Nodal Spin Density Wave and band topology of the FeAs based materials

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The recently discovered FeAs-based materials exhibit a $(\pi,0)$ Spin Density Wave (SDW) in the undoped state, which gives way to superconductivity upon doping. Here we show that due to an interesting topological feature of the band structure, the SDW state cannot acquire a full gap. This is demonstrated within the SDW mean-field theory of both a simplified two band model and a more realistic 5-band model. The positions of the nodes are different in the two models and can be used to detect the validity of each model.

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I. INTRODUCTION

Since the discovery of superconductivity in La$_{1-x}$Fe$_x$As at $T_c = 26$K, there has been mounting excitement associated both with the rapidly increasing $T_c$ when La is substituted by other lanthanoids, as well as the similarity with the cuprate superconductors. As with the cuprates, the FeAs materials are quasi 2D square lattice based transition metal compounds, which are magnetically ordered at stoichiometry. On doping, in both cases, the magnetism is replaced by superconductivity.

However, there are several significant differences. Most importantly, the FeAs stoichiometric compounds are not insulating. Also, the magnetic order here is along the $(\pi,0)$ direction, and has a small moment. In contrast to the cuprates, where only the $d_{x^2-y^2}$ orbital of the five Cu d-orbitals is important, the multi-orbital nature of the FeAs materials have been emphasized in several recent calculations. In this paper we point out a topological aspect of the band structure, closely connected with the multi-orbital nature of the material, that has important ramifications for the phases in this system. In particular we show that a symmetry enforced band degeneracy at high symmetry points in the Brillouin zone leads to a band structure with nontrivial topology. This can be quantified in terms of a ‘vorticity’ quantum number. An example of vorticity $\pm 1$ is the Dirac node. Here the vorticity takes on values $\pm 2$. While such degenerate points occur in the band structure of other multi-orbital systems, here they actually occur close to the Fermi level. In this article we discuss both a simplified 2-band model and a realistic 5-band model where this is explicitly realized.

An important consequence of this nontrivial band topology is that it leads to an unusual Spin Density Wave (SDW) state that is necessarily gapless. Specifically, the SDW wavevector connects hole pockets with vorticity $= \pm 2$ with electron pockets with zero vorticity. This mismatch forces nodes in the SDW gap function even in the presence of perfect nesting. Away from nesting the nodes are offset from the fermi energy, resulting in fermi pocket. We term such magnetic order ‘nodal-SDW’. We emphasize that the topological feature required for the nodal SDW state exists both in other simplified models in the literature as well as first-principles band structures.

In the following we first derive and study a simplified two-orbital tight-binding model motivated by the quantum chemistry. Other studies have also focused on two orbital models. However it has been argued that one needs at least three orbitals to accurately reproduce the LDA band structure and Fermi surfaces, e.g. location of the hole pockets in the Brillouin Zone. We then directly study the more general and realistic 5-band model based on LDA calculation. We consider the stoichiometric compound (zero doping), and study the mean-field SDW phase. This mean field analysis confirms the existence of nodes in the SDW gap function in both models. We also established the topological stability of the nodes. The location of the nodes in momentum space, and the associated fermi surface topologies, however, are different in the two models. This can be used to detect the validity of 2-band or 5-band model. A recent numerical renormalization group study by us has found precisely this nodal structure in the two-band model. The general requirements for the existence of these nodes are also discussed.

II. NODAL SDW IN THE 2-BAND MODEL

A. 2-band microscopic model and band structure

The Fe atoms form a square lattice whose principal axes are denoted as $x$ and $y$, and the crystal structure axes are labeled as $X$ and $Y$[Fig. 1(b)]. Let us first assume that Fe 3$d_{xz}$ and 3$d_{yz}$ are the relevant orbitals to describe the low energy physics of this material. Because of the tetragonal symmetry they are locally degenerate, and we use their linear combinations 3$d_{x^2-y^2}$ and 3$d_{y^2}$ as our basis since they have clear symmetry when hybridized with the nearest As 4$p$ orbitals. Other $d$ orbitals will be ignored here, but included in a later section.

In a simple chemistry picture[Fig. 1(a)] all symmetry allowed Fe 3d-As 4p hybridizations are assumed to domi-
nate over direct Fe 3d hybridization. This naturally leads to large nearest-neighbor (NN) orbital-changing hopping \( t_1 \) (see Fig. 1(b)), note that \( t_1 \) has opposite signs between vertical and horizontal bonds), next-nearest-neighbor orbital-preserving hoppings \( t_2 \) and \( t'_2 \). If we further assume that the hybridizations between 3d_{xz,yz} and 4p_z, shown in Fig. 1(a) dominate, we expect \( t_2 \sim t_1 \gg |t'_2| \), while the direct hopping \( t'_1 \) is expected to be much smaller than these two\(^{16}\).

