Pairing symmetry in the iron-pnictide superconductor KFe$_2$As$_2$

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Abstract - The pairing symmetry is one of the major issues in the study of iron-based superconductors. We adopt a ten-orbital model by using the maximally localized Wannier functions based on the first-principles band structure calculations combined with the $J_1$-$J_2$ model for KFe$_2$As$_2$, the phase diagram of pairing symmetries is constructed. We find that the pairing symmetry for KFe$_2$As$_2$ is a nodal $(s_+^2 + s_{2+}^2)$-wave in the folded Brillouin zone with two iron atoms per unit cell. This pairing symmetry can explain the experiments observed nodes, and it also can be tested by future experiments.

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The discovery of the superconducting iron-pnictide material (1111-type $Re$OFeAs, $Re =$ rare earth) [1] in 2008 has triggered great research interests which led to synthesize similar iron-based superconductors, such as 122-type $B$Fe$_2$As$_2$ ($B =$ Ba, Sr, or Ca) [2], 111-type $A$FeAs ($A =$ alkali metal) [3], 11-type $\alpha$-FeSe(Te) [4], and new-type $K$Fe$_2$As$_2$ [5] materials. Their crystal structures are tetrahedral with divalent iron square planes. A characteristic feature of these superconducting systems is that the band structure near the Fermi energy is derived from Fe-3$d$ orbitals with only modest hybridization of ligand-p orbitals [6]. Most of these compounds were reported to show superconductivity after doping or under high pressure and have the same robust tetrahedral layer structure.

To uncover the mechanism of superconductivity in these materials, the determination of pairing symmetry of the superconducting order parameter is a good starting point. In most of the electron-doped and weakly hole-doped 1111 and 122 compounds, the band structure calculations show that there are disconnected quasi-two-dimensional (2D) hole and electron pockets [7,8]. The former ones are centered at the $\Gamma$-point, while the latter ones are located at the $M$-point of the Brillouin zone (BZ) of two iron atoms per unit cell. The strong scattering between the electron and hole pockets corresponds to a nesting wave vector [9]: $q \approx (\pi, \pi)$, which could lead to superconductivity with the so-called $S^\pm$ pairing symmetry [8]. The order parameter with this pairing symmetry is nodeless, and has a sign changed from the hole to the electron pocket. Such a $S^\pm$ pairing symmetry is gaining increasing experimental supports [10,11]. For a heavily hole-doped compound like KFe$_2$As$_2$, the angle-resolved photoemission spectroscopy (ARPES) measurements [12,13] indicated that the electron pockets near $M$ points were replaced by the ellipse-like hole pockets while the hole pockets near the $\Gamma$-point became larger and closer to $\pi/2$ in the folded BZ of two iron atoms per unit cell. The superconducting transition temperature of this compound is $T_c \sim 3.6$ K, which is much lower than those in other iron-based superconductors. Under this situation $q \sim (\pi, \pi)$ is no longer the nesting wave vector and the superconductivity pairing interactions could come from small $q$ scattering. Although both experimental observations [14–21] and theoretical investigations [22–26] give nodal gap structures in KFe$_2$As$_2$, the pairing symmetry of this compound is still controversial. Specifically, experiments on small-angle neutron scattering [14] indicate nodal lines perpendicular to the $c$-axis while experiments on thermal conductivity [15,16] and superfluid density [17] show a $d$-wave-like nodal structure. Theoretically, based on the weak coupling approaches, a functional renormalization group study showing the dominant $d$-wave state [22] is most favorable, while Fermi surface (FS) restricted random phase approximation type spin-fluctuations analysis [23] and an analytical study in which the interactions are approximated by their lowest angular harmonics [24,25] have revealed that $s$-wave and $d$-wave
Each face of the Fe square lattice, respectively.

are chosen to ensure the calculation with an accuracy of

individual atom sizes smaller than 0.5 Å to obtain sufficient accuracy throughout the calculations. The crystal energy is set to zero.

We now turn to discuss the superconducting pairing symmetry in KFe$_2$As$_2$. Because of the strong hole doping in KFe$_2$As$_2$, the electron pockets at the M-point are replaced by small hole pockets, and the hole pockets at the Γ-point are very large in the folded BZ of two iron atoms per unit cell, as shown in fig. 1(b). The nesting between Γ-point and M-point is absent. Therefore, we start with a t-J$_1$-J$_2$-type model:

\[
\hat{H} = \sum_{i,j} \epsilon_{n} n_{ij} + \sum_{i,j} \sum_{\mu,\nu,\sigma} \epsilon_{\mu} c_{i\mu\sigma}^{\dagger} c_{j\nu\sigma}^{\dagger} c_{j\mu\sigma} c_{i\nu\sigma} + J_1 \sum_{\langle i,j \rangle} \langle S_{i\mu} \cdot S_{j\nu} - \frac{1}{4} n_{i\mu} n_{j\nu} \rangle + J_2 \sum_{\langle \langle i,j \rangle \rangle} \langle S_{i\mu} \cdot S_{j\nu} - \frac{1}{4} n_{i\mu} n_{j\nu} \rangle,
\]  

