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Duality in spin fluctuation in correlated electron systems

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ABSTRACT

An origin of high-temperature superconductivity for cuprate superconductors is investigated on the basis of the two-dimensional Hubbard model. The Coulomb interaction is a candidate that can bring about high-temperature superconductivity because its characteristic energy is of the order of eV. It is not trivial whether the on-site Coulomb interaction U leads to a pairing interaction between two electrons. We argue that the antiferromagnetic fluctuation and the kinetic charge fluctuation are responsible for high-temperature superconductivity. The kinetic charge fluctuation is induced by large U to get the kinetic energy gain in the strongly correlated region. We consider electron correlation beyond the Gutzwiller ansatz, by taking account of inter-site correlation such as doublon–holon correlation and kinetic correlation. We show that high-temperature superconductivity is possible in the strongly correlated region, where U is greater than the bandwidth, by using the variational Monte Carlo method.

1. Introduction

High-temperature superconductors have been studied intensively since the discovery of high-temperature cuprates [1]. The electron correlation between electrons is important because parent compounds without carriers are insulators. It is primarily important to clarify electronic states in the CuO_2 plane contained in cuprate high-temperature superconductors. The mechanism of superconductivity has been investigated, but it remains unresolved. It is obvious that interaction with large energy scale is necessary and responsible for realization of high-temperature superconductivity. The Coulomb interaction has obviously a large characteristic energy scale and is a candidate of interaction that induces high-temperature superconductivity.

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) [1–14]. The single-band Hubbard model [15–17] is obtained by neglecting oxygen atoms in the CuO_2 plane. It is an open question whether the on-site Coulomb repulsion indeed induces superconductivity in correlated electron systems. It remains controversial for the two-dimensional Hubbard model [18–23]. The studies for the ladder Hubbard model have indicated positive results on superconductivity [24–29]. These results suggest the existence of pairing interaction influenced by the on-site Coulomb repulsive interaction.

A system described by the Hubbard model is a typical strongly-correlated system. The two-dimensional (2D) Hubbard model has been investigated intensively for several decades [15,30–35]. The Hubbard model was first introduced to describe a metal–insulator transition [15]. Since the discovery of cuprate high-temperature superconductors, many researchers tried to explain the occurrence of superconductivity in cuprates in terms of the 2D Hubbard model. The results of quantum Monte Carlo methods, which are believed to be exact unbiased methods, do not support the existence of high-temperature superconductivity in this model [18–20]. In our opinion this is because the Coulomb interaction U is not large in quantum Monte Carlo calculations where the accessible U is very restricted because of its nature of method. Based on the variational Monte Carlo method, the finite superconducting gap with d-wave symmetry is obtained for $6 \leq U/t$ in the 2D Hubbard model [36–41].

It is necessary to improve the wave function in the variational Monte Carlo method since the Gutzwiller function only accounts for the on-site correlation. The Gutzwiller function is a starting function that should be improved to take account of correlation effects. We discuss several methods to improve the wave function, and show that an $\exp(-\lambda K)$-type function [42] can be a best function with the lowest variational energy. The variational energy is lowered greatly and can be close to the exact value.

We discuss the properties of antiferromagnetism and superconductivity in strongly-correlated region by using improved wave functions. It may be believed that the antiferromagnetic correlation is enhanced as U is increased and this will hold for large U where U is greater than the bandwidth. This is, however, not correct when

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holes are doped as will be shown on the basis of improved wave functions. The antiferromagnetic correlation is suppressed when U is extremely large being larger than the bandwidth. A superconducting correlation is developed in this region as the antiferromagnetic correlation is suppressed with the increase of U. The development of superconducting correlation is understood as induced by spin fluctuation which is inspired by the kinetic charge fluctuation to conquer antiferromagnetism. This spin fluctuation in strongly correlated region must be distinguished from that in weakly correlated region. The latter is the conventional spin fluctuation that has been discussed extensively in literatures [43,44]. We expect some relation between these two spin fluctuations.

In next section we discuss an improvement of wave function in correlated electron systems. In Section 3 we examine the stability of antiferromagnetic state and pairing state, based on our wave functions. We give a summary in the last section.

2. Hamiltonian and wave functions

The single-band Hubbard model is given by

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

where t_{ij} are transfer integrals and U is the on-site Coulomb energy. The transfer integral t_{ij} is non-zero $t_{ij} = -t$ for nearest-neighbor pair $\langle ij \rangle$ and $t_{ij} = -t'$ for next-nearest neighbor $\langle\langle ij \rangle\rangle$. 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 wave function should include correlation between electrons. The well-known Gutzwiller wave function is given by $\psi_G = P_G \psi_0$ where P_G is the Gutzwiller operator defined by

$$P_G = \prod_j \left(1 - (1-g) n_{j\uparrow} n_{j\downarrow}\right) \tag{2}$$

with the variational parameter g in the range of $0 \le g \le 1$. P_G controls the double occupancy to take account of electron correlation. ψ_0 is a trial one-particle state that is taken to be the Fermi sea ψ_{FS}, the antiferromagnetic state (spin-density wave state) ψ_{AF} or the BCS state ψ_{BCS}. When $\psi_0 = \psi_{BCS}$, we multiply P_{N_e} which is a projection operator that extracts only the state with a fixed total electron number N_e.

