correlation

to get the kinetic energy gain to lower the ground state energy. This indicates that the spin fluctuation becomes large in the large- U region.

In this paper we investigate the stability of AF ordered state using the wave functions that take account of kinetic correlation and doublon-holon correlation. We show the results obtained by the variational Monte Carlo method.

2. Model and Wave Functions

The Hubbard Hamiltonian is written as

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

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 .

The simple wave function is given by the Gutzwiller function:

$$\Psi_G = P_G \Psi_0, \quad (2)$$

where P_G is the Gutzwiller operator

$$P_G = \prod_j (1 - (1 - g) n_{j\uparrow} n_{j\downarrow}) \quad (3)$$

with the parameter g in the range of $0 \leq g \leq 1$. Ψ_0 is a trial function of the noninteracting state. To investigate the superconducting state, we use the BCS wave function Ψ_{BCS} for Ψ_0 with the gap parameter Δ . The condensation energy is defined as

$$E_{\text{cond}} = E(\Delta = 0) - E(\Delta = \Delta_{\text{opt}}) \quad (4)$$

for the optimized gap function Δ_{opt} .

We take into account intersite correlation effects in the wave function by multiplying a correlation operator $e^{-\lambda K}$:

$$\Psi_\lambda = e^{-\lambda K} \Psi_G, \quad (5)$$

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 to be optimized [37–39]. This wave function is a first approximation to the wave function used in quantum Monte Carlo method [40].

The other way to improve the wave function is to consider the doublon-holon correlation that is controlled by the operator given by [41]

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

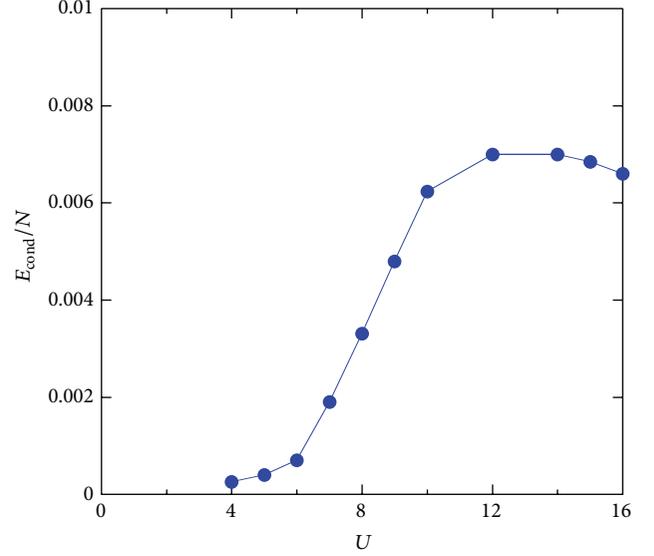


FIGURE 1: Superconducting condensation energy as a function of U for the Gutzwiller function. The system is 10×10 lattice with $t' = -0.2$ and the electron number is $N_e = 84$. We impose the periodic boundary condition in one direction and antiperiodic boundary condition in the other direction.

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 of $0 \leq \eta \leq 1$. The doublon-holon wave function is written as

$$\Psi_\eta = P_{\text{dh}} \Psi_G. \quad (7)$$

We evaluate physical quantities for the Gutzwiller function Ψ_G and optimized wave functions Ψ_λ and Ψ_η using the variational Monte Carlo method [42, 43].

3. Antiferromagnetism and Superconductivity

We first show the superconducting condensation energy and optimized superconducting gap function Δ as a function of U in Figures 1 and 2, respectively. These results were obtained by using the Gutzwiller function with a BCS trial function. The results show that Δ increases as U is increased and will have a maximum at some U . This indicates that the superconducting state becomes more stable in the strongly correlated region for larger U . The region with U being greater than the bandwidth is called the strongly correlated region [41, 44]. It is difficult to observe a clear sign of superconductivity in weakly correlated region; for example, U is less than $6t$, by numerical calculations. This is consistent with the results obtained by quantum Monte Carlo methods [17, 39, 45].