Given the empirically observed SDW order, we take \( t_2 - t'_2 > |t_1| \), which leads to nested electron and hole pockets at \( (\pi, 0) \).

To simplify the notation we will use \( d_1 \) and \( d_2 \) for electron operators associated with the XZ and YZ orbitals. The tight binding Hamiltonian has only one Fe atom per unit cell, and we choose the Brillouin zone accordingly. Many other studies work with a two Fe atom unit cell, a comparison requires an appropriate folding of the Brillouin zone of the present study. Its Fourier transform is (independent of spin)

\[
H_0 = \sum_{\vec{k}} \left( \begin{array}{cc} a_{1,\vec{k}}^\dagger & a_{2,\vec{k}}^\dagger \end{array} \right) K(\vec{k}) \left( \begin{array}{c} a_{1,\vec{k}} \\ a_{2,\vec{k}} \end{array} \right)
\]

where the sum is over \( k_x \in [-\pi, \pi], \ k_y \in [-\pi, \pi], \) the \( 2 \times 2 \) matrix \( K(\vec{\kappa}) \) is

\[
K(k_x, k_y) = 2t_1 (\cos k_x - \cos k_y) \tau_1 - 2(t_2 - t'_2) \sin k_x \sin k_y \tau_2
+ [2(t_2 + t'_2) \cos k_x \cos k_y + 2t'_1 (\cos k_x + \cos k_y)] \cdot \mathbf{1}
\]

and \( \tau_{1,2,3} \) are Pauli matrices. As argued previously we expect \( t_2 \gg t_1 \gg t'_2, t'_1 > 0 \). The two energy eigenvalues of Eq. (2) are:

\[
E_{\pm}(\vec{k}) = 2(t_2 + t'_2) \cos k_x \cos k_y + 2t'_1 (\cos k_x + \cos k_y)
\]

\[
\pm 2 \sqrt{t_1^2 (\cos k_x - \cos k_y)^2 + (t_2 - t'_2)^2 \sin^2 k_x \sin^2 k_y}
\]

In Fig. 2(a) we plot the band structure Eq. (3). At half-filling the fermi level will cut out two hole-like fermi surfaces around \( (0, 0) \) and \( (\pi, \pi) \), and two electron-like fermi surfaces around \( (\pi, 0) \) and \( (0, \pi) \) (see Fig. 2(b)). Note the band touchings at \( (0, 0) \) and \( (\pi, \pi) \). This endows the hole.

Fermi surfaces with 'vorticity' \( \pm 2 \), where the spinor describing the admixture of 3d_{xz,yz} and 3d_{yz} orbitals rotates twice on encircling these Fermi surfaces. The simultaneous presence of inversion and time reversal symmetry in this band structure allows us to choose at each \( k \) point, real spinor wavefunctions which are hence confined to a plane. Vorticity in this spinor field is therefore topologically protected - the singularity at the vortex center forces the orbital degeneracy at \( (0, 0) \) and \( (\pi, \pi) \). In contrast, the electron Fermi surfaces are topologically trivial, with no winding as shown in Figure 2(b). This topological characterization of the fermi pockets is also present in more realistic LDA calculations, although it has not been previously commented upon.

At half filling, the total electron pocket area equals the total hole pocket area. If the pockets are every small, i.e. \( t_2 \approx t_1 \), Taylor expansion of Eq. (3) gives four nearly circular fermi pockets with same area. Therefore the electron and hole pockets are nested at momentum \( (\pi, 0) / (0, \pi) \).

It is interesting to consider for a moment the case \( t'_1 = 0 \). Then, the model decouples into two independent \( t_2 - t'_2 \) checkerboard models. Each give rise to one hole and one electron pocket, separated by \( (\pi, \pi) \) from the other electron-hole pocket pair. Unexpectedly, the electron and hole pockets are precisely nested with momentum \( (\pi, 0) / (0, \pi) \), as long as \( t'_1 = 0 \), even when the pockets are large and non-circular. One can check that at the half filling Fermi energy \( E_F = \pm 2t_1/\sqrt{t_2+t'_2} \), the fermi surface wavevectors \( \vec{k}_F \) of the two bands: \( E_-(\vec{k}_F) = E_F \) and \( E_+(\vec{k}_F + (\pi, \pi)) = E_F \) satisfy exactly the same condition:

\[
[(t_2 + t'_2)^2 \cos^2 k_y - t_1^2] [(t_2 + t'_2)^2 \cos^2 k_y - t_1^2]
= (t_2 + t'_2)^2 (t_2 - t'_2)^2 \sin^2 k_F \sin^2 k_F.
\]
along the $k_y$ ($k_z$) direction and the perfect nesting is lost.