It is necessary to improve the Gutzwiller wave function because only the on-site correlation is considered in the Gutzwiller ansatz. The one way to improve the wave function is to take account of nearest-neighbor doublon–holon correlation [45–48]. The wave function with doublon–holon correlation is given by $\psi_{d-h} = P_{d-h} P_G \psi_0$ with

$$P_{d-h} = \prod_j \left(1 - (1-\eta) \prod_{\tau} [d_j (1 - e_{j+\tau}) + e_j (1 - d_{j+\tau})]\right). \tag{3}$$

Here, d_j is the operator for the doubly-occupied site given by $d_j = n_{j\uparrow} d_{j\downarrow}$, and e_j is the empty site operator given as $e_j = (1 - n_{j\uparrow})(1 - n_{j\downarrow})$. η is a variational parameter in the range of $0 \le \eta \le 1$. We put $\eta = 1$ in the non-interacting case. A Jastrow factor is defined as

$$P_J = \exp\left(-\frac{1}{2} \sum_{i \ne j} h_{ij} n_i n_j\right), \tag{4}$$

where $n_i = n_{i\uparrow} + n_{i\downarrow}$ and $\{h_{ij}\}$ are variational parameters. We can take into account inter-site correlations by multiplying P_J such as $P_J P_{d-h} P_G \psi_0$.

In the other way, we can take account of inter-site correlation by multiplying the kinetic operator to the Gutzwiller function to improve the wave function. A typical wave function of this type is written as [42,49]

$$\psi_\lambda \equiv \psi^{(2)} = e^{-\lambda K} P_G \psi_0, \tag{5}$$

where K is the kinetic term in the Hamiltonian: $K = \sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma}$ and λ is a variational parameter to be optimized to lower the energy. This wave function is further improved by multiplying the Gutzwiller operator again:

$$\psi^{(3)} \equiv P_G \psi_\lambda = P_G e^{-\lambda K} P_G \psi_0. \tag{6}$$

The expectation values for these wave functions are evaluated by using the variational Monte Carlo method.

We calculate the ground state energy to check the validity of our wave functions. Recently, a variational wave function was proposed by introducing large number of variational parameters in the Gutzwiller–Jastrow factor and the one-particle function [50,51]. The energy evaluated by a wave function with many variational parameters is lowered considerably compared to that by the Gutzwiller function ψ_G. The wave function ψ_λ gives a good estimate of the energy, and $P_G \psi_\lambda$ and $e^{-\gamma K} P_G \psi_\lambda$ give best ground-state energy. We show variational energy calculated on 4×4 lattice in Table 1. The many-parameter wave function in [50] is a nice wave function with much lowered variational energy. The variational energy by our wave functions are also lowered greatly compared to the Gutzwiller wave function and exhibits a best ground-state energy.

It is seen that the energy is not so improved only by multiplying the doublon–holon correlation factor P_{d-h} to the Gutzwiller function. The trial wave function $P_{d-h} P_G \psi_0$ was used to develop the physics of Mott transition [45] following the suggestion that the Mott transition occurs due to doublon–holon binding [52]. We before examined the Mott transition with the wave function $e^{-\lambda K} P_G \psi_0$ [53] because the variational energy by this wave function is much lower than that of the doublon–holon wave function.

Table 1
Variational energies for 4×4 lattice, $N_e = 16$, $U/t = 5$ and $t'/t = 0$. The boundary conditions are periodic in one direction and antiperiodic in the other direction. The nearest-neighbor (n.n.) Jastrow function in the third row means that we considered only the nearest-neighbor Jastrow correlation factor $\exp(-\sum_{\langle ij \rangle} h_{ij} n_i n_j)$. The result in the fourth row is from Ref. [50]. The exact result was obtained by using the exact diagonalization method.

Wave function	Energy	Comments
$P_G \psi_{FS}$	−11.654	
$P_{d-h} P_G \psi_{FS}$	−11.856	$g = 0.46$, $\eta = 0.89$
$P_J P_{d-h} P_G \psi_{FS}$	−11.863	n.n. Jastrow function
$P_J P_{d-h} P_G \mathcal{L}^{S=0} P_{pair}$	−12.459	Ref. [50]
$e^{-\lambda K} P_G \psi_{FS}$	−12.366	$g = 0.15$, $\lambda = 0.115$
$P_G(g') e^{-\lambda K} P_G(g) \psi_{FS}$	−12.479	$g = 0.035$, $g' = 0.60$
$e^{-\lambda K} P_G e^{-\mu K} P_G \psi_{FS}$	−12.487	
Exact	−12.530	

3. Spin fluctuation induced by kinetic charge fluctuation

Here we examine the stability of the antiferromagnetic state as a function of U when holes are doped in the 2D Hubbard model. As we mentioned in Section 1, the antiferromagnetic correlation is suppressed in the strongly correlated region. We discuss this and its relation to superconductivity in this section.

We show the antiferromagnetic (AF) order parameter Δ_{AF} as a function of U in Fig. 1. This is a typical behavior of Δ_{AF} and the AF energy gain ΔE_{AF} also shows a similar behavior. The calculation was carried out, by employing the wave function ψ_λ, on a 10×10 lattice. When U is small, Δ_{AF} increases with the increase of U and has a maximum at $U_m \simeq 8t - 10t$ that is of the order of

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