

# 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  $\epsilon_p - \epsilon_d$  is increased.

## Keywords

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

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## 1. Introduction

The study of high-temperature superconductors has been addressed extensively since the discovery of cuprate superconductors [1]. The  $\text{CuO}_2$  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  $\text{CuO}_2$  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.

## 2. Hamiltonian

The three-band Hamiltonian with d and p electrons is

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

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.  $p_{i\pm\bar{x}/2,\sigma}$  and  $p_{i\pm\bar{x}/2,\sigma}^+$  denote operators for the p electrons at the site  $R_{i\pm\bar{x}/2}$ , and in a similar way  $p_{i\pm\bar{y}/2,\sigma}$  and  $p_{i\pm\bar{y}/2,\sigma}^+$  are defined.  $n_{i\sigma}^d$  and  $n_{i+\bar{\mu}/2,\sigma}^p$  ( $\mu = x, y$ ) 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 copper sites, where  $\langle ij \rangle$  denotes a next nearest-neighbor pair of copper sites. The energy unit is given by  $t_{dp}$  in this paper. We use the notation  $\Delta_{dp} = \varepsilon_p - \varepsilon_d$ . 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  $\mu$ . The non-interacting part is written as

$$H_0 = \sum_{k\sigma} \begin{pmatrix} d_{k\sigma}^+ \\ p_{xk\sigma}^+ \\ p_{yk\sigma}^+ \end{pmatrix} \begin{pmatrix} \varepsilon_{dk} - \mu & \varepsilon_{xk} & \varepsilon_{yk} \\ -\varepsilon_{xk} & \varepsilon_p - \mu & \varepsilon_{pk} \\ -\varepsilon_{yk} & \varepsilon_{pk} & \varepsilon_p - \mu \end{pmatrix} \tag{2}$$

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  $p_{i+\bar{\mu}/2,\sigma}$  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:

$$\psi_G = P_G^d \psi_0 \tag{3}$$

where  $P_G$  is the Gutzwiller projection operator given by

$$P_G^d = \prod_i [1 - (1-g)n_{i\uparrow}^d n_{i\downarrow}^d] \tag{4}$$

with the variational parameter in the range from 0 to unity:  $0 \leq g \leq 1$ . 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

$$P_G = P_G^d P_G^p, \tag{5}$$

where

$$P_G^p = \prod_i [1 - (1-g_p)n_{i+\bar{x}/2\uparrow}^p n_{i+\bar{x}/2\downarrow}^p] [1 - (1-g_p)n_{i+\bar{y}/2\uparrow}^p n_{i+\bar{y}/2\downarrow}^p] \tag{6}$$

with the parameter  $g_p$  in the range  $0 \leq g_p \leq 1$ .  $\psi_0$  is a one-particle wave function. We can take various kinds of states for  $\psi_0$ ; 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:

$$\psi = \exp(\lambda K)\psi_G \quad (7)$$

where  $K$  is the kinetic part of the total Hamiltonian  $H$  and  $\lambda$  is a variational parameter [9]. The ground state energy is lowered appreciably by the introduction of  $\lambda$  [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  $\psi_G$  cannot describe an insulating state at half-filling because we have no kinetic energy gain in the limit  $g \rightarrow 0$ . 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  $g \rightarrow 0$  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  $\psi_0$ . The one-particle state  $\psi_0$  contains the variational parameters  $\tilde{t}_{dp}$ ,  $\tilde{t}_{pp}$ ,  $\tilde{t}'_d$ ,  $\tilde{\epsilon}_d$  and  $\tilde{\epsilon}_p$ :

