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# Exact diagonalization studies on two-band minimal model for iron-based superconductors

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ABSTRACT

In order to explore a superconducting mechanism on iron-based superconductors, we numerically study a two-band minimal model considering two degenerate $d_{xz}$ and $d_{yz}$ orbitals on Fe atom. We perform exact diagonalization on a two-band and two-leg square ladder totally composed of 10 lattice sites, which is computationally equivalent to 4-leg 20-sites square-Hubbard-ladder. Consequently, we find that a robust pairing occurs in a wide parameter range when the intra-orbital repulsive interaction becomes smaller than the inter-orbital one. Moreover, the obtained binding energy can grow into much larger value than that obtained in the single band Hubbard model depending on the parameter range.



## 1. Introduction

Since the discovery of iron-based superconductors, their high-$T_c$ mechanism has been one of the most intensively studied issues in condensed matter field. A common question in this field is now whether $T_c$ rises up or not above ~55 K, which is the highest $T_c$ seen in $SmFeAsO_{1-x}F_x$ [1]. So far, several mechanisms have been suggested, e.g., one of which ascribes a possible pairing glue to a magnetic fluctuation associated with the Fermi surface nesting [2]. However, these mechanisms have been still elusive, because there remain several unsolved problems in understanding the electronic states.

One of the most struggling mysteries is a big discrepancy between the experimental magnetic moment value per Fe and the one obtained by first principle calculations in a mother compound, e.g., LaOFeAs [3]. Nakamura et al. suggested that the negative $U$ correction resolves the problem [4]. This result characterizes a uniqueness of the materials. In addition, X-ray inelastic scattering revealed the softening of the phonon modes associated with Fe–As bonding [5]. This implies a strong electron–phonon coupling beyond our expectation based on first-principle calculations. Very recently, BCS type of isotope effects only on Fe atoms have been reported [6]. Thus, it is found that spin, charge, and lattice degree of freedoms are cooperatively involved to exhibit the unique properties.

Besides the insights described above, it is clear that Fe has multi-orbital degree of freedom. This uniqueness is remarkable in contrast to cuprate High-$T_c$ superconductors. Thus, several theoretical works have studied the multi-band characters. In this paper, we focus on a two-band model suggested by Daghofer et al. [7] as a minimal model to study the multi-band features [8] and perform the exact diagonalization on the model. It is noted that if one applies exact numerical schemes, e.g., the exact diagonalization or the density matrix renormalization group, then two-band model is a calculation limit. Thus, our strategy is to take into account two-orbitals and their intra- and inter-band interactions in an exact manner and explore the pairing mechanism on the minimal model.

The contents of the present paper are as follows: in Section 2, the two-band minimal model is given with an explanation of the parameters, and the numerical calculation method including the measurement of the binding energy is briefly described. In Section 3, the numerical results are shown, and possible mechanisms are discussed in Section 4. Section 5 is devoted to summary.

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## 2. Two-band minimal model

There have been debates how many bands are essential to study the superconductivity mechanism in iron-based superconductors [2,9]. However, it is an accepted idea that the most active bands are two degenerate bands, i.e., $d_{xz}$ and $d_{yz}$ orbitals on Fe atoms. Thus, we make an exact analysis on the two-band model and would like to give an information on the pairing mechanism.

### 2.1. Model hamiltonian

The kinetic terms of the model Hamiltonian $H_{\rm kin}$ suggested by Daghofer et al. is given as follows [7],

