Coexistence and competition of spin-density-wave and superconducting order parameters in iron-based superconductors

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Abstract

We theoretically study the coexistence of spin density wave (SDW) and superconductivity (SC) in ironpnictide superconductors based on a three-orbital model, focusing on the momentum-space and real-space distributions of SDW and SC order parameters in the coexistence region. We show that a SDW-SC coexisting state lies in the T - n phase diagram, in qualitative agreement with those of $\text{NaFe}_{1-x}\text{Co}_x\text{As}$ and $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$. In the SC state the pairing wavefunction has $s_{\pm}$ symmetry with $s_{x^2y^2}$ and $s_{x^2+y^2}$ components. In the coexisting state, the SDW and SC order parameters display strong orbital-selective competitions in momentum space, which also result in real-space modulation and spin singlet-triplet mixing in the Cooper pairing amplitude. We expect that the obtained features may be observed in future experiments.

Keywords: iron-base superconductor, spin density wave, orbital-selective competition, singlet-triplet mixing

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1. Introduction

Conventionally, magnetic order competes with superconducting (SC) phase since the effective molecular magnetic field breaks the Cooper pairs, precluding the coexistence of a magnetically ordered state with an SC one. Nevertheless, lots of theoretical studies have shown the possibility of a coexisting antiferromagnetism (AFM) and SC phase [1]. The interplay between AFM and SC in unconventional compounds, such as cuprates and heavy fermion compounds, is an intriguing problem of substantial current interest [2, 3, 4, 5]. In particular, addressing the nature of the coexistence of these two condensations on a microscopic scale is of special importance given the antithetical nature of magnetism and SC [6, 7, 8]. While the coexisting SDW and SC phases may have a significant impact on the mechanism of SC [9], the subtle interacting nature between magnetism and SC is still far from well understood. In recent years many experiments have shown that in ironpnictide compounds [10] the SC order can coexist with a SDW order [11, 12, 13, 14, 15, 16, 17, 17, 18, 19, 20, 21, 22, 23, 24, 25], which gives a unique SC ground state and attracts great attentions.

The coexistence of SDW order with SC order in many ironpnictide compounds has been verified in numerous experiments, including the neutron scattering measurements [12, 26, 13, 14, 15], nuclear magnetic resonance [16, 17, 17, 18, 19], scanning tunneling microscope (STM) [20, 21] and angle-resolved photoemission spectroscopy (ARPES) experiments [24, 25], providing robust evidence for the microscopic coexistence of SDW and SC long-range orders, which also compete for the same electronic states. The competition between the two coexisting orders has been revealed by neutron scattering measurements on the Co-doped [12, 26] and Ni-doped [27] Ba-122 compounds, which showed a reduction of the magnetic Bragg peak intensity upon entering the SC state, and by ARPES measurements on the K-doped Ba-122 compound which showed

that the SDW gap shrinks in magnitude as the system enters the SC phase [28]. Some experiments[29, 30, 31, 32] also suggested that the coexisting phase
 30 may be mesoscopic or nanoscale electronic phase separation rather than microscopic coexistence. It is still unclear how to unify the apparently contrasting experimental results.

It was predicted that microscopic coexistence of an SDW and SC is possible when the SC wavefunctions on different portions of the Fermi surface have
 35 different signs, that is, have $s_{\pm}$ symmetry [33]. The coexistence may cause angular variation of the gap function and even give rise to nodes in the limit of strong AFM ordering [34, 35]. It is also argued that an incommensurate SDW is more likely to coexist with SC than for a commensurate SDW [36, 37]. In contrast, for s_{++} gap symmetry where the phase of the SC order parameter is
 40 a constant, coexistence is only possible when the SC gap has nodes [34], and the coexisting cannot be microscopic [9]. Then it is an important theoretical task to clarify the electronic structure of the coexistence phase, such as how the SC gap or Cooper pairing amplitude distribute in momentum space, and how the two orders coexist and compete in the same electronic structure. Although
 45 many research efforts have been made to clarify the symmetry and structure of the SC gap, suggesting a $s_{\pm}$ symmetry with $\cos k_x \cos k_y$ structure [38], there have been fewer quantitative studies on the symmetry and detailed structure of the SC pairing wavefunction and its evolution as the SDW order emerges and coexists with it.

