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# Hole distribution in the three-band Hubbard model of high- $T_c$ cuprates

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## Abstract

Based on the three-band Hubbard model, we studied the distance and orientation dependence of the interaction between two small ferromagnetic polarons induced by extra holes doped in the  $\text{CuO}_2$  plane. Through the binding energy calculation of the three-hole-doped system, we have shown that the favourable hole distribution pattern is mainly determined by the sum of all pairs of two-hole energy changes. In the case of four-hole doping, we get a schematic phase diagram in parameter space for the stable configuration.

## 1. Introduction

In undoped high- $T_c$  cuprates, the ground state is an antiferromagnetic (AF) Mott insulator with nearest-neighbour (nn)  $\text{Cu}^{2+}$ – $\text{Cu}^{2+}$  AF exchange interaction in the  $\text{CuO}_2$  plane. Upon doping, holes enter into the oxygen p-orbit in the  $\text{CuO}_2$  plane, which induce an equivalent ferromagnetic (FM) coupling for the  $\text{Cu}^{2+}$  ions adjacent to the partially empty oxygen orbit [1], thus resulting in a small FM cluster of five mainly parallel copper spins (named polaron) in the  $\text{CuO}_2$  plane [2, 3]. These spin-polarized clusters have been demonstrated by experiments [4, 5]. In the low-doping region, the local AF order is destroyed while the long-range AF order is reserved with lower Neel point. There exists a critical doping concentration at which an insulator–metal transition takes place. With increasing doping concentration, the single-hole polarons start to build up a conducting network, i.e. the gap states become more and more extended and build up a conducting network [6]. For example, doping  $\text{La}_2\text{CuO}_4$  with Sr, the AF–spin-glass transition happens at a doping density of about 2% and the onset point of the metal–insulator transition is at 5%. A review on theoretical and experimental result about the properties at finite doping is given in [7]. Also, a number of doped holes tend to organize themselves into different configurations. Extensive neutron scattering measurements revealed that the extra holes may form a quasi-one-dimensional (1D) structure called a stripe, where each of them runs parallel to one of the principal lattice directions, e.g. in the (10) direction [8–10] or (11)

direction [11–13]. Recently, using scanning tunnelling microscopy (STM), two-dimensional checkerboard modulation has been observed under a magnetic field [14], and also in zero field [15] in Bi2212 and in lightly hole-doped  $\text{Ca}_{2-x}\text{Na}_x\text{CuO}_2\text{Cl}_2$  [16].

Much theoretical work has studied the possibility of real-space stripe patterns or checkerboard patterns in doped high-temperature superconductors. Emery *et al* [17] and some later work [18] propose that phase separation and inhomogeneous spatial charge ordering arises from a competition between the short-range attractive interactions and long-range Coulomb repulsion between holes. However, White and Scalapino [19] have shown that the presence of striped phases as the ground state of large  $t$ - $J$  clusters does not require long-range Coulomb forces to stabilize the stripes. Also, striped states with charge-density waves (CDWs) along the stripes can give approximate checkerboard patterns [20]. Anderson [21] and Huang *et al* [22] suggest that the observed checkerboard patterns may well be induced by the long-range Coulomb repulsion, but require a rather small dielectric constant. Lemanski and coworkers [23] give the restricted phase diagram of a simple spinless Falicov–Kimball model and it displays rich behaviour, illustrating both possibilities in different regions, and predict that Kivelson–Emery scenario of phase separation [17] does not require the long-range Coulomb interaction to stabilize stripes. Some other theoretical works [24] have proposed their own microscopic model to interpret the recent experimental result. In the three-band Hubbard model of high- $T_c$  cuprates, a diagonal stripe pattern has been examined by Hartree–Fock (HF) method [6] and it was found that the four-lattice stripe state is stable at 1/8 doping level by using a variational Monte Carlo method [25]. To our knowledge, the recently observed checkerboard pattern has not been discussed in the three-band Hubbard model.

