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Comparison of experimental data on the spin resonance frequency and gap magnitudes in Fe-based superconductors

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ABSTRACT

Here we review experimental data on the peak in inelastic neutron scattering (INS) and superconducting gaps extracted from various experimental techniques. Comparison of energy scales gives the confidence that the observed peak in INS for most materials is the true spin resonance.

1. Introduction

Fe-based superconductors (FeBS) represent a non-cuprate class of high-T_c systems with the unconventional superconducting state, which origin is still debated. In general, FeBS can be divided into the two subclasses, pnictides and chalcogenides [1]. Different mechanisms of Cooper pairs formation result in different superconducting gap symmetries and structures [2]. In particular, the RPA-SF (random-phase approximation spin fluctuation) approach gives the extended *s*-wave gap that changes sign between hole and electron Fermi surface sheets ($s_\pm$ state) as the main instability for the wide range of doping concentrations [3–7]. On the other hand, orbital fluctuations promote the order parameter to have the sign-preserving s_{++} symmetry [8]. Thus, probing the gap structure can help in elucidating the underlying mechanism. In this respect, inelastic neutron scattering (INS) is a useful tool since the measured dynamical magnetic susceptibility $\chi(\mathbf{q},\omega)$ in the superconducting state carries information about the gap structure. For the $s_\pm$ state as well as for an extended non-uniform *s*-wave gap, nesting wave vector $\mathbf{q} = \mathbf{Q}$ connects Fermi sheets with the different signs of gaps. This fulfills the resonance condition for the interband susceptibility, and the spin resonance peak is formed at a frequency ω_R [9,10] in contrast to the s_{++} state where a gradual increase of spin response should take place unless additional scattering mechanisms are assumed [11,12].

2. Analysis of experimental data

In Ref. [13], we studied the magnetic response of FeBS with two different superconducting gap scales, $\Delta_L > \Delta_S$. Spin resonance appears in the $s_\pm$ state below the indirect gap scale $\widetilde{\Delta}$ that is determined by the sum of gaps on two different Fermi surface sheets connected by the scattering wave vector $\mathbf{Q}$. For the Fermi surface geometry characteristic to the most of FeBS materials, the indirect gap is either $\widetilde{\Delta} = \Delta_L + \Delta_S$ or $\widetilde{\Delta} = 2\Delta_L$. This gives the simple criterion to determine whether the experimentally observed peak in inelastic neutron scattering is the true spin resonance – if the peak frequency ω_R is less than the indirect gap $\widetilde{\Delta}$, then it is the spin resonance and, consequently, the superconducting state has the $s_\pm$ gap structure.

Sometimes it is not always clear experimentally which gaps are connected by the wave vector $\mathbf{Q}$. Even without knowing this exactly, one can draw some conclusions. For example, if one of the gaps is Δ_L, then there are three cases possible: (1) $\omega_R \leq \Delta_L + \Delta_S$ and the peak at ω_R is the spin resonance, (2) $\omega_R \leq 2\Delta_L$ and the peak is most likely the spin resonance but the definitive conclusion can be drawn only from the calculation of the dynamical spin susceptibility for the particular experimental band structure, and (3) $\omega_R > 2\Delta_L$ and the peak is definitely not a spin resonance. In the latter case, the peak could be coming from the s_{++} state [11,12], where it forms at frequencies *above* 2Δ due to the redistribution of the spectral weight upon entering the superconducting state when a special form of scattering in the normal state is assumed.

Here we combine data on the peak frequency ω_R and maximal and minimal gap sizes Δ_L and Δ_S available in the literature. Results are presented in Table 1 and illustrated in Fig. 1. Unfortunately, for many materials either the INS data or gaps estimations are absent. Latter is shown by question marks in the Table. This gives a whole set of tasks for future experiments. Here are some conclusions, which we can make based on the available data:

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Table 1
Comparison of peak energies in INS and larger and smaller gaps in various FeBS. Data on gap sizes Δ_L and Δ_S extracted from the Andreev reflections data, tunneling spectra and STS, optical spectroscopy, muon spin rotation (μSR), the BCS fit of $H_{c1}(T)$, and angle-resolved photoemission spectroscopy (ARPES) are presented. If the peak frequency and gaps satisfy condition $\omega_{INS} < \Delta_L + \Delta_S$, gaps are marked by green color, and if they satisfy condition $\omega_{INS} < 2\Delta_L$, gaps are marked by yellow color. Red color is used in the case of $\omega_{INS} > 2\Delta_L$ [14–73].

