Superconducting symmetry of three-dimensional $t$-$J$ model on simple cubic lattice

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Motivated by the finding of nearly isotropic superconductivity in (Ba,K)Fe$_2$As$_2$, we use renormalized mean field theory to investigated the $t$-$J$ model on three-dimensional simple cubic lattice. A tunable anisotropic parameter is introduced to dictate the coupling on $z$ direction. The symmetry of the superconducting order is studied in detail. Calculation shows that for the isotropic case, pairing parameters on the three perpendicular directions have $\frac{\pi}{3}$ phase shift to each other. However, when the interaction on $z$ direction is suppressed, the corresponding amplitude of the pairing parameter decreases rapidly, furthermore, two-dimensional $d$-wave state pairing is favored when the anisotropic rate less than 0.75.

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I. INTRODUCTION

The key feature of copper oxides is the layered structure and led to speculation that reduced dimensionality is a necessary prerequisite for superconductivity at temperatures above 40K [1]. Although two dimensional (2D) models, such as $t$-$J$ model or Hubbard model, have captured essential of superconductivity, and successfully explained properties of the un-doped insulator and occurrence of gap in superconductors, 2D models alone can not describe and explain all observations of experiments [2, 3, 4, 5, 6, 7, 8]. Despite how large the ratio between out-of-plane and in-plane resistivity is, at the phase transition temperature $T_c$, both resistivities drop to zero simultaneously, this indicates the phase transition is of three dimensional [8], meanwhile, the observed antiferromagnetism is definitely a 3D phenomenon [9]. Some works provided evidence that superconductivity in the infinite-layer compounds ACu$_2$O$_2$ [10] is of three-dimensional nature which do not contain a charge-reservoir block and the distance from one unit cell to the next is the shortest among all the cuprates. Experimental data [2, 3, 4, 5, 6, 7, 8] shows that the decrease of doping concentration is accompanied by a raise of anisotropy which is defined as the ratio of the correlation lengths parallel and perpendicular to the CuO$_2$ plane in cuprates superconductivity. For materials Y$_{123}$, Y$_{121}$ [11, 12] and HgbBa$_2$Ca$_{0.86}$Sr$_{0.14}$Cu$_2$O$_{6-\delta}$ [10], coherence length and the anisotropy ratio imply that they are anisotropic 3D superconductors, these phenomena are supported by good 3D scaling analysis [10]. Recently observed [13, 14, 15] superconductivity in iron arsenic-based compounds has attracted many attention. Our motivation of investigating three dimensional isotropic superconductivity come directly from the measurements of the electrical resistivity in single crystals of (Ba,K)Fe$_2$As$_2$ in a magnetic field up to 60T [16]. Yuan et al found that the superconducting properties are in fact quite isotropic, appear more three dimensional than that of the copper oxides. Their results indicates that reduced dimensionality in these compounds is not necessarily a prerequisite for high temperature superconductivity.

3D anisotropic $t$-$J$ model has already been studied before [17, 18, 19]. By using mean-field Hamiltonian and carrying out expansion of free-energy, two main results were obtained [17]. One is that transition temperature decreases weakly with both increasing of 3D coupling strength and doping concentration, the other one is that in all cases $d$-wave pairing almost has the lowest energy. However, in simple cubic lattice (SCL), each site has six nearest neighbors(nm) settled in three perpendicular directions, no direction is special, if superconducting behavior is possible, its symmetry can not be conventional $d$-wave.

With the help of renormalized mean-field theory [20, 21](RMFT), We found that for isotropic case, pairing parameters on the three perpendicular directions have $\frac{\pi}{3}$ phase shift to each other. While as interaction in $z$ direction is suppressed, corresponding amplitude of pairing parameter drops quickly from infinite value to zero. By tuning coupling integral in $z$ direction, our calculation shows that superconducting symmetry are functions of the anisotropic parameter and doping concentration. Moreover, as the anisotropic parameter decreases from 1 to 0.75, symmetry of pairing parameters change from $\frac{\pi}{3}$ of 3D to $d$-wave of 2D. This may give some understanding of 3D-2D crossover.