50 In this paper, we present the phase diagram of a three-orbital t - J_1 - J_2 model describing ironpnictide compounds. We show that the SC pairing occurs mainly in the degenerate xz and yz orbitals, and the pairing wavefunction is a superposition of $s_{x^2y^2}$ and $s_{x^2+y^2}$ waves in both the SC and the SDW-SC coexisting phases. In the coexistence region, the electronic structure displays a strong

55 orbital-dependent character in the momentum-space spectral distribution and
a clear orbital-selective competition between the SDW and SC order parameters.
The coexistence and competition between SDW and SC also result in spin
singlet-triplet mixing and spatial modulation of the SC pairing wavefunction,
and the modulation displays a strong direction dependence and orbital selectiv-
60 ity. Our theoretical results are in good agreement with relevant experimental
observations for the finite-temperature phase diagrams in $\text{NaFe}_{1-x}\text{Co}_x\text{As}$ and
 $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$. The distributions of SDW and SC order parameters in
momentum space appeal for further ARPES experiments, while the real-space
modulation of the pairing amplitude may be observed by high-resolution scan-
65 ning tunneling microscopy experiments.

The rest of this paper is organized as follows: we first outline the model
Hamiltonian and the self-consistent mean-field equations for the SDW and SC
order parameters in section 2. The numerical solutions of these equations are
present in section 3, which give the phase diagram, the competition between SD-
70 W and SC, the electronic structure and the spatial modulation of the superfluid
density. Finally we draw our conclusions in section 4.

2. Model Hamiltonian and Mean-Field Equations

We consider a three-orbital t - J_1 - J_2 model with the tight-binding hopping
integrals, nearest-neighbour and next-nearest-neighbour exchange interactions,
75 and Hund's rule coupling. Considering the references [39] and [40], the Hamil-

tonian reads

$$\begin{aligned}
H = & \sum_{\mathbf{k}, \alpha, \beta, \sigma} T^{\alpha, \beta}(\mathbf{k}) d_{\mathbf{k}, \alpha, \sigma}^\dagger d_{\mathbf{k}, \beta, \sigma} \\
& + \sum_{\mathbf{r}, \mathbf{r}', \alpha, \beta} J_{\mathbf{r}, \mathbf{r}'}^{\alpha \beta} \left[\mathbf{S}(\mathbf{r}, \alpha) \cdot \mathbf{S}(\mathbf{r}', \beta) - \frac{1}{4} n(\mathbf{r}, \alpha) n(\mathbf{r}', \beta) \right] \\
& - J_H \sum_{\mathbf{r}, \alpha \neq \beta} \mathbf{S}(\mathbf{r}, \alpha) \cdot \mathbf{S}(\mathbf{r}, \beta),
\end{aligned} \tag{1}$$

where the operator $d_{\mathbf{r}, \alpha, \sigma}^\dagger$ ($d_{\mathbf{r}, \alpha, \sigma}$) creates (annihilates) an electron at site $\mathbf{r}$ with orbital index $\alpha = xz, yz, xy$ and spin σ . Its Fourier transformation is denoted by $d_{\mathbf{k}, \alpha, \sigma}^\dagger$ ($d_{\mathbf{k}, \alpha, \sigma}$). The corresponding charge and spin density operators are
80 denoted by $n(\mathbf{r}, \alpha) = \sum_{\sigma} d_{\mathbf{r}, \alpha, \sigma}^\dagger d_{\mathbf{r}, \alpha, \sigma}$ and $\mathbf{S}(\mathbf{r}, \alpha) = \frac{1}{2} \sum_{s, s'} d_{\mathbf{r}, \alpha, s}^\dagger \sigma_{ss'} d_{\mathbf{r}, \alpha, s'}$, respectively, where σ represents the Pauli matrices. Following reference [40], the tight-binding matrix $T(\mathbf{k})$ has the following matrix elements

$$\begin{aligned}
T^{1,1} &= 2t_2 \cos k_x + 2t_1 \cos k_y + 4t_3 \cos k_x \cos k_y - \mu, \\
T^{2,2} &= 2t_1 \cos k_x + 2t_2 \cos k_y + 4t_3 \cos k_x \cos k_y - \mu, \\
T^{3,3} &= 2t_5 (\cos k_x + \cos k_y) + 4t_6 \cos k_x \cos k_y - \mu + \Delta_{xy}, \\
T^{1,2} &= T^{2,1} = 4t_4 \sin k_x \sin k_y, \\
T^{1,3} &= \bar{T}^{3,1} = 2it_7 \sin k_x + 4it_8 \sin k_x \cos k_y, \\
T^{2,3} &= \bar{T}^{3,2} = 2it_7 \sin k_y + 4it_8 \sin k_y \cos k_x.
\end{aligned}$$

The exchange interaction $J_{\mathbf{r}, \mathbf{r}'}^{\alpha \beta}$ equals to $J_1^{\alpha \beta}$ if $\mathbf{r}$ and $\mathbf{r}'$ are nearest neighbour, $J_2^{\alpha \beta}$ if $\mathbf{r}$ and $\mathbf{r}'$ are next-nearest neighbour, and vanishes otherwise. In principle,
85 the exchange couplings $J_{1(2)}^{\alpha \beta}$ should be matrices in orbital space. However, for clarity and simplicity, we take $J_{1(2)}^{\alpha \beta} = J_{1(2)}$, i.e., all of the matrix elements take the same value.