Instead of investigating a specific distributed pattern of the polarons for a given doping concentration, here we will start from the three-band Hubbard model under the HF approximation to compare the ground-state energy of the static distribution of several extra holes for the given parameters in the low-doping limit where the system is in the insulating state. Also, we will determine which distribution is the preferable one in a given parameter region, i.e. the phase diagram in parameter space. We base this on the idea that each excess hole slightly perturbs the electronic structure in its vicinity by forming some separated small polarons where all holes are completely localized when more holes are doped [2, 3]. We focus on investigating the interaction between two small polarons. The interaction depends on the relative distance and orientation and the parameter values of the model Hamiltonian. Also, we assume that the binding energy of a many-hole-doped system equals the sum of the two-hole binding energy over all pairs of holes (hereafter named the S-method for simplicity). This rather crude approximation is verified to be effective in getting a favourable hole distribution pattern. We apply our idea to the four-hole-doped case and get a schematic phase diagram.

The paper is organized as follows. In section 2 the Hamilton and the relevant Green's functions in the HF approximation are introduced. In section 3, the main formulae and methods used in the calculation are given. Also, we test the validity of the S-method by comparing the energy change values by a self-consistent method and the S-method for certain three-hole-doped systems. Then, in section 4, the distance and orientation dependence of the energy change in two-hole-doped system are shown. For the four-hole-doped case, by the S-method, the favourable configurations with different parameter values are discussed. Also, in section 5, we summarize our conclusions.

## 2. HF approach and Green's function

We start from the three-band Hubbard model which takes the  $d_{x^2-y^2}$  band of the Cu ions and the  $p_{x(y)}$  bands of the oxygen ions into account. Within the HF approximation, the Hamiltonian

can be simplified to  $H^{\text{MF}} = \sum_{\sigma} H_{0\sigma}^{\text{MF}} + H_{\text{int}}^{\text{MF}}$ , where

$$H_{0\sigma}^{\text{MF}} = \sum_m (\varepsilon_d + U \langle n_{m-\sigma}^d \rangle) n_{m\sigma}^d + \varepsilon_p \sum_{m'} n_{m'\sigma}^p + t \sum_{\langle m, m' \rangle} (d_{m\sigma}^\dagger p_{m'\sigma} \text{H.c.}) \quad (1)$$

$$H_{\text{int}}^{\text{MF}} = -U \sum_m \langle n_{m\uparrow}^d \rangle \langle n_{m\downarrow}^d \rangle. \quad (2)$$

The notation is standard, except that  $\langle m, m' \rangle$  denotes Cu and its four nearest-neighbour (nn) oxygen ions. The nn Cu–O hopping  $t$  is always set to unity. The parameters are usually assumed to be  $U \approx 8$ ,  $\varepsilon = \varepsilon_p - \varepsilon_d \approx 3$ ,  $\varepsilon_d \approx 0$ , and  $\varepsilon_p \approx 3$ . In the undoped case, the oxygen sites are doubly occupied while the copper site is singly occupied, and thus the copper spins are aligned antiferromagnetically through super-exchange interaction. In order to describe the AF ordered state, the unit cell is doubled. Due to the mean-field renormalization effect, the two copper on-site energies in the magnetic unit cell are given by  $\varepsilon_{1\sigma} = \varepsilon_d + U \langle n_{1-\sigma}^d \rangle$ ,  $\varepsilon_{2\sigma} = \varepsilon_d + U \langle n_{2-\sigma}^d \rangle$ . Considering the symmetry of AF state, it follows immediately that  $\langle n_{1\sigma}^d \rangle = \langle n_{2-\sigma}^d \rangle$ . Therefore we can use the notation  $\langle n_{\sigma}^d \rangle$  and consider these quantities as modulated with twice the lattice period. In  $k$  space, the Hamiltonian  $H_{0\sigma}^{\text{MF}}$  for a fixed spin direction, say  $\sigma = \uparrow$ , is written as a matrix which can be found in [3].