B. Mean Field Study of the SDW order in the 2-band model

Now we include on-site interactions in an extended two-band Hubbard model with $H = H_0 + H_I$ where, as in Ref.9,

$$H_I = \frac{U}{2} \sum_i (n_{i1}^2 + n_{i2}^2) + (U - 2J) \sum_i n_{i1} n_{i2}$$

$$+ J \sum_i d_{i1,\alpha}^\dagger d_{i1,\beta} d_{i2,\beta} d_{i2,\alpha}$$

$$+ J \sum_i (d_{i1,\alpha}^\dagger d_{i1,\beta} d_{i2,\alpha} d_{i2,\beta} + h.c.)$$

(5)

where the first and second terms are the intra-orbital and inter-orbital Coulomb repulsions. The third term the Hund’s coupling and the fourth term is the inter-orbital pair hopping. First principles calculations suggest that the FeAs material is in the intermediate coupling regime and we choose $t_1 = 1$, $t'_1 = 0.2$, $t_2 = 1.7$, $t'_2 = 0.3$ for our Hopping Hamiltonian $H_0$, where we estimate $t_1 \sim 0.3eV$ to get the right bandwidth. Also, we use $U = 4$ (1.2eV), $J = 0.4$, a factor of three smaller than in to get reasonable SDW transition temperatures and moments compatible with experiments.

For small $t'_1$, where good nesting prevails and in the presence of repulsive onsite interactions, it is natural to consider SDW order at wave-vector $(\pi, 0)$. Then, $H_{SDW} = M_{ab} \sum_i (-)^i (d_{i1, a}^\dagger d_{i1, b} - d_{i1, a} d_{i2, b})$ where the spin direction is assumed to be along the $S_2$ axis. Because of the multi orbital nature of the system, different flavors of SDW are allowed, described by the Hermitian matrix $M_{ab}$, which may be parameterized by four real numbers $M_{ab} = [\phi_0 \tau_0 + \phi_1 \tau_1 + \phi_2 \tau_2 + \phi_3 \tau_3]_{ab}$ where $(\tau_0)_{ab} = \delta_{ab}$. We perform the finite temperature mean-field study by using a trial density matrix of the mean-field Hamiltonian $H_{MF} = H_0 + H_{SDW}$. We construct a trial free energy based on this mean-field density matrix: $F_{trial}(\phi_0, \phi_1, \phi_2, \phi_3) = F_{MF} + \langle H_I - H_{SDW} \rangle_{MF}$ where $F_{MF}$ is the free energy of the free fermion system described by $H_{MF}$. The Feynman inequality implies that we need to minimize $F_{trial}$ over the mean field parameters $\phi_i$ keeping the electron density fixed.

Implementing this we find that the model $H_0 + H_I$ has a unique SDW phase at low temperature characterized by $\phi_0 \neq 0, \phi_1 \neq 0$. The symmetry of this phase is consistent with the regular ($\pi, 0$) magnetic order depicted in Fig.4. If we denote the order parameter operators $\hat{m}_{ab} = d_{i1, a}^\dagger d_{i1, b} - d_{i1, a} d_{i2, b}$, in Fig.3(a) we plot these magnetizations as a function of temperature and it is clear that $\langle \hat{m}_{11} \rangle \gg \langle \hat{m}_{22} \rangle$. The fact that the $\phi_2$ and $\phi_3$ orders are not mixed in can be understood from symmetry. Under reflections $P_y$ about the y-axis crossing the plaquette center, $\phi_0$ and $\phi_1$ transform differently from $\phi_3$. Under time reversal, $\phi_2$ order transforms differently from a SDW, and in fact describes a spin-orbital locked state.