Both experimental [41, 42] and theoretical [43, 44, 45] studies have shown

that the parent phases of most ironpnictides have a long-range stripe SDW or-
 90 der with a wavevector $\mathbf{Q} = (\pi, 0)$ or $(0, \pi)$. However, we note that recently
 there are also some experimental and theoretical evidences for more complicat-
 ed magnetic structures in the phase diagram. For example, double- Q phases
 consisting of superposition of ordering at two vectors $\mathbf{Q}_1$ and $\mathbf{Q}_2$ have been
 seen in experiments [46, 47, 48] and studied in theory [49, 50]. A comprehensive
 95 investigation of possible magnetic structures is beyond the scope of this work,
 therefore only the experimentally dominating stripe order would be considered
 in the following. To explore the coexistence of such a SDW and SC orders, we
 decouple the interaction Hamiltonian in a mean-field manner:

$$H_m = \sum'_{\mathbf{k}} (\Phi(\mathbf{k}, \uparrow)^\dagger, \Phi(-\mathbf{k}, \downarrow)^T) A(\mathbf{k}) \begin{pmatrix} \Phi(\mathbf{k}, \uparrow) \\ \Phi(-\mathbf{k}, \downarrow)^{\dagger T} \end{pmatrix}, \quad (2)$$

where the prime in the superscript of the summation means that the momentum
 $\mathbf{k}$ should run over the reduced Brillouin zone,

$$\Phi(\mathbf{k}, \sigma)^\dagger = (d_{1,\mathbf{k},\sigma}^\dagger, d_{2,\mathbf{k},\sigma}^\dagger, d_{3,\mathbf{k},\sigma}^\dagger, d_{1,\mathbf{k}+\mathbf{Q},\sigma}^\dagger, d_{2,\mathbf{k}+\mathbf{Q},\sigma}^\dagger, d_{3,\mathbf{k}+\mathbf{Q},\sigma}^\dagger),$$

and

$$A(\mathbf{k}) = \begin{bmatrix} T(\mathbf{k}) + V_c & M & \Delta(\mathbf{k}) & \tilde{\Delta}(\mathbf{k} + \mathbf{Q}) \\ M^\dagger & T(\mathbf{k} + \mathbf{Q}) + V_c & \tilde{\Delta}(\mathbf{k}) & \Delta(\mathbf{k} + \mathbf{Q}) \\ \Delta^\dagger(\mathbf{k}) & \tilde{\Delta}^\dagger(\mathbf{k}) & -T(\mathbf{k}) - V_c & M \\ \tilde{\Delta}^\dagger(\mathbf{k} + \mathbf{Q}) & \Delta^\dagger(\mathbf{k} + \mathbf{Q}) & M^\dagger & -T(\mathbf{k} + \mathbf{Q}) - V_c \end{bmatrix},$$

with $V_c = V_c^\dagger$ denoting the homogeneous potential due to the charge density and
 100 $M = M^\dagger$ the staggered potential due to the SDW. The pairing potential with
 zero total momentum, that is, between $(\mathbf{k}, \uparrow)$ and $(-\mathbf{k}, \downarrow)$, is $\Delta(\mathbf{k})$, and that

between $(\mathbf{k} + \mathbf{Q}, \uparrow)$ and $(-\mathbf{k}, \downarrow)$ is $\tilde{\Delta}(\mathbf{k})$. All the elements $T(\mathbf{k})$, V_c , M , $\Delta(\mathbf{k})$ and $\tilde{\Delta}(\mathbf{k})$ are 3×3 matrices and hence the total matrix $A(\mathbf{k})$ is a 12×12 matrix. The mean fields encoded in V_c , M , $\Delta(\mathbf{k})$ and $\tilde{\Delta}(\mathbf{k})$ are determined self-consistently through a set of equations.

The self-consistent equations for V_c are

$$V_c^{\mu\mu} = -4 \sum_{\beta} (J_1^{\mu,\beta} + J_2^{\mu,\beta}) n_{\beta\beta}, \quad (3a)$$

$$V_c^{\mu\nu} = \frac{3}{2} J_H n_{\nu\mu}, \quad (\mu \neq \nu), \quad (3b)$$

where $n_{\alpha\beta} \equiv \frac{1}{N} \sum_{\mathbf{k}} \langle d_{\alpha,\mathbf{k},\sigma}^\dagger d_{\beta,\mathbf{k},\sigma} \rangle$, with N denoting the total number of Fe sites.