Now we calculate the Green's function according to

$$G^{0\sigma}(\vec{k}) = \left[ (E - H_{0\sigma}^{\text{MF}})^{-1} \right]. \quad (3)$$

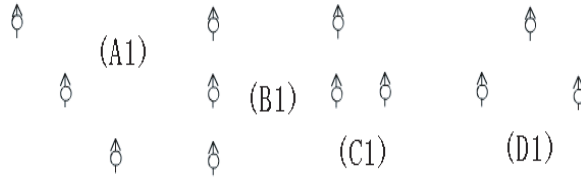
Defining  $\eta^2 = D(E)/16t^2$ , where  $D(E) = D_1(E)D_2(E)$ ,  $D_i(E) = (E - \varepsilon_i)(E - \varepsilon_p) - 4t^2$  ( $i = 1, 2$ ), and  $\varepsilon_{1,2} = \varepsilon_d + U \langle n_{\downarrow, \uparrow}^d \rangle$ . Therefore in  $k$  space the Green's function for Cu ion with spin  $\uparrow$ , i.e. the (11) component of (3) is given by:

$$G_{00}^{0\uparrow}(\vec{k}) = \frac{(E - \varepsilon_p) D_2(E)}{16t^4 \left[ \cos^2\left(\frac{k_x + k_y}{2}a\right) \cos^2\left(\frac{k_x - k_y}{2}a\right) - \eta^2 \right]}. \quad (4)$$

For  $\sigma = \downarrow$ , the Green's function can be expressed by the same formula as equation (4) with only one change: replacing  $D_2(E)$  by  $D_1(E)$ . The corresponding real-space Green's functions can be obtained by doing Fourier transformation. For simplicity, the diagonal matrix element  $G^{0\sigma}(\vec{r}_1, \vec{r}_2)$  with  $|(\vec{r}_1 - \vec{r}_2)_x| = |(\vec{r}_1 - \vec{r}_2)_y| = l$  will be denoted as  $G^{0\sigma}(l)$ . If we plot the imaginary part of the Green's function  $G^{0\sigma}(0)$  versus energy  $E$ , we obtain information on the band structures. Symmetric linear combinations of the oxygen states lead to the decoupling of two dispersive bands of oxygen type. Four bands remain: the upper and lower Hubbard bands of mainly copper character and two broader bands of mainly oxygen type between them. In the undoped case, the lowest three bands are occupied (in an electron description). The charge-transfer gap (CT gap) denotes the energy difference between the lowest unoccupied level of the upper Hubbard band and the highest occupied level of the upper oxygen band.

### 3. Main formula

In the undoped region, the long-range AF order remains. When one hole is doped at the site neighbouring (0,0), we assume that the copper spin at the site (0,0) is spontaneously flipped, changing the spin densities from  $\langle n_{\sigma}^d \rangle_{00}$  to  $\langle n_{\sigma}^d \rangle_{00}$ . This scenario has already been used by several authors [2, 3]. The perturbation is  $V^{\sigma} = U(\langle n_{-\sigma}^d \rangle_{00} - \langle n_{-\sigma}^d \rangle_{00})$ . Through the Dyson equation  $(1 - G^{0\sigma}(0)V^{\sigma})G^{\sigma}(0) = G^{0\sigma}(0)$ , we can obtain the perturbed Green's function  $G^{\sigma}(0)$ , and hence the band structure of the disturbed lattices can be calculated. The calculations in which the further neighbours have been taken into account showed that, as in [3], the spin polarization increases slightly, but a smaller increase in the binding energy was found. So, the localized perturbation theory is a good approximation.



**Figure 1.** Three-hole-doped distributed patterns.

For the two-hole-doped case, two FM spin polarons will be formed, e.g. one at the site  $(i, i)$ , and the other at  $(j, j)$ .  $G^{0\sigma}$  and  $V^\sigma$  can be written as a  $2 \times 2$  matrix [26]:

$$G^{0\sigma} = \begin{pmatrix} G^{0\sigma}(0) & G^{0\sigma}(|i-j|) \\ G^{0\sigma}(|i-j|) & G^{0\sigma}(0) \end{pmatrix}, \quad (5)$$

$$V^\sigma = U \begin{pmatrix} \Delta\langle n \rangle & 0 \\ 0 & \Delta\langle n \rangle \end{pmatrix} \quad (6)$$

where  $\Delta\langle n \rangle \equiv \langle n_{-\sigma}^d \rangle - \langle n_{\sigma}^d \rangle$ . The equations for the new spin density  $\langle n_{\sigma}^d \rangle$  should be solved self-consistently. Upon doping, the number of localized states with energy  $E^L$  in the energy gap is determined by the poles of Green function  $G^\sigma$ , i.e. the  $E^L$  satisfy the equation  $(1 - G^{0\sigma}V^\sigma) = 0$ . If  $n$  spins flipped, there would be  $n$  localized states split off from the upper oxygen band into the CT gap. The electrons are removed from these localized states [2]. Therefore the Fermi energy ( $E_F$ ) lies between the upper band edge and the localized state.

