Influence of electronic correlations on orbital polarizations in the parent and doped iron pnictides

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Abstract

Orbital polarization and electronic correlation are two essential aspects in understanding the normal-state and superconducting properties of multi-orbital FeAs-based superconductors. In this paper, we present a systematic study on the orbital polarization of iron pnictides from weak to strong Coulomb correlations within the Kotliar–Ruckenstein slave boson approach. The magnetic phase diagram of the two-orbital model for LaFeAsO clearly shows that a striped antiferromagnetic metallic phase with orbital polarization exists over a wide doping range, in addition to the Slater-type insulator, Mott insulator and paramagnetic phases. A reversal of the orbital polarization occurs in the intermediate correlation regime in the absence of the crystal field splitting; however, a small crystal field splitting considerably enhances the orbital polarization, and stabilizes the $xz$-type orbital order. We argue that the ferro-orbital polarization is characteristic of a density wave, and leads to a pseudogap-like behavior in the density of states.

(Some figures may appear in colour only in the online journal)

1. Introduction

Since the discovery of high-$T_c$ superconductivity (SC) in doped iron pnictides\cite{1–3}, the iron-based high-$T_c$ SC material has been the subject of intensive research for the past two years. Among various factors influencing the normal-state and SC-state properties of iron pnictides, electronic correlation and orbital polarization are essential. The parent phases of cuprates are Heisenberg antiferromagnets (AFMs) and insulators, and the important role of the electronic correlation and dominant single-orbital hole with $x^2-y^2$ symmetry are well established and verified. Unlike the high-$T_c$ cuprates, the parent phase of iron pnictide SC is a bad metal\cite{2}, and usually exhibits spin-density wave (SDW)-type or striped AFM (SAFM) ordering\cite{3, 4}. The role of the electronic correlation and how many Fe 3d orbitals are involved in the iron pnictides are two essential aspects for understanding various properties in the SAFM metallic and SC phases.

To date, the experimental evidence on the role of electronic correlation in the parent phase and SC phases is controversial. Indeed, the metallic conductivity\cite{1, 2}, small magnetic moment of Fe spins\cite{4}, x-ray absorption spectroscopy (XAS) and resonant inelastic x-ray scattering (RIXS) of Fe in undoped iron pnictides seem to suggest a weak correlation between Fe 3d electrons\cite{5}. From the resonant x-ray emission spectroscopy (RXES) of Fe 3d $L_2,L_3$ edges, Kurmaev \textit{et al}\cite{6} suggested that the 111 phase is a weakly or at most moderately correlated system. However, many more experimental clues have demonstrated the band narrowing effect, suggesting the importance of the 3d electronic correlation\cite{5–7}. In fact, in addition to the band narrowing effect, the existence of intermediate magnetic moments in the 1111, 122 and 111 phases also shows...
the importance of the electronic correlation. Therefore one should employ an approach applicable for a general Coulomb interaction so as to uncover the roles of electronic correlations in the electronic states and the magnetic configurations in undoped and doped iron pnictides. Recently a few authors have attempted to uncover the role of the electron correlation in iron pnictides theoretically [8–13]. These authors found that an intermediate electronic correlation could reasonably address the SAFM metallic ground state together with a small magnetic moment in undoped iron pnictides. They showed that the electron correlation plays a considerable quantitative role in the spin-density wave ground state.

On the other hand, there is still active debate in the literature over how many orbitals are involved and what the orbital symmetry of the bands near $E_F$ is in the parent and doped iron pnictides. Theoretically, two-orbital [10, 14], three-orbital [15], four-orbital [16] and even five-orbital [17, 18] tight-binding models have been proposed. Most of the multi-orbital tight-binding models captured the major Fermi surface and dominant band-structure characters near $E_F$ of the 1111 and 122 phases. It is essential to distinguish the validity of these models to reveal the symmetry character and the number of orbitals involved. The orbital polarization could provide useful information on the orbitals involved in various iron pnictides. Some works have tried to answer this orbital related problem. For example, Kubo and Thalmeier [10] found a weak orbital polarization in the weak correlation approximation. However, it remains unclear how the electronic correlation affects the orbital polarization, and which physical elements mostly influence the orbital polarization in iron pnictides. This calls for further study both in theory and in experiment.