The self-consistent equations for M are

$$M^{\mu\mu} = \sum_{\mathbf{r}-\mathbf{r}',\beta} J_{\mathbf{r},\mathbf{r}'}^{\mu,\beta} e^{i\mathbf{Q}\cdot(\mathbf{r}-\mathbf{r}')} \tilde{n}_{\beta\beta} - \sum_{\nu \neq \mu} J_H \tilde{n}_{\nu\nu}, \quad (4a)$$

$$M^{\mu\nu} = -J_H^{\mu\nu} \tilde{n}_{\nu\mu}, \quad (\mu \neq \nu), \quad (4b)$$

where $\tilde{n}_{\alpha\beta} \equiv \frac{1}{N} \sum_{\mathbf{k}} \langle d_{\alpha,\mathbf{k},\sigma}^\dagger d_{\beta,\mathbf{k}+\mathbf{Q},\sigma} \rangle$.

The self-consistent equations for $\Delta(\mathbf{k})$ are given through $\Delta(\mathbf{k}) = \sum_{\mathbf{r}} P(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}}$, with

$$P^{\alpha\alpha}(\mathbf{r} - \mathbf{r}') = -J_{\mathbf{r},\mathbf{r}'}^{\alpha\alpha} [\phi_{\alpha\alpha}(\mathbf{r} - \mathbf{r}') + \phi_{\alpha\alpha}(\mathbf{r}' - \mathbf{r})], \quad (5a)$$

$$P^{\mu\nu}(\mathbf{r} - \mathbf{r}') = -J_{\mathbf{r},\mathbf{r}'}^{\nu\mu} [\phi_{\mu\nu}(\mathbf{r} - \mathbf{r}') + \phi_{\nu\mu}(\mathbf{r}' - \mathbf{r})], \quad (\mu \neq \nu), \quad (5b)$$

where $\phi_{\alpha\beta}(\delta) \equiv \frac{1}{N} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\delta} \langle d_{\alpha,-\mathbf{k},\downarrow}^\dagger d_{\beta,\mathbf{k},\uparrow} \rangle$. Similarly, the equations for $\tilde{\Delta}(\mathbf{k})$ are given through $\tilde{\Delta}(\mathbf{k}) = \sum_{\mathbf{r}} \tilde{P}(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}}$, with

$$\tilde{P}_{\alpha\alpha}(\mathbf{r} - \mathbf{r}') = -J_{\mathbf{r},\mathbf{r}'}^{\alpha\alpha} [\tilde{\phi}_{\alpha\alpha}(\mathbf{r}' - \mathbf{r}) + e^{-i\mathbf{Q}\cdot(\mathbf{r}-\mathbf{r}')} \tilde{\phi}_{\alpha\alpha}(\mathbf{r} - \mathbf{r}')], \quad (6a)$$

$$\tilde{P}_{\mu\nu}(\mathbf{r} - \mathbf{r}') = -J_{\mathbf{r},\mathbf{r}'}^{\nu\mu} [\tilde{\phi}_{\nu\mu}(\mathbf{r}' - \mathbf{r}) + e^{-i\mathbf{Q}\cdot(\mathbf{r}-\mathbf{r}')} \tilde{\phi}_{\mu\nu}(\mathbf{r} - \mathbf{r}')], \quad (\mu \neq \nu) \quad (6b)$$

where $\tilde{\phi}_{\alpha\beta}(\delta) \equiv \frac{1}{N} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\delta} \langle d_{\alpha,-\mathbf{k},\downarrow} d_{\beta,\mathbf{k}+\mathbf{Q},\uparrow} \rangle$.

115 From these equations one could obtain the finite-temperature properties and phase diagrams of ironpnictide compounds. Usually there are many solutions of the set of self-consistent equations. In these cases we have to compare the corresponding free energies defined as

$$F \equiv \frac{\text{Tr} [(H - H_m) e^{-H_m/(k_B T)}]}{\text{Tr} [e^{-H_m/(k_B T)}]} - k_B T \ln \text{Tr} [e^{-H_m/(k_B T)}] \quad (7)$$

to determine which solution has the lowest free energy and hence gives the
120 genuine physical state and corresponding properties.