The total energy change of this two-hole-doped system due to the perturbation of the Hamiltonian is given by  $\Delta E(2) = \Delta E^{\text{int}} + \Delta E^{\text{loc}}$ , where  $\Delta E^{\text{int}} = 2(\langle n_{\uparrow}^d \rangle \langle n_{\downarrow}^d \rangle - \langle n_{\uparrow}^d \rangle \langle n_{\downarrow}^d \rangle)$  is the variation coming from the  $H_{\text{int}}^{\text{MF}}$ , and  $\Delta E^{\text{loc}}$  arises from the change in density of state and the formation of the split-off states [27]:

$$\Delta E^{\text{loc}} = \sum_{\sigma} \int_{-\infty}^{E_F} E \Delta N_{\sigma}(E) dE$$

$$\Delta E^{\text{loc}} = \sum_{\sigma} E^L - \frac{1}{\pi} \sum_{\sigma} \sum_{\alpha} \int_{\text{band}} \arctan \left( \frac{\text{Im}(G^{0\sigma}(0)V^{\sigma}(\alpha, \alpha))}{\text{Re}((1 - G^{0\sigma}(0)V^{\sigma}(\alpha, \alpha)))} \right) dE \quad (7)$$

where  $E^L$  signify the energies of the occupied localized states measured from the neighbouring band edges. In order to get the energy band edge, we use the criterion  $0 \leq \eta^2 \leq 1$  [3, 28].  $V^{\sigma}(\alpha, \alpha)$  denote the diagonal element of the perturbation matrix.

The matrix approach can be generalized to three, four, etc, hole-doped cases. But here we propose an approximate method. Let us define the binding energy of an  $n$ -hole-doped system as relative quantities from which the large-distance limit case has already been subtracted,  $\Delta E_b(n) = \Delta E(n) - n\Delta E(1)$ , where  $\Delta E(n)$  is the energy change of the  $n$ -hole-doped system and  $\Delta E(1)$  denotes the energy change of the one-hole-doped case at the same parameter set. By the S-method, we neglect the three-body interaction energy, and the binding energy  $\Delta E_b(n)$  is assumed to be the sum of the two-hole binding energies of all pairs of them, i.e.  $\Delta E_b(n) = \sum_{(ij)} \Delta E_b(2)$ . So, in the S-method, the energy change  $\Delta E'(n)$  of an  $n$ -hole-doped system can be calculated from the following formula:

$$\Delta E'(n) = \left( \sum_{(ij)} \Delta E(2) \right) - (n^2 - 2n)\Delta E(1). \quad (8)$$

To illustrate the validity of the S-method, we calculate the energy change  $\Delta E(n)$  by the self-consistent method and the S-method for a certain three-hole-doped system in figure 1.

**Table 1.** The energy change calculated by the self-consistent method (the left column under the corresponding parameter) and the ‘S-method’ (the right column under the corresponding parameter) for different hole distribution patterns of a three-hole-doped system.

Pattern	$(U, \epsilon)$					
	(6, 2.5)		(6, 3)		(7, 3)	
	$\Delta E(3)$	$\Delta E'(3)$	$\Delta E(3)$	$\Delta E'(3)$	$\Delta E(3)$	$\Delta E'(3)$
A1	-0.799 05	-0.811 61	-0.693 75	-0.702 46	-0.852 51	-0.861 7
B1	-0.804 32	-0.835 96	-0.681 44	-0.694 32	-0.862 01	-0.896 03
C1	-0.817 04	-0.846 10	-0.690 28	-0.695 70	-0.873 23	-0.907 47
D1	-0.799 92	-0.822 02	-0.697 62	-0.705 72	-0.858 76	-0.877 97
L.P		-0.790 29		-0.672 6		-0.849 3

**Table 2.** The energy change and the Cu-spin polarization for the undoped and doped cases with two holes in a certain parameter set.

