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Electron Correlation in High Temperature Cuprates

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Abstract

Electron correlation plays a key role in high-temperature cuprate superconductors. Material-parameter dependence of cuprates is important to clarify the mechanism of high temperature superconductivity. In this study, we examine the ground state of the three-band Hubbard model (d-p model) that explicitly includes oxygen p orbitals. We consider the half-filled case with the large on-site Coulomb repulsion U_d by using the variational Monte Carlo method. The ground state is insulating when U_d is large at half-filling. The ground state undergoes a transition from a metal to a Mott insulator when the level difference ε_p-ε_d is increased.

Keywords

High-Temperature Superconductor, Electron Correlation, Mott Insulator, Metal-Insulator Transition, Charge-Transfer Insulator

1. Introduction

The study of high-temperature superconductors has been addressed extensively since the discovery of cuprate superconductors [1]. The CuO_2 plane in cuprates plays a key role for the appearance of superconductivity [2-10] and the electron correlation in this plane is important [11-16].

Relationship between material parameters and critical temperature T_C is important to clarify the mechanism of high temperature superconductivity. We consider two kinds of material parameters. The first category includes transfer integrals t_{dp}, t_{pp} and the level of d and p electrons. These parameters determine the band structure and the Fermi surface. The t_{dp} is the transfer integral between nearest d and p orbitals in the CuO_2 plane, and t_{pp} is that between nearest p orbitals. The other category is concerning with the strength of interactions such as the Coulomb interaction, U_d and U_p, and the electron-phonon interaction. The transfer integrals play an important role to obtain a finite bulk limit of the superconducting condensation energy [12,13,17]. The parameter values were estimated in the early stage of research of high temperature cuprates [18-21].

In this paper, we investigate the ground state of the three-band d-p model in the half-filled case. When the Coulomb interaction U_d is large, the ground state is presumably insulating. We show, in fact, that there is a transition from a metallic state to an insulating state as the level difference between d and p electrons is increased.

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2. Hamiltonian

The three-band Hamiltonian with d and p electrons is

$$H = \varepsilon_d \sum_{i\sigma} d^+_{i\sigma} d_{i\sigma} + \varepsilon_p \sum_{i\sigma} (p^+_{i+\tilde{x}/2,\sigma} p_{i+\tilde{x}/2,\sigma} + p^+_{i+\tilde{y}/2,\sigma} p_{i+\tilde{y}/2,\sigma}) + t_{dp} \sum_{i\sigma} [d^+_{i\sigma} (p_{i+\tilde{x}/2,\sigma} + p_{i+\tilde{y}/2,\sigma} - p_{i-\tilde{x}/2,\sigma} - p_{i-\tilde{y}/2,\sigma}) + h.c.]$$
$$+ t_{pp} \sum_{i\sigma} (p^+_{i+\tilde{y}/2,\sigma} p_{i+\tilde{x}/2,\sigma} - p^+_{i+\tilde{y}/2,\sigma} p_{i-\tilde{x}/2,\sigma} - p^+_{i-\tilde{y}/2,\sigma} p_{i+\tilde{x}/2,\sigma} + p^+_{i-\tilde{y}/2,\sigma} p_{i-\tilde{x}/2,\sigma} + h.c.) + t'_d \sum_{\langle ij\rangle\sigma} \left(d^+_{i\sigma} d_{j\sigma} + h.c. \right)$$
$$+ U_d \sum_i n^d_{i\uparrow} n^d_{i\downarrow} + U_p \sum_i \left(n^p_{i+\tilde{x}/2\uparrow} n^p_{i+\tilde{x}/2\downarrow} + n^p_{i+\tilde{y}/2\uparrow} n^p_{i+\tilde{y}/2\downarrow} \right) \tag{1}$$

