Superconducting Properties of Two-Orbital $t-t'-J-J'$ Models

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Abstract

Motivated by the recent contradiction of the superconducting pairing symmetry in the angle-resolved photoemission spectra (ARPES) and the nuclear magnetic resonance (NMR) data in the FeAs superconductors, we present the theoretical results on the phase diagram, the temperature dependent Fermi surfaces in normal state, the ARPES character of quasiparticles and the spin-lattice relaxation $1/T_1$ of the two-orbital $t-t'-J-J'$ models. Our results show that most of the properties observed in iron-based superconductors could be comprehensively understood in the present scenario qualitatively, indicating that the pairing symmetry of the ironpnictides is anisotropic nodeless $d_{x^2-y^2}+S_{x^2-y^2}$-wave, mainly originating from the band structures and the Fermi surface topology.

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I. INTRODUCTION

Following the discovery of the first high temperature superconductivity in the copper-based compounds two decades ago [1], a second class of high temperature superconductors has been recently reported in iron-based pnictides [2, 3, 4, 5, 6, 7], in which the transition temperature $T_c$ can be as high as 55K [8]. Intensively experimental [9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19] and theoretical [20, 21, 22, 23, 24, 25] efforts have been devoted to understand the nature of new superconductors. Resemble to cuprates, layered iron pnictides consist of the conducting FeAs layers and the ReO layers (Re represents the rare earth elements, such as La, Ce, Pr, Nd, Sm, and etc) which provide carriers to the FeAs layers. The antiferromagnetic spin density wave (SDW) order is suppressed upon substituting a few percent O with F, and the new compounds become the superconductor (SC) below $T_c$. On the other hand, there are a few of considerable differences between cuprates and iron pnictides. For example, the first difference is that the undoped iron-oxypnictides with the SDW order exhibit poor metallic conduction, rather than the Neel AFM insulator in undoped cuprates; the second one is that the spin and magnetic moment of Fe are much smaller than expected, completely different from the Cu spin in cuprates, etc. These facts suggest that there exists significant difference between the ground states of ironpnictides and cuprates.

First-principle electronic structure calculations provide the first evidence of the difference. It has been shown [26, 27, 28, 29, 30, 31] that in LaFeAsO, the most of the spectral weight close to the Fermi energy is contributed from the Fe 3$d$ orbital, and the Fermi surfaces (FS) of LaFeAsO consists of two hole-type circles around Γ point and two electron-type co-centered ellipses around M point [32]. This implies that the multiorbital character is dominant in the undoped FeAs superconductor, contrast to the single-orbital character in cuprates. Up to date, many tight-binding multi-orbital models have been proposed to reproduce the Fermi surface (FS) character and the band structures near Fermi level $E_F$ in ReFeAsO$_{1-x}$F$_x$ and Ba$_{1-x}$K$_x$Fe$_2$As$_2$. To this end, once the electron-phonon mechanism is precluded by Boeri et al. [33], the electronic mechanisms are proposed as the driving force of the SC paring, such as the Coulomb interaction between Fe 3$d$ electrons [22, 23, 24, 34] or the antiferromagnetic exchange coupling between the nearest neighbor Fe sites and the next nearest neighbor site, such as the two-orbital models [35, 36, 37], three-orbital ones [23], and four-orbital ones.
Among these models, the two-orbital $t\text{-}t^\prime\text{-}J\text{-}J'$ model is minimal, and can reproduce the key characters of ironpnictides, such as the complex Fermi surface and the multi-orbital degeneracy of the Fe $3d$ electrons and the band structures near $E_F$, as well as the stripe antiferromagnetic or spin-density-wave ground state.

