Properties of a two-orbital model for oxypnictide superconductors: Magnetic order, $B_{2g}$ spin-singlet pairing channel, and its nodal structure

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A recently proposed two-orbital model for the Fe-based superconductors is studied using the Lanczos method on small clusters as well as pairing mean-field approximations. Our main goals are (i) to provide a comprehensive analysis of this model using numerical techniques with focus on the magnetic state at half-filling and the quantum numbers of the state with two more electrons than half-filling and (ii) to investigate the nodal structure of the mean-field superconducting state and compare the results with angle-resolved photoemission data. In particular, we provide evidence that the dominant magnetic state at half-filling contains spin “stripes,” as observed experimentally using neutron scattering techniques. Competing spin states are also investigated. The symmetry properties of the state with two more electrons added to half-filling are also studied: depending on parameters, either a spin-singlet or spin triplet state is obtained. Since experiments suggest spin-singlet pairs, our focus is on this state. Under rotations, the spin-singlet state transforms as the $B_{2g}$ representation of the $D_{4h}$ group. We also show that the $s^\pm$ pairing operator transforms according to the $A_{1g}$ representation of $D_{4h}$ and becomes dominant only in an unphysical regime of the model where the undoped state is an insulator. We obtain qualitatively very similar results both with hopping amplitudes derived from a Slater-Koster approximation and with hoppings selected to fit band-structure calculations, the main difference between the two being the size of the Fermi surface pockets. For robust values of the effective electronic attraction producing the Cooper pairs, assumption compatible with recent angle-resolved photoemission spectroscopy (ARPES) results that suggest a small Cooper-pair size, the nodes of the two-orbital model are found to be located only at the electron pockets. Note that recent ARPES efforts have searched for nodes at the hole pockets or only in a few directions at the electron pockets. Thus, our results for the nodal distribution will help us to guide future ARPES experiments in their search for the existence of nodes in the Fe-based superconductors. More in general, the investigations reported here aim to establish several of the properties of the two-orbital model. Only a detailed comparison with experiments will clarify whether this simple model is or not a good approximation to describe the Fe pnictides.

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I. INTRODUCTION

A. Current status of experimental and theoretical investigations

The discovery of a new family of superconducting materials with Fe-As layers in their structure1–8 has triggered a large effort in the condensed matter community. LaO$_1$–xF$_x$FeAs is a much studied example of this family of compounds. The $\sim$55 K record critical temperature$^5$ in SmO$_{1–x}$F$_x$FeAs is second only to those observed in the Cu-oxide high temperature superconductors. In addition, there are several aspects of the physics of the Fe-based superconductors that suggest the possibility of an exotic pairing mechanism at work:

1. Evidence is accumulating that phonons may not be sufficient to understand the superconductivity of these compounds.9–11 Moreover, the importance of correlations between the electrons has been remarked in several investigations.12–22 In fact, it has been claimed that these oxypnictide superconductors may bridge the gap between MgB$_2$ and the Cu-oxide superconductors.23,24 In addition, a pseudogap was detected, similarly as in the cuprates.25–28 Coexistence or proximity of magnetism and superconductivity has also been reported.20–32 Although the parent undoped compound is not a Mott insulator, these results suggest that the influence of electron-electron repulsions cannot be neglected. Perhaps the intermediate range of $U/t$, where $U$ is the typical Hubbard repulsion scale and $t$ is the typical hopping amplitude in a tight-binding description, is the most representative of the Fe-based superconductors. $U$ cannot be too large, otherwise the system would develop a gap and the undoped compound would be insulating, contrary to the experimentally observed properties of the undoped limit that suggest bad metallic behavior. But poor-metal characteristics imply that $U$ cannot be too small either, otherwise the undoped system would be a good metal. In addition, the mere presence of a spin-density-wave magnetic state shows that correlations must be important.

2. Several experimental investigations suggest the presence of nodes in the superconducting gap.33–43 This is reminiscent of the nodes that appear in the $d$-wave superconducting state of the high-$T_c$ cuprates. However, other investigations indicate nodeless superconductivity.44–50 As a consequence, this issue is still controversial.

3. The undoped parent compound has long-range spin order in the ground state.51 This magnetic state corresponds
to spin “stripes” having the Fe spins along one of the Fe-Fe crystal axes pointing all in the same direction and being antiferromagnetically coupled in the perpendicular direction. According to neutron scattering experiments, in LaOFeAs the transition to this magnetic state occurs at 134 K and the magnetic moment is 0.36\(\mu_B\), which is smaller than anticipated.\(^{52}\) For NdOFeAs,\(^{53}\) the critical temperature is 141 K and the magnetic moment is even smaller, 0.25\(\mu_B\). However, recently by means of resistivity, specific heat, and magnetic susceptibility measurements, the antiferromagnetic critical temperature of SrFe\(_2\)As\(_2\) was reported to be as high as 205 K, with a more robust Fe magnetic moment of value of 1.7\(\mu_B\).\(^{24}\) Also, CaFe\(_2\)As\(_2\) was investigated using neutron diffraction, and a critical temperature of 173 K with a moment of 0.8\(\mu_B\) was reported.\(^{55}\) Thus, although originally it was believed that the undoped material had a very weak magnetic state, the most recent results suggest that the spin-striped order may be more robust.

On the theory front, several band-structure calculations have shown that the Fermi surface (FS) of these and related compounds is made out of two small hole pockets centered at the \(\Gamma\) point and small electron pockets at the \(X\) and \(Y\) points, in the notation corresponding to a square lattice of Fe atoms.\(^{56-60}\) These calculations have also shown that the 3\(d\) levels of Fe play the dominant role in establishing the properties of these materials near the Fermi level. To address theoretically the physics of these compounds, particularly the superconducting state, model Hamiltonians are needed and several proposals for the dominant pairing tendencies have been made.\(^{61-72}\) In particular, a two-orbital model based on the \(d_{xy}\) and \(d_{yz}\) orbitals was recently presented.\(^{73}\) Several other investigations have addressed this model for the Fe-based superconductors, using a variety of approximations.\(^{74-85}\) Classifications of the possible superconducting order parameters for the two-orbital model have been made.\(^{86-89}\)

As already mentioned, a variety of experimental results suggests that the Cooper pairs are spin singlets.\(^{38,40,60}\) Thus, it is important to find the range of parameters leading to spin singlets in model Hamiltonians since several calculations produce either singlet or triplet superconductivity depending on the couplings and bandwidths used. For this experimentally based reason, our focus here will be mainly on singlet superconductivity.

**B. Why the two-orbital model?**

In this paper, a detailed study of the two-orbital model for the oxypnictide superconductors is carried out using Lanczos and pairing mean-field (MF) techniques. This effort provides a comprehensive view of the model, considerably expanding our recent research on the subject\(^{76}\) by varying the several couplings of the model and studying the main tendencies. When two electrons are added to the half-filled ground state, a spin-singlet state that transforms in a nontrivial manner under rotations is shown to dominate in the regime of couplings that is argued to be the most relevant to describe the superconductors. In addition, the nodal structure of the Fe-based superconducting state obtained using these spin-singlet pairs is here studied for this model using the pairing mean-field approximation. Our results are compared with recent angle-resolved photoemission spectroscopy (ARPES) experiments, and suggestions to further refine the search for nodes in those experiments are discussed.

Currently there is no consensus on what is the minimal model capable of capturing the essential physics of the oxypnictides. Band structure calculations in the local-density approximation (LDA) indicate that the bands that form the observed electron and hole pockets are strongly hybridized but they have mostly Fe 3\(d\) character.\(^{62,91}\) Several authors argue that the hybridization of the Fe 3\(d\) is so strong that all five \(d\) orbitals have to be considered to construct a minimal model. For instance, a five-orbital model has been proposed.\(^{61}\) The tight-binding term respects the FeAs lattice symmetries and the hopping parameters have been obtained from fittings against the LDA calculations. The parameters used reproduce the FS for the electron doped system (i.e., electronic density \(n=6.1\)) but an extra hole pocket around \(M\) [in the notation of the extended Brillouin zone (BZ)] appears for the undoped case and upon hole doping. For this reason, the model may not be suitable to study the magnetic properties of the undoped system. In addition, the number of degrees of freedom in five-orbital models makes its study very difficult using numerical techniques. However, LDA calculations have shown that, although heavily hybridized, the main characters of the bands that determine the FS are \(d_{xy}\) and \(d_{yz}\), with a small contribution of \(d_{xz}\) at the most elongated portions of the electron pockets.\(^{60,85}\) This fact has been the main justification for the proposal of two,\(^{73,76}\) and three-orbital\(^{57}\) models. The two-orbital model can have its hopping parameters fitted such that the shape of the FS, both in the undoped and electron and hole doped cases, is well reproduced in the reduced or folded BZ. However, it has been argued by some authors\(^{67}\) that the two hole pockets around \(\Gamma\) have to arise from the \(d_{xy}\) and \(d_{yz}\) orbitals that are degenerate with each other at \(\Gamma\), as obtained in LDA. In the two-orbital model, one of the hole pockets forms around \(M\) in the extended BZ which gets mapped onto \(\Gamma\) upon folding. The \(d_{xy}\) and \(d_{xz}\) orbitals that form the \(M\)-point pocket are degenerate at \(M\) and, upon the folding, give rise to higher energy bands at the \(\Gamma\) point. For this reason one of the hole pockets in the two-orbital model may not have the correct linear combination of orbitals, potentially leading to incorrect conclusions. In addition, it is also argued that the contribution of the \(d_{xy}\) orbital to the electron pockets may play an important role that should not be ignored which motivated the proposal of the three-orbital model.\(^{57}\) However, the three-orbital model cannot eliminate a spurious hole pocket around \(M\). Thus, a fourth-orbital needs to be added to accomplish this task and, again, the number of degrees of freedom makes this model too complex to be studied numerically.