where U_d and U_p indicate the on-site Coulomb interaction among d and p electrons, respectively. $d_{i\sigma}$ and $d^+_{i\sigma}$ are operators for the d electrons. $p_{i\pm\tilde{x}/2,\sigma}$ and $p^+_{i\pm\tilde{x}/2,\sigma}$ denote operators for the p electrons at the site $R_{i\pm\tilde{x}/2}$, and in a similar way $p_{i\pm\tilde{y}/2,\sigma}$ and $p^+_{i\pm\tilde{y}/2,\sigma}$ are defined. $n^d_{i\sigma}$ and $n^p_{i+\tilde{\mu}/2,\sigma}(\mu = x, y)$ are number operators for d and p electrons, respectively. We have introduced the parameter t'_d that is the transfer integral of d electrons between next nearest-neighbor cooper sites, where <ij>denotes a next nearest-neighbor pair of copper sites. The energy unit is given by t_{dp} in this paper. We use the notation $\mathbf{\Delta_{dp}} = \varepsilon_p$-$\varepsilon_d$. The number of sites is denoted as N_s, and the total number of atoms is denoted as $N_a = 3N_s$. Our study is within the hole picture where the lowest band is occupied up to the Fermi energy μ. The non-interacting part is written as

$$H_0 = \sum_{k\sigma} \left(d^+_{k\sigma} p^+_{xk\sigma} p^+_{yk\sigma} \right) \begin{pmatrix} \varepsilon_{dk} - \mu & \varepsilon_{xk} & \varepsilon_{yk} \\ -\varepsilon_{xk} & \varepsilon_p - \mu & \varepsilon_{pk} \\ -\varepsilon_{yk} & \varepsilon_{pk} & \varepsilon_p - \mu \end{pmatrix} \begin{pmatrix} d_{k\sigma} \\ p_{xk\sigma} \\ p_{yk\sigma} \end{pmatrix} \tag{2}$$

where $\varepsilon_{xk} = 2it_{dp}\sin(k_x/2)$, $\varepsilon_{yk} = 2it_{dp}\sin(k_y/2)$, $\varepsilon_{pk} = -4t_{pp}\sin(k_x/2)\sin(k_y/2)$ and $\varepsilon_{dk} = -4t'_d\cos(k_x)\cos(k_y)$. $p\mu_{k\sigma}$ and $d_{k\sigma}$, are Fourier transforms of $p_{i+\tilde{\mu}/2,\sigma}$ and $d_{i\sigma}$, respectively. The eigenvectors of this matrix give the corresponding weights of d and p electrons.

3. Mott State and Wave Function

3.1. Gutzwiller Function

We adopt the Gutzwiller ansatz for the wave function:

$$\psi_G = P^d_G \psi_0 \tag{3}$$

where P_G is the Gutzwiller projection operator given by

$$P^d_G = \prod_i \left[1 - (1-g) n^d_{i\uparrow} n^d_{i\downarrow} \right] \tag{4}$$

with the variational parameter in the range from 0 to unity: $0 \le g \le 1$. The operator P_G controls the on-site electron correlation on the copper site. When we take into account U_p, the correlation among p electrons is also considered. In this case P_G is

$$P_G = P^d_G P^p_G, \tag{5}$$

where

$$P^p_G = \prod_i \left[1 - (1-g_p) n^p_{i+\tilde{x}/2\uparrow} n^p_{i+\tilde{x}/2\downarrow} \right] \left[1 - (1-g_p) n^p_{i+\tilde{y}/2\uparrow} n^p_{i+\tilde{y}/2\downarrow} \right] \tag{6}$$

with the parameter g_p in the range $0 \le g_p \le 1$. ψ_0 is a one-particle wave function. We can take various kinds of states for ψ_0; for example, the Fermi sea or the Hartree-Fock state with some order parameters.

3.2. Optimized Wave Function

There are several ways to improve the Gutzwiller function. One method is to consider an optimization operator:

$$\psi = \exp(\lambda K)\psi_G \tag{7}$$

where K is the kinetic part of the total Hamiltonian H and λ is a variational parameter [9]. The ground state energy is lowered appreciably by the introduction of λ [11]. This type of wave function is an approximation to the wave function in quantum Monte Carlo method [22-24].