In this newly discovered superconductor, the most intriguing issues are the pairing mechanism and pairing symmetry. To date, various possibilities of the SC mechanism and pairing symmetry for $Fe$–pnictide superconductor are proposed theoretically and experimentally. The pairing symmetries range from spin singlet $d$-wave to $s$-wave, or the mixture of $S_{x^2-y^2}$ and $d_{x^2-y^2}$, or spin triplet $p$-wave. At present, the nature of the SC gap observed experimentally is very different from authors to authors and from samples to samples, ranging from one gap to two gaps, and from isotropic or anisotropic fully gap to line node gap. On the one hand, the angle-resolved photoemission spectroscopy (ARPES) measurements, a direct measurement to the quasiparticle spectra and the SC gap, observed that all the gaps are nodeless around their respective Fermi surface sheets, which is different from the situation of the cuprates. On the other hand, however, the spin-lattice relaxation rate in the nuclear magnetic resonance (NMR) experiments strongly suggest the existence of nodes in the gap, which share partial features of cuprates and MgB$_2$. The question thus arises whether the contradiction between the ARPES and the NMR data is due to the sample qualities or it reflects the two sides of the new superconductors?

In this paper, we start from the minimal two-orbital $t\text{-}t^\prime\text{-}J\text{-}J'$ model, which has the same topology as the band structure of the iron based superconductors, and obtain the mean-field phase diagram of the extended $t\text{-}t^\prime\text{-}J\text{-}J'$ model, the quasiparticle spectra and its ARPES manifestation, and the spin-lattice relaxation rate $1/T_1$. Our results demonstrate that the various pairing symmetries are stable in the mean-field phase diagram, and the $T^3$-like behavior in the spin-lattice relaxation rate may coexist with the anisotropic nodeless SC gap, as observed in ARPES and NMR experiments.
II. MODEL HAMILTONIAN AND METHOD

Based on the band structures results and theoretical analysis, the twofold-degenerate $d_{xz}/d_{yz}$ orbits are essential for the ironpnictide superconductors. We depict such physical processes with the two-orbital Hubbard model,

$$
\hat{H} = \sum_{<ij>\alpha\beta} t_{ij}^\alpha \hat{c}^\dagger_{i\alpha\sigma} \hat{c}_{j\beta\sigma} + \sum_{<ij>>\alpha\beta} t_{ij}' \hat{c}^\dagger_{i\alpha\sigma} \hat{c}_{j\beta\sigma}
+ U \sum_{i\sigma} \hat{c}^\dagger_{i\alpha\sigma} \hat{c}_{i\alpha\sigma} \hat{c}^\dagger_{i\alpha\sigma} \hat{c}_{i\alpha\sigma} + U' \sum_{i\sigma\sigma'} \hat{c}^\dagger_{i\alpha\sigma} \hat{c}_{i\alpha\sigma} \hat{c}^\dagger_{i\alpha\sigma'} \hat{c}_{i\alpha\sigma'}$

$$
- J_H \sum_{i\sigma\sigma'} \hat{c}^\dagger_{i\alpha\sigma} \hat{c}_{i\alpha\sigma} \hat{c}^\dagger_{i\alpha\sigma} \hat{c}_{i\alpha\sigma'} + J_H \sum_{i\alpha \neq \alpha'} \hat{c}^\dagger_{i\alpha\sigma} \hat{c}_{i\alpha'\sigma} \hat{c}^\dagger_{i\alpha'\sigma} \hat{c}_{i\alpha\sigma}
$$

(1)

Here $\hat{c}^\dagger_{i\alpha\sigma}$ creates a $d_{xz}$ ($\alpha=1$) or $d_{yz}$ ($\alpha=2$) electron with orbital $\alpha$ and spin $\sigma$ at site $R_i$. $t$ and $t'$ denotes the hopping integrals of the nearest-neighbor (NN) and the next-nearest-neighbor (NNN) sites, respectively. $U$, $U'$ and $J_H$ are the intra-orbital, inter-orbital Coulomb interactions and the Hund’s coupling. Formally, the $t$-$t'$-$J$-$J'$ model can be derived from Eq.(1) in the atomic limit [49], although far from strict. The $t$-$t'$-$J$-$J'$ model reads,

