

Magnetic Interactions, Superconductivity, and Spin-Resonance Peak in Iron-Based Materials

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Abstract—Different mechanisms of superconductivity result in specific symmetries and structures of the gap in multiband systems. Here we review the spin fluctuation mechanism of Cooper pairing and discuss the spin resonance feature in the superconducting state of iron-based materials.

Keywords: Fe-based superconductors, spin resonance peak, spin fluctuation mechanism of pairing

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INTRODUCTION

Weakly doped pnictides are antiferromagnetic metals and the most promising candidate for the theory of superconductivity is the spin fluctuation mechanism of Cooper pairing [1–4]. The leading superconducting instability in a wide range of dopings is characterized by the extended s -wave gap having the opposite signs on hole and electron Fermi surface pockets – the so-called s_{\pm} state [4–7]. On the other hand, orbital fluctuations results in the s_{++} state with the gap having the same sign on all Fermi surface sheets [8]. By determining the gap structure, one can deduce the microscopic mechanism of superconductivity. In this respect, inelastic neutron scattering plays a special role since the imaginary part of the dynamical spin susceptibility $\chi(\mathbf{q}, \omega)$ measured there carries information about the gap structure in the superconducting state. That is, the sign-changing s_{\pm} gap leads to the formation of the spin resonance peak at or near the commensurate antiferromagnetic wave vector $\mathbf{q} = \mathbf{Q}$ connecting Fermi surface sheets with different signs of gaps on them [9, 10].

Here we review the spin fluctuation mechanism of superconductivity and discuss the spin resonance in the superconducting state of iron-based materials. Based on the gap function calculated within the spin fluctuation theory of pairing, we show that the resonance peak shifts to lower frequencies and loses some intensity with increasing the gap anisotropy [11–14].

MODEL

As the kinetic energy H_0 , we use the five-orbital tight-binding model from [15] that is based on the DFT band structure calculations within LDA for the prototypical iron pnictide, LaFeAsO. H_0 is described by a tight-binding model spanned by five Fe d -orbitals. Total number of electrons is given by $n = n_0 \pm x$, where electron filling $n_0 = 6$ corresponds to the fully occupied d^6 -orbital and x is the doping concentration. For the electron-doped and undoped systems, the Fermi surface consists of two small hole pockets, α_1 and α_2 , around the $\Gamma = (0, 0)$ point, and two small electron pockets, β_1 and β_2 , around the $X = (\pi, 0)$ and $Y = (0, \pi)$ points in the one-electron Brillouin zone, respectively. Upon hole doping a new hole Fermi surface pocket, γ , emerges around the (π, π) point.

Explicit form of H_0 is

$$H_0 = \sum_{\mathbf{k}\sigma} \sum_{l'l'} [(\epsilon_l - \mu_0) \delta_{ll'} + t_{ll'}(\mathbf{k})] d_{\mathbf{k}l\sigma}^{\dagger} d_{\mathbf{k}l'\sigma}, \quad (1)$$

where $d_{\mathbf{k}l\sigma}$ is the annihilation operator of the electron with momentum \mathbf{k} , spin σ , and orbital index l , $t_{ll'}(\mathbf{k})$ is the hopping matrix element, ϵ_l is the one-electron energy, and μ_0 is the chemical potential. Later we use numerical values of hopping matrix elements $t_{ll'}(\mathbf{k})$ and one-electron energies ϵ_l from [15]. Similar model for iron pnictides was proposed in [16].

There is an important consequence of the multiorbital nature of the system. The single-particle noninteracting Green's function is diagonal in the band space but not in the orbital space. It makes sense to

transform to the band basis that is constructed using operators of electron's creation and annihilation, $b_{\mathbf{k}\mu\sigma}^\dagger$ and $b_{\mathbf{k}\mu\sigma}$, with the band index μ . Green's function for H_0 is then diagonal in the band basis,

$$G_{\mu\sigma}(\mathbf{k}, i\omega_n) = 1/(i\omega_n - \varepsilon_{\mathbf{k}\mu\sigma}), \quad (2)$$

where ω_n is the Matsubara frequency and $\varepsilon_{\mathbf{k}\mu\sigma}$ is the energy. The transition from the orbital to the band basis is implemented with the aid of the orbital matrix elements $\varphi_{\mathbf{k}l}^\mu$, $|\sigma\mathbf{k}\rangle = \sum_\mu \varphi_{\mathbf{k}l}^\mu |\sigma\mu\mathbf{k}\rangle$. In this case,

$$d_{\mathbf{k}l\sigma} = \sum_\mu \varphi_{\mathbf{k}l}^\mu b_{\mathbf{k}\mu\sigma}.$$