We note that the Gutzwiller function ψ_G cannot describe an insulating state at half-filling because we have no kinetic energy gain in the limit $g \to 0$. A wave function for the Mott state has been proposed for the single-band Hubbard model by adopting the doublon-holon correlation factor [25]. In this paper, instead, we consider the optimized Gutzwiller function in Equation (7) in the limit $g \to 0$ as a Mott insulating state. This is an insulator of charge-transfer type [26] and is a metal-insulator transition in a multi-band system [27].

3.3. Mott State in the Single-Band Case

Here we examine the Mott insulating state for the single-band Hubbard model [28]. We show the ground-state energy per site as a function of U in **Figure 1**, obtained by using the wave function in Equation (7). The curvature of the energy, as a function of U, changes near $U \sim 8$ and the parameter g vanishes simultaneously. The state with vanishing g would be an insulating state because of vanishingly small double occupancy.

3.4. Variational Parameters of the Band Structure

In the three-band case, we have additional band parameters as variational parameters in ψ_0. The one-particle state ψ_0 contains the variational parameters $\tilde{t}_{dp}$, $\tilde{t}_{pp}$, $\tilde{t}'_d$, $\tilde{\varepsilon}_d$ and $\tilde{\varepsilon}_p$:

$$\psi_0 = \psi_0(\tilde{t}_{dp}, \tilde{t}_{pp}, \tilde{t}'_d, \tilde{\varepsilon}_d, \tilde{\varepsilon}_p) \tag{8}$$

In the non-interacting case, $\tilde{t}_{dp}$, $\tilde{t}_{pp}$ and $\tilde{t}'_d$ coincide with t_{dp}, t_{pp} and t'_d, respectively. The expectation values of physical quantities are calculated by employing the variational Monte Carlo method [6,7].

4. Mott State of Charge-Transfer Type

Our study on the Mott state of the three-band model is based on the wave function in Equation (7). The ground-state energy per site $E/N_s - \varepsilon_d$ as a function of the level difference Δ_{dp} is shown in **Figure 2**. The parameters are $t_{pp} = 0.4$, $t'_d = 0.0$ and $U_d = 8$. We set $U_p = 0$ for simplicity because U_p is not important in the low doping case and also in the half-filled case. The parameter g for the optimized function ψ vanishes at $\Delta_{dp} \approx 2$ while that for the Gutzwiller function ψ_G remains finite even for large Δ_{dp}. The result shows that there is a transition from a metallic state to an insulating state at the critical value of $\Delta_{dp} \sim\approx (\Delta_{dp})_c \sim 2$.

We find that the curvature of the energy, as a function of Δ_{dp}, is changed near $\Delta_{dp} \sim 2$. The energy is well fit-

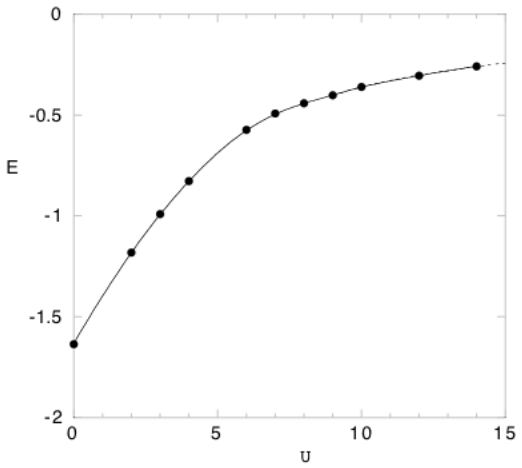

Figure 1. Ground state energy of the 2D single-band Hubbard model as a function of U at half-filling. The system size is 6 × 6.