$$
H = H_{t-t'} + H_{J-J'}
$$

(2)

with the kinetic energy term,

$$
H_{t-t'} = \sum_{k\sigma} [ (\varepsilon_{kxz} - \mu) \hat{c}^\dagger_{k1\sigma} \hat{c}_{k1\sigma} + (\varepsilon_{kyz} - \mu) \hat{c}^\dagger_{k2\sigma} \hat{c}_{k2\sigma} + \varepsilon_{kxy} (\hat{c}^\dagger_{k1\sigma} \hat{c}_{k2\sigma} + \hat{c}^\dagger_{k2\sigma} \hat{c}_{k1\sigma}) ]
$$

with the notations

$$
\varepsilon_{kxz} = -2t_1 \cos k_x - 2t_2 \cos k_y - 4t_3 \cos k_x \cos k_y,
$$

$$
\varepsilon_{kyz} = -2t_2 \cos k_x - 2t_1 \cos k_y - 4t_3 \cos k_x \cos k_y,
$$

$$
\varepsilon_{kxy} = -4t_4 \sin k_x \sin k_y.
$$

Here the components of $t_{ij}^\alpha$ are $t_{11}^x = t_1 = -1$ and $t_{22}^x = t_2 = 1.3$, and these of $t_{ij}'^\alpha$ are $t_3 = t_4 = -0.85$ [40]. The electron is filled with $n=2$ (or half-filling) on a two-dimensional square lattice. The interaction term reads,

$$
H_{J-J'} = J \sum_{<ij>\alpha\beta} (\vec{S}_{ia} \cdot \vec{S}_{j\beta} - \frac{1}{4} n_{ia} \cdot n_{j\beta}) + J' \sum_{<<ij>>\alpha\beta} (\vec{S}_{ia} \cdot \vec{S}_{j\beta} - \frac{1}{4} n_{ia} \cdot n_{j\beta})
$$

(3)

where $J$ and $J'$ are the NN and the NNN antiferromagnetic couplings, through the concrete values of $J$ and $J'$ are still in debate. Haule et al. estimated that $J/J' \sim 2$ [50]. In this
paper, we assume $J=0.7$ and $J'=0.3$. $\hat{S}_i^\alpha$ is the spin operator of the electron in the $\alpha$-orbit, and $n_{i\alpha}$ is the particle number operator. The orbital indices $\alpha$ and $\beta$ run over 1 and 2.

Introducing the following order parameters,

\begin{align*}
\Delta_{m_{x/y}}^1 &= J < c_{im\uparrow}^\dagger c_{jm\downarrow}^\dagger >, \quad (j = i \pm \hat{x}/\hat{y}) \\
\Delta_{m_{x\pm y}}^2 &= J' < c_{im\uparrow}^\dagger c_{jm\downarrow}^\dagger >, \quad (j = i \pm (x \pm y)) \\
P_{m_{x/y}}^m &= < c_{ima\sigma}^\dagger c_{jm\sigma} >, \quad (j = i \pm \hat{x}/\hat{y}) \\
P_{m_3}^3 &= < c_{ima\sigma}^\dagger c_{jm\sigma} >, \quad (j = i \pm (x \pm y))
\end{align*}

(4)

the interaction term in Eq.(4) could be decoupled within the framework of the mean-field approximation [40]. Slightly different from Seo et al. mean-field ansatz, we consider the contributions of the kinetic order parameters $P_{x/y}$ and $P_3$, since the itinerant character of the Fe 3d electrons is considerable. So one could obtain the mean-field Hamiltonian and the ground state energy. Minimizing to the ground state energy gives rise to the self-consistent equations for the order parameters $\Delta$ and $P$,