The band structure resulting from this SDW is shown in Fig.3(d), where electron and hole pockets in the same direction as the SDW axis are visible for each pair of Fermi surfaces. Even with perfect nesting, the Fermi surfaces are not fully gapped, instead there are Dirac nodes as in Fig.3(b). In the absence of nesting these Dirac nodes are at slightly different energies and the half-filled system has small Fermi pockets. As shown below, the presence of such pockets are required under fairly general conditions. This is the main point of the current study. The presence of such pockets are detectable by ARPES, and also, due to the velocity anisotropy present for the nodes, via conductivity measurements. Based on Drude’s formula we compute the DC conductivities in $x$ and $y$ directions for a mean-field SDW state with nodes along the $x$ direction and with a $T = 0$ magnetic moment of 0.3$\mu_B$ per Fe atom. We find $\sigma_{xx}/\sigma_{yy} = 6.2$. Any state with broken rotation symmetry would have conductivity anisotropy, but the large value here stems from the nodal structure discussed.

For the other SDW type orders, $\phi_2$ or $\phi_3$, the nodes are along the direction orthogonal to the SDW axis. Note that although the nodal structure of our SDW gap func-
tion resembles that of a $p$-wave symmetry, the SDW order that we found is completely on-site and inversion symmetric.

C. No-full-gap ‘theorem’ in the two band model

In the following we argue that the Dirac nodes are topologically stable as long as the SDW order satisfies three conditions (a brief account of this argument was presented in Ref.1, 4): (1) collinear order (denote the magnetization direction by $\hat{n}$) (2) inversion (about the Fe site $I$) symmetry and (3) Effective time reversal symmetry $\mathcal{T}\mathcal{R} = \mathcal{S}\mathcal{R}(\hat{n} \rightarrow -\hat{n}) \circ \mathcal{T}\mathcal{R}$ obtained by combining time reversal and spin reversal ($\mathcal{T}\mathcal{R}$ is time-reversal and $\mathcal{S}\mathcal{R}(\hat{n} \rightarrow -\hat{n})$ is the $180^\circ$ spin rotation which flips the direction of magnetization). These three conditions are naturally satisfied by a $(\pi,0)$ collinear SDW which is consistent with experiments, and the mean-field SDW that we find also satisfies these conditions.

Since we focus on the consequences of the nontrivial band structure, we begin by turning on a very weak SDW order: $\hat{M} = \sum_{\vec{k}} \sigma_{\alpha\beta} M_{\alpha\beta}(\vec{k}) d^\dagger_{\alpha\vec{k}} d_{\beta\vec{k}+(\pi,0)}$ (where we have rotated the magnetization to the $S_z$ direction). We therefore need to consider degenerate perturbation theory in the unfolded Brillouin zone scheme, with a single Fe atom per unit cell (here unit translations along the $x$ and $y$ axes are followed by reflections in the $xy$ plane). The two band model has a hole pocket at $\Gamma = (0,0)$ and another one at $(\pi,0)$, the LDA calculation predicts two hole pockets around the $\Gamma$ point. The electron pockets although centered around the same locations in both cases, acquire a $d_{xz} + d_{xy}$ character at $(0,\pi)$ and a $d_{yz} + d_{xy}$ character at $(\pi,0)$ in the LDA calculations. Hence they are also rather different from the two band model that does not include the $d_{xy}$ orbitals. A 5-band hopping Hamiltonian including all the iron $d$-orbitals is required to capture the fermi surface topology of the LDA calculation.

In this section we will show that even in the five band model, the SDW is necessarily gapless (nodal-SDW), despite these important differences. An important role here is played by the fact that the two hole pockets at the $\Gamma$ point are derived from the $d_{xz}, d_{yz}$, which are precisely the orbitals that enter the two band model. In this case we will prove that there must be at least two Dirac nodes close to fermi level in the SDW phase.

A. The mean-field study of SDW in the 5-band model

We again apply the trial density matrix method to study the $(\pi,0)$ SDW instabilities of the 5-band model. We take the 5-band hopping Hamiltonian $H_0$ from Kuroki et al.\cite{Kuroki} (Eq.(1) and Table I). We then turn on a on-site interaction in the following form:

$$H_I = U \sum_{i,a} n_{ia\uparrow} n_{ia\downarrow} + (U - 2J) \sum_{i,a<b} n_{ia} n_{ib}$$

$$+ J \sum_{i,a,b} d_{ia,a}^\dagger d_{ib,b}^\dagger d_{ia,b} d_{ib,a}$$

$$+ J \sum_{i,a,b} (d_{ia,a}^\dagger d_{ib,a} + h.c.) \tag{6}$$

where $a, b = 1, 2, \ldots, 5$ label the 5 orbitals \{d_{3z^2-r^2}, d_{xz}, d_{yz}, d_{x^2-y^2}, d_{x'y'}\}. We have parameterized the inter-orbital Coulomb interaction by $U - J$. While this is strictly expected to hold within the $t_{2g}$ and $e_g$ levels,\cite{Kuroki} to reduce the number of interaction...
parameters, we assume it for the five-band model as well.