As the interaction part of the model, we take the on-site Coulomb (Hubbard) electron-electron repulsion written for the multiorbital systems [15–19],

$$H_{\text{int}} = U \sum_{f,l} n_{f\uparrow} n_{f\downarrow} + J \sum_{f,l,l'} \sum_{\sigma,\sigma'} d_{f\uparrow\sigma}^\dagger d_{f'l'\sigma'}^\dagger d_{f\downarrow\sigma} d_{f'l'\sigma'} + U' \sum_{f,l,l'} n_{f\uparrow} n_{f'l'} + J' \sum_{f,l,l'} d_{f\uparrow}^\dagger d_{f'l'}^\dagger d_{f\downarrow} d_{f'l'}, \quad (3)$$

where $n_{f\uparrow} = n_{f\uparrow} + n_{f\downarrow}$, $d_{f\uparrow}$ is the electron annihilation operator, $n_{f\uparrow} = d_{f\uparrow}^\dagger d_{f\uparrow}$ is the number of particles operator, f is the site index, l and l' are orbital indices, U and U' are intra- and interorbital Hubbard repulsions, J is the Hund's exchange, and J' is the pair-hopping. Usually, parameters obey the spin-rotational invariance (SRI) that leads to relations $U' = U - 2J$ and $J' = J$ thus reducing the number of free parameters in the theory.

The interactions in the Hamiltonian have a complicated orbital structure. To compactify the expressions we define the local matrix interaction in orbital space, $U_{nm}^{ll'}$, $d_{f\uparrow\sigma}^\dagger d_{f'm'\sigma'}^\dagger d_{f\downarrow\sigma} d_{f'm'\sigma'}$, which accounts for all the quartic terms. It will be used later for calculations of susceptibility.

SPIN FLUCTUATION THEORY OF PAIRING

The original proposal of superconducting pairing arising from magnetic interactions was put forward by Emery [20] and by Berk and Schrieffer [21], who were interested primarily in transition metal elements and nearly ferromagnetic metals. Such systems are considered to be close to a ferromagnetic ordering transition in the Stoner sense, so that their susceptibility may be approximated by $\chi = \chi_0/(1 - U\chi_0)$, where χ_0 is the "bare" susceptibility at zero momentum and U is a Hubbard matrix element assumed to be large since $U\chi_0 \simeq 1$. Physically this means that a spin-up electron traveling through the medium polarizes the spins around it ferromagnetically lowering the system's energy. The spin-triplet pairing interaction for such a correlated electron gas is therefore attractive, while the

singlet interaction turns out to be repulsive [21]. The "exchanged" excitations in such a picture are not well-defined collective modes such as phonons or magnons, but rather "paramagnons" defined by the existence of a peak-like structure in the imaginary part of the small- \mathbf{q} susceptibility [22].

While there are many types of spin fluctuation theories, they share more commonalities than differences. Indeed, in the singlet channel exchange of spin fluctuations always leads to a repulsive interaction, and therefore can only result in superconducting states with the sign-changing gap. If this interaction is sufficiently strong at some particular momentum, it will necessarily lead to the superconductivity. The superconducting interaction in the singlet channel is determined by the Cooper vertex $\Gamma_{\uparrow\downarrow}$, which is given by the RPA series. The expression for the $+$ – $-$ component of the bare spin susceptibility takes the form [5]

$$\chi_{0,+}^{ll',mm'}(\mathbf{q}, i\Omega) = -T \sum_{\omega_n, \mathbf{p}, \mu, \nu} \varphi_{\mathbf{p}m}^\mu \varphi_{\mathbf{p}l}^{*\mu} G_{\mu\uparrow}(\mathbf{p}, i\omega_n) \times G_{\nu\downarrow}(\mathbf{p} + \mathbf{q}, i\Omega + i\omega_n) \varphi_{\mathbf{p}+\mathbf{q}l'}^\nu \varphi_{\mathbf{p}+\mathbf{q}m'}^{*\nu}$$