To further uncover the roles of the electronic correlation and orbital polarization in high-$T_c$ iron pnictide SCs, we apply the Kotliar–Ruckenstein slave boson (KRSB) method [19] on the two-orbital Hubbard model. The KRSB approach and its extension may provide a useful tool to treat the multi-orbital Hubbard model over a wide correlation range. It also has a few advantages in dealing with multiple orbitals, nontrivial magnetic configurations and spatial correlations. Our recent numerical ansatz developed for the multi-orbital KRSB solution overcomes the convergence of many parameters in minimizing the ground state energy, and is suitable for treating an arbitrary Coulomb interaction in the presence of inter-orbital hoppings or hybridizations and various magnetic configurations.

In the rest of this paper, we briefly introduce the model Hamiltonian and KRSB methods in section 2. In section 3, we first present the magnetic phase diagram of the two-orbital model and demonstrate that in intermediate and strong electronic correlation the SAFM metallic phase with small magnetic moment is stable against the paramagnetic (PM), ferromagnetic (FM) and Néel AFM phases, accompanied with a small orbital polarization, or a ferro-orbital density wave (F-ODW) order. In addition, at half-filling there also exists a PM metallic for a small $U$, a Slater-type insulator for a comparatively strong $U$, and a Mott insulator for a strong $U$. A small crystal field splitting arising from the lattice distortion further stabilizes the SAFM and ferro-orbital ground state. The evolution of the orbital occupation with the electron correlation shows that the contribution of the $d_{z^2}$ orbital is larger than that of the $d_{x^2-y^2}$ orbital. These results clearly show the importance of the intermediate electronic correlation and small orbital polarization in the parent and doped phases of iron pnictides. Section 4 is devoted to the discussion and summary.

2. Model Hamiltonian and methods

We start with a two-orbital model Hamiltonian $H = H_0 + H_I$ applied for iron pnictides in real space with

$$H_0 = - \sum_{i,j,\alpha,\beta,\sigma} (\epsilon_{i\alpha} \delta_{\alpha\beta} c_{i\alpha\sigma}^\dagger c_{j\beta\sigma} + \text{h.c.}) + \sum_{i,\alpha,\sigma} (\epsilon_{i\alpha} - \mu) n_{i\alpha\sigma} \quad (1)$$

$$H_I = U \sum_{i,\sigma} n_{i\uparrow\sigma} n_{i\downarrow\sigma} + \sum_{i,\sigma,\sigma',\alpha,\beta} (U' - 2J_H \delta_{\alpha\beta}) n_{i\alpha\sigma} n_{i\beta\sigma'} \delta_{\sigma\sigma'} - J_H \sum_{i,\alpha,\beta \neq \alpha} (c_{i\alpha\uparrow}^\dagger c_{i\alpha\downarrow}^\dagger c_{i\beta\downarrow} c_{i\beta\uparrow} - c_{i\alpha\downarrow}^\dagger c_{i\alpha\uparrow}^\dagger c_{i\beta\uparrow} c_{i\beta\downarrow}), \quad (2)$$

where $c_{i\alpha\sigma}^\dagger$ creates an electron with orbital index $\alpha$ and spin $\sigma$ at lattice site $i$, $\epsilon_{i\alpha}$ is the energy level of the $\alpha$ orbital, and $n_{i\alpha\sigma}$ is the corresponding occupation number operator. The hopping integral for the orbitals $\alpha$ and $\beta$ is denoted by $t_{i\alpha\beta}$. The intraband (inter-band) Coulomb repulsion and Hund’s rule coupling are denoted by $U'$ and $J_H$, respectively. Here we set $U' = U = 2J_H$ and $J_H = 0.2U$. To investigate the ground state electronic and magnetic properties of iron pnictides, we adopt the hopping parameters of Raghu et al [14] for the two-orbital situation in the present slave boson scheme. The unit of the hopping parameters $t_i$ is taken as 0.3 eV; such a choice can give rise to the correct bandwidth in LaFeAsO [20]. In the two-orbital situation, the orbitals 1 and 2 refer to the $d_{x^2-y^2}$ and $d_{z^2}$ components, respectively.

