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Mixed-state effect on the low-energy spin dynamics in optimally-doped iron pnictide superconductors

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ABSTRACT

Based on a phenomenological model with $s_{\pm}$ pairing symmetry, the mixed-state effect on the low-energy spin dynamics in optimally-doped iron pnictide superconductors is studied by solving Bogoliubov–de Gennes equations. Our results of the spin susceptibility at $\mathbf{q}=\mathbf{Q}$ in the normal, superconducting and mixed states agree qualitatively with recent neutron scattering experiments. We also propose that the field-induced intensity change in both momentum and real space can be used to further verify the $s_{\pm}$ pairing symmetry in the iron pnictides.

1. Introduction

The discovery of high-transition temperature superconductivity in iron pnictide superconductors [1] raised the possibility of an unconventional superconducting (SC) pairing mechanism in this kind of materials. Theoretically, one commonly believed idea is that the Cooper pairs are formed via spin fluctuations, leading to the $s_{\pm}$ pairing symmetry where the paring order parameter (OP) changes sign between the electron and hole pockets [2–7]. Experimentally, in optimally-doped $Ba_{1-x}K_xFe_2As_2$, $BaFe_{2-x}(Co,Ni)_xAs_2$ and $FeTe_{1-x}Se_x$, neutron scattering (NS) experiments observed a resonance peak at wave vector $\mathbf{Q}=(\pm\pi,0)$ and $(0,\pm\pi)$ [defined in the 1Fe/cell Brillouin zone (BZ)] in the SC state [8–14], which was interpreted as the evidence for the $s_{\pm}$ symmetry [15–18]. Later, some NS experiments studied the effect of a magnetic field on the low-energy spin dynamics [19–21]. Specifically in Ref. [22], a perpendicular magnetic field applied in optimally-doped $BaFe_{1.9}Ni_{0.1}As_2$ reduces the intensity and energy of the resonance while broadens its width. A natural question arises: Is the evolution of the resonance with the magnetic field consistent with the $s_{\pm}$ scenario? In this paper we address this issue and propose a method to test it. Here the mixed-state effect on the spin dynamics is studied by solving the Bogoliubov–de Gennes (BdG) equations in the presence of a perpendicular magnetic field and then conducting the real-space random-phase approximation (RPA) to calculate the spin susceptibility χ. Previously, for the iron pnictides without the magnetic field, χ has been calculated in momentum space [15–18]. However in the presence of a magnetic field, the translational symmetry is broken and χ has to be calculated in real space which requires much more computational time and resources. Therefore a theoretical investigation of the mixed-state effect on the spin dynamics in the iron pnictides is still lacking and needs to be done urgently. In our previous work [23], we have shown that the mixed-state effect cannot be simplified solely as magnetic impurities. Considering only the amplitude suppression of the SC OP near the vortex cores (without taking into account the phase variation) is also not sufficient. On the contrary, in our BdG approach, we can take both the amplitude suppression and the phase variation of the SC OP into account self-consistently, and based on our previous calculation [23–25], we found that the vortex-core states are very robust against finite size effects. Therefore our approach is currently the most accurate way to study the mixed-state effect in the iron pnictides. By studying this, we find that the spin excitation spectra for the $s_{\pm}$ symmetry are consistent with the NS experiments no matter the magnetic field is present or not. In addition, the field-induced intensity change can be used to further verify the $s_{\pm}$ pairing symmetry in the iron pnictides.

2. Method

We adopt an effective two-orbital model on a two-dimensional $N\times N$ lattice which captures the basic Fermi surface structures of the iron pnictides [26], with a phenomenological form for the

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intraorbital pairing terms. The Hamiltonian can be written as [24,27,28]

$$H_0 = -\sum_{ij,\alpha\beta,v} t'_{ij,\alpha\beta} c^\dagger_{i\alpha v} c_{j\beta v} + \sum_{j\beta v}\left[-\mu + U\langle n_{j\beta\bar{v}}\rangle + (U-2J_H)\langle n_{j\bar{\beta}v}\rangle + (U-3J_H)\langle n_{j\bar{\beta}v}\rangle\right] n_{j\beta v} + \sum_{ij,\alpha\beta}(\Delta_{ij,\alpha\beta} c^\dagger_{i\alpha\uparrow} c^\dagger_{j\beta\downarrow} + H.c.). \quad (1)$$