The Cooper vertex has the form

$$\Gamma_{\uparrow\downarrow}^{l_1 l_2 l_3 l_4}(\mathbf{k}, \mathbf{k}', \omega) = \left[\frac{3}{2} \widehat{U}_s \widehat{\chi}_s(\mathbf{k} - \mathbf{k}', \omega) \widehat{U}_s + \frac{1}{2} \widehat{U}_s - \frac{1}{2} \widehat{U}_c \widehat{\chi}_c(\mathbf{k} - \mathbf{k}', \omega) \widehat{U}_c + \frac{1}{2} \widehat{U}_c \right]_{l_1 l_2 l_3 l_4},$$

where $\widehat{\chi}_{s,c} = (\widehat{1} \mp \widehat{\chi}_0 \widehat{U}_{s,c})^{-1} \widehat{\chi}_0$ is the spin (s) and charge (c) RPA susceptibilities, $\widehat{U}_{s,c}$ are the interaction matrices in the spin and charge channels [15], and l_1 to l_4 are the orbital indices.

Hubbard interaction is local in the orbital basis that makes it easier to calculate susceptibility and Cooper vertex in this basis. However, gap equations are easier to solve in the band basis (especially near the Fermi surface), therefore, we transform the Cooper vertex into a band basis via matrix elements $\varphi_{\mathbf{k}l}^\mu$,

$$\Gamma^{\mu\nu}(\mathbf{k}, \mathbf{k}', \omega) = \sum_{l_1, l_2, l_3, l_4} \varphi_{\mathbf{k}l_2}^\mu \varphi_{-\mathbf{k}l_3}^{*\mu} \Gamma_{\uparrow\downarrow}^{l_1 l_2 l_3 l_4}(\mathbf{k}, \mathbf{k}', \omega) \varphi_{\mathbf{k}'l_1}^\nu \varphi_{-\mathbf{k}'l_4}^\nu.$$

Calculations show that $\Gamma^{\mu\nu}$ rapidly decreases with increasing ω in the range of frequencies that are much lower than the bandwidth. Although the equation for the superconducting gap depends on $\text{Im}\Gamma^{\mu\nu}$, the momenta \mathbf{k} and \mathbf{k}' making the main contribution to the pairing should correspond to the small frequencies at which these momenta appears to be close to the Fermi surface. Similarly to the case where the coupling constant for the electron-phonon interaction is determined by the frequency integral of the Eliashberg

function $\alpha^2 F(\omega)$, using the Kramers–Kronig relationship, we obtain

$$\int_0^\infty d\omega \frac{\text{Im}\Gamma^{\mu\nu}(\mathbf{k}, \mathbf{k}', \omega)}{\omega} \quad (4)$$

$$= \text{Re}\Gamma^{\mu\nu}(\mathbf{k}, \mathbf{k}', \omega = 0) \equiv \tilde{\Gamma}^{\mu\nu}(\mathbf{k}, \mathbf{k}').$$

Thus, the problem of the effective pairing interaction calculation reduces to finding the real part of $\Gamma^{\mu\nu}$ at the zero frequency, which substantially simplifies further calculations.

If we represent the order parameter $\Delta_{\mathbf{k}}$ as a product of the amplitude Δ_0 and the angular part $g_{\mathbf{k}}$, we can determine the dimensionless coupling λ as a result of the eigenvalue problem solution with the eigenvalues λ and eigenvectors $g_{\mathbf{k}}$ [5, 15]:

$$\lambda g_{\mathbf{k}} = - \sum_{\nu} \oint_{\nu} \frac{d\mathbf{k}'_{\parallel}}{2\pi} \frac{1}{2\pi v_{F\mathbf{k}'}} \tilde{\Gamma}^{\mu\nu}(\mathbf{k}, \mathbf{k}') g_{\mathbf{k}'}, \quad (5)$$

where $v_{F\mathbf{k}}$ is the Fermi velocity, the contour integral is taken over the parallel to the ν th Fermi surface component of momenta \mathbf{k}'_{\parallel} , and the band μ is unambiguously determined by which of the Fermi surfaces the momentum \mathbf{k} belongs to. Positive λ 's correspond to attraction and the maximal one of them represents the state with the highest T_c , i.e., the most favorable pairing symmetry with the corresponding gap function determined by $g_{\mathbf{k}}$. By arranging λ 's in the descending order, we can determine which symmetries and gap structures are most favorable and which will be competing with each other.

SPIN RESONANCE PEAK

Since different mechanisms of Cooper pairs formation result in different superconducting gap symmetries and structures in FeBS [4], one way to elucidate the mechanism of pairing is to determine the details of the order parameter. For example, as discussed above, spin fluctuation approach gives the s_{\pm} state as the main instability for the wide range of doping concentrations [5–7, 15, 16, 23–25], while orbital fluctuations promote the s_{++} state [8].