3. Numerical Results

In what follows we present the finite-temperature solution of the model Hamiltonian (1). Throughout this paper we consider the electron doping case, i.e., the electron concentration $n \geq 4$. According to the SC phase diagram in
125 the J_1 - J_2 parameter space [39, 51], we take the AFM exchange interactions as $J_1 = 0.02\text{eV}$ and $J_2 = 0.06\text{eV}$, which support a $s_{\pm}$ pairing symmetry. The Hund's rule coupling is taken as $J_H = 0.35\text{eV}$ according to the estimation in reference [52].

3.1. Coexisting State and Phase Diagram

130 By investigating the equations of the order parameters self-consistently, we map out the phase diagram in the doping-temperature plane in figure 1. Without doping, i.e., at $n = 4.0$, as the temperature decreases the system undergoes a paramagnetic-SDW transition at a high temperature and a SDW-SC transition at a low temperature, where the low-temperature SC coexists with SDW order.
135 With the electron doping away from $n = 4.0$, the low-temperature coexisting phase ceases at $n_c \approx 4.1$, and the system enters into the pure SC phase. The

SC dome vanishes around $n = 4.3$. Such a global phase diagram is qualitatively in agreement with the experimental data very well [53].

From our phase diagram shown in figure 1 one could clearly see that the SDW order can coexist with the SC order in the underdoped region at low temperatures, consistent with many experiments in several families of iron-based SC's [12, 13, 14, 15, 16, 17, 17, 18, 19, 20, 21, 23, 24, 25] and theoretical predictions [33, 34, 35]. However, we notice that most ironpnictide parent compounds are not SC down to very low temperatures. Two factors may suppress the SC in the parent compound: (i) quantum fluctuations beyond the mean-field solution and/or (ii) large magnetic moments on Fe sites or smaller exchange interactions, especially the next-nearest-neighbour AFM interaction J_2 . A suitable choice of J_1, J_2 and J_H may enhance SDW while suppress SC in the parent compound and the SC only emerges at finite doping. However, in this work we would not search for such a set of suitable parameters since our focus is on the electronic structure in the coexisting region, which would not change qualitatively as long as the pairing symmetry does not qualitatively change.

We also plot the SDW and SC order parameters at two different temperatures in figure 2. We find that the pairing wavefunction is a superposition of $s_{x^2y^2}(\propto \cos k_x \cos k_y)$ and $s_{x^2+y^2}(\propto \cos k_x + \cos k_y)$ waves, which belong to the same representation of the lattice point group and hence naturally coexist. The relative amplitude of the two waves depends on the relative strength of J_1 and J_2 : the nearest-neighbour exchange interaction J_1 supports the $s_{x^2+y^2}$ wave while the next-nearest-neighbour exchange interaction J_2 supports the $s_{x^2y^2}$ wave. The interorbital pairing amplitudes are quite small, therefore the intraorbital Cooper pairing dominates in the SC wavefunction, forming a orbital-triplet as proposed by Ong and Coleman [54]. Furthermore, the SC pairing amplitude in the xy orbital is not plotted in figure 2 since it is smaller than that in the

xz and yz orbitals by approximately one order in magnitude. As entering into
 165 the coexistence phase, the degeneracy of the pairing amplitudes in xz and yz
 orbitals is lifted by the striped SDW order, as seen in figures 2(a) and 2(b). This
 degeneracy lifting reflects the different SC-SDW coupling strengths in different
 orbitals. This orbital-selective competition between SC and SDW orders will be
 investigated in more details in the following.

170 3.2. Competition between SDW and SC orders

In the coexisting region, the SDW and the SC orders also compete with each
 other. This competition could be seen in both the doping- and the temperature-
 dependence of the order parameters. As seen in figures 2(a) and 2(b), for fixed
 temperature, as the system goes from the pure SC state at large doping into
 175 the coexisting state at low doping, the SC order parameter in the xz orbital is
 suppressed rapidly while that in the yz orbital is suppressed only a little. This
 shows that the competition between the stripe SDW order and the SC order is
 orbital-selective.

In figure 3, we plot the temperature dependence of the SDW and SC order
 180 parameters at two different electron concentrations. The SDW order parameters
 emerge below the transition temperature T_{SDW} , but instead of monotonically
 increasing with decreasing temperature as in the pure SDW state, they dip
 at the onset of SC, as shown in figures 3(a) and 3(b). The reduction of the
 total moment ranges from 100% at $n = 4.1$, $\approx 23\%$ at $n = 4.095$, $\approx 13\%$ at
 185 $n = 4.09$, to $\approx 2\%$ at $n = 4.075$. This reduction behavior of the SDW moment is
 reminiscent of the orthorhombicity and magnetic moment suppression observed
 in underdoped $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ [22, 23] and $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ [55] in trans-
 port and neutron scattering experiments, signalling macroscopic competition
 between the SDW and the SC orders. In a recent ARPES experiment on un-
 190 derdoped $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ [28], Yi *et al.* observed that the SDW gap shrinks in

magnitude as the system enters the SC phase. These experimental observations are in good agreement with our results based on the three-orbital t - J_1 - J_2 model. In particular, at $n \approx 4.1$ we observe that there is a reentrance of the paramagnetic phase below 50K (magnetic long-range order is completely suppressed by SC), in agreement with the previous theory [9] and the experimental data on $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ [56]. The opening of the SC gap removes states at the Fermi level that otherwise would contribute to the magnetic order, leading to a reduction of the magnetic long-range order after the onset of SC.

