Proposal:	4-01-1206	(Council:	4/2012		
Title:	Paramagnon in a KxFe2-ySe2 superconductor					
This proposal is a new proposal						
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Samples:	KFeSe					
Instrument		Req. Days	All. Days	s From	То	
IN8		8	7	26/10/2012	02/11/2012	
Abstract:						

A recent time-of-flight experiment on a superconducting KxFe2-ySe2 sample revealed not only spin resonance mode at 14 meV around the (0.5,0.25,0) wave vector, but also a ring-like low energy (LE) mode at 9 meV which connects the equivalent resonance positions in the HK0 scattering plane. This feature does not show a temperature dependence upon entering the superconducting state. We suspect that this new excitation is a paramagnon resulting from the nesting of the electron pockets at M point. In order to confirm its magnetic character we propose to study its temperature dependence in the normal state and its dispersion with the out-of-plane wave vector.

Introduction.

The recently discovered family of alkali iron selenide superconductors $A_x \operatorname{Fe}_{2-y} \operatorname{Se}_2$ show a comparatively high superconducting (SC) transition temperature of $T_c = 31 \text{ K}$ on the one hand [1], and a strong antiferromagnetic order ($T_N > 500 \text{ K}$) on the other hand [2]. It was shown by multiple experimental probes that both ground states originate from chemically different, spatially separated phases. The former presumably has $A_{0.3}\operatorname{Fe}_2\operatorname{Se}_2$ stoichiometry [4], whereas the latter was found to have $A_2\operatorname{Fe}_4\operatorname{Se}_5$ stoichiometry, exhibiting an $\sqrt{5} \times \sqrt{5}$ iron vacancy superstructure [2]. This magnetic phase is insulating, whereas the SC/metallic phase shows a distinctly different Fermi surface compared to its 122 iron arsenide analogues, consisting mainly of large electron pockets at the *M* point [$Q = (\frac{1}{2}, 0)$] [5].

The unconventional nature of superconductivity was recently revealed when observing spin fluctuations peaked at $\mathbf{Q}_{\text{res}} = (\frac{1}{2}\frac{1}{4})$ in the normal state, which get redistributed into a resonant mode excitation at $\hbar\omega_{\text{res}} = 14 \text{ meV}$ in the SC state [6]. Below $\hbar\omega_{\text{res}}$ a spin gap with zero intensity should exist. However, in a recent time-of-flight spectroscopy study on a $K_{0.77}$ Fe_{1.85}Se₂ sample an additional low energy mode around $\hbar\omega_2 = 9 \text{ meV}$ was observed in both normal state and superconducting state [7]. In reciprocal space the intensity forms a ring centered at $M(\frac{1}{2}\frac{1}{2})$ and passing through the wave vectors of the resonant mode at $\mathbf{Q}_{\text{res}} = (\frac{1}{2}\frac{1}{4})$. Goal of the proposed experiment was to investigate whether this feature is magnetic by measuring the temperature dependence and *L*-dependence of its intensity. Before the date of the experiment the same investigation was already conducted at the Puma spectrometer (FRM2, Garching) on a $K_{0.77}$ Fe_{1.85}Se₂ sample by our group (see Ref. 7). It revealed the LE mode to be a phonon, since the intensity increases upon warming to T = 100 K. Therefore, we decided to concentrate on measuring the spectrum at the resonance position at $\mathbf{Q}_{\text{res}} = (\frac{1}{2}\frac{1}{4})$ in the superconducting and in the normal state, which is part of a study, that has been initiated in a previous experiment at In8 [8]. Being previously restricted to energies below 16 meV due to kinematical constraints, we decided to measure in the (H H/2 L) scattering plane. Since the resonance signal has no *L*-dependence, we can freely alter the *L*-component and reach energy transfers up to E = 36 meV. The sample was Rb_{0.8}Fe_{1.6}Se₂, as previously used. The final wave vector was chosen to $k_{\rm f} = 4.1$ Å⁻¹. The sample environment comprised a standard orange cryostat.

Results of Experiment

It was planned to measure the spin fluctuations at $Q_{res} = (\frac{1}{2}\frac{1}{4})$ by performing momentum scans in the normal (at T = 35 K) and in the SC state (at T = 1.5 K). The trajectory were slightly off the scattering plane, progressing with a step of $d\mathbf{Q} = (0.018 \ 0.003 \ \Delta L)$. By this we wanted to avoid contaminations from spin waves associated with the block-AFM $\sqrt{5} \times \sqrt{5}$ ordering of Rb₂Fe₄Se₅, that are emerging from the superstructure peaks at the nearby wave vectors (0.3, 0.1) and (0.7, 0.1). Nonetheless, in the discussion here the trajectory will be treated as if it goes along ($\Delta H \ \Delta H/2 \ \Delta L$). The stepsize along the *c* direction ΔL can be chosen freely. This freedom was important in order to avoid possible contaminations on both sides of the center at $(\frac{1}{2}\frac{1}{4}L)$.