II. FORMULATION

In SCL, anisotropic $t$-$J$ model can be written as $H = P_dH_tP_d + H_s$ with

$$H_t = -t \sum_{\langle nn \rangle} c_{i\sigma}^\dagger c_{j\sigma} - t\lambda \sum_{\langle nn \rangle} c_{i\sigma}^\dagger c_{j\sigma} + h.c.,$$

$$H_s = J \sum_{\langle nn \rangle} \vec{S}_i \cdot \vec{S}_j + J\eta \sum_{\langle nn \rangle} \vec{S}_i \cdot \vec{S}_j,$$

(1)

where $P_d = \prod(1 - n_i n_j)$ is the Gutzwiller projection operator [22, 23] which removes totally the doubly occupied states, $t$ and $J$ are the electron hoping interaction
and antiferromagnetic exchange interaction, respectively. $c_{i\sigma}^\dagger$ is to create an electron with spin $\sigma$ at site $i$, and $\hat{S}_i$ is a spin operator. Summation $\langle mn \rangle$ runs over all $nn$ in $xy$ plane, while summation $\langle nn' \rangle$ runs over all $nn$ in direction $z$ which is perpendicular to $xy$ plane. For convenience, all anisotropic parameters are put into $z$ direction terms, $\lambda$ and $\eta$ are anisotropic parameters with range $[0,1]$, $\lambda = \eta = 1$ corresponding to the isotropic case.

In RMFT the wavefunction of the Hamiltonian is assumed to be the projected state $|\Psi\rangle = P_B|\Psi_{BCS}\rangle$, $|\Psi_{BCS}\rangle = \prod_k (u_{\uparrow k}^\dagger + v_{\uparrow k}^\dagger c_{\uparrow k}^\dagger |0\rangle)$, where $\hat{k}$ is constrained in the reduced Brillouin zone, and the two coefficients satisfy $|u_{\uparrow k}|^2 + |v_{\uparrow k}|^2 = 1$. The projection operator can be taken into account by a set of renormalized factors $\{20, 26\}$ defined as $\langle c_{\sigma i}^\dagger c_{\sigma j}\rangle \approx g_{i\sigma} \langle c_{\sigma i}^\dagger c_{\sigma j}\rangle_0$, $\langle \hat{S}_i \cdot \hat{S}_j\rangle \approx g_s \langle \hat{S}_i \cdot \hat{S}_j\rangle_0$, where $\langle \rangle_0$ denotes expectation value of unprojected state $\Psi_{BCS}$, and $\langle \rangle$ denotes expectation value of physical state $\Psi$. Then one has $\langle H\rangle_0 = \langle H\rangle_0 + g_s H + g_h H_L$.

In homogeneous case the renormalized factors $\{20, 26\}$ take the form of $g_l = 2\phi/(1 + \phi)$ and $g_s = 4/(1 + \phi^2)$. Considering even-parity case in which $u_{\downarrow k}^\dagger v_{\downarrow k}^\dagger = u_{\uparrow k}^\dagger v_{\uparrow k}^\dagger$ and $|v_{\uparrow k}|^2 = |v_{\downarrow k}|^2$, the expectation value of the effective hamiltonian has the same form as that of 2D

$$\langle H\rangle_0 = 2g_l \sum_k \varepsilon_k |v_{\uparrow k}|^2 + N_s^{-1} \sum_{k,k'} V_{k,k'} \langle |v_{\uparrow k}|^2 |v_{\uparrow k'}|^2 + u_{\uparrow k}^\dagger v_{\uparrow k'}^\dagger u_{\uparrow k'}^\dagger \rangle, \quad (2)$$

where $N_s$ is the total number of sites and

$$\varepsilon_k = -t_{\uparrow k}^3,$$
$$V_{k,k'} = \frac{3}{4} g_s J \gamma_{\uparrow k},$$
$$\gamma_{\uparrow k} = \frac{1}{2} (\cos k_x + \cos k_y + \lambda \cos k_z),$$
$$\gamma_{\downarrow k} = \frac{1}{2} (\cos k_x + \cos k_y + \eta \cos k_z). \quad (3)$$

In order to investigate superconducting property, one should introduce two mean-field parameters such as particle-particle(pairing) parameter $\Delta_{\tau} = \langle c_{\uparrow i}^\dagger c_{\uparrow i + \tau}^\dagger - c_{\uparrow i}^\dagger c_{\uparrow i + \tau} \rangle_0$ and particle-hole parameters $\xi_{\tau} = \sum_{\sigma\sigma'} \langle c_{\sigma i}^\dagger c_{\sigma^\prime i + \tau} \rangle_0$. By minimizing the quantity $W = \langle H' - \mu \sum_{\sigma\sigma'} c_{\sigma i}^\dagger c_{\sigma^\prime i} \rangle_0$ with respect to $u_{\uparrow k}$ and $v_{\uparrow k}$, where $\mu$ is denoted as chemical potential, one gets the coupled gap equations

$$\Delta_{\tau} = -N_s^{-1} \sum_k \cos k_{\tau} \gamma_{\uparrow k} / E_{\uparrow k}, \quad \xi_{\tau} = -N_s^{-1} \sum_k \cos k_{\tau} \gamma_{\downarrow k} / E_{\downarrow k}, \quad (4)$$

where $\tau$ indicates the three perpendicular directions $x, y, z$, $E_{\uparrow k} = \sqrt{\varepsilon_k^2 + |\Delta_{\uparrow k}|^2}$, $\Delta_{\uparrow k} \propto \cos k_x + \Delta_y \cos k_y +$$

$$\eta \Delta \cos k_z, \quad \xi_{\uparrow k} = -\xi_{\downarrow k} \propto \cos k_x + \cos k_y + \eta \cos k_z, \quad \xi_{\tau} = \mu + N_s^{-1} \langle \frac{\partial H'}{\partial \mu} \rangle_0.$$