Here i,j are the site indices, $\alpha,\beta = 1,2$ are the orbital indices, v represents the spin, μ is the chemical potential and $n_{j\beta v} = c^\dagger_{j\beta v} c_{j\beta v}$ is the number operator. U and J_H are the onsite intraorbital Hubbard repulsion and Hund's coupling, respectively. Here we have the interorbital Coulomb interaction $U' = U - 2J_H$ according to symmetry [29]. $\Delta_{ij,\alpha\beta} = \frac{V_{ij}\delta_{\alpha\beta}}{2}(\langle c_{j\beta\downarrow} c_{i\alpha\uparrow}\rangle - \langle c_{j\beta\uparrow} c_{i\alpha\downarrow}\rangle)$ is the intraorbital spin-singlet bond OP, where V_{ij} is the next-nearest-neighbor $[i = j \pm \hat{x} \pm \hat{y}]$ (NNN) attraction we choose to achieve the $s_\pm$ pairing symmetry. In the presence of a magnetic field B perpendicular to the plane, the hopping integral is $t'_{ij,\alpha\beta} = t_{ij,\alpha\beta}\exp\left[i\frac{\pi}{\Phi_0}\int_j^i \mathbf{A}(\mathbf{r})\cdot d\mathbf{r}\right]$, where $\Phi_0 = hc/2e$ is the SC flux quantum, and $\mathbf{A} = (-By, 0, 0)$ is the vector potential in the Landau gauge. Following Ref. [26], we have

$$t_{ij,\alpha\beta} = \begin{cases} t_1 & \alpha = \beta, i = j \pm \hat{x}(\hat{y}), \\ \frac{1+(-1)^j}{2} t_2 + \frac{1-(-1)^j}{2} t_3 & \alpha = \beta, i = j \pm (\hat{x} + \hat{y}), \\ \frac{1+(-1)^j}{2} t_3 + \frac{1-(-1)^j}{2} t_2 & \alpha = \beta, i = j \pm (\hat{x} - \hat{y}), \\ t_4 & \alpha \neq \beta, i = j \pm (\hat{x} \pm \hat{y}), \\ 0 & \text{otherwise}. \end{cases} \quad (2)$$

Eq. (1) can be diagonalized by solving the BdG equations $H = C^\dagger M C$, where $C^\dagger = (\cdots, c^\dagger_{j1\uparrow}, c_{j1\downarrow}, c^\dagger_{j2\uparrow}, c_{j2\downarrow}, \cdots)$, subject to the self-consistency conditions: $\langle n_{j\beta\uparrow}\rangle = \sum_{k=1}^{L} |Q_{m-1k}|^2 f(E_k)$, $\langle n_{j\beta\downarrow}\rangle = 1 - \sum_k |Q_{mk}|^2 f(E_k)$ and $\Delta_{ij,\alpha\beta} = \frac{V_{ij}}{2}\delta_{\alpha\beta}\sum_k (Q^*_{mk} Q_{nk} + Q^*_{n+1k} Q_{m-1k}) f(E_k)$. Here $L = 4N^2, m = 4(j_y + Nj_x) + 2\beta, n = 4(i_y + Ni_x) + 2\alpha - 1$ and Q is a unitary matrix that satisfies $(Q^\dagger M Q)_{kl} = \delta_{kl} E_k$. Here we used $i = (i_x, i_y)$ and $j = (j_x, j_y)$, with $i_x, j_x, i_y, j_y = 0, 1, \ldots, N-1$. μ is determined by the doping concentration x through $\frac{1}{N^2}\sum_{j\beta v} n_{j\beta v} = 2 + x$.

The bare spin susceptibility in real space is [30].

$$\chi^{-+0}_{\substack{\delta\alpha \\ \gamma\beta}}(i,j,\omega) = -\langle\langle c^\dagger_{i\delta\downarrow} c_{i\alpha\uparrow} | c^\dagger_{j\gamma\uparrow} c_{j\beta\downarrow}\rangle\rangle_{\omega+i\eta} = \sum_{k,l=1}^{L} Q_{pk} Q_{nl} (Q^*_{ol} Q^*_{mk} - Q^*_{ok} Q^*_{ml}) \frac{f(E_k) + f(E_l) - 1}{\omega - E_k - E_l + i\eta}, \quad (3)$$

where $o = 4(j_y + Nj_x) + 2\gamma - 1$ and $p = 4(i_y + Ni_x) + 2\delta$. Including interactions within RPA, the full susceptibility can be calculated through

$$\chi_{\substack{\delta\alpha \\ \gamma\beta}}(i,j,\omega) = \chi^0_{\substack{\delta\alpha \\ \gamma\beta}}(i,j,\omega) + \sum_v \sum_{rstu} \chi^0_{\substack{\delta\alpha \\ rt}}(i,v,\omega) U^I_{\substack{rt \\ su}}(v,v) \chi_{\substack{su \\ \gamma\beta}}(v,j,\omega). \quad (4)$$