Then, the justifications for continuing studying a minimal model with just two orbitals, as carried out in the present paper, are the following: (i) The correct shape of the FS is reproduced in the reduced Brillouin zone, both in the doped and undoped cases. (ii) The main characters of all the bands that determine the FS are \(d_{xy}\) and \(d_{xz}\) except for a small portion of the electron pockets that has \(d_{yz}\) character. Then, it is worthwhile to understand the role, if any, that this orbital...
plays in the magnetic and superconducting states. (iii) The two-orbital model is the only one that can be studied exactly with numerical techniques using the minimal size cluster needed for a spin-striped state.\textsuperscript{73} Thus, we believe that it is very important to establish which properties of the oxypnictides are properly captured by this model and which one is not. The role that the correct shape of the FS plays can be investigated as well and also the pairing symmetry and nodal structure involving only the $d_{x^2-y^2}$ and $d_{xy}$ orbitals. It is interesting to note that although two superconducting gaps may appear in a two-orbital model,\textsuperscript{92} symmetry forces the magnitude of the gaps to be the same in this case.\textsuperscript{89}

C. Organization

The organization of the paper is as follows. In Secs. II and III, the two-orbital model is derived. The emphasis is on the Slater-Koster (SK) procedure to evaluate the hopping amplitudes, but the model derived by this method is more general: it coincides with the two-orbital Hamiltonian proposed earlier,\textsuperscript{73} and the values of the hoppings can be obtained also by fitting band-structure calculations.\textsuperscript{73} Both sets of hopping parameters will be used in Secs. II–V. The qualitative aspects of the magnetic and pairing states are shown to be the same for both sets of hopping amplitudes. In Sec. IV, results for the ground states of the undoped model (half-filled) and the case of two more electrons than half-filling will be discussed using the Lanczos technique. The emphasis is on the dominant magnetic states and on the pairing tendencies, which are either in the spin-singlet or triplet channels depending on couplings. Moreover, the spin-singlet case is shown to correspond to the $B_{2g}$ representation of the $D_{4h}$ lattice symmetry group of the model. Section V contains a pairing mean-field analysis of the nodal structure of the model. The two-orbital nature of the problem causes the number and location of the nodes to be a more complex topic than for just one orbital. A qualitative comparison with experiments is included here. Section VI contains our main conclusions. The possible sources of the $B_{2g}$ pairing and the $s\pm$ pairing operator are discussed in Appendixes A and B.

II. MODEL DISCUSSION AND DERIVATION OF HOPPING AMPLITUDES

To study numerically the properties of LaO$_{1-x}$F$_x$FeAs and related compounds, it is necessary to construct a simple model, one that contains a minimum amount of degrees of freedom but still preserves the main physics of the problem. Since all the materials in the family have in common the Fe-X planes ($X=\text{As, P, ...}$), as a first approximation we will just focus on those planes, similarly as it occurs in theoretical studies of the Cu-O planes in the cuprate superconductors. In addition, band-structure calculations\textsuperscript{56–60} have shown the relevance of the Fe 3$d$ levels and that mainly two bands determine the Fermi surface (see Sec. I). Based on these considerations, here we will include only the $d_{x^2-y^2}$ and $d_{xy}$ Fe orbitals in our discussion. To estimate the hopping amplitudes for the tunneling from one Fe to another and, thus, define a tight-binding model, we will calculate their hybridization with the three $p$ orbitals of As following the Slater-Koster formalism.\textsuperscript{90} From the Fe-As hopping integrals, we will calculate the effective Fe-Fe tight-binding hopping parameters following a standard perturbative approach. Thus, the hopping parameters in this model will be functions of the overlap integrals between the orbitals and the distance between the atoms. While this procedure is not as accurate as band-structure calculations, it provides a simple to understand approach that has \textit{ab initio} characteristics, which can be easily reproduced since the calculations are analytical, and they also illustrate how the geometry of the problem affects the hoppings.

However, before proceeding, we remark that another avenue to obtain the hopping amplitudes is via fittings of the band-structure calculations.\textsuperscript{73} In our description of results below, data for both the SK hoppings and those that fit band structures will be presented. An important result is that both sets of hoppings lead to similar qualitative results, both in the undoped case, regarding the magnetic state, as for two electrons added, regarding the pairing tendencies.

The unit cell in the FeAs planes contains two Fe atoms since the As atoms are above and below the plane defined by the Fe atoms in alternating plaquettes [Fig. 1(a)]. However, after the calculation previously described only the Fe atoms will be considered in a simple two-orbital Hamiltonian. Since these Fe atoms form a planar square lattice, it is natural to orient the lattice as in Fig. 1(b).

To guide the discussion, consider a cluster with four Fe and five As atoms [Fig. 2(a)]. The coordinates of the atoms are needed to calculate hopping amplitudes, and they are
provided in Table I, where \( k, l, \) and \( c \) are obtained from the materials structure. The nearest-neighbor (NN) Fe-Fe distance is \( l=2.845 \text{ Å}, \) thus \( k=l/2=1.427 \text{ Å} \). The distance between Fe and As is \( s=2.327 \text{ Å} \) (Ref. 57) [see Fig. 2(b)]. The next-nearest-neighbor (NNN) Fe-Fe distance along the square diagonal is \( d=\sqrt{2l}=4.037 \text{ Å} \) [see Fig. 2(c)] and \( r=d/2=2.018 \text{ Å} \). According to Fig. 2(d), \( c=\sqrt{s^2-r^2}=\sqrt{8^2-2^2}=1.158 \text{ Å} \). The director cosines \( l, m, \) and \( n \) for each of the Fe atoms,93 with respect to the As located at \((0,0,-c)\), are given in Table II.

### A. Overlap integrals between the Fe \( d_{xz} \) and \( d_{yz} \) orbitals and the As \( p_x \) and \( p_y \) orbitals

According to the SK analysis, for the orbitals considered here we obtain the following results for the center integrals,

\[
E_{x,yz} = \sqrt{3} l n p d \sigma - 2 l m n p d \pi \tag{1}
\]

\[
E_{x,xy} = \sqrt{3} l n p d \sigma - 2 l m n p d \pi \tag{2}
\]

\[
E_{x,zz} = \sqrt{3} l n p d \sigma + n (1 - 2 l^2) p d \pi \tag{3}
\]

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<tr>
<td>As4</td>
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### Table II. Director cosines of the Fe atoms with respect to As0 in Fig. 2(a).

The corresponding hopping amplitudes are

\[
|t_{x,yz}| = |t_{y,xy}| = a = \sqrt{3} \frac{c^2}{s^2} (p d \sigma) - 2 \frac{k^2}{s^2} (p d \pi), \tag{5}
\]

\[
|t_{x,zz}| = |t_{y,yy}| = b = \sqrt{3} \frac{c^2}{s^2} (p d \sigma) + \frac{c}{s} \left(1 - 2 \frac{k^2}{s^2}\right) (p d \pi). \tag{6}
\]

Now let us compute the hopping amplitudes for a square lattice made up only of Fe atoms. For the NN effective Fe-Fe hopping \( t_{NN} \) we will consider the pair of atoms Fe1 and Fe2. For the hopping between the \( d_{cz} \) orbitals, there are two possible paths using the As \( p_z \) as a bridge. Their contribution is given by (1) \( d_{cz} \text{Fe}_1 p_z \text{As}_0 d_{cz} \text{Fe}_2 \) and (2) \( d_{cz} \text{Fe}_1 p_z \text{As}_0 d_{cz} \text{Fe}_2 \). From Fig. 3(a), we observe that these paths contribute with \(-a\) each. Regarding the use of the \( p_z \) of As as a bridge, in this case there are also two paths: (3) \( d_{cz} \text{Fe}_1 p_z \text{As}_0 d_{cz} \text{Fe}_2 \) and (4) \( d_{cz} \text{Fe}_1 p_z \text{As}_0 d_{cz} \text{Fe}_2 \). From Fig. 3(b), these paths contribute with \(b^2\) each. Reasoning in an analogous manner, four similar paths are found for the NN
hopping between orbitals $d_{xz}$: (1) $d_{x}^{zz}Fe_{1}p_{z}As_{y}d_{y}^{zz}Fe_{2}$ and (2) $d_{y}^{yz}Fe_{1}p_{y}As_{y}d_{y}^{yz}Fe_{2}$, which from Fig. 3(a) they give a contribution $-a^2$ each, and (3) $d_{x}^{zz}Fe_{1}p_{z}As_{y}d_{y}^{zz}Fe_{2}$ and (4) $d_{y}^{yz}Fe_{1}p_{y}As_{y}d_{y}^{yz}Fe_{2}$, which from Fig. 3(b) they give a contribution $b^2$ each. Combining all these results, and to second order in perturbation theory, the Fe-Fe nearest-neighbor hopping amplitude is given by

$$t_{NN}^{xz} = t_{NN}^{yz} = (-2a^2 + 2b^2)/\Delta = 2(b^2 - a^2)/\Delta,$$

where $\Delta$ is the difference between the on-site energies of the $d$ and $p$ orbitals. Notice that by mere geometrical reasons, it is not possible to have a nearest-neighbor hopping from $d_{yz}$ to $d_{xz}$.

For the hopping $t_d$ along the Fe lattice plaquette diagonal, namely, the NNN Fe-Fe hopping, let us consider the hopping from $Fe_1$ to $Fe_2$, and from $Fe_2$ to $Fe_4$. It can be easily shown that $d_{xz}^{zz}Fe_{1}p_{z}As_{y}d_{x}^{yz}Fe_{4}$ contributes by an amount $b^2$ to $t_{NN}^{xz}$, while $d_{xz}^{zz}Fe_{1}p_{z}As_{y}d_{x}^{yz}Fe_{2}$ contributes $a^2$ to $t_{NN}^{xy}$. The same result is obtained if the hopping from $Fe_2$ to $Fe_4$ is considered. Combining these numbers, then we obtain $t_{NN}^{xz} = t_{NN}^{xy} = (a^2 + b^2)/\Delta$.

Along the plaquette diagonal we can also obtain interorbital hopping. From $Fe_1$ to $Fe_2$ the contribution is $-ab$, while from $Fe_2$ to $Fe_4$ it is $ab$. Thus, the hoppings along the $x+y$ and $x-y$ directions are different by a sign from the interorbital hopping. The fact that the plaquette diagonals are equivalent by symmetry implies that the absolute values of the hoppings must be the same along these diagonals, but the signs can be different as shown here. More explicitly, we obtain $t_{NN}^{xz} = t_{NN}^{yz} = ab/\Delta$, and $t_{NN}^{xy} = -ab/\Delta$.

B. Overlap between $d_{xz}$ and $d_{yz}$ with $p_z$

The consideration of the $p_z$ orbitals adds two center integrals to the present analysis:

$$E_{x,z} = \sqrt{3}n^2ixz(dxsz) + l(1-2n^2)(pdxz)$$

$$E_{y,z} = \sqrt{3}n^2ipyz(dxpz) + m(1-2n^2)(pdxz)$$

which means that an additional hopping must be considered

$$|t_{x,z}^{xz}| = |t_{x,z}^{yz}| = g = \sqrt{3}k_2c^2/s(pdxz) + k / s \left(1 - 2c^2/s\right)(pdxz).$$

Using the values for $k$, $s$, and $c$ calculated before,

$$g = 0.263(pd2s) + 0.31(pd2\pi).$$

The signs are indicated in Figs. 4(a) and 4(b).

