Experimental report

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Proposal: **4-03-1764** **Council:** 4/2023

Title: Low-energy excitations near a field-induced multi-quantum critical point in Nb1-yFe2+y

Research area: Physics

This proposal is a new proposal

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Samples: NBFe2

Instrument	Requested days	Allocated days	From	To
ORIENTEXPRESS	1	1	30/06/2023	01/07/2023
THALES	7	7	28/06/2023	05/07/2023

Abstract:

Our previous neutron scattering of ferromagnetic (FM) Nb1-yFe2+y revealed that chemical composition (y) tuning leads to a FM quantum-critical point masked by an emerging spin-density wave (SDW). This scenario could be connected to many exciting phenomena, including field-induced quantum-critical lines, quantum tri-critical points, and quantum multicritical points. The latter could be reached in Nb1-yFe2+y by transverse-field tuning of a nearly stoichiometric sample. Here, we propose to follow this strategy and measure the transverse-field evolution of low-energy excitations across the suspected quantum multi-critical point. The results would form an important test for, e.g., order-by-disorder models that predict the emergence of modulated order at the border of ferromagnetism. We apply for 7 days of beamtime at ThALES.

Low-energy excitations near a field-induced multi-quantum critical point in $Nb_{1-y}Fe_{2+y}$

1. Scientific background

The transition metal Laves phase compound $NbFe_2$ presents a rare opportunity to study the border of itinerant ferromagnetism (FM) at low temperature at ambient pressure (Fig. 1a). Slight iron excess of the order of 1% induces FM, whereas the stoichiometric compound exhibits spin density wave order (SDW), and slightly Nb-rich $NbFe_2$ remains a paramagnet (PM) down to low temperatures and displays signatures of Fermi-liquid breakdown [1]. Empirical observation in other materials as well as theoretical arguments [2, 3] suggest that the masking of itinerant FM quantum critical points (QCPs) by SDW order may be intrinsic in many clean systems. $NbFe_2$ is most suitable to investigate the underlying mechanism by detailed studies of the magnetic excitation spectrum.