$U$	$\epsilon$	(0, 0) (2, 2)				$\Delta E(2)$	(0, 0) (24, 24)	1 hole
		$\langle n_{\uparrow}^d \rangle$	$\langle n_{\downarrow}^d \rangle$	$\langle n_{\uparrow}^{d'} \rangle$	$\langle n_{\downarrow}^{d'} \rangle$		$\Delta E(2)$	$\Delta E(1)$
6	3	0.229 19	0.979 65	0.742 04	0.322 11	-0.458 99	-0.446 84	-0.224 2
7	3	0.163 13	0.983 59	0.767 62	0.234 59	-0.577 82	-0.566 2	-0.282 55
8	3	0.119 82	0.985 00	0.788 43	0.172 94	-0.606 69	-0.635 46	-0.317 05
9	3	0.090 72	0.985 36	0.803 34	0.130 69	-0.648 81	-0.672 3	-0.336 02

Each symbol represents a polaron and other Cu ions and O ions are all omitted. The vertical and horizontal units are  $2a$ . The results are listed in table 1. The left column under the corresponding parameter  $(U, \epsilon)$  represents the self-consistent results  $\Delta E(3)$ , and the right column under the same parameter  $(U, \epsilon)$  represents the results  $\Delta E'(3)$  by the S-method. A1, B1, C1, D1 are the corresponding pattern labels in figure 1. L.P denotes the independent-polaron case in which three polarons are an infinite distance apart.

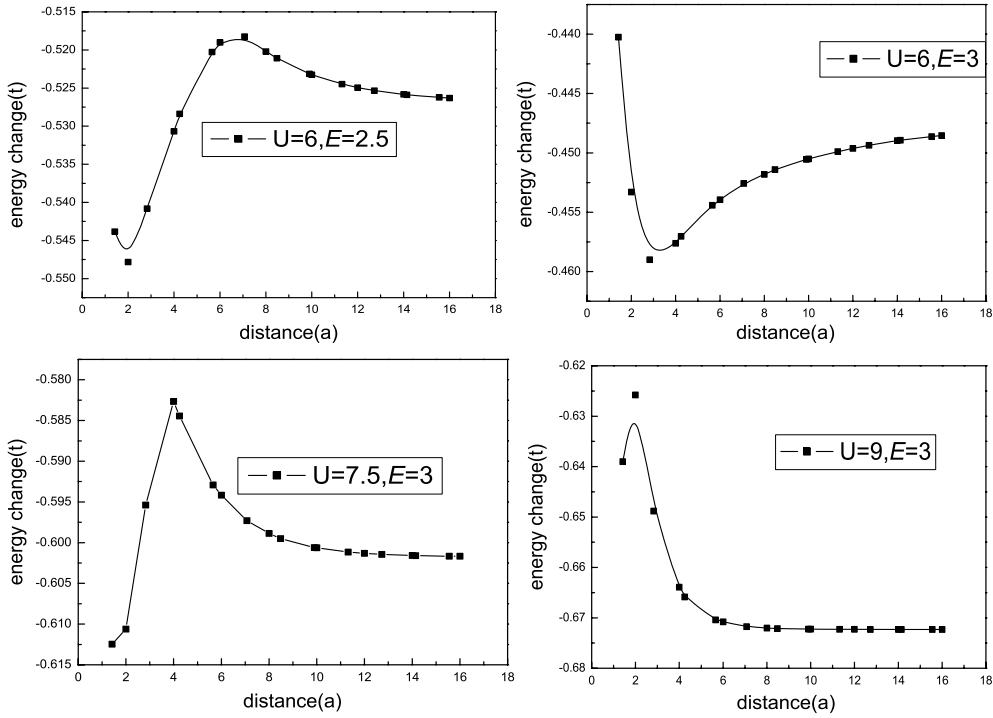
By comparing the  $\Delta E_b(3)$  calculated by the self-consistent method and the S-method, respectively, from the results listed in table 1, we can see that, in some cases, the three-body interaction energy ( $\Delta E(3) - \Delta E'(3)$ ) amounts to more than 50% of the  $\Delta E_b(3)$  given by the S-method. However, neglecting the three-body interaction energy, the order of the energy change  $\Delta E'(3)$  by the S-method is the same as the order of This is equivalent to the conclusion that only the pair interaction determines the favourable hole distribution pattern by just comparing  $\Delta E'(n)$  of different  $n$ -hole-doped configurations by the S-method. Thus, from the plot of the two-body energy change versus distance, it is easy to determine the stable distributed pattern of doped holes in the  $\text{CuO}_2$  plane.