To reflect the multi-orbital character of iron pnictides, we extend the single-orbital KRSB approach [19] to the two-orbital Hubbard models for various magnetic configurations. In the multi-orbital Hubbard model, a few auxiliary boson field operators representing the possibilities of various electron occupations are introduced, such as $e, p, d, b, t$ and $q$, which denote the possibilities of no, single, orbital-singlet double, spin-singlet double, triplicate and quaternary occupations, respectively. With these auxiliary boson fields, an original fermion operator can be expressed as

$$c_{i\alpha\sigma}^\dagger = Q_{i\alpha\sigma}^{-1/2} \left( p_{i\alpha\sigma}^\dagger e_i + h_{i\alpha}^\dagger p_{i\alpha\sigma} + \sum_{\sigma'} d_{i\alpha\sigma\sigma'}^\dagger p_{i\sigma'\sigma} + t_{i\alpha\sigma}^\dagger h_{i\sigma\sigma} \right) + \sum_{\sigma'} t_{i\alpha\sigma\sigma'}^\dagger d_{i\alpha\sigma\sigma'} + q_{i\alpha\sigma}^\dagger I_{\alpha\sigma} (1 - Q_{i\alpha\sigma})^{-1/2} f_{i\alpha\sigma}^\dagger. \quad (3)$$

Here $f_{i\alpha\sigma}^\dagger$ is the new slaved fermion operator and $Q_{i\alpha\sigma}$ is an auxiliary particle number operator [19]. Projecting the original fermion operators into these boson field and fermion field operators, one could not only obtain an effective Hamiltonian, but also get the ground state energy in the
saddle point approximation with the normalization condition and the fermion number constraints [19]. Here we employ a generalized Lagrange multiplier method to enforce these constraint conditions [21], thus the inter-orbital hoppings and crystal field splitting can be treated on the same footing. The fermion occupation number is constrained with the penalty function method [21].

To enforce the normalization condition, we have a boundary constrained condition:

\[ 1 \geq \sum_{\alpha, \sigma} n_{\sigma}^2 + \sum_{\alpha} b_{\alpha}^2 + \sum_{\alpha, \sigma} d_{\alpha, \sigma}^2 + \sum_{\alpha, \sigma} f_{\alpha, \sigma}^2 + q^2. \] (4)

We use an optimizing method to get the minimized ground state energy. To search for possible ground states, we study four different magnetic configurations, including the PM or nonmagnetic, FM, Néel AFM and SAFM phases so as to find the stable ground state. As the penalty factor is sufficiently large, the particle number constraint is satisfied. Nevertheless, the problem of the boundary constrained condition is still difficult. In numerically searching the global minima of the ground state energy, we employ the search method [22], together with the gradient method and the Rosenbrock method [23]. If the optimizing point is on the boundary, we move one step inward on the high-dimensional ellipsoid on the equipotential surface. Since the first axis of the new local orthogonal coordinate system of the Rosenbrock method is directed in the negative gradient direction, the corresponding algorithm is straightforward.

### 3. Numerical results

We first obtain the magnetic phase diagram of the two-orbital system through comparing the energies of the PM (or nonmagnetic), FM, Néel AFM and SAFM configurations. In the present symmetric orbital situation, the penalty factors adopted for the two degenerate orbitals are identical. This will save a great deal of computation time in minimizing the total energy.