$$\begin{aligned} H_{\rm kin} = & -t_1 \sum_{\boldsymbol{i},\sigma} \left( c^\dagger_{\boldsymbol{i},x,\sigma} c_{\boldsymbol{i}+\hat{\boldsymbol{x}},x,\sigma} + c^\dagger_{\boldsymbol{i},y,\sigma} c_{\boldsymbol{i}+\hat{\boldsymbol{y}},y,\sigma} + \text{H.c.} \right) \\ & - t_2 \sum_{\boldsymbol{i},\sigma} \left( c^\dagger_{\boldsymbol{i},y,\sigma} c_{\boldsymbol{i}+\hat{\boldsymbol{x}},y,\sigma} + c^\dagger_{\boldsymbol{i},x,\sigma} c_{\boldsymbol{i}+\hat{\boldsymbol{y}},x,\sigma} + \text{H.c.} \right) \\ & - t_3 \sum_{\boldsymbol{i},\sigma} \left( c^\dagger_{\boldsymbol{i},x,\sigma} c_{\boldsymbol{i}+\hat{\boldsymbol{x}}+\hat{\boldsymbol{y}},x,\sigma} + c^\dagger_{\boldsymbol{i},x,\sigma} c_{\boldsymbol{i}+\hat{\boldsymbol{x}}-\hat{\boldsymbol{y}},x,\sigma} + c^\dagger_{\boldsymbol{i},y,\sigma} c_{\boldsymbol{i}+\hat{\boldsymbol{x}}+\hat{\boldsymbol{y}},y,\sigma} + c^\dagger_{\boldsymbol{i},y,\sigma} c_{\boldsymbol{i}+\hat{\boldsymbol{x}}-\hat{\boldsymbol{y}},y,\sigma} + \text{H.c.} \right) \\ & - t_4 \sum_{\boldsymbol{i},\sigma} \left( c^\dagger_{\boldsymbol{i},x,\sigma} c_{\boldsymbol{i}+\hat{\boldsymbol{x}}+\hat{\boldsymbol{y}},y,\sigma} + c^\dagger_{\boldsymbol{i},y,\sigma} c_{\boldsymbol{i}+\hat{\boldsymbol{x}}+\hat{\boldsymbol{y}},x,\sigma} + \text{H.c.} \right) \\ & + t_4 \sum_{\boldsymbol{i},\sigma} \left( c^\dagger_{\boldsymbol{i},x,\sigma} c_{\boldsymbol{i}+\hat{\boldsymbol{x}}-\hat{\boldsymbol{y}},y,\sigma} + c^\dagger_{\boldsymbol{i},y,\sigma} c_{\boldsymbol{i}+\hat{\boldsymbol{x}}-\hat{\boldsymbol{y}},x,\sigma} + \text{H.c.} \right), \end{aligned} \tag{1}$$

where $c^\dagger_{\boldsymbol{i},\alpha,\sigma} (c^\dagger_{\boldsymbol{i},\alpha,\sigma})$ is the annihilation- (creation-) operator with spin $\sigma(=\uparrow,\downarrow)$ in the orbitals $\alpha = x, y$ ($d_{xz}$ and $d_{yz}$ orbitals, respectively) at site $\boldsymbol{i}$ of a two-dimensional square lattice as seen in Fig. 1, and $\hat{\boldsymbol{x}}$ and $\hat{\boldsymbol{y}}$ are unit vectors along the axes.

The original interaction Hamiltonian $H_{\rm int}$ consists of the following terms [7]:

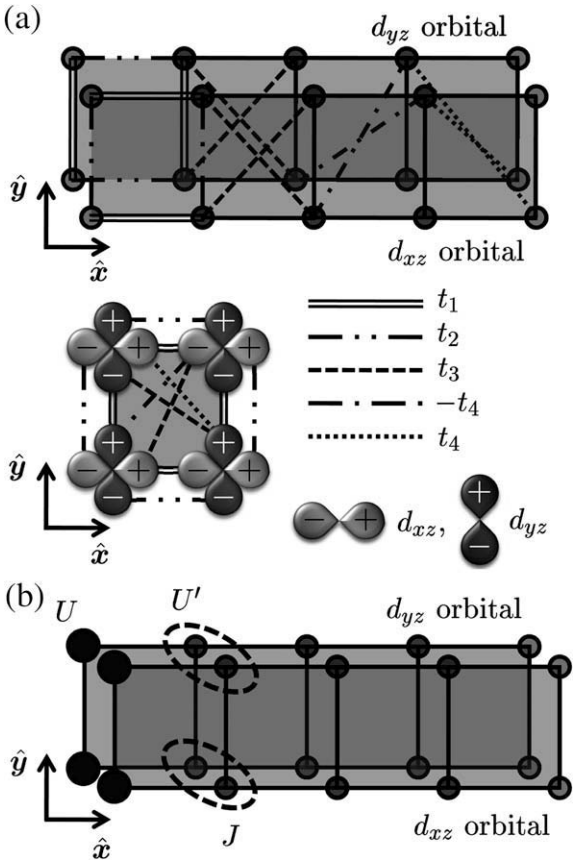


**Fig. 1.** Schematic figures of the simulated system, i.e., (a) $d_{xz}$ and $d_{yz}$ orbitals and the corresponding hopping parameters and (b) the interaction terms.