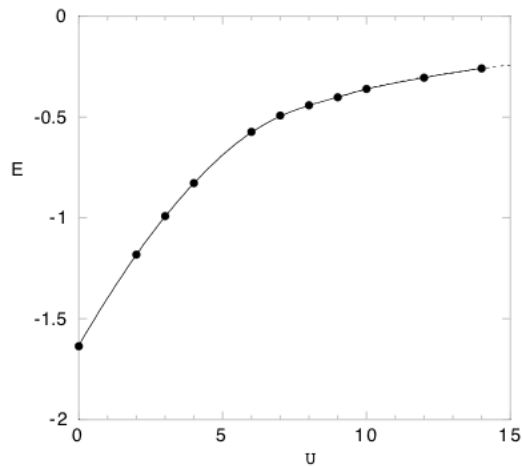
$$\psi_0 = \psi_0(\tilde{t}_{dp}, \tilde{t}_{pp}, \tilde{t}'_d, \tilde{\epsilon}_d, \tilde{\epsilon}_p) \quad (8)$$

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].

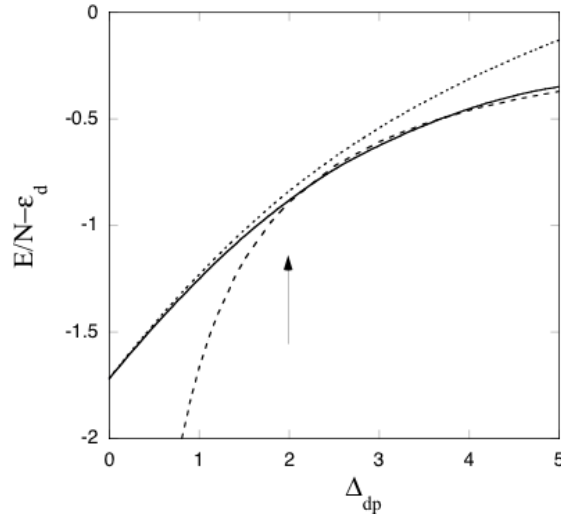
## 4. Mott State of Charge-Transfer Type

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  $E/N_s - \epsilon_d$  as a function of the level difference  $\Delta_{dp}$  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  $\psi$  vanishes at  $\Delta_{dp} \approx 2$  while that for the Gutzwiller function  $\psi_G$  remains finite even for large  $\Delta_{dp}$ . The result shows that there is a transition from a metallic state to an insulating state at the critical value of  $\Delta_{dp} \approx (\Delta_{dp})_c \sim 2$ .

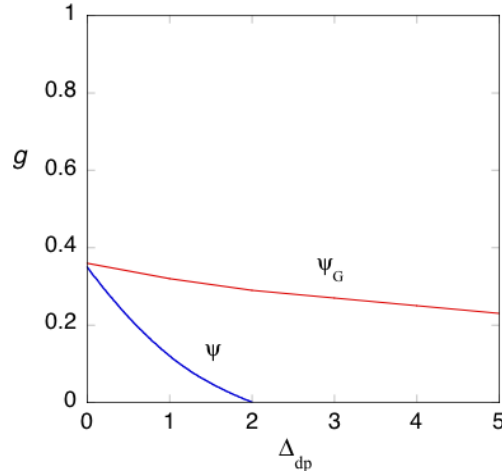
We find that the curvature of the energy, as a function of  $\Delta_{dp}$ , is changed near  $\Delta_{dp} \sim 2$ . The energy is well fit-



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



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



**Figure 3.** The Gutzwiller parameter  $g$  as a function of  $\Delta_{dp}$  for  $\psi_G$  and the optimized wave function  $\psi$ .  $g$  for  $\psi$  decreases and vanishes as  $\Delta_{dp}$  is increased.

ted by  $1/\Delta_{dp}$  when  $\Delta_{dp}$  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  $J_K$ :

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

In the insulating state, the energy gain is proportional to  $J_K$ , which is consistent with our result. We show the Gutzwiller parameter  $g$  as a function of the level difference  $\Delta_{dp}$  in **Figure 3**.  $g$  for the Gutzwiller

function  $\psi_G$  decreases gradually when  $\Delta_{dp}$  is increased. In contrast,  $g$  for the optimized function  $\psi$  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  $\Delta_{dp}$  is increased. The critical value of  $\Delta_{dp}$  would depend on  $U_d$  and band parameters.

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