Thus, we obtain an additional contribution to the NN hopping $t_{NN}$ so that $t_{NN}^{xz} = 2g^2/\Delta'(-2g^2/\Delta')$ along the $y$ (x) axis. Reciprocally, $t_{NN}^{yz} = 2g^2/\Delta'(-2g^2/\Delta')$ along the $x$ ($y$) axis. Along the diagonal, $t_d = -g^2/\Delta'$ for both orbitals is noted. Also note that $p_z$ generates an interorbital hopping given by $-g^2/\Delta'$ ($g^2/\Delta'$) along the $x+y$ ($x-y$) directions. $\Delta'$ is the difference between the on-site energies of the $d$ and $p_z$ orbitals. From Ref. 59, the gaps are $\Delta = 1.25$ eV and $\Delta' = 5$ eV, but other values for these gaps are also considered below.

**C. Direct Fe-Fe hopping**

Since the distance between Fe atoms is $l = 2.854$ Å, comparable to the Fe-As distance, the contributions to the electron hoppings coming from the direct overlap between the $d$ orbitals of the Fe atoms should also be considered. Following SK, $E_{x,x} = 3l^n^2/\Delta(d\sigma) + (l^2 + n^2 - 4l^2n^2/\Delta(d\sigma) + (m^2 + l^2n^2)dd\delta, E_{y,y} = 3l^n^2/\Delta(d\sigma) + (m^2 + n^2 - 4m^2n^2)dd\sigma)$, and $E_{x,y} = 3l^2m^2/\Delta(d\sigma) + 2l^2m^2n^2dd\sigma$. Notice that all the Fe atoms have $n = 0$ and $l = 1, m = 0(l = 0, m = \pm 1)$ if they are neighbors along the $x$ ($y$) direction. Thus, the interorbital hopping vanishes, and we obtain $t_{x,x}^{d} = -dd\sigma(t_{x,x}^{y} = dd\sigma)$ along the direction $x$ ($y$) and $dd\sigma$ along $y$ ($x$). These same expressions can be used to obtain the diagonal Fe-Fe hopping parameters. We find that $t_d^{x,x} = -(dd\sigma' + dd\delta)/2$, where $\sigma' = \pm (dd\sigma' - dd\delta)/2$ with the minus (plus) sign for the $(\hat{x} + \hat{y})$ $(\hat{x} - \hat{y})$ direction and the prime indicates second-nearest-neighbor overlap integrals.

**III. EFFECTIVE TWO-ORBITAL TIGHT-BINDING MODEL**

A. Hopping term

Considering the results of Sec. II C, the kinetic-energy term of the effective tight-binding Hamiltonian involving the $d_{xz}$ and $d_{yz}$ orbitals, defined on the square lattice formed only by the Fe atoms, is given by

$$H_{TB} = -t_{x} \sum_{i,\sigma} (d_{i,x}\sigma d_{i+1,x}\sigma + d_{i,y}\sigma d_{i+1,y}\sigma + H.c.)$$

$$-t_{y} \sum_{i,\sigma} (d_{i,y}\sigma d_{i+1,y}\sigma + d_{i,y}\sigma d_{i+1,y}\sigma + H.c.)$$

$$-t_{z} \sum_{i,\sigma} (d_{i,z}\sigma d_{i+1,z}\sigma + d_{i,y}\sigma d_{i+1,y}\sigma + H.c.)$$

$$+t_{x} \sum_{i,\sigma} (d_{i,x}\sigma d_{i+1,y}\sigma + d_{i,y}\sigma d_{i+1,x}\sigma + H.c.)$$

$$-t_{y} \sum_{i,\sigma} (d_{i,y}\sigma d_{i+1,y}\sigma + d_{i,y}\sigma d_{i+1,y}\sigma + H.c.)$$

$$-\mu \sum_{i} (n_i^x + n_i^y).$$

![FIG. 4. (Color online) (a) Hoppings between the $d_{xz}$ orbitals in Fe and the $p_z$ orbitals in As for the cluster considered in Fig. 2(a). (b) Hoppings between the $d_{yz}$ orbitals in Fe and the $p_z$ orbitals in As for the cluster considered in Fig. 2(a). Continuous (dashed) lines indicate positive (negative) values.]
In this Hamiltonian, the operator \( d^\dagger_{i,\alpha} \) creates an electron with spin z-axis projection \( \sigma \), orbital \( \alpha \), and on the site \( i \) of a square lattice. The chemical potential is given by \( \mu \) and \( n_i^\alpha \) are number operators. The index \( \mu = \hat{x} \) or \( \hat{y} \) is a unit vector linking nearest-neighbor sites. The hoppings, within the SK approach, are given by
\[
\begin{align*}
t_1 &= -2[(b^2 - a^2)/(\Delta + g^2/\Delta')] - d d \delta, \\
t_2 &= -2[(b^2 - a^2)/(\Delta - g^2/\Delta')] - d d \pi, \\
t_3 &= -(a^2 + b^2 - g^2/\Delta')] - (d d \pi' + d d \delta)/2, \\
t_4 &= -(ab/\Delta - g^2/\Delta') - (d d \pi' - d d \delta)/2.
\end{align*}
\]
(15)
The explicit expressions for these hopping amplitudes in terms of the overlap integrals using the parameters for FeAs can be easily found and they will not be provided here. The two-orbital model proposed by Raghu et al.\(^{73} \) has the same form as the one presented above, but the hoppings are obtained by fitting band structures.\(^{60} \)

It is interesting to note that if only the direct overlap between the \( d \) orbitals is considered, i.e., ignoring the indirect hopping through the \( p \) As orbitals, the form of Eq. (14) does not change. Thus, the form of \( H_{TB} \) arises from the symmetry properties of the \( d_{xz} \) and \( d_{yz} \) orbitals rather than from the location of the As ions. However, the indirect Fe-Fe hopping through the As atoms plays a key role in providing the relatively large value of the diagonal hopping \( t_3 \) vs the NN hoppings which, as discussed below, stabilizes the magnetic stripe order. For example, if we only consider the direct hopping then \( t_1/t_2 = d d \pi'/d d \pi \), where \( d d \delta = 0 \) was assumed.\(^{95} \) Since \( d d \pi' \ll d d \pi \), then \( |t_1| \approx |t_2| \). However, if we consider the indirect hopping then \( |t_1| \approx |t_2|/2 \).

To analyze the influence of the several parameters, let us consider two special cases. Setting \((pd\sigma) = 1.0 \text{ eV}, pd\pi = -0.2 \text{ eV}, \Delta = 1.0 \text{ eV}, \text{ and } \Delta' = 1 \text{ eV in Eqs. (15)-(18)}\) and neglecting the direct Fe-Fe coupling i.e., using \( d d \pi' = d d \pi = 0 \), we obtain \( t_1 = 0.058 \text{ eV}, t_2 = -0.22 \text{ eV}, t_3 = -0.21 \text{ eV}, \text{ and } t_4 = -0.08 \text{ eV} \). With these values, the band structure, shown in Fig. 5, is qualitatively similar to the band-structure calculations, although the pockets are larger in size. Another example can be obtained by using the calculated values of the energy gaps, which are \( \Delta = 1.25 \text{ eV} \) and \( \Delta' = 5 \text{ eV} \).\(^{89} \) In Fig. 6, the band structure is shown for \((pd\sigma) = 1 \text{ eV}, \text{ and } pd\pi = -0.2 \text{ eV} \). The chemical potential is \( \mu = 0.081 \text{ eV} \) which corresponds to half-filled orbitals. Results are plotted along the path \((0,0) \to (\pi,0) \to (\pi,\pi) \to (0,0) \).

B. Interactions

In this section, the Coulombic interaction terms are added to the tight-binding Hamiltonian (14) to form the full two-orbital model. These Coulombic terms are\(^{76} \)
\[
H_{\text{int}} = U \sum_{i} n_{i,\alpha \uparrow} n_{i,\alpha \downarrow} + (U'/2) \sum_{i} n_{i,\alpha \downarrow} n_{i,\alpha \downarrow} - 2 \sum_{i} \mathbf{S}_{i,\alpha} \cdot \mathbf{S}_{i,\alpha},
\]
(16)
where \( \alpha = x, y \) denotes the orbital, \( \mathbf{S}_{i,\alpha} \) is the spin (electronic density) in orbital \( \alpha \) at site \( i \), and we have used the

![FIG. 5. (Color online) (a) Energy vs momentum for the noninteracting tight-binding Hamiltonian in Eq. (14) using \( t_1 = 0.058 \text{ eV}, t_2 = -0.22 \text{ eV}, t_3 = -0.21 \text{ eV}, \text{ and } t_4 = -0.08 \text{ eV} \). These hopping amplitudes are obtained from the Slater-Koster formulas using \((pd\sigma) = 1 \text{ eV and } (pd\pi) = -0.2 \text{ eV}, \text{ supplemented by } \Delta = \Delta' = 1 \text{ eV for simplicity, and } \mu = -0.03 \text{ eV, which corresponds to half-filled orbitals. Results are plotted along the path } (0,0) \to (\pi,0) \to (\pi,\pi) \to (0,0). (b) Fermi surface for the half-filled system.](image)

![FIG. 6. (Color online) (a) Energy vs momentum for the noninteracting tight-binding Hamiltonian (14) using \( t_1 = -0.1051 \text{ eV}, t_2 = -0.1472 \text{ eV, } t_3 = -0.1909 \text{ eV, and } t_4 = -0.0874 \text{ eV, obtained using the parameters } (pd\sigma) = 1 \text{ eV, } (pd\pi) = -0.2 \text{ eV, } d\pi = 0.2 \text{ eV, } dd\delta = -0.02 \text{ eV, } \Delta = 1.25 \text{ eV, and } \Delta' = 5 \text{ eV. The chemical potential is } \mu = 0.081 \text{ eV, which corresponds to half-filled orbitals. Results are plotted along the path } (0,0) \to (\pi,0) \to (\pi,\pi) \to (0,0). (b) Fermi surface for the half-filled system.](image)
C. Pairing

Diagonalizing exactly the full two-orbital Hamiltonian on a $8\times8$ cluster with periodic boundary conditions, it was observed in previous investigations that in regions of parameter space the ground state with two extra electrons above half-filling is a spin triplet. In this case, the relevant pairing operator is given by

$$\Delta^i(k) = \sum_\sigma (d_{i,k,x}^\dagger d_{i,k,-x,\sigma} - d_{i,k,-x}^\dagger d_{i,k,x,\sigma}),$$

(17)

where \(\sigma = \uparrow\) or \(\downarrow\) denotes the spin projection 1 or -1, respectively, while the 0 projection operator is

$$\Delta^i(0) = \sum_\mu (d_{i,k,x}^\dagger d_{i,k,x,\mu} + d_{i,k,x}^\dagger d_{i,k,x,\mu}) - d_{i,k,x}^\dagger d_{i,k,x,\mu} - d_{i,k,x} d_{i,k,x,\mu}^\dagger,$$

(18)

or, in momentum space,

$$\Delta^i(k) = (\cos k_x + \cos k_y)(d_{k,x}^\dagger d_{k,-x,\sigma} + d_{k,-x}^\dagger d_{k,x,\sigma}),$$

(19)

$$\Delta^i(k) = (\cos k_x + \cos k_y)(d_{k,x}^\dagger d_{k,-x} + d_{k,-x}^\dagger d_{k,x}) - d_{k,x}^\dagger d_{k,-x} - d_{k,-x}^\dagger d_{k,x}.$$  

(20)

This operator is invariant under the $A_{2g}$ irreducible representation of the group $D_{4h}$, it is odd under orbital exchange, and it is a spin triplet.