3.3. Momentum-resolved SDW and SC order parameters

To understand how the two orders coexist and compete with each other in the same electronic structure, we now analyze the spectral distribution in the momentum space in some details. It is defined in an energy window $\omega \equiv E - \mu \in (\omega_<, \omega_>)$ by

$$D_\alpha(\mathbf{k}; \omega_<, \omega_>) \equiv \int_{\omega_<}^{\omega_>} \rho_\alpha(\mathbf{k}, \omega) d\omega, \quad (8)$$

where $\rho_\alpha(\mathbf{k}, \omega)$ is the spectral function in the α orbital and $\omega_<(\omega_>)$ is the lower (upper) edge of the energy window. This quantity can resolve the spectral distribution in orbital, momentum and energy spaces, giving more detailed information about the states than a conventional momentum-integrated DOS or Fermi surface. It reflects the momentum distribution of the states in a special orbital in the energy window $(\omega_<, \omega_>)$. We are interested in the spectral distribution in an energy window near the Fermi level since it reflects the distribution of states available for low-energy physics such as Cooper pairing. Conventionally this information is reflected by Fermi surface. However, Fermi surface cannot always be characterized clearly and correctly, especially in strongly interacting systems [57]. On the other hand, the spectral distribution in momentum space near the Fermi level could always be well defined and provide more details about the low-energy states than Fermi surface. We plot $D_\alpha(\mathbf{k}, -10\text{meV}, 0)$ in figures

4(a)-4(c) at $n = 4.05$ in the paramagnetic phase, which clearly show two hole pockets near $(0, 0)$ and one electron pocket near $(\pi, 0)$ or $(0, \pi)$ with different orbital characters. We can expect that all low-energy physics, such as SC pairing, its competition with SDW and spatial modulation (which will be discussed later) should exhibit similar orbital characters with the momentum-space spectral distribution. It is indeed the case as observed in this paper.

At low temperatures and in underdoping compounds, SDW order could form as a result of AFM interactions. This magnetic order opens gap and changes the low-energy states. Due to the imperfect nesting of the Fermi surface, the SDW gap does not always lie on the Fermi surface and hence does not remove all the states near the Fermi energy, allowing the SC order to emerge. In figures 4(d)-4(f) we plot $D_\alpha(\mathbf{k}, -10 \text{ meV}, 0)$ in the SDW phase at $n = 4.05$ and $T = 60 \text{ K}$. In comparison with the paramagnetic phase, the change in the xz orbital is more considerable than that in the yz orbital. This feature explains why in the coexisting phase the SC order in the xz orbital is strongly suppressed while that in the yz orbital is only suppressed a little: the SDW ordering removes most of the states in the xz orbital near the Fermi energy, leading to a strong suppression of Cooper pairing in the xz orbital.

We now turn to another question in ironpnictides: what is the distribution of the Fe $3d$ electrons that contribute to the SDW order in the momentum space? To answer it, we define the momentum distribution of the SDW order as

$$m_\alpha(\mathbf{k}) = \Re \left[\langle d_{\alpha, \mathbf{k}, \uparrow}^\dagger d_{\alpha, \mathbf{k} + \mathbf{Q}, \uparrow} \rangle \right], \quad (9)$$

from which the magnetic moment, or the SDW order parameter, is given by its average over the momentum space:

$$m = \frac{2\mu_B}{N} \sum_{\mathbf{k}} \sum_{\alpha} m_\alpha(\mathbf{k}), \quad (10)$$

240 where N is the total number of Fe sites. The distribution of momentum-resolved SDW order parameter in the SDW phase at $n = 4.05$ and $T = 60\text{K}$ is plotted in figures 4(g)-4(i). We see that the distribution $m_{xz}(\mathbf{k})$ is deeply concentrated at the hole pockets in the y direction, where the corresponding spectral distribution is strongly suppressed, as seen in figure 4(d). On the other hand, the
245 distributions $m_{yz}(\mathbf{k})$ and $m_{xy}(\mathbf{k})$ are broad and do not change the topology of the corresponding spectral distribution, as seen in figures 4(e) and 4(f). Such features has important effects on the SC order distribution in the momentum space, which will be discussed below.