## 4. Result

### 4.1. Two-hole-doped case

Table 2 gives the result of the two-hole-doped case. We can see that, when two holes are at an infinite distance, the energy change is equal to two times  $\Delta E(1)$ , which is the energy change of the one-hole-doped case with the same parameters. When the distance between them is finite, an effective interaction potential between them can be obtained.

As an example, in table 2 we list the energy change of two holes positioned at two points,  $(0, 0)$ ,  $(2, 2)$  and  $(0, 0)$ ,  $(24, 24)$  respectively, under different parameter sets  $(U, \epsilon)$ . It is obvious



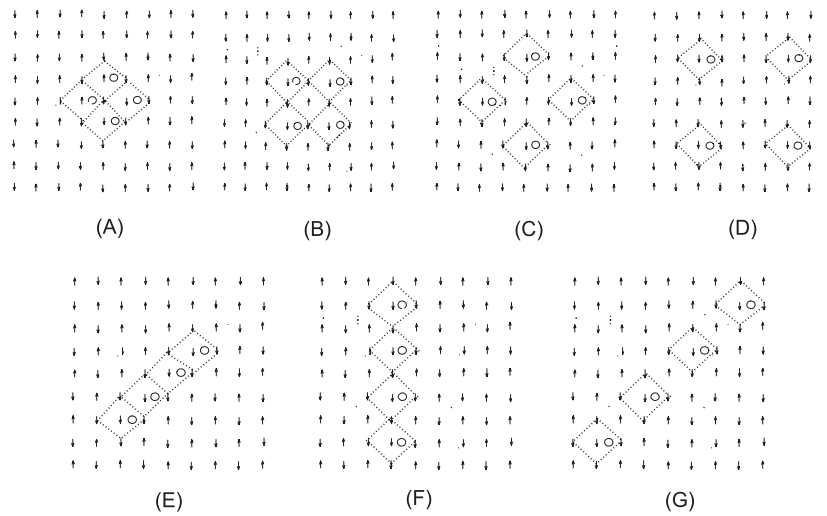
**Figure 2.** The energy change for the two-hole-doped system as a function of the relative distance between the two induced polarons in a certain parameter set.

that, even with the same parameter set, the energy changes  $\Delta E$  for two different distances between two holes are different. After calculations of the energy change for a number of different distances and different parameter sets are carried out, the  $\Delta E$  versus distance curves can be plotted in figure 2. From the 3rd and 5th (or 4th and 6th) columns, we can see that the Cu spin and its four nn Cu spins adjacent to the doped hole will be aligned ferromagnetically, as reported in previous works [2, 3, 6]. In the large- $U$  limit, the potential between two polarons is repulsive and decays with increasing relative distance. In the case of moderate  $U$ , the interaction can be attractive, i.e. the two holes can be in a stable state when they are distributed in a certain distance range.