However, in our previous effort we have also identified regions of parameter space where the state with two extra electrons is a spin singlet, which appears to be compatible with the results of experiments that favor singlet states over triplets. The dominant pairing operator for the singlet is given by

$$\Delta^i(0) = \sum_\alpha (d_{i,-x}^\dagger d_{i,-x,\alpha} + d_{i,-x}^\dagger d_{i,-x,\alpha}) + d_{i,-x}^\dagger d_{i,-x,\alpha},$$

(21)

which in momentum space becomes

$$\Delta^i(k) = \sum_\alpha (\cos k_x + \cos k_y)d_{k,-x}^\dagger d_{k,-x}.$$

(22)

This operator transforms as the $B_{2g}$ irreducible representation of the $D_{4h}$ point group, it is even under orbital exchange, and it is a spin singlet. As explained in Sec. I, the experimental results favoring spin-singlet pairing lead us to focus our effort on this spin-singlet operator in Secs. IV A–IV C.

IV. EXACT DIAGNOSIS RESULTS

A. Method

In this section, the Lanczos or exact diagonalization (ED) method will be used to obtain the ground state of the two-orbital model, both at half-filling and also for a system with two electrons more than half-filling. Due to the exponential growth of the Hilbert space with increasing cluster sizes, here our effort must be restricted to a tilted $\sqrt{8}\times\sqrt{8}$ cluster. Using translational invariance, the Hilbert space can be reduced to 21 081 060 states at half-filling and 16 359 200 for two electrons away from half-filling. Taking into account the additional symmetries of spin inversion as well as rotations, the dimension of the Hilbert space becomes ~2 600 000. The employed Lanczos scheme is standard and requires up to 11 Gbytes of memory when only translational invariance is used. Note that the two-orbital eight-site cluster has a similar Hilbert-space size as a 16-site one-band Hubbard lattice, and they are similarly computationally demanding. The focus of our effort is on ground states for a fixed set of quantum numbers corresponding to the symmetries that were implemented. We use both the hoppings from the SK approach and
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also the hoppings that fit band-structure calculations and find qualitatively consistent results for both sets.

b. results using slater-koster derived hoppings

1. fermi surfaces, spin order, and spin of the pairs

in the sk approach, the parameter pdσ is here kept fixed equal to 1, providing the scale and the free parameter pdπ is varied. to constrain the values of pdπ, let us return to the tight-binding hamiltonian. figure 9 shows how the fermi surface evolves by changing pdπ. these figures are in the unfolded brillouin zone, i.e., for one fe atom per unit cell. for a negative ratio pdπ/pdσ, hole pockets around momenta (0, 0) and (π, π) and electron pockets around (0, π) and (0, π) are observed. however, for a vanishing ratio pdπ=0, additional electron pockets appear at (π/2, π/2), while the pockets around (0, π) and (π, 0) disappear fast by further increasing pdπ to positive values. as discussed before,76 the robust nnn hopping t3 at negative pdπ/pdσ induces tendencies toward a (0, π)/(π, 0) magnetic ordering at half-filling, as shown by the spin structure factor in fig. 10(a). this is in good agreement with neutron scattering experiments. thus, it is clear that the realistic regime corresponds to negative pdπ, and an opposite sign of pdπ and pdσ is also what would be expected from the tabulated values.95

as it can be observed in fig. 10(a), the onsite repulsion u enhances the spin “striped” ordering, which is already dominant even at u=0 (although in this noninteracting case a power-law decay in the spin correlations is expected rather than genuine long-range order). increasing hund’s coupling j at a fixed u [see fig. 10(b)] produces a similar effect because it leads to larger localized moments, allowing for a stronger overall collective spin ordering. however, for positive pdπ, the diagonal hopping t3 is no longer strong enough to drive the (π, 0) order, and the spin structure factor peaks at (π, π) instead [fig. 11(a)]. figure 11(b) shows the spin structure factor for pdπ/pdσ=0.2, u=0.5, and j/u=1/8 when two more electrons are added to half-filling. the (0, 0) order is weakened in the doped system.

in our previous effort,76 we investigated the pairing symmetry for two added electrons in the region of hoppings -0.5=pdπ=-0.2, varying u, and for the special case j/u =1/4. the spin of the state with two additional electrons can be determined by comparing the ground state energy for a total z component of the spin s_z=0 to s_z=1. if these two energies are degenerate, the state is a triplet (it was also tested that the ground state of s_z=2 is not degenerate with s_z=0 and 1, thus excluding higher spin states). the hubbard

FIG. 9. (Color online) Noninteracting (U=J=0) Fermi surface in the unfolded Brillouin zone at the pdπ/pdσs indicated. The realistic regime is pdπ/pdσ<0 since hole pockets around (0,0) and (π, π) and electron pockets around (0, π) and (0, π) are observed.

FIG. 10. (Color online) Spin structure factor S(k) at half-filling obtained with ED on a $\sqrt{8} \times \sqrt{8}$ cluster for pdπ/pdσ=-0.2. (a) Results corresponding to several U’s and J/U=1/8. (b) Results varying J at fixed U=1.

FIG. 11. (Color online) Spin structure factor S(k) for (a) half-filling and pdπ/pdσ=0.1, U=0.5, J/U=1/8 and (b) pdπ/pdσ =-0.2, U=0.5, J/U=1/8 at half-filling and with two additional electrons. These are ED results on a $\sqrt{8} \times \sqrt{8}$ cluster.
that increasing the Hund coupling pair repulsion $U$ was found to drive the spin of the two electrons added to the half-filled system from triplet at small $U$ to singlet at larger $U$ for the $pd\sigma$'s investigated. The critical $U_c$ needed for the transition was found to be the lowest at $pd\pi=-0.2$. This value of $pd\pi$ moreover leads to a Fermi surface with hole and electron pockets similar to that obtained with band structure after folding [see Ref. 76 and Fig. 9(b)]. For large $|pd\pi|/pd\sigma|$, on the other hand, the Fermi surface has far larger electron pockets around $(0,\pi)$ than those found in band calculations or experiments [see Fig. 9(a)]. Consequently, we will mainly focus on $pd\pi/|pd\sigma|=-0.2$ below.

In Fig. 12, the regions where singlet and triplet pairings dominate, depending on $U$ and $J$, are shown. [The notation “singlet 9” and “singlet 2” refer spin-singlet states with $B_{2g}$ and $A_{1g}$ symmetries, as discussed in more detail in the “pairing symmetry” section below as well as in Eq. (A8).] The trends observed for $J/U=1/4$ remain stable for other realistic values of $J$. Additionally, qualitatively we have observed that increasing the Hund coupling $J$ promotes a robust triplet pairing. Due to the relation used between $U$, $U'$, and $J$, two electrons on the same site, but in different orbitals, no longer feel any Coulomb repulsion for the maximal $J=2U/5$. As a consequence, values of $J/U=0.4$ are here considered unphysical.

2. Pairing symmetry

To investigate the symmetry under rotations of the pairing states, the half-filled ground state is compared to states with two additional electrons. The symmetry sector of the half-filled ground state must be contrasted with the symmetry of the doped state, and the symmetry operation leading from one to the other gives us an indication for the pairing symmetry. This method was very successful in establishing the $d$-wave character of the pairing in the $t-J$ model for the cuprates.\(^{97}\) In addition, we also added a pair of electrons with a well-defined symmetry under rotations to the half-filled ground state and calculate the overlap between the resulting state and the ground state obtained for half-filling plus two electrons.

From this analysis, we found that the dominant pairing operator for spin-singlet pairs is interorbital and given by\(^{76}\)

$$\Delta_0^s = \frac{1}{2N_{\text{sites}}} \sum_{i,a,\mu} (d_{i-a,\delta,\mu,a_i} - d_{i-a,\delta,\mu,-a_i}).$$

where $i=1,\ldots,N_{\text{sites}}$ denotes the lattice site, $\mu = x, y$ are the unit vectors connecting NN sites, and $a=x, y$ are the $x\delta$ and $y\delta$ orbitals, respectively. This operator transforms as $B_{2g}$ and it is 9 in the detailed list provided in Ref. 89. In addition to the $B_{2g}$ pairing between nearest-neighbor sites, we also find a small overlap for the corresponding $B_{2g}$ onsite pairing 8 (reaching at most 10% of the intersite overlap) and some overlap for the NNN $B_{2g}$ pairing. In contrast to the small onsite contribution, the NNN pairing is sizable, but its exact strength compared to NN pairing is difficult to ascertain with the small cluster used.

