The minimum model for the iron-based superconductors

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A single band $t$-$U$-$J_1$-$J_2$ model is proposed as the minimum model to describe the superconductivity of the newly discovered iron-based superconductors $R(O_{1-x}Fe_x)FeAs$ and $RO_{1-x}FeAs$ ($R = La, Ce, Sm, Pr, Nd, Gd$). With the mean-field approach, it is found that the pairing occurs in the $d$-wave channel. In the likely parameter region of the real materials, by lowering temperature, the system enters firstly the $d_{xy}$ superconducting phase with $D_{4h}$-symmetry and then enters the time-reversal-symmetry-broken $d_{xy} + id_{x^2-y^2}$ superconducting phase with $C_{4h}$-symmetry.

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It is well known that the most exciting finding after cuprates in the family of superconductors is the discovery of $ROFeAs$ ($R = La, Ce, Sm, Pr, Nd, Gd$). Soon after the announcement of the 26K superconductivity in $LaOFeAs$ by Kamihara et al.\[1\], several groups discovered a number of compounds with superconducting transition temperatures up to 52K.\[2, 3, 4, 5\]. Interestingly, even without $F$, those compounds may show superconductivity by introducing some oxygen vacancies.\[6\]. It is argued that this family of superconductors may share some common features with the cuprate superconductors and a number of models\[7, 8, 9, 10, 11, 12\] have been proposed to account for the mechanism of its superconductivity. Band structure calculations\[13, 14, 15, 16\] show that six $d$ bands of totally ten $d$ bands cross the Fermi surface but another group claimed that the parent compound could be a bad metal\[17\] with quite low density of states at the Fermi surface. A sound experiment combined with computation show that in the parent compound there is a phase transition from normal metal to stripe-type spin density wave (SDW) around 150K.\[18\]. This SDW state was subsequently demonstrated by the neutron scattering experiments\[19, 20\]. A theoretical analysis\[12\] and ab initial computation\[16\] indicate that the stripe SDW phase is induced by the frustrated spin-exchange interactions and the possible pairing symmetry is $d_{xy}$. These observations somehow hint that the antiferromagnetic fluctuation may play an important role for the superconductivity.

Although the band calculations indicate that six bands (hybridized $2d_{xy}, 2d_{yz}, 2d_{zx}$) cross the Fermi surface, the carriers very likely come from those bands lying in the $a$-$b$ plane, i.e., those composed of $d_{xy}$- and $d_{x^2-y^2}$-orbitals. However, the numerical result\[21\] strongly suggests that the $d_{x^2-y^2}$ band is far above the Fermi surface and $d_{xy}$-orbital indeed contribute a major weight to the Fermi pocket. The quasi one-dimensional $d_{yz}$ and $d_{zx}$ bands, though may extend slightly in the iron plane through hybridization with $p$-orbit of $As$, are unlikely to dominate the superconductivity. The above arguments directly lead to the hypothesis that a single band model may qualitatively describe the mechanism of the superconductivity in this family of compounds. Therefore, in this Letter, we propose the following Hamiltonian as the minimum model to account for the superconductivity in electron doped $ROFeAs$:

$$H = -t \sum_{\sigma, <i,j>} C_{i,\sigma}^\dagger C_{j,\sigma} + U \sum_j n_{j,\uparrow} n_{j,\downarrow} + J_1 \sum_{<i,j>} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{<<i,j>>} \vec{S}_i \cdot \vec{S}_j,$$

where $\sigma$ indicates the spin indices; $C_{i,\sigma}^\dagger (C_{i,\sigma})$ is the creation (annihilation) operator of electrons; $n_{j,\sigma}$ is the particle number operator and $<i,j>$ and $<<i,j>>$ indicate nearest neighbor and next nearest neighbor, respectively; $U$ describes the Hubbard repulsion and $J_{1,2} > 0$ represent the exchange constants. The recent ab initial calculation\[16\] suggested that $J_2$ is considerably larger than $J_1$ due to the superexchange processes through $As$ atoms.