Figure 1 displays the zero-temperature magnetic phase diagram in the \( U-n \) plane. We consider the full Hund’s coupling \( J_{H} \), which equals 0.2\( U \). One notices that only the PM metallic phase is stable when the on-site Coulomb interaction \( U < U_{c1} \approx 1.2 \text{ eV} \). When \( U > U_{c1} \), the SAFM phases are stable over wide doping and interaction ranges. This SAFM region can be divided into a high magnetic moment one (denoted as SAFM(HM)) with \( m > 1 \mu_B \) and a low magnetic moment one (denoted as SAFM(LM)) with \( m < 1 \mu_B \). The latter lying in \( U_{c1} < U < U_{c2} \) is the most interesting and is marked with shading since the magnetic moments of most parent and doped phases of iron pnictides, including the 1111, 122 and 111 phases, fall into this region. In the present phase diagram, it is also shown that the SAFM(LM) regime is limited to the intermediate strength \( U \) in a narrow range, as seen the marked area in figure 1.

Especific interest is found around the particle-filling number \( n = 2 \). The SAFM(LM) regime ranges from \( U_{c1} = 1.2 \text{ eV} \) to \( U_{c2} = 2.4 \text{ eV} \) at half-filling. One notices that the phase diagram is not symmetrical about the half-filling (\( n = 2 \)); this is due to the presence of the next nearest-neighbor hopping. When \( U > U_{c1} \), the system with half-filling enters the Slater-type insulating phase, in which the insulating gap fully opens due to the formation of SAFM ordering and spin modulation [24]. In this SAFM insulating phase the energy gap and the exchange splitting between the spin-down and spin-up subbands, and the sublattice magnetic moment increase with the increase of \( U \). In this Slater-type insulating regime, both the energy gap and the spin exchange splitting are much smaller than \( U \). Distinctly different from the Mott insulator in the nonmagnetic situation, the present band narrowing factor \( Z \) is not zero, and slightly increases with increase of \( U \). In particular, it is worth pointing out that in this Slater-type insulating case \( Z \) is no longer proportional to the quasiparticle weight at \( E_F \), since the system goes beyond the Fermi liquid regime. Hence \( Z \) could not be used as the criterion of the metal–insulator transitions.

When the electronic correlation becomes so strong that \( U > 5 \text{ eV} \), the system enters another full gapped region, i.e., the conventional Mott insulating phase. We separate the phase boundary between the Slater insulating phase and the Mott insulating one from the local maximum of the band narrowing factor \( Z \), which gradually increases with the increase of \( U \) in the Slater region and then slightly decreases with \( U \) in the Mott region. In the Mott insulating region, with the further increase of the Coulomb interaction \( U \), the sublattice magnetic moment almost saturates; the energy gap and the spin exchange splitting still gradually increase with increase of \( U \) and are almost comparable with \( U \). In comparison with the conventional paramagnetic Mott phase, this Mott phase is SAFM ordering, which can be equivalent to the Heisenberg \( J_1-J_2 \) model. As shown in the following, orbital polarization is observed in wide doping and interaction regimes, while no orbital polarization is seen at \( n = 2 \) when the correlation becomes sufficiently strong.

For more clarity, we plot the correlation dependence of the ground state energies in the PM phase and the SAFM phase in Figure 2. Also an energy difference, \( E_{PM} - E_{SAFM} \),
between these two phases is displayed. One finds that when the electronic correlation is weak, or \( U < U_{c1} \), the energy difference is very small and negative. So the PM phase is stable against the SAFM one. When the correlation reaches intermediate strength so that \( U > U_{c1} \), the energy difference becomes large and positive, and the SAFM phase becomes more stable than the PM one. Furthermore, one could estimate the magnitudes of the magnetic couplings between iron spins. The magnetic coupling strength crucially depends on the doping concentration and electron correlations, as seen in figure 2. For a typical parent compound LaOFeAs, the on-site Coulomb correlation between Fe 3d electrons is estimated to be about 2–3 eV [25]. When \( U = 2 \) eV, this gives rise to a magnetic coupling strength of about 7 meV at \( n = 2 \), of the same order of magnitude as the spin coupling between Fe ions in LaOFeAs deduced from neutron scattering experiments [4].