Here we omitted the superscript $-+$. The interaction vertex $U^I_{\substack{rt \\ su}}(i,j)$ is nonzero only when $i = j$ and satisfies

$$U^I_{\substack{rr}} = U, U^I_{\substack{rt}} = J_H, U^I_{\substack{rt}} = U - 2J_H, U^I_{\substack{rr}} = J_H, \quad (5)$$

where $r \neq t$. The spin susceptibility measured by NS experiments is proportional to $\chi''(\mathbf{q},\omega)$, where

$$\chi''(\mathbf{q},\omega) = \frac{1}{N^2}\sum_{ij,\alpha\gamma} \mathrm{Im}\chi_{\substack{\alpha\alpha \\ \gamma\gamma}}(i,j,\omega)\cos[\mathbf{q}\cdot(i-j)] = \sum_{i-j} f(i-j,\omega)\cos[\mathbf{q}\cdot(i-j)], \quad (6)$$

with $f(i-j,\omega) = \frac{1}{N^2}\sum_{j,\alpha\gamma} \mathrm{Im}\chi_{\substack{\alpha\alpha \\ \gamma\gamma}}(i-j,j,\omega)$ being the average real-space spin–spin correlation function.

The parameters are chosen as $t_{1-4} = 1, 0.4, -2, 0.04$. $N = 32$ and magnetic unit cells are introduced where each unit cell accommodates two SC flux quanta. V_{ij} $[i = j \pm \hat{x} \pm \hat{y}]$ is chosen to be -2. Hereafter, we fix $x = 0.1$, corresponding to the optimally-doped $BaFe_{1.9}Ni_{0.1}As_2$, which enables us to compare the results directly with those in Ref. [22]. The temperature T is set to be 0 and $0.7\Delta_0$. Here Δ_0 is the SC OP we solved at $(B = 0, T = 0)$. At $T = 0.7\Delta_0$, the self-consistently calculated SC OP is zero, indicating that the system is in the normal state. After solving the BdG equations at $(B = 0, T = 0)$, we found that for the NNN intraorbital pairing, $\Delta_{ij,\beta\beta} = \frac{\Delta_0}{4}$ $[i = j \pm \hat{x} \pm \hat{y}]$, thus in momentum space, the pairing OP can be written as $\Delta_{\mathbf{k}} = \frac{\Delta_0}{2}(\cos k_x + \cos k_y)$ and only intraband pairing exists since the pairing function on the two orbitals are exactly the same. Here $\mathbf{k}$ is defined in the 2Fe/cell BZ. In Fig. 1 we plot the Fermi surface in the 2Fe/cell BZ together with the nodal lines for $\cos k_x + \cos k_y$. As we can see, the nodal lines do not intersect any Fermi surface, leading to full gap opening on all the pockets. The value of $\cos k_x + \cos k_y$ on each pocket is shown in Fig. 2. The SC OP changes sign between the hole and electron pockets and on each pocket, it shows minor anisotropy. Thus the NNN intraorbital pairing we adopted can indeed generate the $s_\pm$ pairing symmetry. In the following we calculate $\chi''(\mathbf{q},\omega)$ at $(B = 0, T = 0.7\Delta_0)$, $(B = 0, T = 0)$ and $(B \neq 0, T = 0)$, corresponding to the normal, SC and mixed states, respectively.

3. Results

For the $s_\pm$ pairing, we choose U and J_H to be 2 and $0.2U$, respectively. With this choice of parameters, the system stays paramagnetic no matter it is in the normal, SC or mixed state. Meanwhile

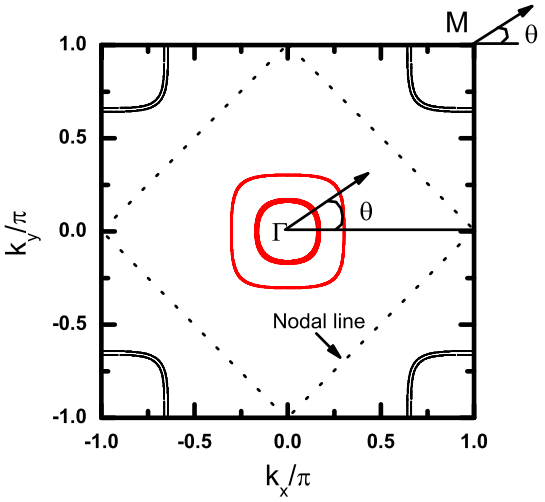

Fig. 1. The Fermi surface of our tight-binding model in the 2Fe/cell BZ. There are two hole pockets (red) around Γ and two electron pockets (black) around M. The dotted lines mean $\cos k_x + \cos k_y = 0$. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)