This result suggests that there is some effect which induces an attractive interaction to form electron pairings in strongly correlated region. We examine the stability of AF ordered state in this region. For this purpose we employ the kinetic correlation function $\Psi_\lambda = e^{-\lambda K} \Psi_G$ and the doublon-holon correlation function $\Psi_\eta = P_{\text{dh}} \Psi_G$. We compare the ground state energy for Ψ_G , Ψ_η , and Ψ_λ in Table 1. Among these wave

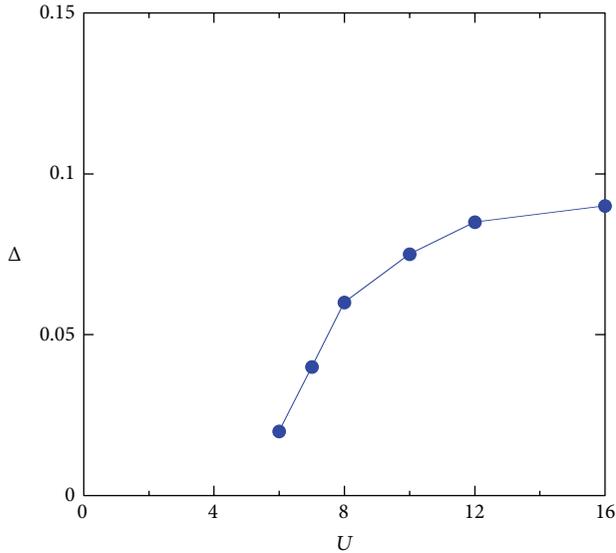


FIGURE 2: Optimized superconducting gap function as a function of U for the BCS Gutzwiller function. The conditions are the same as in Figure 1.

TABLE 1: Ground state energy per site for wave functions ψ_G , doublon-holon function ψ_η and ψ_λ . The parameters are $N_e = 86$, $U = 10$, $t' = -0.2$ on 10×10 lattice with periodic boundary conditions. Δ_{AF} is the antiferromagnetic order parameter.

Wave function	E/N	g	Δ_{AF}	η	λ
ψ_G	-0.5859	0.21	0.0	1.0	0
$\psi_G(AF)$	-0.5953	0.21	0.2	1.0	0
$\psi_\eta = P_{dh}\psi_G$	-0.6179	0.21	0.0	0.78	0
$\psi_\lambda = e^{-\lambda K}\psi_G$	-0.6643	0.06	0.0	1.0	0.06

functions, ψ_λ shows the lowest ground state energy. This indicates that the intersite correlation induced by the kinetic operator K is important in the correlated region. In Figure 3 we show the kinetic energy which is the expectation value of the kinetic term as well as the ground state energy as a function of λ for ψ_λ . The kinetic energy is lowered appreciably by the kinetic correlation operator $e^{-\lambda K}$.

When U is large, there is a competition between antiferromagnetic energy gain and kinetic energy gain to lower the total energy. The AF energy gain, being proportional to the AF exchange coupling $J \propto t^2/U$, is reduced gradually as U is increased. We show this in Figure 4 where the energy gain of the AF state with reference to the normal state is shown as a function of U . When U is increased more than the bandwidth, the antiferromagnetism is suppressed and its energy gain is decreased as U is increased. This indicates that there is a large AF spin fluctuation in this region. This shows a possibility of AF fluctuation induced electron pairing in the strongly correlated region.

4. Summary

We have investigated the two-dimensional Hubbard model by adopting the wave function that takes into account

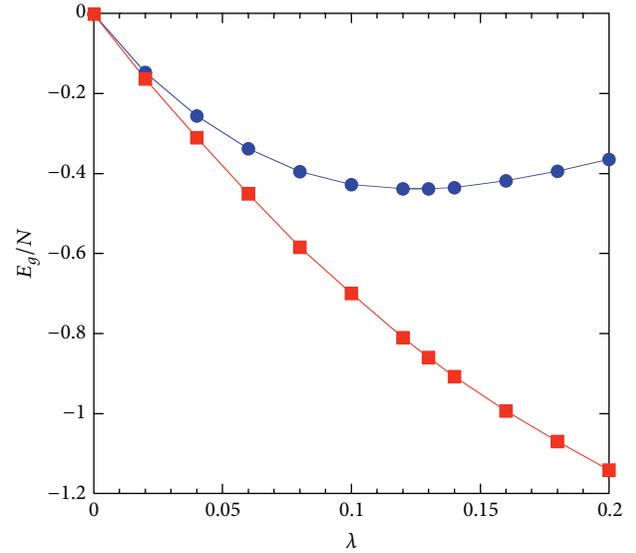


FIGURE 3: Ground state energy (circles) and the kinetic energy (squares) as a function of λ , evaluated using ψ_λ . The parameters are $U = 10$, $t' = -0.2$, and $N_e = 100$.