The only other singlet pairing for which we have found a substantial overlap is 2 in the above mentioned list, although, as discussed below, its region of stability at large $U$ does not have the correct properties expected for the FeAs superconductors. This operator is intraorbital with $A_{1g}$ symmetry, and it is given by

$$\Delta_2^s = -\frac{1}{2N_{\text{sites}}} \sum_{i,a,\mu} (d_{i,a,\delta,\mu,a_i} - d_{i,a,\delta,\mu,-a_i}).$$

Applying the pairing operators $\Delta_0^s$ to the half-filled ground state $|\phi_0\rangle$, we find that the resulting vector $\Delta_0^s|\phi_0\rangle$ has a very small norm $\lesssim 0.15$ for pairings $i=3, 4, 5,$ and 6 in the list of Ref. 89, while it reaches $0.6-0.8$ (depending on $U$ and $J$) for 1, 2, 7, 8, and 9. Then, at least qualitatively, we conclude that only the latter pairs can be created easily in the half-filled ground state. To provide more quantitative information, we then calculate the overlap between $\Delta_0^s|\phi_0\rangle$ and the ground state found for half-filling plus two additional electrons $|\phi_2\rangle$. We only find substantial overlaps for the operators $9 (B_{2g})$ and 2 ($A_{1g}$) given in Eqs. (23) and (24), while $\Delta_0^s|\phi_0\rangle$ is always orthogonal to the two-electron ground state $|\phi_2\rangle$, at least for the range of parameters investigated. As it can be observed in Fig. 13, the $B_{2g}$ pairing $\Delta_0^s$ occurs at small intermediate Coulomb repulsion $U$, which is the expected suitable regime to describe noninsulating materials with bad metallic properties. Only for large $U \approx 2.8$ eV, where a hard gap in the density of states indicates insulating behavior,\(^{67}\) we do find the pairing [Eq. (24)] with $A_{1g}$ symmetry. In this regime we find some admixture of the corresponding onsite pairing (1) and the longer-range $A_{1g}$ NNN pairing, which, as shown in Eq. (A8), corresponds to the much discussed $s^{\pm}$ pairing state.\(^{49,61,62,65}\)

Figure 12 shows more explicitly the regions of dominance of the states 9 ($B_{2g}$) and 2 ($A_{1g}$) in the $U$ vs $J/U$ plane. Thus, the $B_{2g}$ symmetric operator seems to be the most realistic in the regime $pd\pi/|pd\sigma|=-0.2$ and $0.5 \leq U \leq 1$, which is the appropriate region of parameters to qualitatively describe the FeAs-based superconductors.\(^{98}\)

C. Results with hopping parameters fitted to band-structure calculations

1. Results at nonzero $J$

We have also investigated the two-orbital model using hopping parameters obtained from a fit to band-structure cal-
culation results.\textsuperscript{73} It is interesting to observe that this set of parameters also leads to $(0,\pi)/(\pi,0)$ antiferromagnetic order at half-filling (see Fig.\ 14), which is again enhanced by increasing $U$ at fixed $J$ or increasing $J$ at fixed $U$. As for SK hoppings, Fig.\ 15 shows that the magnetic order is only slightly reduced by the doping with two electrons. In Fig.\ 16, we report the spin of the state with two electrons added to the half-filled state and find qualitatively similar behavior as with the SK approach: $U$ promotes singlet pairing, in the previously discussed “9” ($B_{2g}$) and “2” ($A_{1g}$) channels, and $J$ favors triplet pairing.

We have performed an analogous analysis of the electron pairing as in Sec. IV B 2 and again find the interorbital singlet operator [Eq.\ (23)] to dominate at intermediate $U$ and $J$. Table III gives the pairing amplitudes for operators [Eqs.\ (23) and (24)] for several $(U,J)$ parameter sets. As before, the Coulombic parameters were chosen to give a spin-singlet state for two electrons added to half-filling but are expected to be small enough to remain in the metallic regime. As for SK hoppings, the pairing symmetry for these singlet states is $B_{2g}$, i.e., the interorbital singlet Eq.\ (23) dominates here as well.

Interorbital pairing is favored over intraorbital pairing by the kinetic energy because the interorbital Coulomb repulsion $U'$ is weaker than the repulsion $U$ within the orbitals. To test this assumption, we analyze pairing amplitudes for the special case $J=0$ but instead of using $U=U'$, we use $U'<U$, i.e., we deviate from the relation $U'=U-2J$. The resulting pairing symmetry is still the same $B_{2g}$ interorbital singlet [Eq.\ (23)], as deduced from the amplitudes in Table IV.

\textbf{2. Results at $J=0$ and $U=U'$}

Finally, let us discuss the special case $J=0$, $U=U'$ for $U=2.8$ (in eV units), which are the couplings used in Ref.\ 73. In contrast to $J=0.05$ and $U'=2.6$, we here find that the

\begin{table}[h]
\centering
\begin{tabular}{ccc}
\hline
$U$ & $J$ & $\langle \phi_2 | \Delta^+_i | \phi_0 \rangle$ \\
\hline
1.4 & 0.10 & 0.64 \\
2.8 & 0.00 & 0.66 \\
2.8 & 0.05 & 0.66 \\
2.8 & 0.10 & 0.66 \\
4.0 & 0.50 & 0.65 \\
10.0 & 1.25 & 0.58 \\
\hline
\end{tabular}
\caption{Overlap between the ground state $| \phi_2 \rangle$ for two electrons added to half-filling and the states $\Delta^+_i | \phi_0 \rangle$ that are obtained by applying pairing operators [Eqs.\ (23) and (24)] to the ground state at half-filling. Data are for a kinetic-energy operator obtained from band-structure fitting with $t_1=-1.0$, $t_2=1.3$, and $t_3=t_4=-0.85$ (in eV units) (Ref.\ 73).}
\end{table}
The magnetic phase diagram for the present model was also studied using a mean-field approximation.\textsuperscript{80} At half-filling, it was claimed that the Coulomb repulsion rather than stabilizing a state with NN correlations stabilizes a state with NN correlations. For comparison, we also include results obtained for a linear combination of states with perfect Ising-type (0, π) and (π, 0) orders in the z direction. These results are useful to judge the expected order-of-magnitude values for the correlations investigated. The numbers on Table VI show that the numerical results for the two-orbital model are compatible with those of the Ising spin-stripe state, particularly considering that quantum fluctuations will reduce the spin correlations of such a state. As a consequence, our present investigations favor the spin-stripe magnetic state, although further work is needed to fully confirm these conclusions.

V. DISCUSSION OF NODAL STRUCTURE IN THE MEAN-FIELD APPROXIMATION

In this section, the results of a pairing mean-field analysis of the two-orbital Hamiltonian will be discussed.

### TABLE V. Energy of the lowest eigenstates for two electrons and \( J=0, U=U'=2.8 \), and pairing operators giving the largest overlap when applied to the half-filled state. Hoppings are those from band-structure fitting.

| Energy | Pairing No. | \( \langle \phi_2|\Delta|\phi_0 \rangle \) |
|--------|-------------|---------------------------------|
| 1      | −8.45322    | 2                               |
| 2      | −8.45150    | 9                               |
| 3      | −8.4132     | 7                               |

\[ |\psi_i\rangle = \frac{1}{N_{\text{sites}}} \sum_i S_i \cdot S_{i+1} |\phi_0\rangle, \] (25)

\[ |\psi_i\rangle = \frac{1}{N_{\text{sites}}} \sum_i S_i \cdot S_{1+i} |\phi_0\rangle. \] (26)

Our numerical ED results indeed give very small negative values for the NN spin correlation. However, we expect the two states to lead to different results for \( \langle \psi_i|\psi_j \rangle \) and \( \langle \psi_i|\psi_{i'} \rangle \). \( \langle \psi_i|\psi_j \rangle \) is expected to be positive and \( \langle \psi_i|\psi_{i'} \rangle \) to be negative in the spin-striped phase, while both should be zero or very small in the OM phase. Table VI shows the results for strong \( (U=4) \), intermediate \( (U=1) \), and weak \( (U=0.5) \) on-site Hubbard repulsions. For \( U=4 \), we clearly find \( \langle \psi_i|\psi_j \rangle < 0 \) and \( \langle \psi_i|\psi_{i'} \rangle > 0 \). While these numbers become weaker for the less spin ordered states at smaller \( U \), they are still consistent with the \( (0, \pi) \) or \( (\pi, 0) \) ordering. For comparison, we also include results obtained for a linear combination of states with perfect Ising-type \( (0, \pi) \) and \( (\pi, 0) \) orders in the \( z \) direction. These results are useful to judge the expected order-of-magnitude values for the correlations investigated. The numbers on Table VI show that the numerical results for the two-orbital model are compatible with those of the Ising spin-stripe state, particularly considering that quantum fluctuations will reduce the spin correlations of such a state. As a consequence, our present investigations favor the spin-stripe magnetic state, although further work is needed to fully confirm these conclusions.
merical results of Secs. I–IV and experimental data will be used to guide this mean-field approximation. Experiments indicate that the pairs in the Fe-based superconductors are spin singlets\textsuperscript{38,40,96} and our previous numerical results did provide a dominant spin-singlet pairing operator, as discussed in Sec. IV C 3. It is also important to note that the pairing operator that we obtained mixes different orbitals. A numerical study of the orbital composition of the bands that determine the FS in our two-orbital model indicates that the bands that constitute the pockets are an admixture of $xz$ and $yz$ orbitals. Thus, it is not surprising that the dominant pairing operator creates pairs made of electrons in different orbitals. One of the main goals of the analysis discussed below will be to find out the nodal structure of the mean-field Hamiltonian.

A. Location of the nodes

1. Reminder of one-band model results

For the simple case of $d$-wave superconductivity in a single-orbital model, characterized by the dispersion relation $\xi(k)=-2t'(\cos k_x+\cos k_y)-4t''\cos k_x\cos k_y-\mu$, the gap function is given by $\Delta(k)=\Delta(\cos k_x-\cos k_y)$. In this case, the mean-field Hamiltonian reduces to a $2\times 2$ matrix linking $k$ with $-k$ which is simply given by

$$H_{MF} = \begin{pmatrix} \xi(k) & \Delta(k) \\ \Delta(k) & -\xi(k) \end{pmatrix}. \tag{27}$$

To obtain the position of the nodes in the gap, we merely need to find the values of $k_x$ and $k_y$ where the eigenvalues of the matrix [Eq. (27)] are zero. These are the same values that solve the equation $\det(H_{MF})=0$, i.e., $\xi(k)^2+\Delta(k)^2=0$, which is satisfied only if each term vanishes independently. This occurs at the points where the noninteracting Fermi surface described by $\xi(k)=0$ intersects the diagonal lines along which $\Delta(k)=0$, i.e., $k_x=k_y$ and $k_x=-k_y$. This procedure establishes the well-known location of the four $d$-wave nodes of a single-band model.