We only consider the on-site SDW order, because the interactions taken to be on-site. Then, the \((\pi,0)\) SDW order parameter with spins assumed to point along the \(z\) axis induces the following mean field term in the Hamiltonian:

\[
H_{SDW} = \sum_i e^{i\pi x_i} \sum_{a,b=1}^5 M_{ab}(d_{i,a}\sigma^z d_{i,b})^\dagger \tag{7}
\]

which is parameterized by \(M_{ab}\), a Hermitian matrix with 25 real parameters. The orbital structure can leads to many different SDW states which break symmetry in different ways. Energetically, we find that the preferred state always has the same symmetry as the regular \((\pi,0)\) SDW shown in Fig 4. That is, the state breaks time reversal \((TR)\) and 180° spin rotation about an axis perpendicular to the ordering direction \(SR\), but preserves their combination \((TR')\). The state is invariant under inversion \((I)\) which is a 180° rotation in the \(x-y\) plane, the \(P_x\) reflection around the \(x\)-axis crossing an Fe atom (which actually combines with \(z \rightarrow -z\) reflection and is a 3-D 180° rotation around the \(x\)-axis), and similarly the \(P_y\) reflection \((P_x \circ P_y = I)\). At the end of this subsection we comment on other possible states, that break different symmetries.

We now discuss details of the mean field solution, as the on-site interaction strength is varied. Since this is not accurately known, we note the resulting ordered moment and Fermi surface topology in each case, which may be directly compared with experiments. The Hund’s coupling \(J\) is assumed to be about 20% of \(U\).

1. \(U=1.0\text{eV}, J=0.2\text{eV}\). The temperature evolution of the net SDW magnetization \(M = \langle \sum_a d_{i,a \uparrow}^\dagger d_{i,a \downarrow} - d_{i,a \downarrow}^\dagger d_{i,a \uparrow} \rangle\) (assuming \(g=2\) this is in unit of Bohr magneton) from mean field theory is shown in Fig 5(a). The mean field transition temperature obtained is \(T_c = 0.026\text{eV}\) while the zero temperature magnetic moment obtained is \(\sim 0.23\mu_B\). The latter is consistent with neutron scattering experiments on \(LaOFeAs\). In Fig 5(c) we present the Fermi surfaces of the zero temperature half-filled SDW phase with these parameters. Note that the double degenerate point at \((0,0)\) of the 5-band hopping Hamiltonian is split into two Dirac nodes, \(C\) and \(C'\), on the \(k_y\) axis. The electron pocket at \((0,\pi)\) still intersect with Fermi level and contributes significantly to the density of states. However, on increasing the interaction strength this feature is suppressed. Stronger repulsive interactions will tend to gap out more of the Fermi surface and the electron pockets at \((0,\pi)\) can be fully gapped out. We note that the area occupied by electron pocket is 3.5% of the magnetic Brillouin zone (defined by \(-\pi/2 < k_x < \pi/2\) and \(-\pi < k_y < \pi\)). The hole pockets, of course, occupy the same area.

2. \(U=1.2\text{eV} \quad \text{and} \quad J=0.25\text{eV}\). In this case we obtain a somewhat larger low temperature moment \(\sim 1.04\mu_B\). In Fig 5(d) we plot the Fermi surfaces of the zero temperature SDW. As compared to the previous cases, we see that the Fermi surfaces around \((0,\pi)\) disappears and the Fermi level adjusts itself to form one hole pocket around \((0,0)\) and four electron pockets. The hole pocket occupies 2.2% of the magnetic Brillouin zone while the area of the electron pockets on the \(k_x\) axis is 0.1% each, and of those on the \(k_y\) axis is 1.0% each.

The electron pockets on \(k_x\) axis and on \(k_y\) axis are fundamentally different in that the \(k_x\)-pockets arise from the Dirac nodes \(A\) and \(A'\) below them, and thus pro-
tected. On the other hand the \( k_y \)-pockets can be easily gapped out by turning on interactions because they are simple band bottoms (after \( B(B') \) and \( C(C') \) annihilate each other, which already happens in the current case).