These gap equations should be solved simultaneously with doping concentration $\delta = \sum_{k} \xi_{\tau} / E_{\uparrow k}$. After iterative self-consistent solving, for a set of given $\delta, \lambda, \eta$ and $\mu$, one can obtain all those particle-particle and particle-hole parameters simultaneously. Superconductivity symmetry is determined by the phase shift of different pairing parameters $\Delta_{\tau}$ and the superconducting parameter $\Delta_{\tau\tau}$.

III. SYMMETRY OF SUPERCONDUCTIVITY FOR ISOTROPIC AND ANISOTROPIC CASES

For isotropic SCL, $\eta = \lambda = 1$. In half-filled case, $\mu, \varepsilon_k = 0$, there is a trivial solution with $\Delta_{\tau} = 0$ corresponding to projected fermi-liquid. $\xi_{\tau}$ changes its sign at the surface and the average energy of per site is $
abla = -4J / N_s \sum_{k} \varepsilon_{\uparrow k} / E_{\uparrow k} \approx 0.050J$. For non-trivial solution, by using Eq. (2), the energy per site can be written as $\omega = \frac{3}{2} g_{s} J \sum_k E_{\uparrow k}$, here relations $|u_{\uparrow k}|^2 = \frac{1}{2} (1 + \xi_{\uparrow k} / E_{\uparrow k})$ and $u_{\uparrow k}^\dagger = \Delta_{\tau} \approx \frac{1}{2} \eta \Delta_{\tau} \approx \frac{1}{2} \eta$. By assuming $E_{\uparrow k} = c (\cos k_x^2 + \cos k_y^2 + \cos k_z^2)^{1/2}$ and substituting it into gap equations, one can get $\Delta = \frac{1}{2} \eta \Delta_{\tau} \approx \frac{1}{2} \eta \Delta_{\tau}$.

Substituting the solutions into energy expression, one can get $\omega = \frac{3}{2} \eta \Delta_{\tau} \approx 0.398$ and the energy of per site is $\omega = \frac{3}{2} \eta \Delta_{\tau} \approx 0.712J$, which is lower than the energy of the projected fermi liquid state and is more favored and stable. In the non-trivial case parameters should satisfy following equations simultaneously

$$\xi_{\tau}^2 + |\Delta_{\tau}|^2 = c^2,$$
$$\Delta_{\tau} = \frac{\Delta_{\tau}^2}{h c} + 2 \xi_{\tau} \xi_{\tau} = 0. \quad (6)$$

\begin{figure}[h]
\centering
\includegraphics[width=\columnwidth]{figure1.pdf}
\caption{Parameters amplitude as functions of doping concentration $\delta$. $\xi = \xi_{\uparrow k}$ denotes amplitude of particle-hole parameter, $\Delta = |\Delta_{\uparrow k}|$ denotes pairing parameter, and $\Delta_{\tau}$ is superconducting parameter defined as $g_l \Delta_{\tau}$.}
\end{figure}
It has SU(2) degeneracy, the most important solution is

\[ \xi_\tau = \frac{\sqrt{3}}{3} c = 0.229, \]

\[ |\Delta_x| = \frac{\sqrt{6}}{3} c = 0.324, \]

\[ \Delta_x = |\Delta| \exp i\theta, \]

\[ \Delta_y = |\Delta| \exp (i\theta + 2/3\pi), \]

\[ \Delta_z = |\Delta| \exp (i\theta + 4/3\pi), \] (7)

It clearly shows that the phase shift of different \( \Delta_{\tau} \) is \( \frac{2\pi}{3} \). By changing the sign of \( \xi_\eta \) and taking the phase difference of any two pairing parameters as \( \frac{1}{3}\pi \), one can obtain another solution and if one sets one or two of the three \( \xi \) as zero other solutions can also be obtained. All these solutions have the same energy. Among these energetically degenerated states the \( \frac{2\pi}{3} \) symmetric state has the best kinetic energy \( \langle H_t \rangle_0 \). Upon doping degeneracy will be lifted, superconducting state favors the best kinetic energy state, which is the \( \frac{2\pi}{3} \) symmetry state. This is also the reason why we call this solution as the most important one.

