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Mean-field state population study for iron-based superconductors

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ABSTRACT

The occupation number distribution in momentum space are theoretically studied within a two-orbital model, which can be unified describing the low-energy physics of the iron pnictides and iron chalcogenides. The mean-field approximation of Hubbard interaction is employed. By tuning the hopping parameters, the difference between the iron pnictides and iron chalcogenides in their occupation number distribution behavior can be clearly observed. The results show that when the pairing interaction tends to zero, the occupation number $n(\mathbf{k}) \approx 0$ at Γ point for iron chalcogenides while $n(\mathbf{k}) \approx 2$ at Γ point for iron pnictides. By increasing the strength of the pairing interaction to a large value, the change of $n(\mathbf{k})$ at Γ point for iron chalcogenides (pnictides) is remarkable (unremarkable). In addition, we find that the effect of the nearest-neighbor coupling between the two layers, contained in the S_4 model [Hu and Hao, (2012) [33]], is very weak.

1. Introduction

Iron-based superconductors [1–3], as a new family of high-T_c superconducting materials, have been the focus of intense interest in condensed matter physics since its first experimental discovery in 2008 [4]. The discovery of iron-based superconductors not only breaks the widely accepted concept that iron is antagonistic against superconductivity, but also exposes a rich variety in candidate materials and in pairing interaction [5]. Iron-based superconductors possess several unique properties, such as high upper critical field, high-T_c superconductivity [6–9], isotropic superconducting gaps around Fermi surfaces [10–14], robustness to impurity [15,16], excellent grain boundary character, and so on. Since the report of $T_c = 26$ K in $LaFeAsO_{1-x}F_x$ [4], several ten superconducting materials have been reported in layered iron pnictides [3,6,17,4,18] or chalcogenides [19]. Very recently, a monolayer FeSe deposited on $SrTiO_3$ substrate [8,20] exhibits a dramatic increase in its superconducting transition temperature T_c up to 110 K [21] compared to the bulk FeSe whose critical temperature $T_c \approx 9.4$ K [22]. This novel electronic property is because of the extraordinary potential of interface engineering.

These iron-based materials contain a common building block of square lattice of Fe^{2+} ions which take tetrahedral coordination with pnictide or chalcogenide ions. However, their electronic structures, in particular, the Fermi surface topologies, are quite different in the materials that reach high T_c. The hole pockets are absent in iron chalcogenides but present in iron pnictides [8]. Comparing with the well known cuprates [23], the complex Fermi surface of the iron-based superconductors is determined by several bands [24–35] since their parent compounds are metallic [36]. Their complicated multiple-*d*-orbital electronic structures results in the considerable controversy over the choice of the appropriate microscopic Hamiltonian. Therefore, it is important to understand superconductivity in multiorbital systems in general terms [32]. The pairing interaction [24–27] is related to the structure of Fermi surface, the hybridization between orbitals, competition and/or cooperation between spin-fluctuation and orbital-fluctuation, and the symmetry of the system. Based on the B_{2g} symmetry and mean-field approximation, Moreo et al. [37] have discussed the dependence of both intra-band and inter-band pairings on the hybridization among orbitals in the pnictides superconductors. Recently, Hu and Hao [33] proposed an effective two-orbital model Hamiltonian near half filling which unifies the iron pnictides and iron chalcogenides. They demonstrated that the underlying electronic structure for their high-T_c superconductivity is protected by the S_4 symmetry. By tuning the hopping parameters, their model is capable of quantitatively explaining the experimental results by angle-resolved photoemission microscopy [10,38,39].

In this work, we study the quasiparticle occupation number distribution in momentum space by employing a minimal two-orbital model reduced from the S_4-symmetry model [33], which can be unified describing the low-energy electronic structure of the iron pnictides and iron chalcogenides. We treat the Hubbard interaction

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via the mean-field approximation. Our results show that the occupation states depend on the hopping parameters and the pairing interactions. The difference between the iron pnictides and iron chalcogenides could be clearly revealed in their occupation number distribution behavior in the momentum space. For instance, on one side, when the pairing interaction is absent, the occupation number $n(\mathbf{k}) \approx 0$ at Γ point for iron chalcogenides, while $n(\mathbf{k}) \approx 2$ at Γ point for iron pnictides. On the other side, by increasing the strength of the pairing interaction to a large value, the change of $n(\mathbf{k})$ at Γ point for iron chalcogenides is remarkable, while it is unremarkable for the case of iron pnictides. In addition, we find that the effect of the nearest-neighbor coupling between the two layers, contained in the S_4 model, is weak enough to be ignored.