Fig. 1: (a) Momentum scan with a step size of $d\mathbf{Q} = (0.018\ 0.003\ -0.03)$ through $\mathbf{Q}_{res} = (\frac{1}{2}\ \frac{1}{4}\ L = 1.5)$ at E = 14 meV in both SC and normal state. (b) Momentum scan along $d\mathbf{Q} = (\frac{1}{2}\ K\ 2.2)$ at E = 28 meV in both SC and normal state. (c) Momentum scan along L in $(H_0\ H_0/2\ L)$ for $H_0 = 0.27$ (left) and $H_0 = 0.5$ (middle). All solid lines are fits with one or more Gaussian functions.

A typical momentum scan is shown in Fig. 1 (a) for E = 14 meV. The peak in the middle at H = 0.5 are the spin fluctuations which get enhanced when cooling below T_c . However, on the right side is a spurion that creates a slopy background, which makes it difficult to determine the amplitude of the magnetic peak by fitting it with a Gaussian. The momentum scans for other energies were even more contaminated which made it impossible to observe clearly the spin excitations. This became clear when mapping the inelastic intensity over the (H H/2 L) scattering plane as shown in Figure 1 (c) for E = 24 meV. Low statistics momentum scans along L were done for certain $H = H_0$. Especially the center of the spin fluctuations at $H_0 = 0.5$ shows strong contaminations for almost all L values. By doing similar scans for other energies we could find some positions that were "clean". Figure 1 (b) shows a momentum scan along $(\frac{1}{2} K 2.2)$ at E = 28 meV that was feasible by means of the 3D mode at the instrument. It shows a broad peak centered at $K = \frac{1}{4}$ that could also be fitted with two incommensurate Gaussian profiles. Incommensurate excitations at the resonance were also observed in pnictides

 $(Ba(Fe_{1-x}Ni_x)_2As_2$ [9]) and in 11 selenides (FeTe_{1-x}Se_x [10]). Therefore, a closer inspection of this incommensurability would be desirable to see if it is a general property of the pnictides.

At higher energies the magnetic intensity was measured along the ($\Delta H \Delta H/2 \Delta L$) trajectory. Figure 2 (a) shows scans in the SC and in the normal state plus a scan at a very high temperature (T = 150 K), where spin fluctuations are expected to vanish. Unfortunately, there is a concavely shaped background, which renders it impossible to determine the magnetic intensity. However, the flat intensity difference between SC and normal state in Fig. 2 (b) shows that there is no resonant enhancement anymore. The presence of spin fluctuations is established from the intensity difference with the T = 150 K data, that shows a peak in the center. Unfortunately, the concave background in the raw momentum scans persisted for energies up to E = 36 meV. A reason could be the overlap with the spin waves from (0.3, 0.1) that are now reaching into region of the trajectory.



Fig. 2: (a) Momentum scan with a step size of $d\mathbf{Q} = (0.018\ 0.003\ -0.048)$ through $\mathbf{Q}_{\text{res}} = (\frac{1}{2}\ \frac{1}{4}\ 1.72)$ at $E = 30\ \text{meV}$ in the SC $(T = 1.5\ \text{K})$ and in the normal state $(T = 35\ \text{K}$ and $T = 150\ \text{K})$. (b) Intensity difference of the momentum scans in panel (a). (c) Amplitude of the Gaussian fits to the momentum scans, centered at $\mathbf{Q}_{\text{res}} = (0.5\ 0.25\ L)\ vs.$ energy. The solid lines are taken from the previous study covering the energy range below 16 meV.

Summary

Panel (c) of Figure 2 shows the amplitude of the Gaussian fits to the momentum scans through $Q_{res} = (\frac{1}{2}, \frac{1}{4}L) vs$. energy for both normal state and superconducting state, that are corrected for the Fe²⁺ magnetic form factor. The solid lines are taken from the previous study covering the energy range below 16 meV [8]. The data points collected in this study agree with these lines within statistical uncertainty. Both data sets will be combined which will be a first comprehensive assessment of the absolute intensities in both SC and normal state vs. energy for Rb_{0.8}Fe_{1.6}Se₂.

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