Hoping integral \( t \) is used as energy unit, and \( t/J = 3 \) is taking in order to be consistent with the superexchange relation of \( J = 4t^2/U \) in the large Hubbard \( U \) limit. For isotropic SCL case, self-consistent parameters as functions of doping concentration are shown in Fig. 1. Amplitude of all \( \Delta_{\tau} \) are the same which is denoted as \( \Delta \) in the figure. Every \( \xi_\tau \) is real and has the same value of \( \xi \). One can see from Fig. 1 that with doping increasing, amplitude of pairing parameters decreases, while superconducting parameter \( \Delta_x \) varies along a non-monotonic curve. These properties are similar to that of 2D square lattice. The most interesting result is that each \( \Delta_{\tau} \) has imaginary part, \( \theta_{\tau} \) is used to denote phase of \( \Delta_{\tau} \), the pairing parameters have \( \frac{\pi}{3} \) phase shift to each other just as that of half-filled case.

When the interaction in \( z \) direction is suppressed, amplitude of the corresponding parameters will deviate from those of \( xy \) plane. In order to make the situation more simpler, we set \( \eta = \lambda \). For \( \eta = 0.9 \), the doping dependent parameters are presented in Fig. 2. Fig. 2(a) shows that \( \eta \) affects amplitudes of both pairing parameter and particle-hole parameter, with increasing \( \delta \) all pairing parameters decrease with \( |\Delta_x| < |\Delta_{x,y}| \). Anisotropy also affects the symmetry of the \( \Delta_{\tau} \). Fig. 2(b) demonstrates that at half-filled point \( \theta_{x,y} = \theta_x - \theta_y < \frac{\pi}{3} \), and \( \theta_{x,y} \) decreases with increasing \( \delta \). Accompanied by decrease of \( |\Delta_x| \), \( \theta_{x,y} \) approaches to \( \pi \). For \( \eta = 0.8 \), as shown in Fig. 3(a) with \( \delta \) increasing \( |\Delta_x| \) drops more rapidly than \( |\Delta_{x,y}| \) and vanishes at \( \delta = 0.1 \). Symmetry of pairing parameters are shown in Fig. 3(b), \( \theta_{x,y} \) decreases from about 1.08\( \pi \) to \( \pi \) at \( \delta = 0.1 \). For \( \delta > 0.1 \), system apparently behaves as 2D with superconducting order being \( d_{x^2-y^2} \) symmetry. By compare above two anisotropic cases one can reasonably expect that at a given anisotropic parameter, system will behave as 2D in all doping level.

This property can be demonstrated clearly in half-filled case. For anisotropic half-filling, \( E_k = \sqrt{c^2 \cos^2 k_x + c^2 \cos^2 k_y + c^2 \eta^2 \cos^2 k_z} \) where \( c^2 = \xi^2 + |\Delta|^2 \), \( \xi_{x,y} = \xi_{x^2-y^2} + |\Delta|^2 \), \( i \) represents \( x \) or \( y \) direction. For a given \( \eta \) one can obtain the phase difference \( \theta_{x,y} \) and the value of \( \xi_{x,y} \) for the best kinetic energy state. As \( c_3 = c \), it reduces to the isotropic case. As \( c_3 \) approaches to 0, degree of anisotropy is very large and the system turns to a quasi-2D one. From Fig. 4 one can see that by decreasing \( \eta \) from 1, \( \xi_{x,y} \) decreases quickly and reaches zero at about \( \eta = 0.75 \), simultanously the phase difference \( \theta_{x,y} \) increases from \( \frac{\pi}{3} \) to \( \pi \). These results indicate that as the anisotropic parameter decreases to 0.75, \( \Delta_z \) vanishes, and system loses its 3D character.
FIG. 4: For half-filled anisotropic case, with $\eta$ decreasing, amplitude of $c_3 = |\Delta_z|^2 + \xi_z^2$ drops quickly. Phase difference $\theta_{x,y}$ as function of anisotropic coefficient is presented in right picture.

IV. SUMMARY

Experiment shows that 122-type ternary iron arsenides possess three-dimension properties [16], although the microscopic nature of superconductivity in iron-based compound is not clearly at present, and one band model is not enough to describe them, we investigated isotropic and anisotropic $t$-$J$ model on simple cubic lattice to show the superconductivity symmetry from mean-field point of view. For isotropic three-dimensional $t$-$J$ model, superconductivity ground state is not conventional $d$-wave, phase shift of each pairing parameter is exactly $\frac{2}{3}\pi$. For anisotropic cases three-dimensional character is not so obviously, adding a small anisotropic interaction on $z$ direction will induces a great anisotropy in its corresponding mean-field paring parameter and raise serious instability of previous 3D superconducting symmetry. We found that pairing parameter $\Delta_z$ depends strongly on the anisotropic parameter, as anisotropic parameter decrease to 0.75, system appears 2D behavior. From this discussion one can see that 3D character superconductor is sensitive to amplitude of couplings.

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