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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 $NaFe_{1-x}Co_xAs$ and $Ba(Fe_{1-x}Co_x)_2As_2$. 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.

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 [2–5]. 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 [6–8]. 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 [11–25], 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 [12,26,13–15], nuclear magnetic resonance [16–19], 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 scatting 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 [29–32] also suggested that the coexisting phase 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 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 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 elec-

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tronic structure. Although 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.

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 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 selectivity. Our theoretical results are in good agreement with relevant experimental observations for the finite-temperature phase diagrams in $NaFe_{1-x}Co_xAs$ and $Ba(Fe_{1-x}Co_x)_2As_2$. 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 scanning 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 SDW 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-neighbor and next-nearest-neighbor exchange interactions, and Hund's rule coupling. Considering the references [39] and [40], the Hamiltonian reads

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

where the operator $d^{\dagger}_{\mathbf{r},\alpha,\sigma}$ ($d_{\mathbf{r},\alpha,\sigma}$) creates (annihilates) an electron at site $\mathbf{r}$ with orbital index $\alpha = xz, yz, xy$ and spin σ. Its Fourier transformation is denoted by $d^{\dagger}_{\mathbf{k},\alpha,\sigma}$ ($d_{\mathbf{k},\alpha,\sigma}$). The corresponding charge and spin density operators are denoted by $n(\mathbf{r},\alpha) = \sum_{\sigma} d^{\dagger}_{\mathbf{r},\alpha,\sigma} d_{\mathbf{r},\alpha,\sigma}$ and $\mathbf{S}(\mathbf{r},\alpha) = \frac{1}{2}\sum_{s,s'} d^{\dagger}_{\mathbf{r},\alpha,s}\sigma_{ss'} d_{\mathbf{r},\alpha,s'}$, 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 $J^{\alpha\beta}_{\mathbf{r},\mathbf{r}'}$ equals to $J^{\alpha\beta}_1$ if $\mathbf{r}$ and $\mathbf{r}'$ are nearest neighbor, $J^{\alpha\beta}_2$ if $\mathbf{r}$ and $\mathbf{r}'$ are next-nearest neighbor, and vanishes otherwise. In principle, the exchange couplings $J^{\alpha\beta}_{1(2)}$ should be matrices in orbital space. However, for clarity and simplicity, we take $J^{\alpha\beta}_{1(2)} = J_{1(2)}$, i.e., all of the matrix elements take the same value.

Both experimental [41,42] and theoretical [43–45] studies have shown that the parent phases of most ironpnictides have a long-range stripe SDW order 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 complicated 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 [46–48] and studied in theory [49, 50]. A comprehensive 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:

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

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

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

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 $M = M^{\dagger}$ 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

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

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

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

The self-consistent equations for M are

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

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

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

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

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

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