$$\begin{aligned} H_{\rm int} = & U \sum_{\boldsymbol{i},\alpha} n_{\boldsymbol{i},\alpha,\uparrow} n_{\boldsymbol{i},\alpha,\downarrow} + \left( U' - \frac{J}{2} \right) \sum_{\boldsymbol{i}} n_{\boldsymbol{i},x} n_{\boldsymbol{i},y} - 2J \sum_{\boldsymbol{i}} \boldsymbol{S}_{\boldsymbol{i},x} \cdot \boldsymbol{S}_{\boldsymbol{i},y} \\ & + J' \sum_{\boldsymbol{i}} \left( c^\dagger_{\boldsymbol{i},x,\uparrow} c^\dagger_{\boldsymbol{i},x,\downarrow} c_{\boldsymbol{i},y,\downarrow} c_{\boldsymbol{i},y,\uparrow} + \text{H.c.} \right), \end{aligned} \tag{2}$$

where $U$ is the on-site intra-band (for the same $\alpha$) Coulomb repulsion for electrons, $U'$ the on-site inter-band (for different $\alpha$) Coulomb repulsion, $J$ the Hund coupling, and $J'$ the pair-hopping term whose strength $J' = J$. $n_{\boldsymbol{i},\alpha}$ and $\boldsymbol{S}_{\boldsymbol{i},\alpha}$ are the matter density and spin density operators of orbital $\alpha$ at site $\boldsymbol{i}$, respectively. In this paper, we focus on the $U$ and $U'$ dependence of the binding energy. Since these parameter values are still open for argument, we independently vary $U$ and $U'$, respectively, and explore pairing on $U - U'$ space. In addition, for the third term, we omit all the terms except for the Ising-like Hund coupling for simplicity by considering that $U$ and $U'$ are more essential parameters for the present system. Thus, we employ the following reduced interaction Hamiltonian,

$$H_{\rm int,red} = U \sum_{\boldsymbol{i},\alpha} n_{\boldsymbol{i},\alpha,\uparrow} n_{\boldsymbol{i},\alpha,\downarrow} + U' \sum_{\boldsymbol{i}} n_{\boldsymbol{i},x} n_{\boldsymbol{i},y} - 2J \sum_{\boldsymbol{i}} S^z_{\boldsymbol{i},x} S^z_{\boldsymbol{i},y}. \tag{3}$$

### 2.2. Model parameters and measurements

For the hopping parameters, $t_1, t_2, t_3$, and $t_4$ in Eq. (1), we set $t_1 = 0.058t, t_2 = 0.220t, t_3 = -0.208t$, and $t_4 = -0.079t$, which are given in Ref. [7] with $pd\pi/pd\sigma = -0.2$ shown in the caption of Fig. 1 in Ref. [7], where $t$ is a unit of energy being of the order of 0.2 eV corresponding to $(pd\sigma)^2/\Delta_{pd}$ in Ref. [7]. The parameter set well reproduces the Fermi surface, although exact details are different from the band calculation.

Next, we mention about $U, U'$, and $J$. In usual cases, a relation among them is given by the rotational symmetry as $U' = U - 2J$. But, it is elusive if the relation exactly holds or not even on orbitals embedded on the crystalline. In addition, the electronic structure has been not fully understood. Then, we treat $U, U'$, and $J$ as free parameters.

In the present exact diagonalization studies, we calculate the binding energy,

$$E_{\rm b} \equiv E(N_\uparrow + 1, N_\downarrow) + E(N_\uparrow - 1, N_\downarrow) - 2E(N_\uparrow, N_\downarrow), \tag{4}$$

where $E(N_\uparrow, N_\downarrow)$ is the ground state energy for $N_\uparrow$ up and $N_\downarrow$ down spin fermions. This energy has the following meaning. The negative binding energy ($E_{\rm b} < 0$) indicates that an attractive interaction effectively works between two electrons. We evaluate $E_{\rm b}$ defined in Eq. (4) by using the exact diagonalization method on the Earth Simulator [10]. The calculated system is a two-leg square-lattice ladder ($2 \times 5$ sites) with two bands (see Fig. 1). We vary $U$ and $U'$ from 0 to 8 (the step value is 2) with $J = 0$ and 0.5 and examine the half-filling and lightly hole-doping cases. The doping rate $p$ is defined as $p = 0$ when $(N_\uparrow, N_\downarrow) = (10, 10)$, i.e., half-filling and $p = 0.1$ when $(N_\uparrow, N_\downarrow) = (9, 9)$, where $p \equiv N_{\rm hole}/L$, and $N_{\rm hole} \equiv L - N_\uparrow - N_\downarrow$, and $L$ are the number of holes and sites, respectively.

## 3. Numerical calculation results

Fig. 2 shows $U - U'$ contour plots for (a) $p = 0$ and (b) $p = 0.1$ when $J = 0$. From these figures, one finds $E_{\rm b} < 0$ in the two areas, in which $U' > U$ and $U' = U = 0$. Especially in the $p = 0$ case (Fig. 2a), there appears an additional $E_{\rm b} < 0$ region in $U' = 0$ and $U = 2$. These results indicate that a robust pairing emerges when $U' > U$ in the wide parameter range. This may be consistent with the fact that the iron-based superconductor has several varieties, e.g., La can be replaced by other rare-earth ones in LaOFeAs. Moreover, we notice in this case ($U' > U$) that an on-site s-wave pairing