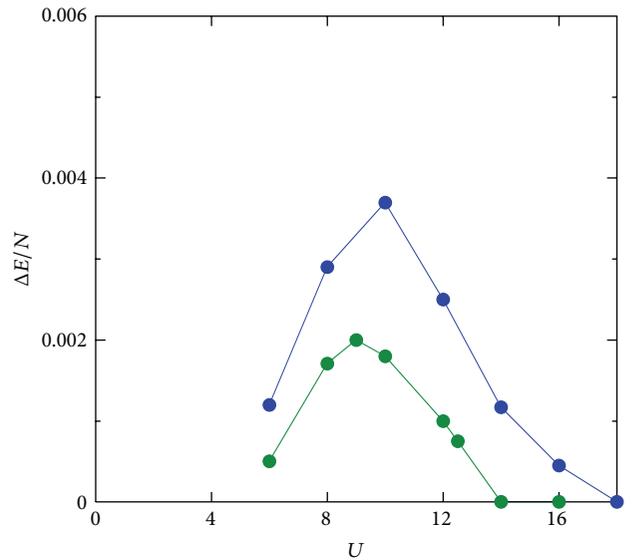


FIGURE 4: Antiferromagnetic condensation energy as a function of U . The system is 10×10 lattice with $t' = -0.2$. The electron number is $N_e = 86$ (lower curve) and $N_e = 84$ (upper curve). In the latter $N_e = 84$ case we have an open shell; that is, the highest occupied electron level is partially filled. We use the periodic boundary condition in both directions.

intersite electron correlation using the variational Monte Carlo method. The condensation energy becomes large in the strongly correlated region, suggesting a possibility of high-temperature superconductivity. The reduction of antiferromagnetic correlation suggests large spin fluctuation in this region. We expect that this spin fluctuation in strongly correlated region induces an attractive interaction which promotes superconductivity. In the weakly correlated region for U/t less than about 6, there is also spin fluctuation because

the AF order is suppressed as U is decreased. In numerical calculations, however, the pairing state is not stabilized in the weakly correlated region. This indicates that only the spin fluctuation effect cannot promote electron pairing and we further need strong correlation to account for high-temperature superconductivity.

It is also important to discuss the role of other parameters in the Hubbard model. In particular, the next-nearest-neighbor transfer t' is important since the density of states crucially depends on t' due to the van Hove singularity of a two-dimensional system. The nearest-neighbor Coulomb interaction V is also important. The on-site Coulomb interaction U is renormalized by V and V will change the nature of antiferromagnetic correlation.

It is necessary to consider three-dimensional electronic models because real cuprate superconductors are three-dimensional layered materials. It is important to investigate the electronic state of layered cuprates because an interlayer interaction may bring about interesting phenomena. They can be regarded as a multiband superconductor and have potential for new phenomena [46–52].

It is also necessary to examine the effect of strong correlation on the electron-phonon interaction [53–56]. There is a possibility that electron-phonon and electron-electron interactions cooperate to realize a high-temperature superconductor. The electron-phonon coupling may induce long-range attractive interaction. We expect that the long-range part of attractive interaction may cooperate with the on-site repulsive interaction to induce superconductivity.

Conflict of Interests

The author declares that there is no conflict of interests regarding the publication of this paper.

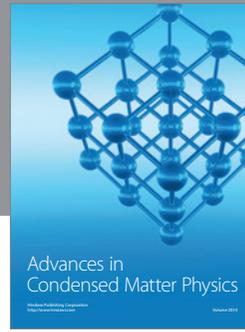
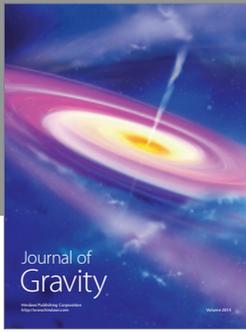
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