(4) \( U = 1.4 \text{eV} \) and \( J = 0.3 \text{eV} \). The zero temperature moment is now large \( \sim 2.3 \mu_B \). Now, the two electron pockets along the \( k_y \) axis are completely gapped out and we only have a small hole pocket around \((0,0)\), and two electron pockets on the \( k_x \) axis nearby (see Fig.4(e)).

Note, for the larger interaction strengths, the area occupied by the residual Fermi surface in the SDW state is very small, typically a few percent. In general, interactions that drive the SDW formation would tend to lower this area. One may naturally expect that this would rapidly lead to a fully gapped state on increasing \( U \). However, as explained in detail in the next section, there is an intrinsic mechanism that blocks such a fully gapped state. A combination of symmetry and band topology necessarily leads to a gapless SDW state, over a wide range of coupling strengths. This provides a ‘natural’ protection of the small pockets that appear here and in LDA calculations, which have now been observed in magnetic oscillation experiments.

**Other Possible Orders:** Before we conclude the mean field study of SDW orders, we comment on other kinds of SDW orders that could be stabilized with onsite interactions. The 25 parameter \( M_{ab} \) matrix admits a plethora of different orders, which may be separated into the following four classes, according to the symmetries of the resulting SDW Hamiltonian \( H_{SDW} \):

(i) \( TR' \) even, \( I \) even and \( P_x, P_y \) even. (6 parameters) This is the SDW state that was considered above. The no-full-gap theorem discussed below, applies to this case.

(ii) \( TR' \) even, \( I \) even and \( P_x, P_y \) odd. (3 parameters)

(iii) \( TR' \) even and \( I \) odd. (6 parameters)

(iv) \( TR' \) odd. (10 parameters) This case is rather exotic because \( TR \) is even but \( SR \) is odd. This is similar to the symmetry of a spin-hall insulator.

To compare the relative stabilities of these different states, we choose \( U = 1 \text{eV} \) and \( J = 0.2 \text{eV} \) and first perform an unbiased minimization of all the 25 parameters. We find that class (i) is always the low free energy solution and with the highest \( T_c = 0.026 \text{eV} \). Even if we suppress order parameter (i) by hand, we find the system has no instability towards (ii), (iii) and (iv) down to 0.0001eV. (Computations were performed on a 40 by 40 lattice with periodic boundary.) We conclude that SDW (i) is the low free energy phase in the model Eq. and is consistent with the ordered pattern observed in experiments. Hence, we do not pursue studying these other kinds of SDW order.

**B. No-full-gap ‘theorem’ in the 5-band model**

In this section we explain why the nodal SDW found in the mean field study appears. We assume that the SDW has the symmetries in (i) above, as found in mean field theory. Briefly, we use reflection symmetry along the \( k_x = 0 \) and \( k_y = 0 \) to label bands with a reflection eigenvalue. Bands connected to the electron pocket and a hole pocket are forced to have opposite eigenvalues and hence do not split in the SDW state along these lines, leading to a gapless state. An important role is played by the band touching at the \( k = (0,0) \) point, as in the two band model. While this reasoning holds for weak SDWs, we extend it to include strong SDW instabilities, where the location of the band intersections can migrate to the \( \Gamma \) point. Even in this case so we show that at least two gapless Dirac nodes will remain.

**Weak SDW Limit:** The reflections \( P_x \) and \( P_y \) around the \( x \) and \( y \) axes passing through the Fe atoms (which actually combine with \( z \to -z \) reflection and are 3-D \( 180^\circ \) rotations), act on the orbital basis of \( \{d_{3Z^2-R^2}, d_{XZ}, d_{YZ}, d_{X^2-Y^2}, d_{XY}\} \) as follows (note that our definition of \( X \) and \( Y \) axes given in Fig.4 is different from the definition in Kuroki, et al. by a \( 90^\circ \) rotation),

\[
T_{P_x} : \begin{pmatrix}
1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 1
\end{pmatrix},
\]

\[
T_{P_y} : \begin{pmatrix}
1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0
\end{pmatrix}
\]

Spin is left invariant as we ignore spin-orbit interactions. We first consider the \( P_x \) reflection symmetry. Along \( k_x \) axis the Bloch Hamiltonian is \( P_x \) symmetric and the wave-function should be eigenstates of \( P_x \) with eigenvalues \( \pm 1 \). We thus can simply present the eigenvalue of \( P_x \) of each band as shown in Fig.4 If we focus on the three bands close to fermi level, we find that the electron pocket is \( P_x \) odd, the large hole pocket is \( P_x \) even and the small hole pocket is \( P_x \) odd. Since the relevant SDW orders are \( P_x \) even, the SDW induced gap along \( k_x \) axis between the electron pocket and the large hole pocket must vanish, i.e. there is a band crossing. These are labeled \( A \) and \( A' \) in the example of Fig.5. We note that the bands corresponding to the large hole pocket and the small hole pocket must have opposite \( P_x \) eigenvalues and as result the nodes must exist no matter whether the electron pocket is \( P_x \) even or odd. The simplest way to understand this is to note the double degenerate wave-functions at \( (0,0) \) are nothing but \( d_x \) and \( d_y \). Hence, these band touchings play a crucial role here, as in the two band model.

