Experimental report

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Proposal: **4-02-551**

Council: 10/2018

Title: Triplett character of resonance modes in Na-doped $BaFe_2As_2$

Research area: Physics

This proposal is a new proposal

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Samples: $Ba_{0.61}Na_{0.39}Fe_2As_2$

Instrument	Requested days	Allocated days	From	To
IN20	6	6	29/07/2019	04/08/2019

Abstract:

Recent neutron scattering experiments show that the spin-resonance modes appearing in the superconducting phase of Fe-based superconductors are more complex than a single singlet-triplet excitation. There is splitting in at least two modes, of which the one at lower energy is anisotropic in spin space and that at higher energy is isotropic. For an optimum electron-doped compound we could recently show that while the high-energy mode behaves in accordance to the singlet-triplet interpretation, the low energy mode exhibits an intrinsic chiral character. Here, we propose to analyse the possible chirality in a hole-doped compound, in which unpolarised neutron scattering finds an extraordinary strong low-energy mode, the strongest resonance reported for any Fe-based superconductor. Is the chiral character of this resonance mode even stronger than that detected for electron doping?

Triplett character of resonance modes in Na-doped BaFe2As2

4-02-551 IN20 from 29/07/2019 to 04/08/2019

The emergence of the so-called spin-resonance modes (SRM) in the superconducting (SC) states of various unconventional superconductors is taken as one of the main arguments in favour of magnetically mediated pairing [1]. However in Fe-based SCs inelastic neutron scattering experiments of the last ~5 years revealed a more complex character of the SRMs in almost every studied compound; for a recent summary see [2]. In particular there are at least two SRMs, with the one at lower energy exhibiting a strong anisotropy in spin space [3].
The SRM is mostly considered [1] as a particle-hole excitation breaking a Cooper pair, and thus as a singlet-triplet excitation. While the magnetic field has no effect on the singlet ground state the excited state should split. Through inelastic neutron scattering this splitting can be directly detected, but from the three split levels only the upper and the lower ones are sensed and both will obtain a chiral character that is opposite to each other.
For 6% Co-doped $BaFe_2As_2$ there is a well-documented splitting in an anisotropic lower-energy mode with some three-dimensional character (as it depends on the l-component of the scattering vector) and a broader resonance at higher energies that is isotropic in spin space [2,3]. Similar observations were reported for Co-doped NaFeAs, for K-doped $BaFe_2As_2$ as well as for Ni- and P-doped $BaFe_2As_2$, see [2], so that split spin-resonance modes must be considered as the ubiquitous response. In a recent polarized INS experiment we studied the behaviour of the SRMs in 6% Co-doped $BaFe_2As_2$ under a horizontal magnetic field, see report 4-02-497. While the upper mode exhibits a splitting of the signals in the two scattering channels in good agreement with the expectation for a singlet-triplet excitation, the lower mode behaves differently. There is no energy splitting induced by the magnetic field, but a strong intensity difference between two spin-flip channels. Since the neutron polarization direction was set parallel to the scattering vector, this intensity difference unambiguously documents an intrinsic chiral character of the lower spin-resonance mode that either is induced by the magnetic field or that is just poled through the field similar to a multiferroic material [4].
In Na-doped $BaFe_2As_2$ there is a second magnetic transition, which is characterized by reorientation of the magnetic moments from in-plane to out-of-plane [5]. This spin-reoriented phase with restoration of tetragonal symmetry appears close to the full suppression of AFM ordering [5,6]. We recently studied the SRMs in three crystals of Na-doped $BaFe_2As_2$ with Na concentrations of 35, 39 and 40% [6]. For 35% and 39% Na there still is long-range AFM order with moments pointing essentially along c at low temperature, while for 40% the long-range AFM ordering is fully suppressed [5]. In spite of the little differences in doping and in the T_c the magnetic response essentially differs. The most remarkable feature is the very strong low-energy resonance mode in Na-39. At this concentration the material still exhibits AFM ordering, which, however, is extremely soft and strongly suppressed in the SC state, this soft magnetism seems to induce the strong low-energy resonance, which in absolute units is the strongest SRM reported for any Fe-based superconductor so far [6]. It was the aim of this polarized experiment to analyse the effect of a magnetic field on the SRMs in the 39% Na-doped $BaFe_2As_2$ in particular to search for similarities with the behaviour discovered for Co doping.

We used the same crystal as in reference [6] with 172mg mass mounted in the [110]/[001] scattering plane. The superconducting transition appears at T_C=29K in zero field. We applied a horizontal magnetic field of up to 3.6T, which still allows for neutron polarization analysis. We applied the field parallel to the scattering vector (0.5,0.5,l) with l=0,1 and we recorded the two neutron spin-flip processes, which sense the different chiral signals. The difference of the two scattering intensities directly evidences a chiral component. It was necessary to recalibrate the spin-flipper for each configuration depending on the angle between the detector arm and the horizontal field. We only used a neutron half-polarization mode in order to improve the intensity profiting from a Si monochromator. However, the recalibration had to be performed with full polarization analysis and the Heusler monochromator. In addition, it was necessary to very carefully drive the magnetic field, since the superconducting material does not allow one to vary the field in the superconducting state. We applied the magnetic field in the normal state and then cooled into the superconducting state without any further variation of the field strength or direction.