Similar to the momentum distribution function of the SDW order parameter,
250 et, we can also define the momentum distribution function of the SC order parameter as

$$\psi_{\alpha}(\mathbf{k}) = \langle d_{\alpha,-\mathbf{k},\downarrow} d_{\alpha,\mathbf{k},\uparrow} \rangle. \quad (11)$$

This function reflects the pairing amplitude in the momentum space, and its Fourier transformation represents the pairing wavefunction in real space. We plot this function in the xz and yz orbitals at $T = 10\text{K}$ for three different
255 electron concentrations in figure 5. From $n = 4.11$ to $n = 4.07$, the system undergoes from a pure SC phase to a coexisting phase, in agreement with the phase diagram in figure 1. We see that the amplitude on the Fermi sheet near the Γ point $(0,0)$ and that on the Fermi sheet near the M point $(\pi,0)$ [or $(0,\pi)$] has different signs, revealing a dominant $s_{\pm}$ pairing symmetry. In the pure SC
260 state in figures 5(a) and 5(b), the amplitudes in the xz and yz orbitals are similar, related by a 90° rotation. As the SDW order emerges, the amplitude in the xz orbital shown in figures 5(c) and 5(e) is strongly suppressed in the region where the corresponding SDW amplitude shown in figure 4(g) is strong. On the other hand, the amplitude in the yz orbital shown in figures 5(d) and
265 5(f) is suppressed rather slightly. This is consistent with the orbital feature

observed in the doping-dependence of the order parameters in figures 2(a) and 2(b). Hence, by comparing the momentum distributions of the SDW and SC order parameters, we can see a clear competition in momentum space between the two long-range orders that coexist in real space.

270 3.4. Spatial modulation of the superfluid density

Inhomogeneous SC state with the symmetry of a pair-density-wave state in which charge, spin, and SC orders are intertwined with each other has been suggested for cuprates [58, 59, 60, 61]. Stripes of superfluid density have also been observed at twin boundaries in Ba(Fe_{1-x}Co_x)₂As₂ [62, 63]. Here we find
 275 that the coexistence of SDW and SC can modulate the pairing amplitude to make it oscillate in the real space. To quantitatively illustrate this phenomenon, we note that in real space the pairing amplitude has the form

$$\langle d_{\alpha,\mathbf{r},\downarrow} d_{\alpha,\mathbf{r}',\uparrow} \rangle = \phi_{\alpha\alpha}(\mathbf{r} - \mathbf{r}') + e^{i\mathbf{Q}\cdot\mathbf{r}'} \tilde{\phi}_{\alpha\alpha}(\mathbf{r} - \mathbf{r}'), \quad (12)$$

$$\langle d_{\alpha,\mathbf{r},\uparrow} d_{\alpha,\mathbf{r}',\downarrow} \rangle = -\phi_{\alpha\alpha}(\mathbf{r} - \mathbf{r}') + e^{i\mathbf{Q}\cdot\mathbf{r}'} \tilde{\phi}_{\alpha\alpha}(\mathbf{r} - \mathbf{r}'), \quad (13)$$

where the two functions ϕ and $\tilde{\phi}$ have been defined after (5b) and (6b), respectively. It's clear that this wavefunction consists of a homogeneous part
 280 $\phi_{\alpha\alpha}(\mathbf{r} - \mathbf{r}')$ and an oscillating part with amplitude $\tilde{\phi}_{\alpha\alpha}(\mathbf{r} - \mathbf{r}')$, and these two parts correspond to spin-singlet and spin-triplet pairings, respectively. So in the coexistence phase the pairing amplitude contains two components: a homogeneous one in the spin-singlet channel and an oscillating one in the spin-triplet channel. The spatial modulation and singlet-triplet mixing in this coexistence
 285 phase are akin to the Fulde-Ferrell-Larkin-Ovchinnikov state [64, 65]. Similar spatial modulation has also been found in a generic one-orbital model [66, 67], where the competition and coexistence of staggered triplet SC with d -wave singlet SC and SDW are obtained. Experimentally, such a mixing may be in-

investigated by Knight shift which measures the electronic spin susceptibility.
 290 Spin-singlet and triplet Cooper pairs should have qualitatively different spin
 susceptibility behaviors and hence could be revealed by Knight shift measure-
 ments.