\begin{align*}
\Delta_{m_{x/y}}^1 &= \frac{J}{N} \sum_k \cos(k_{x/y}) < c_{-km\uparrow}^\dagger c_{km\downarrow}^\dagger > \\
\Delta_{m_{x\pm y}}^2 &= \frac{J'}{N} \sum_k \cos(k_x \pm k_y) < c_{-km\uparrow}^\dagger c_{km\downarrow}^\dagger > \\
P_{m_{x/y}}^m &= \frac{1}{2N} \sum_{k\sigma} \cos(k_{x/y}) < n_{k\sigma} > \\
P_{m_3}^3 &= \frac{1}{2N} \sum_{k\sigma} \cos(k_x) \cos(k_y) < n_{k\sigma} >
\end{align*}

(5)

The inter-orbital pairing parameter $< c_{i1\uparrow}^\dagger c_{j2\downarrow}^\dagger >$ is neglected due to its very small value [40]. This implies that the $p$-wave pairing symmetry is precluded. From Eq.(4), one notices that for each orbital, the hopping along the $x$-direction is not equivalent to that along the $y$-direction. This leads to, for example, $\Delta_{1m_{x}} \neq \Delta_{1m_{y}}$. Due to the equivalence between the $d_{xz}$ and the $d_{yz}$ orbits, the order parameters of the two orbits are symmetric once interchanging the $x$-direction and the $y$-direction. Therefore, throughout this paper, we mainly focus the order parameters in the first orbit. The results on the second orbit can be arrived at if rotating the $x$-axis to the $y$-axis [40].

Within the present scenario, we could obtain not only the groundstate phase diagram, but also the quasiparticle spectra in the normal and the SC states. The temperature dependence
of the Fermi surface in normal state and that of the spin-lattice relaxation rate in the SC state can also be obtained. Among these quantities, the spin-lattice relaxation rate in the NMR experiment is expressed as \[44\]:

\[
\frac{1}{T_{1N}} = \frac{2}{k_B T} \int \int N_s(E)N_s(E')f(E)[1 - f(E')\delta(E - E')dE'dE]
\] (6)

Providing \(1/T_{1N}\) in the normal state satisfies the Korringa law, the spin lattice relaxation rate \(1/T_{1s}\) becomes \[51\]: \(1/T_{1s} \propto (k_B T) \cdot T_{1N}/T_{1s}\).

III. THEORETICAL RESULTS AND DISCUSSIONS

A. Phase diagram

Different from Seo et al.’s phase diagram, we find five stable phases in our phase diagram, which are shown in Fig.1. The first one is the normal phase, denoted N in Fig.1. Obviously,
when the superexchange coupling $J$ and $J'$ are too small to provide the SC pairing glue, the kinetic energy is dominant, and the electrons stay in the normal state. Among the SC phases mediated through the spin exchange couplings, large $J$ and small $J'$ favor the $S_{x^2+y^2}(\propto \cos(kx) + \eta\cos(ky))(\eta > 0)$ SC symmetry, which is the combination of the $S_{x^2+y^2}$ SC symmetry and $d_{x^2-y^2}$ SC symmetry. Here $\eta$ is a constant. Different from Seo et al. \cite{40}, it is not a mixed state of the $S_{x^2+y^2}$ SC state and the $d_{x^2-y^2}$ one, since the relative phase of the coefficients of the $S_{x^2+y^2}$ component and the $d_{x^2-y^2}$ one is fixed, hence it is a pure state. On the other hand, small $J$ and large $J'$ favors the $S_{x^2+y^2} \propto \cos(kx + ky) + \cos(kx - ky)$ SC phase, since the NNN hopping integrals along the $x$-axis and the $y$-axis are identical. As seen in Fig.1a, in the regions where $J$ and $J'$ compete with each other, the third SC phase appears as the combination of the $S_{x^2+y^2}$ and the $S_{x^2y^2}$ symmetries. For the case in this region with $J=3$ and $J'=1.5$, the SC order parameters are $\Delta_{x}^{11}=0.241$, $\Delta_{y}^{11}=0.555$ and $\Delta_{x\pm y}^{2m}=0.060$. And the fourth SC phase appears with the combination of the $d_{x^2-y^2}(\propto \cos(kx) - \eta\cos(ky))(\eta > 0)$ and $S_{x^2y^2}$ symmetries. For the case in this region with $J=0.7$ and $J'=0.3$, the SC order parameters are $\Delta_{x}^{11}=-0.039$, $\Delta_{y}^{11}=0.029$, and $\Delta_{x\pm y}^{2m}=0.012$. The components of the SC order parameters strongly depend on the relative magnitude of $J'$ with respect to $J$ in different SC regions. As we can see the ratio $\Delta_{x}^{11}/\Delta_{y}^{11}=R$ in Fig.1b, the change of the ratio $R$ is discontinuous with the increase of $J'$ at fixed $J$, implying that the quantum phase transitions between these SC phases are the first order.