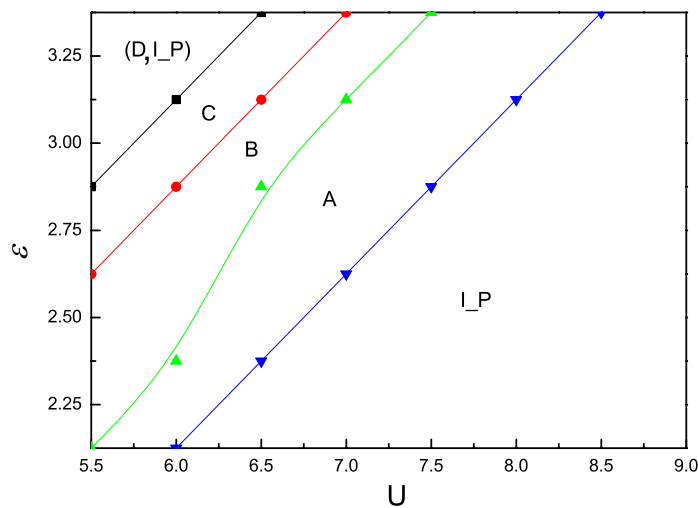
#### 4.2. Four-hole-doped case

When there are four holes doped into the system, six possible distributed patterns are proposed, as shown in figure 3: (i) diagonal checkerboard pattern A ( $\sqrt{2}a \times \sqrt{2}a$ ); (ii) checkerboard pattern B ( $2a \times 2a$ ); (iii) diagonal checkerboard pattern C ( $\sqrt{8}a \times \sqrt{8}a$ ); (iv) checkerboard pattern D ( $4a \times 4a$ ); (v) along the diagonal (11) direction ( $l = \sqrt{2}a$ ) pattern E; (vi) along the vertical (01) direction ( $l = 2a$ ) pattern F; and (vii) along the diagonal (11) direction ( $l = \sqrt{8}a$ ) pattern G.

In the parameter sets of various Coulomb repulsions  $U$  and site energy differences  $\varepsilon = \varepsilon_p - \varepsilon_d$ , by comparing the energy changes  $\Delta E$  of the six patterns and the four independent polarons which are denoted by LP, we obtain the following schematic phase diagram in figure 4. In most intermediate parameter regions, the two-dimensional checkerboard patterns are more favourable. Patterns A, B, C are two-dimensional checkerboard-like structures. For the pattern



**Figure 3.** Representative patterns of the stable hole distribution for a four-hole-doped system: the arrows correspond to the polarization of Cu ions. The circles represent the excess holes in the oxygen sites. Dashed lines label the small polarons.



**Figure 4.** Schematic phase diagram of stable hole distribution for four-hole-doped system: I\_P (independent polarons); A (diagonal checkerboard-like phase) ( $\sqrt{2}a \times \sqrt{2}a$ ); B (checkerboard-like phase) ( $2a \times 2a$ ); C (diagonal checkerboard-like phase) ( $\sqrt{8}a \times \sqrt{8}a$ ); and D (checkerboard-like phase) ( $4a \times 4a$ ).

(This figure is in colour only in the electronic version)

denoted by I\_P, there is a repulsion between two holes when they are at a finite distance. So the more dispersive the holes are, the lower the system energy is, and the ‘evaporating’ effect will happen in the original configuration. In the top-left corner, the favourable pattern is D or I\_P. One-dimensional diagonal (vertical) full-filled (half-filled) stripe patterns do not appear in our phase diagram. We also note that some distributed patterns may have very close energies, e.g.



at the point  $(U, \epsilon) = (6, 3.25)$ , the energy of the stripe pattern G is higher than that of pattern D by only  $0.00744t$ . So, if we consider the fluctuation, the stripe pattern G may also appear.

It should be added that some of the result may be a consequence of the HF approximation and may not survive the addition of fluctuations. Also, we have just included the on-site Coulomb repulsion term  $U$  on Cu. It is energy unfavourable for several extra holes to concentrate on a larger cluster. The ground state of one additional hole is one small polaron with a turned spin. Two or three additional holes would create two or three additional small polarons [2, 3]. The long-range Coulomb repulsion between holes is neglected in the Hubbard model.

## 5. Summary

In summary, we have studied the three-band Hubbard model under the HF approximation in the framework of the self-consistent Green's function method at the temperature  $T = 0$ . We have shown that the favourable hole distribution pattern is mainly determined by the sum of all pairs of two-hole energy changes. In the four-hole-doped system, we have obtained the favourable distribution patterns in the reference parameter set. In the large- $U$  region, isolated small FM polarons are stable. In most intermediate parameter regions, two-dimensional checkerboard-like patterns are favourable.