Similarly there also must be nodes along the \( k_y \) direction by studying the \( P_y \) eigenvalues along the \( k_y \) axis. We find that the electron pocket is \( P_y \) odd, while the large hole pocket is \( P_y \) even and small hole pocket is \( P_y \) odd. Therefore we expect the SDW gap vanishes along \( k_y \) direction between the electron pocket and the large hole.
cause at least there is a rather circular hole pocket around anisotropy of conductivity as in the 2-band model. In the 5-band model, there may not be a large face topologies and shapes are quite different. In particular in the 5-band model, there may not be a large face topologies and shapes are quite different. In particular in the 5-band model.

We compare the nodal SDW in 2-band model and 5-band model. One main difference is that the fermi surface topologies and shapes are quite different. In particular in the 5-band model, there may not be a large anisotropy of conductivity as in the 2-band model because at least there is a rather circular hole pocket around (0, 0). The positions of Dirac nodes and fermi surface topologies, which may be easily measured by single crystal ARPES, can serve as a way to directly detect the validity of 2-band model or 5-band model.

IV. CONCLUSIONS

In this paper, we studied the spin density wave (SDW) ground state of the undoped FeAs compound. We find that the combination of physical symmetry and the topology of the band structure, naturally stabilizes a gapless SDW ground state with Dirac nodes. We first study a popular two-band model due to its simplicity, where this mechanism is manifest. We also study the more realistic five-band model, where the same result obtains. These two rather different models share a key topological feature of the band structure: the double degeneracy at \( \vec{k} = (0, 0) \) enforces a wavefunction winding around this point in the Brillouin zone.

In both models, we perform the mean-field study allowing for all possible collinear magnetic orders at \((\pi, 0)\), and find the inversion and reflection parities of the lowest energy magnetic ordered phase. We then show that the SDW ground state in both models have stable Dirac nodes protected by the inversion symmetry and the topology of the band structure. These Dirac nodes are close to Fermi level and thus may be directly observable in ARPES experiments and might also control the low energy thermodynamic and transport properties of compound. They arise due to the vanishing of the SDW matrix elements along a high symmetry line in the Brillouin zone, which leaves the Fermi surfaces ungapped in this direction. We also proved a general result on the stability of Dirac nodes against pairwise annihilation in an inversion symmetric system (Appendix A) which may be applied to more general situations. While strong interactions tend to increase the SDW gap and reduce the Fermi pocket area, the nodal nature of the SDW does not allow a full gap to open over a wide range of interaction strengths. Hence, one expects to be left with small residual Fermi surface pockets, which naturally explains the small Fermi surface areas (0.52% and 1.38% of the Brillouin zone, which leaves the Fermi surfaces ungapped in this direction. We also proved a general result on the stability of Dirac nodes against pairwise annihilation in an inversion symmetric system (Appendix A) which may be applied to more general situations.

Although we find stable Dirac nodes in the SDW ground state in both the two and five band models, the number and the locations of the fermi pockets are different. These differences can serve as ways to determine which is a better model of the material. Effective low energy theories of the FeAs materials should ideally incorporate the nodal nature of the SDW state, which may also have important consequences for other phases in this system.

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APPENDIX A: ANNIHILATION CONDITION FOR DIRAC NODES

We consider the general question of when a pair of Dirac nodes can come together and annihilate, to give rise to a non-singular band structure. We assume that since \( I \) most differ by a sign, the wavefunction. Hence, these two wavefunctions can be brought together. Now, \( C \) parity , so, the inversion parities \( \sigma \) to fix the inversion eigenvalue of the \( M \) when they are brought together.