Material	T_c (K)	ω_{INS} (meV)	Δ_L, Δ_S (meV)
$BaFe_{1.9}Co_{0.1}As_2$	19	8.3 [14]	5.0, 4.0 (ARPES) [14]
$BaFe_{1.866}Co_{0.134}As_2$	25	8.0 [14]	6.5, 4.6 (ARPES) [14]
$BaFe_{1.81}Co_{0.19}As_2$	19	8.5 [14]	5.6, 4.6 (ARPES) [14]
$BaFe_{1.85}Co_{0.15}As_2$	25	9.5 [15, 16]	6.7, 4.5 (ARPES) [17]
$BaFe_{1.85}Co_{0.15}As_2$	25.5	~ 9.5?	6.6, 5 (ARPES) [18]
$BaFe_{1.8}Co_{0.2}As_2$	24.5	~ 9.5?	9, 4 (Andreev refl.) [19]
$BaFe_{1.85}Co_{0.15}As_2$	25.3	?	5.52-6.98 (Tunneling) [20]
$BaFe_{1.84}Co_{0.16}As_2$	22	8.6 [21]	7 (Tunneling) [22]
$BaFe_{1.9}Ni_{0.1}As_2$	20	9.1 [23]	?
$BaFe_{1.91}Ni_{0.09}As_2$	18	6.5-8.7 [16]	?
$Ba(Fe_{0.65}Ru_{0.35})_2As_2$	20	8 [24]	?
$Ba_{0.6}K_{0.4}Fe_2As_2$	38	14 [25, 26, 27]	12.5, 5.5 (ARPES) [28, 29]
$Ba_{0.6}K_{0.4}Fe_2As_2$	38	14 [25, 26, 27]	7-11.5, 4-7 (ARPES) [30]
$Ba_{0.6}K_{0.4}Fe_2As_2$	38	14 [25, 26, 27]	8.4, 3.2 (Tunneling) [27, 31]
$Ba_{0.6}K_{0.4}Fe_2As_2$	35	14 [26]	10-12, 7-8 (ARPES) [32]
$Ba_{0.6}K_{0.4}Fe_2As_2$	37.5	14 [26]	8.5-9.3, 1.7-2.3 (H_{c1}) [33]
$Ba_{0.67}K_{0.33}Fe_2As_2$	38	15 [34]	?
$Ba_{0.65}K_{0.35}Fe_2As_2$	34	13 [26]	7.4-8, 1.4-2 (Andreev spec.) [35]
$Ba_{1-x}K_xFe_2As_2$	32	14 [26]	9.2, 1.1 (ARPES) [36, 37]
$Ba_{0.55}K_{0.45}Fe_2As_2$	23	?	9.2, 2.7 (Andreev refl.) [38]
$Ba_{0.3}K_{0.7}Fe_2As_2$	22	?	7.9, 4.4 (ARPES) [39]
$Ba_{0.1}K_{0.9}Fe_2As_2$	9	?	2.7-3.6 (ARPES) [40]
$K_{0.8}Fe_2Se_2$	31	?	10.3 (ARPES) [41]
$Cs_{0.8}Fe_2Se_2$	30	?	10.3 (ARPES) [41]
FeSe	8	4 [42]	2.5, 3.5 (Tunneling) [43]
FeSe	8	4 [42]	0.6-1, 2.4-3.2 (Andreev refl.) [44]
$FeTe_{0.5}Se_{0.5}$	14	6-7 [45, 46, 47]	2.61, 0.51-0.87 (μSR) [48, 49]
$FeTe_{0.55}Se_{0.45}$	14	?	5.1, 2.5 (Optics) [50, 51]
$FeTe_{0.6}Se_{0.4}$	14	6.5 [53, 52]	?
$Fe_{1.03}Te_{0.7}Se_{0.3}$	13	?	4 (ARPES) [54]
$Tl_{0.63}K_{0.37}Fe_{1.78}Se_2$	29	?	8.5 (ARPES) [55]
$BaFe_2(As_{0.65}P_{0.35})_2$	30	12 [56, 57]	?
$LaFeAsO_{0.92}F_{0.08}$	29	13 [58]	?
$LaFeAsO_{0.943}F_{0.057}$	25	11-12 [59]	?
$LaFeAsO_{1-x}F_x$	22	?	5.4, 1.4 (Andreev refl.) [60]
LiFeAs	18	8 [61]	5-6, 2.8-3.5 (ARPES) [62, 63, 64]
LiFeAs	18	8 [61]	5.4, 1.4 (Andreev refl.) [65, 66]
LiFeAs	18	8 [61]	5.3, 2.5 (Tunneling) [67, 68, 69]
$NaFe_{0.978}Co_{0.022}As$	18	7.5 [70]	2.8 (Optics) [70]
$NaFe_{0.935}Co_{0.045}As$	18	7 [71]	6.8, 6.5 (ARPES) [72]
$NaFe_{0.95}Co_{0.05}As$	18	~ 7?	6.8, 6.5 (ARPES) [72]
$NdFeAsO_{0.9}F_{0.1}$	53	?	15 (ARPES) [73]