Inelastic neutron scattering (INS) is a useful tool here since the measured dynamical spin susceptibility $\chi(\mathbf{q}, \omega)$ in the superconducting state carries information about the gap structure. There are many reports of a well-defined spin resonance peak in neutron spectra in 1111, 122, and 11 systems appearing only for $T < T_c$ at or around $\mathbf{q} = \mathbf{Q}$ [26–35]. Such a peak is attributed to be a spin resonance that was predicted theoretically [9, 10] as originating from the s_{\pm} superconducting state.

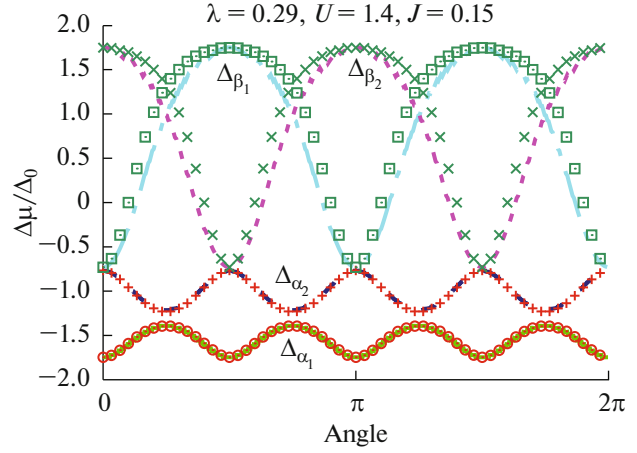


Fig. 1. Angular dependencies of gaps in hole ($\alpha_{1,2}$) and electron ($\beta_{1,2}$) Fermi surface pockets calculated within the spin fluctuation pairing theory (shown by symbols) and obtained by fitting the parameters entering Eq. (6) (shown by curves).

Here, we solve the linearized gap equation within the spin fluctuation theory of pairing and obtain the gap function $g_{\mathbf{k}}$ and the corresponding eigenvalue λ . For $U = 1.4$ eV and $J = 0.1$ eV we obtain $\lambda = 0.24, 0.19$, and 0.08 , which correspond to the A_{1g} gap, $d_{x^2-y^2}$ gap, and d_{xy} gap, respectively. Increase of J doesn't change this hierarchy. In general, the observed situation is typical of iron-based superconductors and was extensively discussed within the leading angular harmonics approximation (LAHA) [24, 25]. For $U = 1.4$ eV, $J = 0.1, 0.15$, and 0.2 eV, the leading instability is the A_{1g} gap that can be parameterized as

$$\Delta_{\mathbf{k}\mu} = \Delta_{\mu}^0 + \Delta_{\mu}^1 (\cos k_x + \cos k_y)/2 + \Delta_{\mu}^2 \cos k_x \cos k_y + \Delta_{\mu}^3 (\cos 2k_x + \cos 2k_y)/2. \quad (6)$$

The resulting gap angular dependence for $U = 1.4$ eV and $J = 0.15$ eV is shown in Fig. 1. The following fitting parameters were obtained (only nonzero values in units of Δ_0 are presented): $\Delta_{\alpha_1}^0 = -23.76$, $\Delta_{\alpha_1}^3 = 26$, $\Delta_{\alpha_2}^0 = -4.76$, $\Delta_{\alpha_2}^3 = 6$, $\Delta_{\beta}^0 = 6.99$, $\Delta_{\beta}^1 = -15.5$, $\Delta_{\beta}^3 = -10$.

To calculate the spin response, the RPA is used with the local Coulomb interaction H_{int} . The sum of the corresponding ladder diagrams that includes electron-hole bubble in the matrix form, $\hat{\chi}_{(0)++}(\mathbf{q}, \omega)$, results in the following expression for the matrix of the RPA spin susceptibility [5],

$$\hat{\chi}_{+-}(\mathbf{q}, \Omega) = [\hat{I} - \hat{U}_s \hat{\chi}_{(0)++}(\mathbf{q}, \Omega)]^{-1} \hat{\chi}_{(0)++}(\mathbf{q}, \Omega),$$

where \hat{I} and \hat{U}_s are the unit and interaction matrices, respectively, in the orbital basis. Explicit form of the