Fig. 1 shows the temperature dependence of the elastic magnetic scattering for small (0.4 T needed to maintain the neutron polarization) and large fields, 3.6 T. Magnetic intensity starts to grow at the Néel temperature at 61 K (hardly visible) and the spin rerorientation at 44.5 K results in a sharp intensity increase, because of the large angle between (0.5 0.5 1) an the out-of-plane direction. The magnetic field does not have a significant impact on these two transitions. However visible differences appear at the superconducting transition. At the larger field the magnetic signal reaches higher values in the normal state before dropping in the superconducting state but at slightly lower temperatures. Furthermore, at 3.6T the magnetic signal gets less suppressed. This is in good agreement with the idea of a general competition between superconductivity and AFM order and the fact that magnetic fields reduce the stability of the superconducting state. Fig. 2 compares the total (sum of the two flipper channels) magnetic scattering observed at the two fields. The sharp low-energy SRM is clearly stronger at the small field. This nicely agrees with the conclusion formulated in [6] that the sharp low-energy SRM compensates for the suppression of the AFM ordered moment.

The key result concerning the chirality of SRMs in Na-doped $BaFe_2As_2$ is shown in Fig. 3 comparing the two polarisation channels at large magnetic field in the superconducting state. The achieved statistics is much below that reached for electron-doped $BaFe_2As_2$ but we may qualitatively confirm the behaviour. The sharp low-energy SRM does not exhibit clear splitting but an enhancement of one chirality while no such effect can be found for the higher energy SRM.

[1] Hirshfeld et al. Rep. Prog. Phys. **74**, 124508 (2011); D. J. Scalapino, Rev. Mod. Phys. **84**, 1383 (2012). **[2]** F. Wasser et al., Sci. Rep. **7**, 10307 (2017) **[3]** P. Steffens et al., PRL **110**, 137001 (2013) **[4]** J. Stein et al., Phys. Rev. Lett. **119**, 177201 (2017). **[5]** F. Waßer et al., PRB *B* **91**, 060505 (2015). ; ibid. physica status solidi (b) 254, 1600181 (2017); Avci et al. nature comm. 5, 3845 (2014). **[6]** F. Waßer et al., PhD dissertation Cologne Univ. (2018); and npj Quantum Mater. **4**, 59 (2019).

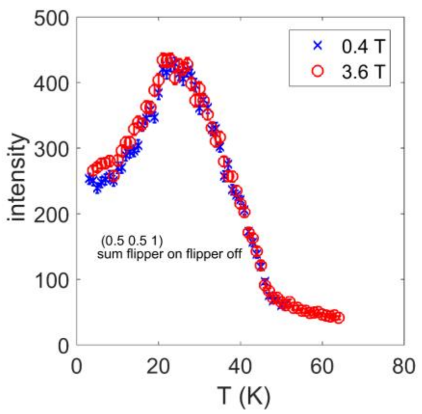

Fig. 1 Dependence of the elastic scattering at small and large fields.

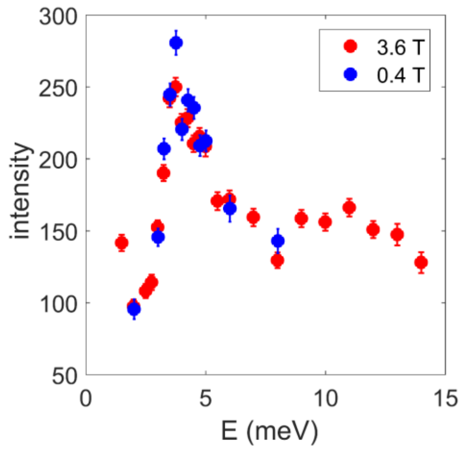

Fig. 3: Comparison of the magnetic scattering (sum of both flipper positions) at small and large fields.

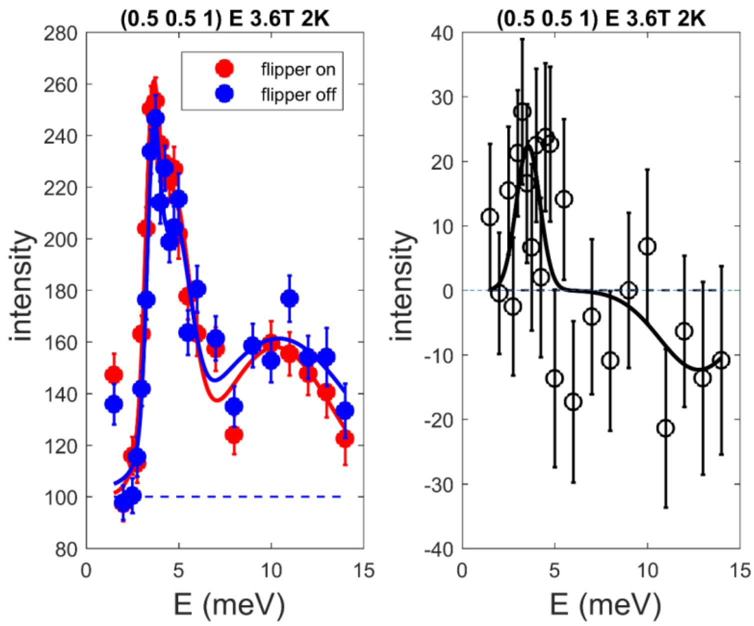

Fig. 3: Energy scans at the (0.5 0.5 1) scattering vector corresponding to the AFM zone center at 3.6T magnetic field. In the left panel one sees the superposition of the two SRMs and a clear difference between the two polarization channels. The right panel presents the difference of the two channels indicating a chiral character of the