2. Nodes in a two-orbital model

For a system with two orbitals, we will proceed in an analogous manner as for one orbital. The MF Hamiltonian matrix in the basis $(d^\dagger_{k,x,1},d^\dagger_{k,y,1},d^\dagger_{-k,x,1},d^\dagger_{-k,y,1})$ is now given by the $4\times 4$ matrix,

$$H_{MF} = \begin{pmatrix} \xi_{xx} & \xi_{xy} & 0 & \Delta_k \\ \xi_{yx} & \xi_{yy} & \Delta_k & 0 \\ 0 & \Delta_k & -\xi_{xx} & -\xi_{xy} \\ \Delta_k & 0 & -\xi_{yx} & -\xi_{yy} \end{pmatrix}. \tag{28}$$

The matrix elements can be obtained by Fourier transforming the tight-binding Hamiltonian $H_{TB}$ given in Eq. (14). We obtain

$$\xi_{xx} = -2t_2 \cos k_x -2t_1 \cos k_x -4t_1 \cos k_y \cos k_y -\mu,$$

$$\xi_{yy} = -2t_1 \cos k_x -2t_2 \cos k_y -4t_5 \cos k_x \cos k_y -\mu,$$

$$\xi_{xy} = -4t_4 \sin k_x \sin k_y,$$

and

$$\Delta_k = V(\cos k_x + \cos k_y), \tag{30}$$

where $V$ is the strength of the pairing interaction.

Note that we can also work in the basis in which $H_{TB}$ is diagonal. In this basis, which is expanded by $(\epsilon_{k,1,1}^1,\epsilon_{k,2,1}^1,\epsilon_{-k,1,1}^1,\epsilon_{-k,2,1}^1)$, $H_{MF}$ becomes

$$H'_{MF} = U^{-1}H_{MF}U$$

given by

$$H'_{MF} = \begin{pmatrix} \epsilon_1 & 0 & V_B & V_A \\ 0 & \epsilon_2 & -V_A & V_B \\ V_B & -V_A & -\epsilon_2 & 0 \\ V_A & V_B & 0 & -\epsilon_1 \end{pmatrix}, \tag{31}$$

where $V_A$ and $V_B$ are given by

$$V_A = 2nu\Delta_k,$$

$$V_B = (u^2-v^2)\Delta_k,$$

and $u$ and $v$ are the elements of the change of basis matrix $U$ given by

$$U = \begin{pmatrix} u & v & 0 & 0 \\ v & -u & 0 & 0 \\ 0 & 0 & v & u \\ 0 & 0 & -u & v \end{pmatrix}. \tag{34}$$

with $U^{-1}=U^T$. Remember that $V_A$, $V_B$, $u$, and $v$ are all functions of the momentum $k$ and $u^2+v^2=1$.

Now let us discuss the physical meaning of $V_A$, $V_B$. According to Eq. (31), $V_A$ is the intraband pairing for band 1, i.e., the band with the highest energy (electron band), while the intraband pairing for band 2 (hole band) is $-V_A$. Thus, there is a relative phase $\pi$ between the two intraband order parameters. In the standard BCS studies for multiband models, it is expected that pairs are formed by electrons in the same band.\textsuperscript{22} In the two-orbital model, as just discussed, we found intraband pairing but we also obtain interband pairing with strength $V_B$. The possibility of interband pairing has been considered previously in several contexts: (i) possibility of $T_c$,\textsuperscript{99} (ii) high T$_c$ cuprates,\textsuperscript{100} and (iii) heavy fermion systems,\textsuperscript{101} where it was shown that if two bands are very close to each other in the vicinity of the Fermi level, interband pairing can occur. The weaker the pairing potential, the closer to the Fermi surface the two bands have to be. When long-range pairing develops the Brillouin zone gets folded and, as a result, the total number of bands doubles. In this representation, which arises by diagonalizing Eq. (28) with $\Delta(k)=0$, the two-orbital model has the dispersion shown in Fig. 17 where each band [panel (a)] and FS [panel (b)] is represented with a different color and the folded (unfolded) portions with dashed (continuous) lines. It can be seen from panel (a) that at the Fermi level there is only intraband crossing indicated by circles. However, there is also interband crossing, indicated by the boxes, above the Fermi energy. The previous numerical results appear to indicate that the effective coupling is sufficiently strong as to produce inter-
band pairing. In Fig. 18 it can be seen that even a small \( V \) opens a gap between the two bands that cross away from the FS. In multiorbital models the opening of these gaps can lower the overall energy.\(^{102} \) Within the standard BCS approach this result may appear counterintuitive and it could be an artifact of the two-orbital model or of the small system size that we have considered. However, there are clear indications that most of the FSs in the five-orbital model have a size that we have considered. However, there are clear indications that other orbitals have to participate in the model and attempt to compare the results with experiments.

The existence and position of nodes in the resulting mean-field band structure can be found by requesting that \( \text{det}(H_{\text{MF}})=0 \), as in the one-orbital case. From Eq. (31), we obtain the following equation:

\[
V_A^2(V_A^2 + 2V_B^2 + \epsilon_1^2 + \epsilon_2^2) + (\epsilon_1\epsilon_2 + V_B^2)^2 = 0.
\] (35)

This equation is satisfied in two possible ways:

1. First, a solution can be found if \( V_A=V_B=0 \), and \( \epsilon_1 =0 \) or \( \epsilon_2 =0 \). This condition for nodes is satisfied if the lines where \( \cos k_x+\cos k_y=0 \), namely, the lines where \( V_A \) and \( V_B \) vanish, intersect any of the noninteracting Fermi surfaces determined by the points where \( \epsilon_1=0 \) or \( \epsilon_2=0 \). It is clear that the line \( \cos k_x+\cos k_y=0 \) intersects each of the four electron-pocket Fermi surfaces in two points per pocket [see Figs. 1(e) and 17(b)]. This means that nodes will appear only in the electron pockets and not in the hole pockets. These are the nodes that arise from a simple extrapolation of the reasoning used to find nodes in the one-orbital model, namely, by finding the intersections of the noninteracting Fermi surface with the trigonometric function, in this case \( \cos k_x + \cos k_y \), contained in the \( \Delta_k \) gap function. The position of the nodes in the electron pockets upon folding of the Brillouin zone [see Figs. 1(d) and 17(b)] is at the points in \( k \) space where the two-electron pockets intersect each other.

Note that the existence of these nodes does not depend on the value of \( V \). They will always be present as it can be seen in Fig. 18 where the nodes along the \( X-Y \) direction appear in all the panels varying \( V \).

2. However, the two-orbital nature of this problem leads to the possibility of additional nodes in unexpected locations. This can be understood by realizing that Eq. (35) can also be satisfied if \( V_A=0 \) and

\[
V_B^2 = -\epsilon_1\epsilon_2.
\] (36)

According to the expression for \( V_B \) in Eq. (32), and assuming that \( \Delta_k \) is nonzero [if it is zero we recover the nodes already described in (1) above], then the condition \( V_B=0 \) is satisfied if \( u=0 \) or \( v=0 \). Due to the normalization \( u^2 + v^2 = 1 \), when \( u=0 \) then it must occur that \( v=1 \) and vice versa. Introducing these values of \( u \) and \( v \) in Eq. (34), it can be shown that the condition that \( H_{\text{MF}}=U^{-1}H_{\text{MF}}U \) is diagonal is satisfied only if \( \xi_{\nu}=0 \). According to Eq. (29), for \( \xi_{\nu} \) to vanish it is necessary to have \( k_x=0 \) or \( \pi \) or \( k_y=0 \) or \( \pi \). Then, additional nodes could be expected along these horizontal or vertical lines in the Brillouin zone. Since the product of the two energies \( \epsilon_1\epsilon_2 \) has to be negative [i.e., the energies cannot vanish, otherwise we recover (1)], the nodes, if they exist, will appear in between the hole and electron pockets at locations in \( k \) space that do not belong to the original tight-binding Fermi surface. To understand this interesting result, consider the ex-

![FIG. 17. (Color online) (a) Energy vs momentum for the noninteracting tight-binding Hamiltonian (14) using the hoppings from band-structure calculations (Ref. 73), \( t_1=-1, t_2=1.3, \) and \( t_3=t_4=-0.85 \) (in eV units). These noninteracting results are shown as continuous lines. Also shown are the additional Bogoliubov bands produced by the pairing interaction considered in this work (dashed lines). The circles (boxes) indicate the bands that contribute electrons to the intraband (interband) pairs at different locations close to the FS (for a discussion see text). (b) Fermi surface for the corresponding noninteracting half-filled system.](image1)

![FIG. 18. (a) Energy vs momentum for the mean-field Hamiltonian using \( t_1=-1, t_2=1.3, \) and \( t_3=t_4=-0.85 \) (in eV units) (Ref. 73). The Bogoliubov bands produced by the pairing interaction considered in this work are also shown, with equal intensity. The four panels correspond to four different values of the pairing attraction: (a) \( V=0 \), (b) \( V=0.5 \), (c) \( V=1 \), and (d) \( V=8 \).](image2)
ample of \( k_x = 0 \). For this special case we obtain
\[
V_B^2 = V^2(1 + \cos k_y)^2,
\]
\[
\epsilon_1 = -2t_2 - 2t_1 \cos k_y - 4t_3 \cos k_y - \mu,
\]
\[
\epsilon_2 = -2t_1 - 2t_2 \cos k_y - 4t_3 \cos k_y - \mu.
\] (37)

Replacing Eq. (37) in Eq. (36), a quadratic equation is obtained that allows us to find the values of \( \cos k_y \) where nodes should appear. Depending on the specific values of \( V \), the hopping amplitudes, and \( \mu \), the quadratic equation can have two solutions (meaning that two nodes appear along the \( k_y = 0 \) axis between the hole and electron pockets), one solution (meaning just one node), or no solution at all (indicating no extra nodes). Thus, once the folding and rotation of the FBZ is performed, nodes can appear along the diagonals of the BZ in Fig. 1(c) for particular values of the parameter in the model.\(^{103} \)

A variety of examples obtained numerically illustrates this nontrivial nodal structure, as shown in Fig. 19: (a) at weak \( V \), several nodes are found either at or close to both the hole and electron pockets. In view of recent photoemission experiments reporting the absence of nodes at the hole pockets (see discussion below), this regime is unlikely to be realized experimentally. (b) is obtained increasing \( V \): in this case the number of nodes has decreased. In addition to those coming from solution (1) in the previous discussion, all at the electron pockets, still solution (2) provides some nodes at the boundaries of the Brillouin zone in this regime. (c) is the most canonical result, obtained at intermediate \( V \), with the nodes only appearing in the electron pockets where \( \cos k_x + \cos k_y = 0 \) intersects the original Fermi surface. Both in (b) and (c) there are no nodes in the \( \Gamma \) centered hole pocket even for this \( B_{2g} \) state. (d) provides the results of (c) but in the folded zone for comparison with experiments.