### B. ARPES and T-Dependence of SC Gaps

The angle-resolved photoemission spectra (ARPES) experiment provides direct information about the quasiparticle spectra in normal state and the symmetry of the SC gaps in the SC phase. We present the SC gap character of the t-t'-J-J' models for the parameters in LaFeAsO in Fig. 2. Notice that the benchmark of the Fermi surface adopted here to plot the SC gap is at $T = 0.2$. Our results show that the SC gap structure exhibits fourfold symmetry, as seen in Fig.2a, in accordance with the Fermi surface topology of the present model. The amplitudes of the SC gaps on the different Fermi surfaces are different, suggesting the nature of a two-gap SC. The SC gap structures are anisotropic and nodeless, as shown in Fig.2a. Though the SC gap structure likes an anisotropic $s-$wave pairing symmetry, it is in fact the symmetry of the $d_{x^2-y^2} + S_{x^2y^2}$-wave. Our result reaches an agreement with recent ARPES experiments by Kondo et al. \cite{41}. We also notice that the relative variation of the
The angle dependence of the SC gaps near the small hole FS (red line) and the large hole FS (orange line) around the Γ point in the polar coordinates. Theoretical parameters: $J = 0.7$, $J' = 0.3$, and doping concentration $x=0.18$.

anisotropic gaps is less than 25\%, so our results do not conflict with Ding et al.’s [43] and Zhou et al.’s [42] reports.

Fig.2b shows the temperature dependence of the SC energy gap $\Delta$ along the $\theta = 0$ and $\theta = 90$ deg. With the increasing of the temperature, the SC order parameter in the small hole-like FS sheets decrease monotonously, as observed in the ARPES experiments [42, 43]. Near $T = 0.04$, both the SC gaps exhibit a small dip, which is attributed to the interactions among the three SC energy scales. Obviously, the nodeless and the anisotropy of the SC gaps originate from the unique gap structure, $\Delta^m = \Delta^2_{x\pm y}(\cos k_x \cos k_y) + (\Delta^1_{x} \cos k_x - \Delta^1_{y} \cos k_y)$. And such a symmetry is also in agreement with the analysis on the SC pairing symmetry [52, 53]. However, one finds that the magnitude of the gap in the large FS is bigger than that in small FS in the Γ point, opposite to the ARPES result. This may be due to the tight-binding parameters of
the two-orbital $t-t'-J-J'$ model, which only describes the topology structure of the Fermi surfaces of the FeAs superconductors, and does not contain all the details of the Fermi surfaces and the band structures in ironpnictide compounds. Hence, we expect that the refined tight-binding parameters will improve our results in the further study.

C. T-dependence of Fermi Surface

The temperature evolution of the FS in the normal state is shown in Fig. 3, when $T$ is higher than the critical temperature of the SC phase transition. The two hole-like and electron-like FS sheets can be clearly identified around the $\Gamma$ and the $M$ points at $x=0.18$, as observed in the ARPES experiments and the first-principle electronic structures calculations. Interestingly, the hole-like FS sheets expand a little with the increasing of the temperature. In contrast, the electron-like FS sheets shrink very acutely. This may demonstrate that the electron-like FS sheets are more important for the occurrence of the SC state, in consistent with Dai et al. prediction. [22].