To derive this result, we use a Berry’s phase formula to fix the inversion eigenvalue of the \( M \) point states before and after node annihilation. This places the required constrain on the inversion eigenvalues, if the nodes are to annihilate. We first define the inversion parity \( \sigma(C) \) of a half loop \( C \) connecting two points \( P \) and \( P' \), which are mapped to one another by inversion. We start with the wavefunction of one of the bands at \( P \), \( |P_I \rangle \), which can be taken to be real given that we have both time reversal and inversion symmetry. This is evolved adiabatically along the contour \( C \) to give the real wavefunction \( |P'_I \rangle \) at point \( P' \). Clearly this is an eigenstate of the Bloch Hamiltonian at this point in the Brillouin zone. A separate way to obtain the eigenstate at \( P' \) is to apply the inversion operation on the state at \( P \): \( I|P_I \rangle \). Again, the inversion operation can be constructed to yield a real wavefunction. Hence, these two wavefunctions can at most differ by a sign,

\[
|P'_I \rangle = \sigma(C)I|P_I \rangle \tag{A1}
\]

which is the inversion parity \( \sigma(C) \) of the curve \( C \). Note that since \( I^2 = 1 \) \( \sigma(C) \) is independent of the direction of \( C \). Although it depends on the band index, the band label is suppressed for clarity.

Now consider two nodes \( N \) and \( N' \) being brought together at \( M \) and choose two points \( P \) and \( P' \) along the perpendicular direction of this path. As shown in Fig. 7, we choose two paths \( C_1 \) and \( C_2 \) connecting \( P \) and \( P' \). Initially, \( C_1 \) + \( C_2 \) encloses a single Dirac node at \( N \), and as a result we must have \( \sigma(C_1) \sigma(C_2) = -1 \) because the wavefunction must wind by \( \pi \) around a Dirac point. Now assume that the nodes annihilate on being brought together. Now, \( C_1 \) + \( C_2 \) encloses no singularity, so, the inversion parities \( \sigma'(C) \) after this operation satisfy \( \sigma'(C_1) \sigma'(C_2) \) = \( +1 \). However, since the wavefunctions along \( C_1 \) evolve smoothly during the annihilation we have: \( \sigma'(C_1) = \sigma(C_1) \). Therefore we must have 

\[ \sigma'(C_2) = -\sigma(C_2). \]

Note, by shrinking the curve \( C_2 \) we can approach the \( M \) point. Then, the inversion parity of the curve simply becomes the eigenvalue under inversion of the wavefunction at the \( M \) point: \((I_1, I_2)\). Therefore we conclude that in the node annihilation process, the inversion eigenvalue of each of the two states at the \( M \) point changes sign. This is only possible if they have opposite signs to begin with, \( I_1 I_2 = -1 \). In that case they can simply pass through each other, and the net result will be a sign change of the inversion eigenvalue of the higher and lower energy states. However, if they both have the same sign, \( I_1 I_2 = +1 \), it is not possible to affect a sign change. In this case, our assumption that the nodes annihilate is invalid - in fact a pair of bands with quadratic dispersion will touch at the \( M \) point.

If the two bands have opposite inversion eigenvalues, then the inversion matrix in the two bands is \( \tau^3 \). And the inversion symmetric real Hamiltonian around \( M \) must be able to expand as \( (a \delta k_x) \tau^1 + (c \delta k_y + c \delta k_x \delta k_y) \tau^3 \) to the quadratic order after choosing the \( k_x \) axis to be along direction connecting the two nodes. We immediately see that depending on the sign of \( c \), the Hamiltonian either has two or zero band touching nodes. This indicates that if the two bands have opposite inversion eigenvalues, the two nodes can always annihilate at \( M \).

Finally we note that the SDW state in the five band model meets the conditions required for the above analysis to hold. Inversion \( \mathcal{I} \) is a symmetry of the system, and the role of time reversal is played by \( TR' = SR(\hat{n} \rightarrow -\hat{n}) \circ TR \) of \( \mathcal{R} \) (defined in text) symmetric system, where \( \hat{n} \) is the direction of collinear SDW. Let us choose the orbital basis \( d_a \) \((a = 1 \ldots n)\) to be eigenfunctions of inversion and label the eigenvalues to be \( I_a \). We then define the \( \mathcal{I} \circ TR \) even basis \( d_a \) in the following fashion: if \( I_a = 1 \) then \( d_a = d_a \), and if \( I_a = -1 \) then \( d_a = i d_a \). For a collinear SDW with \( TR' \) symmetry the Hamiltonian in \( d_a \) is purely real, and so are the eigenfunction in the momentum space. In this basis, the arguments presented above can be made, leading to the conclusion that a pair of Dirac nodes cannot be annihilated at the \( \Gamma \) point. Hence, since we begin with six nodes in all, there will always be a leftover pair that is stable.
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