We note that the Hubbard repulsion $U$ is relatively small in the FeAs compounds compared to those in the cuprates. The correlation effect is not very strong and the FeAs superconductors may share some common feature to the so-called gossamer superconductivity\[22, 23\]. $U$ may have two major effects on the superconductivity: One is to expel the $s$-wave pairing\[24\] and the other is to renormalize the band width and the coupling constants $J_{1,2}\[25\]$. In such a sense, instead of dealing with model (1) we study the following Hamiltonian but keep in mind that $t$ and $J_{1,2}$ are the renormalized constants:

$$H_{eff} = -t \sum_{\sigma, <i,j>} C_{i,\sigma}^\dagger C_{j,\sigma} - J_1 \sum_{<i,j>} b_{i,j}^\dagger b_{i,j} - J_2 \sum_{<<i,j>>} b_{i,j}^\dagger b_{i,j},$$

where

$$b_{i,j} = [C_{i,\uparrow} C_{j,\downarrow} - C_{i,\downarrow} C_{j,\uparrow}]$$

describes the electron pair operator.
Mean-field Hamiltonian. Because of positive $J_{1,2}$ in the system, the electrons favor to form spin-singlet pairs. By introducing the $d$-wave pairing order parameters $d_1 = -< b_{i,i^+} > = < b_{i,i^+} >$, $d_2 = -< b_{i,i^+} >$, we obtain the following mean-field Hamiltonian:

$$
H_{mf} = \sum_k E(k)(\alpha_k^+\alpha_k + \alpha_k^-\alpha_{-k}) + \sum_k (\xi_k - E) + 2J_1 d_1^2 N + 2J_2 d_2^2 N,
$$

with $N$ the number of sites and

$$
E(k) = \sqrt{\xi_k^2 + |\Delta_{1k} + \Delta_{2k}|^2},
$$

$$
\xi_k = -2t(cosk_x + cosk_y) - \mu,
$$

$$
\Delta_{1k} = 2J_1 \gamma_k,
$$

$$
\Delta_{2k} = 2J_2 \delta \eta_k,
$$

where $\gamma_k = cosk_x - cosk_y$, $\delta \eta_k = 2\sin k_x \sin k_y$ and $\mu$ denotes the chemical potential. The Gibbs free energy at a finite temperature $T$ then reads

$$
G(T) = -2K_B T \sum_k ln[2cosh(\frac{E(k)}{2K_B T})]
$$

with $\xi_k = 2J_1 \gamma_k$, $\gamma_k = \frac{1}{2} \sum_k (\xi_k - E) + 2J_1 d_1^2 N + 2J_2 d_2^2 N$.

For a given density of electron number $n$, the order parameters can be determined self-consistently by the following equations:

$$
n = 1 - \sum_k \frac{\xi_k}{E(k)} tanh(\frac{E(k)}{2K_B T}),
$$

$$
1 = \frac{J_1}{N} \sum_k \frac{\gamma_k^2}{E(k)} tanh(\frac{E(k)}{2K_B T}),
$$

$$
1 = \frac{J_2}{N} \sum_k \frac{\delta \eta_k^2}{E(k)} tanh(\frac{E(k)}{2K_B T}).
$$

Ground State. In the ground state, the above self-consistent equations are reduced to:

$$
n = 1 - \sum_k \frac{\xi_k}{E(k)},
$$

$$
1 = \frac{J_1}{N} \sum_k \frac{\gamma_k^2}{E(k)},
$$

$$
1 = \frac{J_2}{N} \sum_k \frac{\delta \eta_k^2}{E(k)}.
$$

Obviously, there are several sorts of solutions for the gap functions. If $d_2 = 0$, we get the conventional $d_{x^2-y^2}$ phase in the ground state; If $d_1 = 0$, we have the $d_{xy}$ phase which is isomorphic to the $d_{x^2-y^2}$ phase by rotating the $k$ space with an angle of $\pi/4$; For both $d_{1,2} \neq 0$, there is an extra free parameter $\theta$ (exp$\{i\theta\} = \frac{J_1 |J_2|}{|J_1| J_2}$) which can not be determined by the self-consistent equations but can be fixed by the lowest energy. Our numerical solution shows that only three superconducting phases are possible with the variation of $t$ and $J_{1,2}$, i.e., the $d_{x^2-y^2}$ phase for larger $J_1/J_2$, the $d_{xy}$ phase for quite smaller $J_1/J_2$ and the $d_{xy} + id_{x^2-y^2}$ phase with $\theta = \pi/2$ in the intermediate parameter range. The third phase is quite interesting because in it the time-reversal symmetry is broken. Its point group symmetry is also reduced to $C_{4h}$ from $D_{4h}$ of the $d_{xy}$ state. Of course there are
also other kinds of mixed solutions such as $d_{xy} + d_{x^2−y^2}$, but the corresponding energy is always higher than that of $d_{xy} + id_{x^2−y^2}$. For large enough $t$, $d_{1,2} = 0$ and the system is in the normal metallic phase. The mean-field phase diagram of the ground state for $n = 1.1$ and fixed $J = \sqrt{J_1^2 + J_2^2}$ is depicted in Fig.1. In the real materials, the band width could be strongly reduced by the Hubbard repulsion and the value of $J_2$ is around $2J_1$ or even larger as suggested by the ab initio calculation\[16\]. In this sense, the superconducting ground state must be either the $d_{xy} + id_{x^2−y^2}$ or the $d_{xy}$ paired state.

Finite Temperature Phase Diagram. For given $t$ and $J_{1,2}$, the thermodynamic phase diagram can be derived from the self-consistent equations by taking the order parameters tending to zero. Fig.2 shows the $T − n$ phase diagram for $t = 2J$ and $J_2 = 0.9J$ (Here $n$ does not mean the true carrier density in the present mean-field approach because we ignore $U$). In the real materials $T_c$ around $n = 1$ could be depressed heavily by $U$). It is found that there are two superconducting phases. One is the $d_{xy}$ phase which breaks the $U(1)$ gauge symmetry and the other is the $d_{xy} + id_{x^2−y^2}$ phase which breaks both the $U(1)$ gauge symmetry and the time-reversal symmetry. The $d_{xy}$ state has a nodal gap function which allows gapless excitations and therefore gains entropy at finite temperatures, while the $d_{xy} + id_{x^2−y^2}$ state is fully gapped with lower energy. The existence of two superconducting phases is due to the competing effect between energy and entropy. It is emphasized the second thermodynamic phase transition could be obtained from the specific heat measurement.

Density of States. One of the important quantities is the low temperature density of states, which can be detected directly by the local probe tunnelling experiments. In our $d_{xy} + id_{x^2−y^2}$ case, it reads:

$$
\rho(\omega) = \int \frac{d\varphi}{2\pi} Re \left\{ \frac{\omega}{\sqrt{\varphi^2 − |\Delta_1|^2 \cos^2(2\varphi) − |\Delta_2|^2 \sin^2(2\varphi)}} \right\}
$$

where $N_F$ is the density of states of the normal phase at the Fermi surface; $\Delta_{1,2} = 2J_{1,2}d_{1,2}$. The numerical result of $\rho(\omega)$ is depicted in Fig.3. Unlike that of the $d_{x^2−y^2}$ superconductors, there is no node in this time-reversal-symmetry-broken superconductor. However, the gap function is strongly anisotropic with a small minimum gap of $|\Delta_1|$ in the spectrum.

In conclusion, a minimum model to account for the mechanism of the iron-based superconductors is proposed. With the mean-field approach, it is found that the most likely superconducting ground state is the $d_{xy}$ or $d_{xy} + id_{x^2−y^2}$ type. At finite temperature, the $d_{xy}$ superconducting state appears first and a second phase transition into the $d_{xy} + id_{x^2−y^2}$ superconducting state occurs in some doping region by lowering the temperature. We emphasize that though the real systems are multi-band superconductors, we believe that our single band model captures the central physics for the mechanism of the superconductivity. The multi-band structure may only induce multi gaps or renormalization of the critical temperature without affecting the mechanism.

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