D. Spin-Lattice Relaxation Rate in NMR

Although many experimental measurements, such as the Andreev reflection [54], the exponential temperature dependence of the penetration depths [55] and the ARPES [42, 43]
observe the nodeless gap function in the SC phase of ReFeAsO$_{1-x}$F$_x$ and Ba$_{1-x}$K$_x$Fe$_2$As$_2$ compounds, the line nodes in the SC gap was also suggested by the NMR experiment\cite{44}. The two characters in the NMR experiment supported the line nodes: lack of the coherence peak and the $T^3$ behavior in the nuclear spin-lattice relaxation rate, $1/T_1$. Using the gap function obtained in this paper, we calculate the spin lattice relaxation rate $1/T_s$, and the numerical result is shown in Fig. 4. We also plot the $T^3$ law (the red line) for a comparison. It is found that over a wide temperature range, the spin lattice relaxation rate in the present model can be fitted by the $T^3$ law, in agreement with the observation of the NMR experiments \cite{44, 56}.

A small coherence peak appears around the critical transition temperature, as clearly seen in the inset of Fig.4. Experimentally, such a small coherence peak may be easily suppressed by the impurity effect or the antiferromagnetic spin fluctuations, similar to the situations in cuprates. This leads to the missing of the Hebel-Slichter coherence peak in the NMR experiment in ironpnictide SC. With the decreasing of the temperature, one find a drop in the spin lattice relaxation rate, $1/T_{1s}$, consistent with the observation of the NMR experiments \cite{44}. Such a behavior deviating from the $T^3$ law may contribute from the multi-gap character of this system, and such a drop reflects the different SC gaps in different orbits. Surely, more meticulous studies are needed in near future. We also notice that Parker etal. found the extended $s_{\pm}$ SC gaps also can give the same NMR relaxation rate in SC pnictides \cite{57}. The inter-band contribution to the spin-lattice relaxation deviating from the $T^3$ law

FIG. 4: (Color online) Temperature dependence of the spin lattice relaxation rate in the t-$t'$-J-J' model. The red arrow indicates the SC critical temperature $T_c$. The red line is the $T^3$ law for comparison. Inset shows the detail near $T_c$. The theoretical parameters are the same as in Fig.2.
was suggested by Parish et al. [58].

Therefore, we find that the numerous unusual properties in the normal state and the SC phase of newly discovered FeAs superconductors could be interpreted in the t-t′-J-J′ model, showing that this model is a good approximate model to describe the iron-based superconductors. Within this scenario, the superimposition and mixing of the pairing electrons in the two orbits contributes to the anisotropic nodeless SC pairing symmetry. Such a pairing symmetry assembles the characters of usual d-wave and s-wave, hence shares the properties of the usual d-wave SC, like cuprates, and the s-wave SC, such as MgB$_2$ [42]. Nevertheless, to compare the theoretical results with the experimental observation quantitatively, more subtle band structures in the t-t′-J-J′ model are needed, though the present two-orbital model gives the qualitatively correct properties. Also the present constrained mean-field approximation should be improved in further study.

IV. SUMMARY

In summary, starting with the t-t′-J-J′ model, we obtain the mean-field parametric phase diagram at the doping concentration x=0.18, and find the normal state and a new SC phase in the phase diagram, different from the literature. With the decrease of the temperature, a nodeless and anisotropic $d_{x^2-y^2}$-wave gap structure emerges. But due to the multi-gap character, the anisotropic gaps open on the hole Fermi surfaces and the electron Fermi surfaces are different. The $T^3$ law of the spin lattice relaxation rate, $1/T_1$, is also interpreted in the present t-t′-J-J′ model.

Acknowledgments

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