2. Model and method

We start from a general effective model, which describes iron-based superconductors obeying the S_4 symmetry,

$$\hat{H}_{eff} = \hat{H}_0 + U \sum_{i,\alpha=1,2} \hat{n}_{i,\alpha\uparrow}\hat{n}_{i,\alpha\downarrow} + U' \sum_i \hat{n}_{i,1}\hat{n}_{i,2} + J'_H \sum_i \hat{\mathbf{S}}_{i,1} \cdot \hat{\mathbf{S}}_{i,2}. \quad (1)$$

Here, $\hat{H}_0$ is an effective S_4-symmetric tight-binding two-orbital model employed in Ref. [33], which can be written as a matrix form

$$\hat{H}_0 = \sum_{\mathbf{k},\sigma} \begin{pmatrix} h_{11}(\mathbf{k}) & h_{12}(\mathbf{k}) & h_{13}(\mathbf{k}) & 0 \\ h_{12}(\mathbf{k}) & h_{22}(\mathbf{k}) & 0 & -h_{13}(\mathbf{k}) \\ h_{13}(\mathbf{k}) & 0 & h_{33}(\mathbf{k}) & -h_{12}(\mathbf{k}) \\ 0 & -h_{13}(\mathbf{k}) & -h_{12}(\mathbf{k}) & h_{44}(\mathbf{k}) \end{pmatrix}, \quad (2)$$

in the base of $\{ c_{\mathbf{k}\sigma},\ c_{\mathbf{k}+\mathbf{Q}\sigma},\ d_{\mathbf{k}\sigma},\ d_{\mathbf{k}+\mathbf{Q}\sigma} \}$ with c and d being the Fermion operators for the two groups. One group includes the d_{xz} orbital in the Fe_1 sublattice and the d_{yz} orbital in the Fe_2 sublattice, and the other group includes the d_{xz} orbital in the Fe_2 sublattice and the d_{yz} orbital in the Fe_1 sublattice, where Fe_1 and Fe_2 label the two sublattices of the iron square lattice [33]. The corresponding lattice structure is shown in Fig. 1. The matrix elements in Hamiltonian (2) can be explicitly written as

$$h_{11/22} = \pm 2t_{1s}(\cos k_x + \cos k_y) \pm 2t_{1d}(\cos k_x - \cos k_y) + 4t_{2s}\cos k_x \cos k_y + 2t_{3s}(\cos 2k_x + \cos 2k_y) + 2t_{3d}(\cos 2k_x - \cos 2k_y) - \mu, \quad (3)$$

$$h_{33/44} = h_{11/22} \mp 4t_{1s}(\cos k_x + \cos k_y) - 4t_{3d}(\cos 2k_x - \cos 2k_y), \quad (4)$$

$$h_{12} = 4t_{2d}\sin k_x \sin k_y, \quad (5)$$

$$h_{13} = 2t_c(\cos k_x + \cos k_y), \quad (6)$$

where t_{is}, t_{id}, and t_c are the hopping parameters, with $i = 1, 2, 3$, labels s and d respectively indicating hoppings of the s-wave type and d-wave type, and c indicating the nearest-neighbor coupling between the two layers [33]. In Eq. (1), U describes the effective Hubbard repulsion interaction within each component, U' describes the one between them, and J'_H describes the effective Hund's coupling. $\alpha = 1, 2$ labels the S_4 isospin. Since the two components couple weakly, U is expected to dominate over U' and J'_H. In the first-order approximation, the model could become a Hubbard model near half filling,

$$\hat{H}_{eff} = \hat{H}_0 + U \sum_{i,\alpha=1,2} \hat{n}_{i,\alpha\uparrow}\hat{n}_{i,\alpha\downarrow}. \quad (7)$$

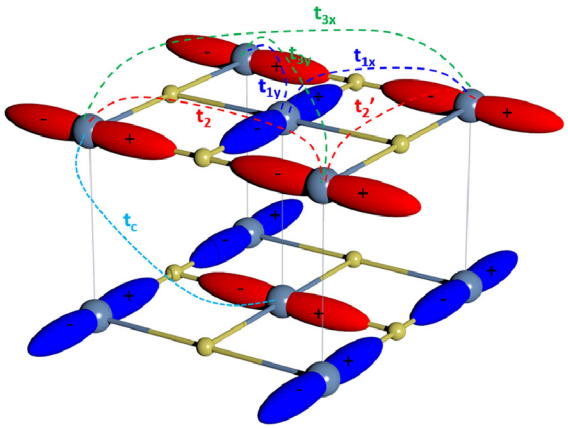

Fig. 1. (Color online) The lattice structure associated with the lattice Hamiltonian $\hat{H}_0$. One cell includes two Fe ions shown as blue and red balls forming two sublattices. The hopping parameters are indicated: t_{1x} and t_{1y} are for the nearest-neighbor hopping; the next-nearest-neighbor hoppings are t_2 and t'_2; and the third next-nearest-hopping is marked by t_{3x} and t_{3y}. The coupling between the two layers is indicated by t_c.