Figure 3 displays the evolution of the sublattice magnetic moments with the increase of electronic correlation. It shows that the system remains PM without any magnetic ordering unless \( U \) is larger than the PM–SAFM(LM) critical point \( U_{c1} \). In the realistic parameter range, i.e., the intermediate correlation regime, the magnetization decreases with increasing doping concentration for \( n < 2 \). This is in agreement with the universal experimental behavior [3, 26]. However, the sublattice magnetic moment for \( n > 2 \) becomes larger than that at \( n = 2 \) in the intermediate correlation regime, which is not consistent with experimental observations [27]. We notice that at half-filling the lower critical value of \( U_{c1} \) for the appearance of a magnetic moment in the sublattice is about 1.2 eV, or \( U_{c1}/t_1 \approx 4 \), which is considerably larger than the mean-field result for the two-orbital model, \( U_{c1}/t_1 \approx 2.9 \) [10, 28]. It is also found that the sublattice magnetic moment increases continuously until \( U \) reaches \( U_{c2} = 2.4 \) eV, and then the system enters the SAFM(HM) region when \( U \) is further increased. Such a behavior was also found by Yu et al in their mean-field solution for the four-orbital model [11]. Further, the upper critical value for the SAFM(HM) region with \( m > 1\mu_B \) is \( U_{c2} = 2.4 \) eV (or \( U_{c2}/t_1 \approx 8 \)) in the half-filling system, also significantly larger than the mean-field result \( U_{c2}/t_1 \approx 5 \) [10, 28, 29]. These results suggest that the quantum fluctuations are well considered within the present KRSB approach.

At half-filling, when \( U > U_{c2} = 2.4 \) eV, the SAFM system enters the high magnetic moment region with \( m > 1\mu_B \) in figure 3, which also can be seen in figure 1. By monitoring the density of states (DOS) near the Fermi surface, we find that the half-filled system becomes Slater-type insulating in the SAFM(HM) region. Notice that when the systems cross over from the SAFM insulating phase to the full-gap Mott one, the sublattice magnetic moments of the systems with \( n = 1.9 \) and 2.1, or 1.95 and 2.05, approach the same values, as seen in figure 3, showing that the electron–hole symmetry is partially restored in the strong correlation regime.

In the present two-orbital model, we can address the orbital polarization problem in the parent and doped phases of LaOFeAs. We find that in the weakly correlated PM phase, due to the equivalence of the present two orbitals, the symmetry of the orbital space is not broken; no orbital polarization is observed. As soon as the system enters the intermediate correlated SAFM phase, a small orbital polarization is observed, as seen in figure 4. Figure 4(a) shows that in the SAFM phase, the orbital polarization considerably depends on the Coulomb correlation and particle filling. When \( n < 2 \), the orbital polarization is negative, or the \( d_{yz} \) component is elevated with the increase of \( U \). This shows that in electron-doped iron pnictides the orbital polarization is \( yz \)-type, implying that the lattice distorts from a tetragonal phase to an orthorhombic one with the lattice parameter in the \( y \)-axis, \( b \), larger than that in the \( x \)-axis, \( a \), which is in disagreement with the experimental data [30, 31]. At \( n = 2 \), orbital polarization only occurs in the intermediate correlation regime, and the polarization is reversed at \( U_0 = 1.9 \) eV; when \( U_{c1} < U < U_0 \) the polarization is dominated by the \( d_{xz} \) component, while it is dominated by the \( d_{yz} \) component as \( U_0 < U < U_{c2} \); when \( U > U_{c2} \), due to the strong correlation...
and large Hund’s coupling, both of the two orbitals are singly occupied, giving rise to a vanishing polarization. This behavior was also found in the conventional mean-field approximation [10, 28]. One may find in figure 4(a) that the \( \alpha \)-type orbital polarization in the intermediate correlation regime at \( n = 2 \) is consistent with the orthorhombic crystal structure of the parent phase in LaFeAsO, in which the lattice parameter in the \( x \)-direction, \( a \), is slightly larger than that in the \( y \)-direction, \( b \) [30, 31].