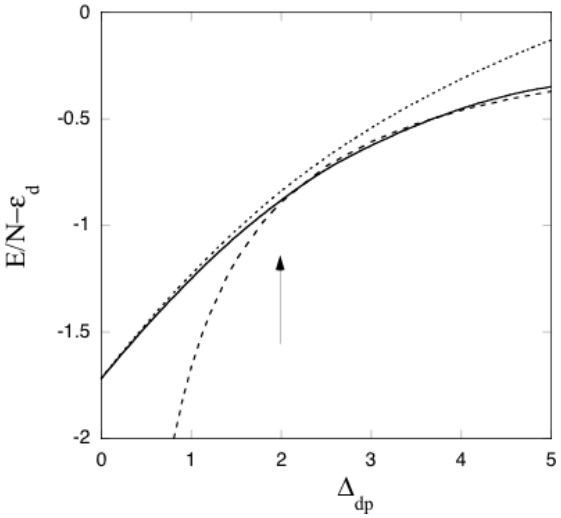

Figure 2. Ground-state energy of the 2D d-p model per site as a function of Δ_{dp} for t_{pp} = 0.4, t'_d = 0.0 and U_d = 8 (in units of t_{dp}) in the half-filled case on 6 × 6 lattice. The arrow indicates a transition point where the curvature is changed. The dotted curve is for the Gutzwiller function ψ_G (with λ = 0). The dashed curve indicates that given by a constant times $1/(\varepsilon_p-\varepsilon_d)$.

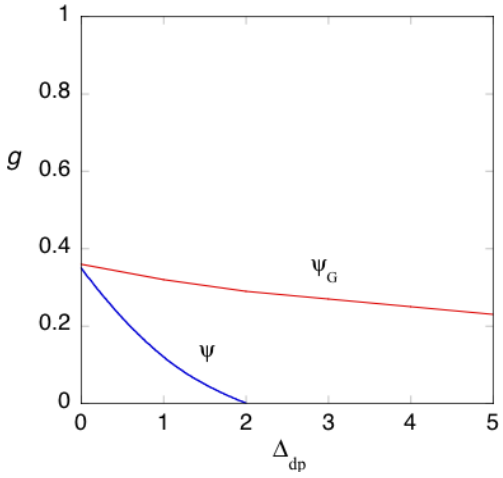

Figure 3. The Gutzwiller parameter g as a function of Δ_{dp} for ψ_G and the optimized wave function ψ. g for ψ decreases and vanishes as Δ_{dp} is increased.

ted by $1/\Delta_{dp}$ when Δ_{dp} is greater than $(\Delta_{dp})_c$. This is shown in **Figure 2** where the dashed curve indicates $1/\Delta_{dp}$. This shows that the most of energy gain comes from the exchange interaction between nearest neighbor d and p electrons. This exchange interaction is given by J_K:

$$J_K = t_{dp}^2\left(\frac{1}{\Delta_{dp}}+\frac{1}{U_d-\Delta_{dp}}\right) \tag{9}$$

In the insulating state, the energy gain is proportional to J_K, which is consistent with our result.

We show the Gutawiller parameter g as a function of the level difference Δ_{dp} in **Figure 3**. g for the Gutzwiller

function ψ_G descreases gradually when Δ_{dp} is increased. In contrast, g for the optimized function ψ shows a rapid decrease and almost vanishes near $(\Delta_{dp})_c$. This is consistent with the behavior of the energy shown in **Figure 2**, indicating that the ground state is an insulator when $\Delta_{dp} > (\Delta_{dp})_c$. When g vanishes, the double occupancy of d holes is completely excluded and we have exactly one hole on the copper site. This is the insulating state of charge-transfer type.

5. Summary

We have investigated the ground state of the three-band d-p model at half-filling by using the variational Monte Carlo method. We have proposed the wave function for an insulating state of charge-transfer type with an optimization operator on the basis of the Gutzwiller wave function. We have shown that this wave function describes a transition from a metallic state to an insulating state as the level difference Δ_{dp} is increased. The critical value of Δ_{dp} would depend on U_d and band parameters.

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