1. In electron-doped $BaFe_{1-x}Co_xAs_2$ system, $NaFe_{1-x}Co_xAs$ system, and FeSe, $\omega_R < \Delta_L + \Delta_S$ and, thus the peak in INS is the true spin resonance evidencing sign-changing gap.
2. Some hole doped $Ba_{1-x}K_xFe_2As_2$ materials satisfy $\omega_R \leq \Delta_L + \Delta_S$ condition, and some satisfy $\omega_R < 2\Delta_L$ condition. Latter comes especially from newer tunneling [27,31] and Andreev reflection [35] data revealing smaller gap values. The fact that $\omega_R < 2\Delta_L$ is still consistent with the sign-changing gap, but as we mentioned before, the calculation of the spin response for the particular experimental band structure is required to make a final conclusion.
3. The only case when $\omega_{INS} > 2\Delta_L$ is $FeTe_{0.5}Se_{0.5}$. According to our analysis, there should be no sign-changing gap structure. But before concluding this since this is the single case only, gap data coming from μSR [48,49] should be double checked by independent techniques.
4. Interesting to note, that ARPES in all cases gives gaps values larger than extracted from other techniques. Natural question arise – whether the ARPES overestimates or all other methods underestimates superconducting gaps?

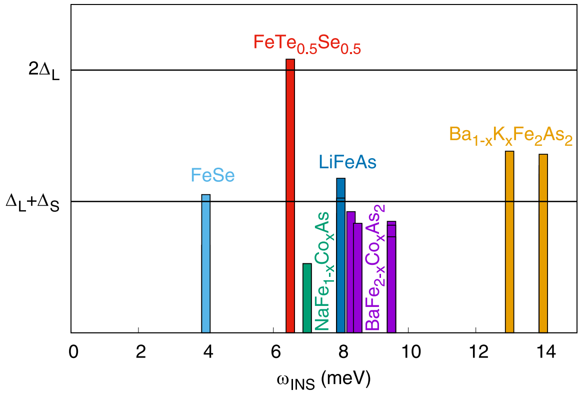

Fig. 1. Data from Table 1 grouped by materials. Each bar height is determined by $\omega_{INS}/(\Delta_L + \Delta_S)$. If it's below $\Delta_L + \Delta_S$ boundary, then case (1) is realized; case (2) occurs once it's below $2\Delta_L$ line, and situation (3) corresponds to the intersection of the $2\Delta_L$ limit.

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