In the system with \( n > 2 \), we find in figure 4(a) that the orbital polarization also reverses sign at about \( U_0 = 1.9 \) eV. This shows that with the increase of doping concentration away from half-filling, the \( \alpha \)-type orbital polarization gradually vanishes, changes its sign at \( U_0 \) and becomes \( \alpha \)-type polarized. This implies that with increasing doping deviating from \( n = 2 \) the crystal structure of the FeAs compound (\( U = 1.8 \) eV) will transit from orthorhombic with \( a > b \) to another orthorhombic phase with the lattice distortion of \( b \) slightly larger than \( a \). However such a sign change in the orbital polarization and the re-entrance to the orthorhombic phase have never been found experimentally. We attribute this to the neglect of the elastic energy and the crystal field splitting in figure 4(a). Also it is possible that more orbitals need to be taken into account.

Meanwhile, we notice that in the half-filled system, the orbital polarization is rather small. Similar behavior was also found in our early mean-field results [28] and Kubo et al’s paper [10]. Such a weak orbital polarization in the intermediate correlation regime at \( n = 2 \), as shown in figure 4(a), is obviously driven by the anisotropic SAFM ordering, since the latter breaks the spatial rotation symmetry of the system, leading to a weak orbital polarization in the SAFM metallic ground state. Although the orbital polarization is rather weak, it may be greatly enhanced by a crystal field splitting, as shown in figure 4(b). One finds that at \( \Delta = 0.09 \) eV the orbital polarization is about ten times larger than that at \( \Delta = 0 \), and the sign does not reverse anymore over a wide correlation regime, while a kink at \( \Delta = 0 \) still exists for various crystal field splittings.

It is well known that such an orbital polarization will result in a lattice distortion, and the lattice distortion will separate the two orbitals through a crystal field splitting and an elastic energy. The consideration of the crystal field splitting and the elastic energy further enhances the orbital polarization and stabilizes the ferro-orbital ordering [28]. Furthermore, our mean-field results showed that a realistic multi-orbital model taking into account more orbitals may greatly enhance the orbital polarization [28, 32]. So we expect that a realistic multi-orbital model taking into account lattice distortion will exhibit a considerable orbital polarization.

Besides, we also display the correlation dependence of the quasiparticle DOS near \( E_F \) for the present two-orbital systems in figure 5. It is found that the DOS increases slowly in the weakly correlated PM regime (\( U < U_{c1} \)). In the intermediate correlation regime, the DOS first steeply decreases and then slightly increases in the metallic SAFM ordered phase with small magnetic moment, showing a pseudogap-like behavior. The larger the crystal field splitting is, the stronger the pseudogap character. This shows that the pseudogap is associated with ferro-orbital polarization or density-wave-type ferro-orbital ordering. The pseudogap in the intermediate correlation regime turns to a full gap in the Slater-type insulating phase when \( U > U_{c2} \). From the analysis of the spin-dependent partial DOS, we find that this full gap is triggered by the spin polarization. When \( U > U_{c3} \), the system enters a conventional Mott insulator phase, and the total DOS completely vanishes.

These results clearly demonstrate that the ferro-orbital polarization is accompanied by the onset of SAFM ordering in the intermediate correlated iron pnictides. In the intermediate correlation regime, the system is metallic. Then a question naturally arises as to what the nature of the ferro-orbital ordering in metallic iron pnictides is. Obviously, such an orbital polarization is essentially itinerant, similar to the

Figure 4. Dependences of the orbital polarizations on the doping concentration (a) and crystal field splitting (b) in the two-orbital model. \( \Delta \) is measured in units of electronvolts. The particle number is \( n = 2 \) in (b).