Furthermore, t_c is smaller than other hopping parameters and can be ignored. Thereby, if we only consider the d_{xz} orbital in the Fe_1 sublattice and the d_{yz} orbital in the Fe_2 sublattice, and the Hubbard interaction U, a reduced effective tight-binding two-orbital model can be written as following form

$$\hat{H}^{one}_{eff} = \hat{H}^{one}_0 + U \sum_i \hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow}, \quad (8)$$

where just S_4 isospin-up (i.e., $\alpha = 1$) is considered, and $\hat{H}^{one}_0 = \sum_{\mathbf{k},\sigma} \begin{pmatrix} h_{11} & h_{12} \\ h_{12} & h_{22} \end{pmatrix}$ in the base of $\{ c_{\mathbf{k},\sigma},\ c_{\mathbf{k}+\mathbf{Q},\sigma} \}$. The tight-binding single-orbital model (8) is what we will use to study the paring operator property and the occupation number distribution in the following discussions. By performing the Fourier transformation and the mean-field approximation, Hamiltonian (8) could be further reduced to a mean-field one

$$\hat{H}_{MF} = \hat{H}^{one}_0 + V \sum_{\mathbf{k}} \Big(c_{-\mathbf{k},\downarrow}c_{\mathbf{k},\uparrow} + c^\dagger_{\mathbf{k},\uparrow}c^\dagger_{-\mathbf{k},\downarrow} + c_{-\mathbf{k}-\mathbf{Q},\downarrow}c_{\mathbf{k}+\mathbf{Q},\uparrow} + c^\dagger_{\mathbf{k}+\mathbf{Q},\uparrow}c^\dagger_{-\mathbf{k}-\mathbf{Q},\downarrow} \Big). \quad (9)$$

Here, we have used the strength of the pairing interaction $V = U\Delta$ and the mean-field parameter $\Delta = (\delta + \delta')$ with $\delta = \frac{1}{N} \times \sum_{\mathbf{k}} \langle c_{-\mathbf{k},\downarrow}c_{\mathbf{k},\uparrow} \rangle = \frac{1}{N}\sum_{\mathbf{k}} \langle c^\dagger_{\mathbf{k},\uparrow}c^\dagger_{-\mathbf{k},\downarrow} \rangle$, and $\delta' = \frac{1}{N}\sum_{\mathbf{k}} \langle c_{-\mathbf{k}-\mathbf{Q},\downarrow}c_{\mathbf{k}+\mathbf{Q},\uparrow} \rangle = \frac{1}{N}\sum_{\mathbf{k}} \langle c^\dagger_{\mathbf{k}+\mathbf{Q},\uparrow}c^\dagger_{-\mathbf{k}-\mathbf{Q},\downarrow} \rangle$.

The four Bogoliubov quasi-particle eigenvalues ($\pm E_A$ and $\pm E_B$) of $\hat{H}_{MF}$ are given in Figs. 2 and 3 for different parameters. Namely, Fig. 2 shows the energy spectrum of iron pnictides, while Fig. 3 shows the energy spectrum of iron chalcogenides. Clearly, (i) when the pairing interaction vanishes, the hole pocket is present (absent) at Γ point in the case of iron pnictides (chalcogenides), see Fig. 2(a) and 3(a) respectively; (ii) due to the nontrivial V different from zero, the $\pm E_B$ bands are separated by a gap restricted to the original Fermi surfaces, see Figs. 2(b) and 3(b). From Figs. 2 and 3, we know that by ignoring t_c and just keeping the three largest parameters t_{1s}, t_{2s}, and t_{2d} in $\hat{H}^{one}_0$, the model (9) is already good enough to capture the main characteristics of the bands contributing to Fermi surfaces [33]. Therefore, in the following discussions, we focus on the reduced mean-field model (9). Similar mean-field approximation can also be performed to the effective Hamiltonian (7), which is not shown for briefness.

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