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Title:	Agnetic excitations in Co-doped LiFeAs				
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Main proposer:	Florian WASSER				
Experimental te	am: Navid QURESHI Florian WASSER Jeoffrey THOMAS Michael RODRIGU Tiamiyu ABDOUL	JEZ FANO ROKIB ADEBAYO			
Local contacts:	Paul STEFFENS				
Samples: LiFe1	-xCoxAs				
Instrument		Requested days	Allocated days	From	То

LiFeAs is a rather peculiar member of the iron-based superconductors, because it is superconducting with any doping. Furthermore, it displays transversally incommensurate magnetic excitations, which are a fingerprint of electron doping. However, when we added more electrons to this compound by 18% Co-doping we expected the incommensurability to increase, but we observed the opposite, a commensurate response. So far the commensurate magnetic scattering observed in Co-doped LiFeAs remains unexplained.

Magnetic Excitations in Co-doped LiFeAs Experimental Report: 4-02-477

LiFeAs is an outstanding member of the iron-based superconductor (FeSC) family as it is superconducting (SC) without any increase of an external control parameter, like pressure, doping or substitution. However, in view of its Fermi surface (FS) [1] and transversal incommensurate magnetic excitations [2] it behaves like an electron doped member of the 122 family. Upon Co-doping, thus with increasing electron doping, SC is suppressed and magnetic excitations become commensurate again, as shown by our experiment on 18 % Co-doped LiFeAs, c.f. the corresponding experimental report 4-02-458 and a recent publication by Li et al. for 12 % Co-doping [3]. These two doping levels are at or beyond the critical end point of SC in the corresponding phase diagram posing the question whether the recurrence of commensurate magnetic excitations happens just there or it is a gradual process liked to the FS evolution upon doping.

In order to address this issue we prepared ~300 mg of intermediate, i.e. 5 %, Co-doped LiFeAs ($T_C \sim 9.5$ K) by co-aligning two single crystals within the [100]/[010] scattering geometry. Due to the severe air-sensitivity the samples were sealed in an Al-can with Ar-atmosphere. Moreover, we attached a Cd-shield around the can to suppress background signal. Note that the magnetic signal in LiFeAs is very weak and becomes even weaker at 18 % Co-doping.

We performed transversal scans through (0.5,0.5,0) at 5, 7.5, 10 and 12.5 meV at temperatures of 1.5, 12 and 70 K to investigate the magnetic excitations, c.f. Fig. 1(a)-(d), respectively. In total five peaks can be observed, one commensurate and two incommensurate. The incommensurate peaks cannot be associated to quasi-particle scattering between electron and hole Fermi surface sheets, as ARPES studies display no overlap at the corresponding wave vectors [4,5]. Furthermore, rocking scans were conducted, which (i) confirmed that the incommensurate peak closer to the commensurate one is pure background signal and (ii) estimated the intensity of the commensurate signal, c.f. Fig. 2 (a). As a result, we can describe the transversal scans by five Gaussians, one for the commensurate signal in between of four purely background peaks. From those fits we explored the width as a function of energy and temperature, c.f. Fig. 2 (b), which seems to be constant in both parameters. Additionally, we normalised the fit amplitudes at 1.5 K through acoustic phonon scattering and compared the energy dependence to that of the undoped host compound, reported in Ref. [6]. Despite the increased nesting conditions, indicated by the commensurate peak and by ARPES reports [4,5], the overall scattering intensity is further reduced by the Co content. This is in line with other FeSCs where overdoping inhibits magnetic excitations although this is interpreted as a result of decreasing nesting conditions. Apparently, nesting conditions alone are not the crucial parameter for the determination of magnetic excitation strength in FeSCs. More likely, the inter-band inter- and intra-orbital scattering rates between the electron and hole FS sheets associated with an orbital dependent pairing mechanism play the dominant role.

Furthermore, we checked the character of magnetic excitations, e.g. at 1.5 K and 5 meV after background subtraction for being (in)commensurate, by fitting the convolution of the experimental resolution with the corresponding model to the data, c.f. Fig. 2 (d). In both cases the overall fits almost coincide, so that there is no evidence for an incommensurate character of the magnetic correlations. Concluding, the incommensurability of magnetic excitations is not linked to the superconducting phase, but to the different sizes of electron and hole pockets on the FS. Increasing the nesting conditions does neither increase T_C nor the strength of magnetic excitations.

Finally we would like to note that the sample environment worked perfectly well throughout the entire experiment. Concerning the IN8 spectrometer there were some positioning errors at the beginning of the experiment, but after a short repair it performed well.

[1] Borisenko et al., PRL, 105, 067002 (2010) [2] Qureshi et al., PRL, 108, 117001 (2012) [3] Li et al., PRL116, 247001 (2016) [4] Dai et al., PRX, 5, 031035 (2015) [5] Miao et al., nat. commun., 6, 6056 (2015) [6] Qureshi et al., PRB, 90, 144503 (2014).



Figure 1: Q-scans at 5, 7.5, 10 and 12.5 meV, respectively shown in (a)-(d) at 1.5 K, 12 K and 70 K. The data were fitted by multiple gaussians, whereas the additional peaks away from (0.5,0.5) are background signal. For each energy transfer one fit is decomposed into it's various gaussian contributions.



Figure 2: (a) Rocking scans over (0.5,0.5) with 10 and 12.5meV energy transfer to pin the magnetic signal, and over (0.2,0.8) at 5meV to assure that this background signal. (b) Intensities resulting from the fits in Fig. 1 at 1.5K, corrected for the monitor, Bose and mag. form factor, normalized on the integrated phonon scattering intensity in order to compare to the pure compound from Ref. [7]. (c) Peak widths resulting from the fits in Fig. 1. (d). Fit of the convolution of the instrumental resolution and a commensurate, as well as an incommensurate magnetic signal. In both cases the overall fits almost coincide, so that there is no evidence for an incommensurate character of the magnetic correlations.