Figure 5. The density of states (DOS) at the Fermi surface as a function of \( U \) for different crystal field splittings.
itiernant FM in 3d transition metals. Hence one expects that the orbital polarization and ferro-orbital ordering in iron pnictides are characteristics of the density wave. As we pointed out in an earlier paper [33], such an itinerant ferro-orbital ordering can occur as soon as a Stoner-like condition is satisfied [33].

4. Remarks and summary

As addressed in the above, the parent phases of iron pnictides, such as the 1111, 122 and 111 phases, fall into As addressed in the above, the parent phases of iron pnictides, such as the 1111, 122 and 111 phases, fall into the intermediate correlated regime [8, 12, 13, 29]. The intermediate correlation could not only address the fact that the energy bandwidth of BaFe$_2$As$_2$ observed in the ARPES experiments [7] is only half of that calculated by the LDA approach, but also contribute the local magnetic moment and the small orbital polarization. Our present slave boson results, together with those of the variational Monte Carlo calculation by Kubo and Thalmeier [29], and Gutzwiller variational wavefunctions by Zhou and Wang [8] and Schickling et al. [12, 13], show that the critical value $U_c$ for the formation of local magnetic moment is much larger than that obtained by the Hartree–Fock mean-field approach [10, 28], and the striped antiferromagnetic ground state and small magnetic moment agree with experimental observations. Recently the magnetic ground state properties of iron pnictides were discussed by Ko and Lee [9] adopting the slave rotor approach and by Yu and Si [34] utilizing the slave spin approach; obviously both of these works focused on the half-filling situation. One finds that in Ko and Lee’s slave rotor results the dependence of the Fe magnetic moment on $U$ at intermediate $J_H$ exhibits nonmagnetic, low and high magnetic moment with $\mu < 1 \mu_B$ and $\mu > 1 \mu_B$, and a saturated magnetic moment regimes. They found that in both the high and saturated magnetic moment regimes the system is insulating, in agreement with our slave boson results, while the two-orbital slave spin results of Yu and Si concentrated on the paramagnetic situation [34], slightly different from the present discussions.

However, just considering the electron correlation effect in the present two-orbital model could not account for the doping evolution of the orbital polarization or the crystal structure in LaFeAsO$_{1-x}$F$_x$ and the sublattice magnetic moments [10, 28], in which both the orbital and the spin polarizations decrease with the increase of doping concentration, no matter whether it is electron doping or hole doping. This obvious disagreement between theory and experiment has not been well addressed in the literature. In this paper we have clearly shown that a small crystal field splitting greatly enhances the orbital polarization and may stabilize the ferro-orbital polarization or orbital ordering, in addition to demonstrating the role of the electronic correlation. One naturally anticipates that consideration of the crystal field splitting or more orbitals could also account for the doping dependence of the sublattice magnetic moment. Recently, Lorenzana et al. [35] showed that in a pure electronic interacting picture, the superposition of different SDW states, e.g. ($\pi$, 0) and (0, $\pi$) ordering, is stable over a wide region in the phase diagram. This disagrees with the experimental observation and implies that they missed some key factors in their theory, which is attributed to the necessity of taking the crystal field splitting into account. Therefore the detailed effect of the crystal field splitting on the magnetism and other orbital properties in the realistic model beyond the two-orbital one deserves further exploration in the correlation scenario.

In summary, we have shown that in the parent and doped phases of iron pnictides, the intermediate electronic correlation favors a striped antiferromagnetic configuration accompanied by a weak ferro-orbital ordering. The consideration of a small crystal field splitting arising from a small structural distortion can greatly enhance the orbital polarization and stabilize the orbital ordering. The orbital polarization is the characteristic of a density wave, and the density of states may exhibit a pseudogap-like behavior.

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