(1)
where \( i,j \) denote the sites in the square lattice of FeAs layers (see fig. 1(b)) and \( \mu, \nu \) the orbitals, and \( t_{ij}^{\text{tr}} \) is the transfer energy obtained from the maximally localized Wannier orbitals [37–39]. As shown in fig. 4, the ten-orbital tight-binding band structure reproduces the density functional theory band structure rather accurately. The last two terms represent exchange interactions between Fe-3d electron spins with parameters \( J_1 \) and \( J_2 \) denoting the intralayer nearest-neighbor (n.n.) and next-nearest-neighbor (n.n.n.) sites exchange interaction, respectively. The symbols \( \langle i,j \rangle \) and \( \langle (i,j) \rangle \) denote the summation over the n.n. and n.n.n. sites, respectively. \( \hat{S}_{\mu \nu} \) is the transfer energy obtained from the maximally localized Wannier orbitals [37–39]. As shown in fig. 4, the ten-orbital tight-binding band structure reproduces the density functional theory band structure rather accurately. The pairing order parameter \( \Delta_{\mu}(k) \) for the orbital \( \mu \) is linear combinations of four intraorbital pairings \( \Delta_{i,\mu}(k) \).

The above equations, eq. (2) and eq. (3), can be solved self-consistently, we obtain the quasiparticle dispersion spectra \( E_{k\mu} \). The pairing gap matrix is determined by minimizing the ground-state energy density [28,29]:

\[
\frac{f}{\sum_{k,\mu,\nu,\sigma} \frac{1}{4} |\phi_b^k (\hat{c}_{k\mu\sigma} \hat{c}_{k\nu\sigma})|^2 - \sum_{\mu,\nu} (E_{k\mu} - E_{k\nu})^2,}
\]

where \( \phi_b^k \) is the eigenvalue of the ten-orbital tight-binding model.

When the effective kinetic energy term is absent, the \( J_1 \) dominating \( s_{x^2−y^2} \)-wave and \( d_{xy} \)-wave pairing symmetries are indeed degenerate. Likewise, the \( s_{x^2+y^2} \)-wave and \( d_{xz} \)-wave dominated by \( J_2 \) are energetically degenerate, and all four pairing states mix together when \( J_3 \) is comparable with \( J_1 \). Taking the effective kinetic-energy term into account, the degeneracy states will be left, and the phase diagram of the pairing symmetries is shown in fig. 5. The phase on the left upper corner has a time reversal breaking phase with the \( (s_{x^2+y^2} + id_{z^2−y^2}) \)-wave dominated by the n.n.n. intralayer pairing interaction \( J_2 \). When the n.n. pairing interaction \( J_1 \) increases and is comparable to the n.n.n. pairing interaction \( J_2 \), the \( d_{x^2+y^2} \)-wave will be suppressed and substituted by the \( s_{x^2+y^2} \)-wave and lead to a \( (s_{x^2+y^2} + id_{z^2−y^2}) \)-wave in the middle part of fig. 5. When the n.n. pairing interaction \( J_1 \) further increases, the \( s_{x^2+y^2} \)-wave will be suppressed and substituted by the \( d_{xy} \)-wave and lead to another kind time-reversal symmetry-breaking state \( (s_{x^2+y^2} + id_{z^2−y^2}) \)-wave. On the left lower corner of the phase diagram, when the n.n. pairing interaction \( J_1 \)
is dominating and has a very small value, the system favors a nodeless $s_{x^2-y^2}$-wave state. From the viewpoint of experiments, the nodes have been observed by several groups [14–21]. Therefore, we conclude that only the $(s_{x^2-y^2} + s_{x^2-y^2})$-wave can give rise to the nodal structure, and only this phase can explain the experiments observed based on the aforementioned discussions. The order parameter in this mixed phase can be written as

$$\Delta_\mu(k) = \Delta_0 \left[ \cos \frac{k_x}{2} \cos \frac{k_y}{2} + \delta (\cos k_x + \cos k_y) \right], \quad (4)$$

where the value $\Delta_0$ is a constant and $\delta$ depends on the n.n. interorbital pairing interaction $J_1$ and the n.n.n. intraorbital pairing interaction $J_2$. When the n.n. intraorbital pairing interaction $J_2$ is comparable to the n.n.n. one $J_3$, the gap zero points will develop. As shown in fig. 6, when $\delta$ reaches a certain value, the contour of the gap zeros will cross the FS topology, which leads to the nodal behavior. This result can be tested by future experiments, such as APRES measurements.

In conclusion, we have constructed a ten-orbital model by using the maximally localized Wannier functions based on the first-principles band structure calculations and combined with the $J_1-J_2$ model, all possible pairing symmetries are examined by solving the BCS equations self-consistently. The mean-field phase diagram of a $t$-$J_1$-$J_2$ model for this compound is constructed. We find that only the $(s_{x^2-y^2} + s_{x^2-y^2})$-wave pairing symmetry can give rise to the nodal structure, and only this wave pairing symmetry can explain those experiments which evidenced a nodal order parameter. This result can be tested by future experiments.

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