Band dispersions obtained with mean-field results are also shown in Fig. 18. We observe how the nodes along the \( \Gamma - X \) and \( X - M \) directions get closer to each other as \( V \) increases from 0 to 0.5 and to 1 and how they have disappeared for \( V = 8 \). It is also interesting to see how the crossing of different bands, indicated by the orange squared boxes in Fig. 17(a), is replaced by a gap as soon as \( V \) is finite [see panel (b) in Fig. 18] which appears to be the effect of the interband interaction.

For completeness, in Fig. 20 we provide the nodal structure for the case of hoppings obtained from the Slater-Koster approximation, which gives large pockets in the band-structure calculations. In the weak coupling case, (a), once again several nodes are obtained. This regime appears unrealistic. Increasing \( V \), panel (b) shows that the nodes only remain in the electron pockets, as found before in Figs. 19(c) and 19(d).

In addition to the analytic discussion, we have also searched numerically, using a large lattice \( 200 \times 200 \) in \( k \)-space, for the zero eigenvalues of the original matrix [Eq. (28)]. These numerical results are in excellent agreement with the analytic discussion, thus showing that the nodal structure of the two-orbital mean-field pairing Hamiltonian has been properly obtained.

3. Comparison with ARPES experiments

How do these theoretical calculations based on the two-orbital model compare with angle-resolved photoemission experiments for the Fe pnictides? In Ref. 45, ARPES results were presented with the focus of the effort on the hole pockets at \( \Gamma \). It was concluded that nodes were not observed in those hole pockets. This result is compatible with our \( B_{2g} \) state since nodes do not appear on the hole pockets, but instead on the electron pockets, at least at intermediate values of the attraction \( V \). In Ref. 46, a similar conclusion was
reached but in this case the electron pockets were also studied. However, in that effort the 122 materials for which the FS depends on \(k_z\) were analyzed, and only a few cuts in momentum-space were investigated. Recent ARPES experiments that suggest a short Cooper-pair size\(^{104}\) would suggest that the regime of large \(V\) in our study of the nodal structure is the most realistic, thus clearly locating all the nodes in the electron pockets. Then, a more detailed ARPES analysis would be needed to fully conclude that there are no nodes in this system, particularly in the electron pockets.\(^{105}\) Other recent ARPES experiments have shown a variety of interesting aspects, such as substantial differences with band-structure calculations,\(^{106}\) which also need to be incorporated in future theoretical studies.

The information provided in this paper for the actual location of the nodes for the \(B_{2g}\) state will help to guide future ARPES experiments. In view of the several other experimental investigations that have reported nodes in the Fe-based superconductors,\(^{33–43}\) we believe this issue is still open and needs further research to arrive to a final conclusion. If future experimental work clearly proves that there are no nodes in the Fe-based superconductors, not only in the hole pockets but more importantly in the electron pockets, then it will be concluded that the two-orbital model used here will not be sufficient to properly describe this family of materials and more orbitals will be needed.\(^{107}\)

VI. CONCLUSIONS

In this paper, we have studied some properties of a two-orbital approach for the Fe-based superconductors. It is important to find out the minimal model capable of reproducing the basic physics of these materials. By studying a relatively simple model, considerable insight could be reached on the inner mechanisms that cause magnetism and superconductivity in these compounds. While models with more than two orbitals would certainly be more accurate, the difficulty in extracting reliable numbers from the models grows fast with the number of orbitals. Two-orbital models are the minimal that allow for a study of simple multiband effects on magnetism and superconductivity, and also allow for the possibility of exploring orbital order in the pnictide materials\(^{108}\) in future works.

Here we have shown that the magnetic properties of the undoped parent compound are properly reproduced by a simple two-orbital model: spin stripes are obtained in agreement with neutron scattering experiments. Regarding electron doping, here we follow the same approach as for the cuprates: it is expected that the pairing channel will be unveiled by simply studying the symmetry properties of the state of two electrons added to the half-filled ground state. This approach worked for the models for Cu-oxide superconductors, leading to the \(d\)-wave state prediction. Within this assumption, the spin-singlet pairing state that dominates in the phase diagram at realistic values of the Hubbard repulsion \(U\) is found to transform according to the \(B_{2g}\) representation of the lattice symmetry group. At large Coulomb repulsion \(U\), too large to describe the metallic state of the undoped compound, we found that the relative symmetry of the undoped and electron doped ground states is the same and, thus, they are connected by a pairing operator that transforms according to \(A_{1g}\). We showed that the NNN pairing operator with this symmetry is the \(s\) state and that this state, according to our numerical calculations, prevails only in an unphysical regime of parameters. On the other hand, for a robust electron-electron effective attraction to form Cooper pairs, assumption compatible with the conclusions of recent ARPES experiments, the \(B_{2g}\) pairing state found for realistic \(U\) has nodes only in the electron pockets. All our main conclusions do not depend qualitatively on the set of hopping amplitudes used: our results appear to be representative of the two-orbital framework in general and not merely of a particular model with particular couplings. Thus, a conclusion of our study is that more refined ARPES experiments in the superconducting state are needed to analyze the possible existence of nodes in the electron pockets. These future experiments will provide crucial information to guide the theoretical search for the minimal model that captures the physics of the Fe pnictides.

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APPENDIX A: EFFECTIVE INTERACTION THAT GENERATES THE \(B_{2g}\) PAIRING OPERATOR

The mean-field superconducting state discussed before could originate from an effective attractive density-density interaction dynamically generated in the original Hamiltonian or induced by particular phononic modes if an electron-phonon coupling is incorporated. The form of this attraction is

\[
H_{\text{attr}} = - V \sum_{i,\mu,\sigma} n_{i,\alpha,i} n_{i+\mu,-\sigma}
\]

and below we prove that indeed it generates the correct pairing term. It is well-known that a similar nearest-neighbor density-density attraction of the form \(-V n_i n_{i+\mu}\) leads to \(d\)-wave superconductivity in a mean-field treatment of the one-band repulsive \(U\) Hubbard model.\(^{109}\) Here we merely generalize this concept to two orbitals.

Let us discuss the mean-field treatment of \(H_{\text{attr}}\). In momentum space, the Fourier transformed of this effective attraction is

\[
H_{\text{attr}} = - \sum_{k,k',\alpha,\sigma} V_{k,k'} d_{k,\alpha,\sigma}^\dagger d_{-k,-\alpha,-\sigma} d_{-k',-\alpha,-\sigma} d_{k',\alpha,\sigma}
\]

where we have requested that the pairing occurs between electrons with opposite momentum (thus, we have dropped a third sum over all wave vectors), in different orbitals, and with opposite spin, as required by the dominant singlet pair-
ing operator obtained from the numerical simulations. The potential is given by

\[ V_{k,k'} = -2V(\cos(k'_x - k_x) + \cos(k'_y - k_y)) \]

\[ = V(k' - k) = \sum_i \tilde{V}_i \eta_i(k) \eta_i(k'), \]

where \( \eta_i(k) \) are the irreducible representations of the group \( D_{4h} \). Since the ED numerical results indicate that the pairing operator is proportional to \( (\cos k_x + \cos k_y) \), which corresponds to the irreducible representation \( A_{1g} \), we will focus on that particular term in the expansion of the full potential \( V_{k,k'} \). Thus, we will consider Eq. (A2) but using the long-range separable potential,

\[ V_{k,k'} = V'(\cos k_x + \cos k_y)(\cos k'_x + \cos k'_y), \]

instead of the full short-range potential.

We will treat the four-fermion term in \( H_{\text{attr}} \) within the usual mean-field approximation, where some pairs of fermionic operators are replaced by numbers, such as \( \langle b_{k,x}^\dagger b_{k,x} \rangle \), to be found self-consistently. Then \( H_{\text{MF}} = H_{\text{TB}} + \sum_{k,k',\alpha} (V_{k,k'}\langle b_{k,\alpha}^\dagger d_{-k',-\alpha}^\dagger \rangle \langle d_{-k',-\alpha} \rangle) \)

\[ + V_{k,k'}\langle b_{k,\alpha}^\dagger d_{-k,\alpha}^\dagger \rangle \langle d_{k,\alpha} \rangle - \sum_{k,k',\alpha} V_{k,k'}\langle b_{k,\alpha}^\dagger \rangle \langle b_{k',\alpha} \rangle. \]

Defining \( \Delta(k) = -\sum_{k',\alpha} V_{k,k'}\langle b_{k',\alpha} \rangle \)

\[ \Delta^\dagger(k) = -\sum_{k',\alpha} V_{k,k'}\langle b_{k',\alpha}^\dagger \rangle, \]

and using the separability of the potential Eq. (A3), we obtain

\[ H_{\text{MF}} = H_{\text{TB}} + \sum_{k,\alpha} [\Delta^\dagger(k) d_{-k,-\alpha} \langle d_{k,\alpha} \rangle] \]

\[ + \Delta(k) \langle d_{k,\alpha} \rangle \langle d^\dagger_{-k,-\alpha} \rangle - \sum_{k,k',\alpha} V_{k,k'} \langle b_{k,\alpha}^\dagger \rangle \langle b_{k',\alpha} \rangle, \]

which leads to the same self-consistent equations as in Sec. V by setting

\[ \Delta^\dagger(k) = \Delta(k) = V'\Delta(\cos k_x + \cos k_y) \]

and \( V = V'\Delta \), where \( \Delta \) should be obtained by solving the gap equation that is obtained from minimizing the energy of the mean-field Hamiltonian with respect to \( \Delta(k) \).

**APPENDIX B: s± Pairing Involving \( d_{zx} \) and \( d_{yz} \) Electrons**

In Sec. IV B 2 we showed that our numerical simulations favored a spin-singlet interorbital pairing state with \( B_{2g} \) symmetry in the physical regime of parameters of the two-orbital model, while a pairing state with symmetry \( A_{1g} \) prevailed only in the unphysical strong coupling regime and at the singular point \( U = U' \), \( J = 0 \). In this appendix we will discuss in more detail the pairing operators with \( A_{1g} \) symmetry in the context of the two-orbital model, and we will show that a \( s \pm \) pairing operator involving only \( d_{zx} \) and \( d_{yz} \) electrons belongs to this group.