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## References

- [1] Yeh N-C 2002 *AAPPS Bull.* **12** 2 and reference there
- [2] Seibold G, Sigmund E and Hizhnyakov V 1993 *Phys. Rev. B* **48** 7537
- [3] Klemm D, Letz M, Sigmund E and Zavt G S 1994 *Phys. Rev. B* **50** 7046
- [4] Wübbeler G and Schirmer O 1992 *Phys. Status Solidi b* **174** K21
- [5] Baranov P G and Badalyan A G 1993 *Solid State Commun.* **85** 987
- [6] Seibold G, Seidel J and Sigmund E 1996 *Phys. Rev. B* **53** 5166
- [7] Dagotto E 1994 *Rev. Mod. Phys.* **66** 763
- [8] Tranquada J M, Buttrey D J, Sachan V and Lorenzo J E 1994 *Phys. Rev. Lett.* **73** 1003  
Tranquada J M, Sternlieb B J, Axe J D, Nakamura Y and Uchida S 1995 *Nature* **375** 561
- [9] Yamada K, Lee C H, Kurahashi K, Wada J, Wakimoto S, Ueki S, Kimura H, Ehdoh Y, Hosoya S, Shirane G, Birgeneau R J, Greven M, Kastner M A and Kim Y J 1998 *Phys. Rev. B* **57** 6165
- [10] Lee Y S, Birgeneau R J, Kastner M A, Endoh Y, Wakimoto S, Yamada K, Erwin R W, Lee S H and Shirane G 1999 *Phys. Rev. B* **60** 3643
- [11] Wakimoto S, Shirane G, Endoh Y, Hirota K, Ueki S, Yamada K, Birgeneau R J, Kastner M A, Lee Y S, Gehring P M and Lee S H 1999 *Phys. Rev. B* **60** R769
- [12] Fujita M, Goka H, Yama K and Matsuda M 2002 *Phys. Rev. Lett.* **88** 167008
- [13] Singer P M and Imai T 2002 *Phys. Rev. Lett.* **88** 187601
- [14] Hoffman J E, Hudson E W, Lang K M, Eisaki H, Uchida S and Davis J C 2003 *Physica C* **388/389** 703–4
- [15] Howald C, Eisaki H, Kaneko N, Greven M and Kapitulnik A 2003 *Phys. Rev. B* **67** 014533
- [16] Hanaguri T, Lupien C, Kohsaka Y, Lee D H, Azuma M, Takano M, Takagi H and Davis J C 2004 *Nature* **430** 1001
- [17] Emery V J, Kovelson S A and Lin H Q 1990 *Phys. Rev. Lett.* **64** 475
- [18] Carlson E W *et al* 1998 *Phys. Rev. B* **57** 14704  
Pryadko L P, Kivelson S A and Hone D W 1998 *Phys. Rev. Lett.* **80** 5651  
Pryadko L P *et al* 1999 *Phys. Rev. B* **60** 7541

- 
- [19] White S R and Scalapino D J 1998 *Phys. Rev. Lett.* **80** 1272  
White S R and Scalapino D J 1998 *Phys. Rev. Lett.* **81** 3227
- [20] White S R and Scalapino D J 2004 *Phys. Rev. B* **70** 220506(R)
- [21] Anderson P W 2004 *Preprint cond-mat/0406038*
- [22] Huang H-X, Li Y-Q and Zhang F C 2005 *Phys. Rev. B* **71** 184514
- [23] Lemanski R, Freericks J K and Banach G 2002 *Phys. Rev. Lett.* **89** 196403
- [24] Chen C-D, Hu J-P, Capponi S, Arrigoni E and Zhang S-C 2002 *Phys. Rev. Lett.* **89** 137004  
Fu H C, Davis J C and Lee D-H 2004 *Preprint cond-mat/0403001*  
Fine B V 2004 *Phys. Rev. B* **70** 224508  
Markiewicz R S 2005 *Phys. Rev. B* **71** 220504
- [25] Yanagisawa T, Koike S, Miyazaki M, Koikegami S and Yamaji K 2002 *Physica C* **378-381** 292-7
- [26] Economou E N 1990 *Green's Function in Quantum Physics* (Berlin: Springer)
- [27] Einstein T L and Schrieffer J R 1973 *Phys. Rev. B* **7** 3629
- [28] Morita T 1971 *J. Math. Phys.* **12** 1744