In the t - J_1 - J_2 model considered in this paper, we find only the nearest-
 neighbour pairing in the x - and y - directions and the next-nearest-neighbour
 295 pairing in the $(x \pm y)$ - directions. The spatial modulation of the pairing wave-
 function in orbital α and direction δ can be measured by the ratio

$$R = \left| \frac{\tilde{\phi}_{\alpha\alpha}(\delta)}{\phi_{\alpha\alpha}(\delta)} \right|. \quad (14)$$

This ratio R is plotted in figure 6 at $T = 10$ K. We see that R is nonzero only
 when the SDW order does not vanish and its value depends on both the pairing
 direction and the orbital. Two features can be observed: (i) the ratio R in the
 300 ferromagnetic y - direction is zero, while that in the AFM x - and the diagonal
 $(x \pm y)$ -directions have the same qualitative behavior in a given orbital; (ii) the
 nonzero ratio R in the yz -orbital increases monotonically with the increasing
 SDW order (i.e., the decreasing n), while that in the xz -orbital first increases
 and then drops. This reflects the fact that the pairing in the xz -orbital is
 305 strongly suppressed by the SDW order, while that in the yz -orbital is only
 suppressed slightly. Such an orbital dependence of the spatial modulation is
 another manifestation of the orbital selectivity of the competition between the
 SC and SDW orders observed in the momentum-space distribution of the order
 parameters.

310 4. Discussions and Conclusions

In the above studies we have shown that the SDW-SC coexistence phase
 demonstrates many unconventional properties. There may be other unusual

behaviors beyond the scope of this work. Recently Hinojosa *et al.* [68] showed that in the coexistence phase, the interpocket spin-triplet pairing may mix with the intrapocket spin-singlet s_{++} -wave, contributing an additional SC gap and breaking the time-reversal symmetry explicitly. Their spin-triplet component may be contained in the spatially oscillating component $\tilde{\phi}$ of the total Cooper pair wavefunction, and the s_{++} one is contained in the $s_{x^2+y^2}$ -wave component in the present situation. However, explicit time-reversal symmetry breaking is not observed in our results. Also, some experiments [29, 30, 31, 32] suggest that the coexistence phase could be electronic phase separation rather than microscopic coexistence. These problems show that the SDW-SC coexistence phase of ironpnictide compounds deserves further investigations.

In summary, we have studied the coexistence of SDW and SC in ironpnictides from a three-orbital model, focusing on the momentum-space distribution of the order parameters and spectral functions. We find that the SC pairing amplitude lies mainly in the two degenerate xz and yz orbitals and has different signs on the hole- and electron-pockets, consistent with the $s_{\pm}$ symmetry. Detailed analysis shows that it is a superposition of $s_{x^2y^2}$ and $s_{x^2+y^2}$ waves in both the SC and the coexistence phases. In the coexistence region the SDW and SC orders show strong orbital-selective competition as reflected in the reduction of the SDW order parameter and gap at the onset of SC, the reduction of the SC order parameter as the SDW order parameter increases, and the momentum-space distribution of the two order parameters. In addition, the coexistence and competition between the SDW and SC orders could give rise to spatial modulation and spin singlet-triplet mixing of the Cooper pair wavefunction. Our theoretical results are in good agreement with relevant experimental data and deserve further experimental observations.

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Figure 1: The mean-field phase diagram of the three-orbital t - J_1 - J_2 model in the n - T plane. SDW, SC and SDW+SC indicate the spin-density-wave, superconducting and their coexisting phases, respectively.

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Figure 2: The SDW and SC order parameters as functions of electron concentration n at 10 K (a) and 50 K (b).

Figure 3: The SDW and SC order parameters as functions of temperature at (a) $n = 4.1$ and (b) $n = 4.09$.

Figure 4: The momentum-space distribution of the spectral weight $D_\alpha(\mathbf{k}; \omega_<, \omega_>)$ of the three orbitals ($\alpha = xz, yz$ and xy) in an energy window $(\omega_<, \omega_>) = (-10 \text{ meV}, 0)$ at $n = 4.05$ in the paramagnetic (PM) phase [(a)-(c)] and the SDW phase [(d)-(f)]. The momentum distribution of the SDW order $m_\alpha(\mathbf{k})$ in the SDW phase at $n = 4.05$ and $T = 60 \text{ K}$ is plotted in (g)-(i).

Figure 5: The momentum-space pairing amplitude $\psi_\alpha(\mathbf{k})$ in the xz and yz orbitals for three different electron concentrations. The system lies in a pure SC phase in (a) and (b), and coexisting phase in (c)-(f). The temperature is 10 K.

Figure 6: The relative amplitude R of the oscillating part with respect to the homogeneous part of the Cooper pair wavefunction in the xz - (solid symbols) and yz - (open symbols) orbitals along the x -, y - and $(x \pm y)$ - directions.