The extensive literature on the \( s \pm \) pairing state indicates that this state does not have nodes on the Fermi surface and that

\[ \Delta^\dagger(k) = -\Delta^2(k + q), \]

where \( 1 (2) \) denotes the electron (hole) Fermi surface and \( q = (\pi,0) \) or \( (0,\pi) \).

From the classification of possible pairing states for the \( d_{zx} \) and \( d_{yz} \) orbitals provided in Ref. 89, we realize that there exist the following four nodeless pairing operators: (i) pairing state 1 which produces on-site intraband pairs which are even under orbital exchange, spin singlets, and transforms according to the \( A_{1g} \) irreducible representation of \( D_{4h} \). Following the steps of Sec. VA for this pairing state we obtain

\[ H_{\text{MF}} = \begin{pmatrix}
\xi_{xx} & \xi_{xy} & \Delta_0 & 0 \\
\xi_{xy} & \xi_{yy} & 0 & \Delta_0 \\
-\Delta_0 & -\xi_{xx} & -\xi_{yy} & 0 \\
0 & 0 & 0 & -\epsilon_1
\end{pmatrix}, \]

where \( \Delta_0 \) is a constant independent of momentum. In the base in which the tight-binding Hamiltonian is diagonal we obtain

\[ H_{\text{MF}} = \begin{pmatrix}
\epsilon_1 & 0 & 0 & \Delta_0 \\
0 & \epsilon_2 & \Delta_0 & 0 \\
0 & -\epsilon_2 & \Delta_0 & 0 \\
0 & 0 & 0 & -\epsilon_1
\end{pmatrix}. \]

This leads to intraband pairing \( \Delta_0 = V \) which is momentum independent and equal for the two bands. This does not correspond to the \( s \pm \) pairing since it does not satisfy Eq. (B1).

Now let us consider nearest-neighbor pairing. We find that the only nodeless pairing operators involving electrons in nearest-neighbor sites also have symmetry \( A_{1g} \) and result from a (ii) symmetric [or (iii) antisymmetric] combination of pairings 2 and 3. The symmetric (antisymmetric) combination corresponds to pairing of the \( d_{zx} \) electrons along the \( x(y) \) direction while the \( d_{yz} \) pairs along the \( y(x) \) direction. Following the steps of Sec. VA we obtain

\[ H_{\text{MF}} = \begin{pmatrix}
\xi_{xx} & \xi_{xy} & \Delta_1 & 0 \\
\xi_{xy} & \xi_{yy} & 0 & \Delta_2 \\
-\Delta_1 & -\xi_{xx} & -\xi_{yy} & 0 \\
0 & 0 & 0 & -\epsilon_1
\end{pmatrix}, \]

where \( \Delta_1 = V \cos k_x (V \cos k_y) \) and \( \Delta_2 = V \cos k_y (V \cos k_x) \) for the symmetric (antisymmetric) combination. In the base in which the tight-binding Hamiltonian is diagonal we obtain...
where $V_1$, $V_2$, and $V_{12}$ are given by
\[ V_1 = u^2 \Delta_1 + v^2 \Delta_2, \]
\[ V_2 = v^2 \Delta_1 + u^2 \Delta_2, \]
\[ V_{12} = uv(\Delta_1 - \Delta_2). \]
Thus, this leads to intraband interactions $V_1$ and $V_2$ which, according to our numerical checks, satisfy $V_i(k) = -V_i(k + q)$ as expected for the $s^\pm$ pairing.

(iv) Finally, we can also focus on pairs of electrons along the diagonals of the square lattice formed by the Fe ions. Following the notation in Ref. 89 the corresponding basis function is $\cos k_x \cos k_y$ that transforms according to $A_{1g}$. This basis provides a pairing operator with a full gap and which is a spin singlet. It is the analog of pairing 2 in Ref. 89. This basis function is $\cos k_x \cos k_y$.

The pairings that transform according to two different irreducible representations of $D_{4h}$, i.e., $B_{12}$ and $B_{2g}$, have the same symmetry and are connected by a pairing operator that pairs electrons along the diagonals of the Fe square lattice formed by the Fe ions.

In the base in which the tight-binding Hamiltonian is diagonal we obtain
\[ H'_{MF} = \begin{pmatrix} \xi_{xx} & \xi_{xy} & \Delta_k & 0 \\ \xi_{xy} & \xi_{yy} & -\Delta_k & 0 \\ \Delta_k & -\Delta_k & -\xi_{xx} - \xi_{xy} & 0 \\ 0 & 0 & \Delta_k & \xi_{xx} + \xi_{xy} \end{pmatrix}, \]
where $\Delta_k = V \cos k_x \cos k_y$, which is exactly the form of the $s^\pm$ pairing interaction proposed in Ref. 65.

In the base in which the tight-binding Hamiltonian is diagonal we obtain
\[ H'_{MF} = \begin{pmatrix} \epsilon_1 & 0 & 0 & \Delta_k \\ 0 & \epsilon_2 & \Delta_k & 0 \\ 0 & \Delta_k & -\epsilon_2 & 0 \\ 0 & 0 & \Delta_k & -\epsilon_1 \end{pmatrix}, \]
Note that this pairing operator corresponds to the $s^\pm$ pairing since it satisfies $V_1(k) = -V_1(k + q)$ and there is no interband pairing. Thus, we have found that the $s^\pm$ pairing operator is possible in the two-orbital model and transforms according to $A_{1g}$. However, the Lanczos numerical calculations presented in the text suggest that in the region of physical interest the undoped ground state has to be connected to the ground state with two extra electrons via a pairing operator that transforms according to $B_{2g}$ and, for this reason, the $s^\pm$ state is not favored. It only can prevail in the strong coupling regime of $U$ and at the unphysical singular point $U = U'$, $J = 0$ where the ground states in the doped and undoped regimes have the same symmetry and are connected by a pairing operator with $A_{1g}$ symmetry.

For completeness, let us also consider a $s^\pm$ pairing operator frequently used in the literature.\cite{49,61,62,65} In this context it is assumed that $\Delta_1 = -\Delta_2 = \Delta_0$ which is independent of the momentum. Let us find whether this result is consistent with the symmetry of the two-orbital model. We start with $H'_{MF}$ and working backward the form of $H_{MF}$ is found. By this procedure we obtain
\[ H'_{MF} = \begin{pmatrix} \epsilon_1 & 0 & 0 & \Delta_0 \\ 0 & \epsilon_2 & -\Delta_0 & 0 \\ 0 & -\Delta_0 & -\epsilon_2 & 0 \\ \Delta_0 & 0 & 0 & -\epsilon_1 \end{pmatrix}, \]
which in terms of the original two orbitals corresponds to
\[ H_{MF} = \begin{pmatrix} \xi_{xx} & \xi_{xy} & \Delta_x & \Delta_{xy} \\ \xi_{xy} & \xi_{yy} & -\Delta_x & -\Delta_{xy} \\ \Delta_x & -\Delta_y & -\xi_{xx} - \xi_{xy} & 0 \\ \Delta_y & -\Delta_y & \xi_{xx} + \xi_{xy} & \Delta_x \\ 0 & 0 & \Delta_x & \xi_{xx} + \xi_{xy} \end{pmatrix}, \]
where
\[ \Delta_x = (u^2 - v^2)\Delta_0, \]
\[ \Delta_y = -(u^2 - v^2)\Delta_0, \]
\[ \Delta_{xy} = 2uv\Delta_0. \]
We have found that $uv$ transforms according to $B_{1g}$ and $u^2 - v^2$ according to $B_{2g}$, then this case corresponds to a linear combination of on-site intraorbital (5) and interorbital (8) pairings that transform according to two different irreducible representations of $D_{4h}$, i.e., $B_{1g}$ and $B_{2g}$. The coexistence of pairs with different symmetries can occur only if the ground state with $N$ particles and/or the ground state with $N + 2$ electrons are/is degenerate or nearly degenerate. Numerically, we have found that the ground states appear to be singlets and the ground states in the doped and undoped regimes have the same symmetry and are connected by a pairing operator with $A_{1g}$ symmetry.

Summarizing, here it was shown that the $s^\pm$ pairing operator that pairs electrons along the diagonals of the Fe square lattice using the $d_{xy}$ and $d_{yz}$ orbitals does transform according to the $A_{1g}$ irreducible representation of the $D_{4h}$ group that characterizes the symmetry of the Fe-As planes in the pnictides. Numerically we found that this is the pairing symmetry that prevails in the strong coupling regime but that in the physical regime the pairing operator must transform according to $B_{2g}$. In addition, we have observed that the often-used momentum-independent approximation for the $s^\pm$ operator does not respect the symmetry of the Fe-As planes.
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Q. Han, Y. Chen, and Z. D. Wang, EPL 82, 37007 (2008).


For small $|\rho d|<0.15$, we find other states. They have $p$ symmetry and their momentum is $(\pi,\pi)$ instead of $(0,0)$. Since these parameters locate us close to the phase transition of the half-filled system at $pd=0$, where the Fermi surface topology changes [see Fig. 9(d)] and the crucial $(0,\pi)$ spin order breaks down [see Fig. 11(a)], we tentatively attribute these exotic results with finite-momentum pairing to finite size effects.


Another way to understand the “nontrivial” nodes in the MF solution is the following: if $\xi_{\pi y}=0$, which happens when $\sin(\tilde{\kappa}_x)=0$...
(for \(i=x\) or \(y\)) as already discussed, then the original Hamiltonian \((28)\) has a simple form. The nodes will occur at values of \((k_x, k_y)\) where the determinant of Eq. \((28)\) with \(\xi_{i\gamma}=0\) vanishes. The resulting equation is given by \(\Delta^2_k + \xi_{xx}\xi_{yy} = 0\). Note now that \(\xi_{ii}\) and \(\xi_{kk}\) are only functions of \(\cos k_x\) or \(\cos k_y\) since one of these cosines is fixed to 1 or \(-1\) due to \(\xi_{ii}=0\). The product \(\xi_{xx}\xi_{yy}\) has to be negative indicating that, if the resulting quadratic equation has real solutions, the nodes will appear at points that lie in between the two noninteracting Fermi surfaces, as derived before.


105 A similar conclusion regarding the importance of further analyzing the electron pockets holds for the ARPES study reported in Ref. 28.


107 We have observed that pairing 8 (\(B_{2g}\) on site) that, as mentioned in the text, appears to coexist with pairing 9 (\(B_{2g}\) nearest neighbors) produces a nodeless gap for some values of \(V\). However, only combinations of pairings 8 and 9 in which \(V\) is stronger for 8 provide a nodeless gap while the numerical results appear to indicate that \(V\) should be smaller for 8.