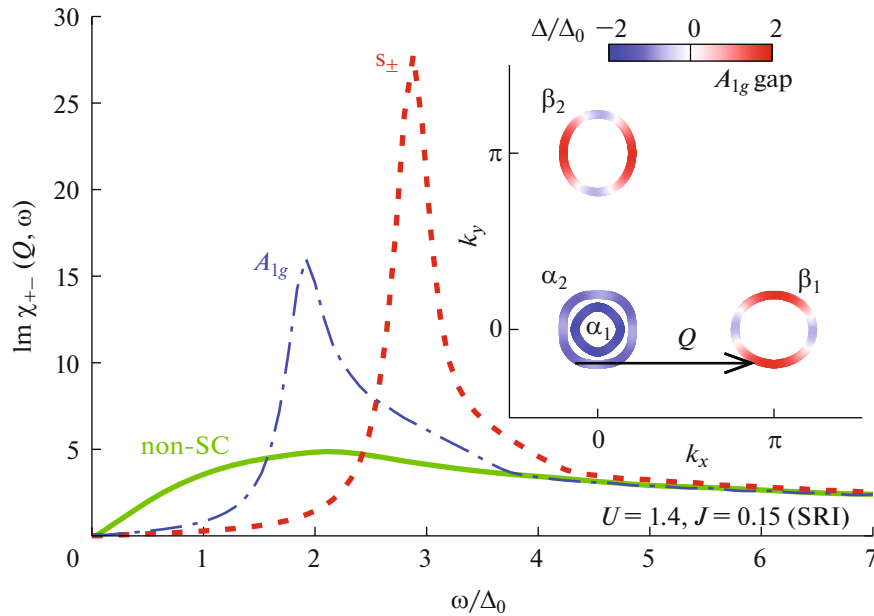


Fig. 2. Frequency dependence of imaginary part of the spin susceptibility at the wave vector \mathbf{Q} in the normal state (non-SC), for the simple s_{\pm} state, and for the A_{1g} gap. Magnitudes of the latter on the Fermi surface and the wave vector \mathbf{Q} are shown in the inset. The A_{1g} gap was normalized by $\Delta_0 = 50$ meV.

latter is given in [15]. Below we present results for the physical susceptibility $\chi_{+-}(\mathbf{q}, \Omega) = \frac{1}{2} \sum_{l,m} \chi_{+-}^{l,mm}(\mathbf{q}, \Omega)$ that was analytically continued to the real frequency axis ω ($i\Omega \rightarrow \omega + i\delta$, $\delta \rightarrow 0+$).

For the s_{\pm} state, a certain set of interaction parameters entering the matrix \hat{U}_s results in the divergence of $\text{Im}\chi_{+-}(\mathbf{Q}, \omega)$. The corresponding peak at a frequency $\omega_R \leq \omega_c$ is the true spin resonance. Frequency $\omega_c = \min(|\Delta_{\mathbf{k}}| + |\Delta_{\mathbf{k}+\mathbf{q}}|)$ depends on gaps in bands separated by the wave vector \mathbf{q} . Therefore, we can call ω_c as the “indirect” or “effective” gap. That is the reason why in the case of unequal gaps in different bands, Δ_L and Δ_S , connected by the wave vector \mathbf{Q} , we have $\omega_c = \Delta_L + \Delta_S$ [11].

Spin response for the A_{1g} gap function with the aforementioned parameters is shown in Fig. 2. $\text{Im}\chi_{+-}$ in the simple s_{\pm} state is also shown there for comparison. The spin resonance peak appears in both cases, but at lower frequencies for the A_{1g} gap because of the smaller effective gap at the same wave vector \mathbf{Q} .

CONCLUSIONS

We have briefly reviewed the spin fluctuation mechanism of pairing for iron-based superconductors. Within the five-orbital model, the dynamical spin susceptibility with the anisotropic gaps has been studied. Using the gap function calculated via the spin fluctuation theory of pairing, we have shown that the spin resonance frequency decreases with the increase

of the gap anisotropy. Such a behavior is connected with the decrease of the effective gap at the scattering wave vector \mathbf{Q} .

As for the experimental verification of the spin resonance appearance, the condition for the spin resonance frequency ω_R in the case of the anisotropic gaps $\Delta_{L,S}$ becomes $\omega_R \leq \min(\Delta_L) + \min(\Delta_S)$. If all values entering here fulfill this condition, then the observed peak is the true spin resonance. Otherwise, a calculation involving the details of the band structure and superconducting gap is required to make a definite conclusion.

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