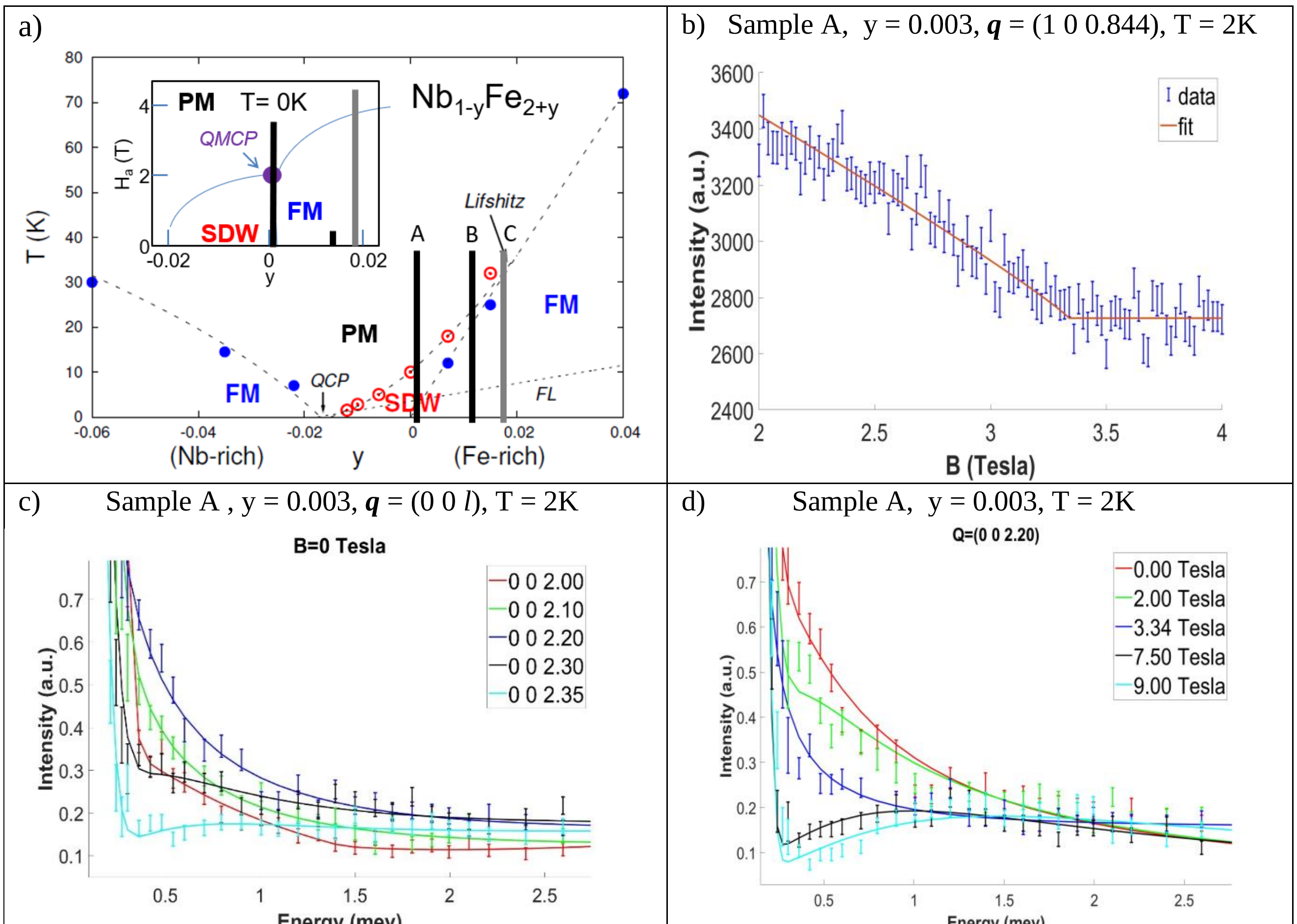

Fig. 1: (a) Phase diagram of $Nb_{2-y}Fe_{2+y}$ indicating the location of Samples A, B (both black lines) and C (grey lines), for which SDW order has been observed. Sample A (nearly stoichiometric) has been measured at ThALES. *(Inset)* T=0K cut of the schematic *y*-*H*||*a*-*T* phase diagram with suspected quantum-critical lines and quantum multi-critical point (QMCP). (*b*) Suppression of an SDW satellite at H_c =3.34 T. (*c*) *l* dependence across $\boldsymbol{q}_{FM}$ and $\boldsymbol{q}_{SDW}$ of the low-*E* spectra in Sample A at low *T* at 0 T. (d) *H*||*a* evolution near $\boldsymbol{q}_{SDW}$ of the low-*E* spectrum in Sample A at low *T*.

Previous neutron scattering measurements we have resolved the SDW ordering wavevector $\boldsymbol{q}_{\mathrm{SDW}}$ [4]. In our inelastic neutron measurements at zero field the excitation spectrum of the FM state softens away from the FM ordering wavevector $\boldsymbol{q}_{\mathrm{FM}}$ and near the magnetic phase transitions the excitation spectrum becomes critical along a line in $\boldsymbol{q}$ space that includes $\boldsymbol{q}_{\mathrm{FM}}$ and $\boldsymbol{q}_{\mathrm{SDW}}$. Both unconventional features reflect the system's proximity to the emerging SDW state that masks the FM QCP.

In Fe-rich $NbFe_2$ a transverse magnetic field ($H||a$) suppresses SDW order at finite T and then the unmasked FM quantum phase transition. The linewidth's $\boldsymbol{q}$ dependence (not shown) at the critical field for the suppression of c-axis FM has a more conventional minimum at $\boldsymbol{q}_{\mathrm{FM}}$ suggesting the possible presence of a field induced FM QCP. The latter could be understood as belonging to a FM quantum critical line in the y-$H||a$ plane at T=0K that ends in a quantum multi-critical point (QMCP) near y=0 (Fig. 1a).

2. Aims of the experiment

The aim was to measure the $H||a$ dependence of the magnetic excitations in a $\boldsymbol{q}$ range including $\boldsymbol{q}_{\mathrm{FM}}$ and $\boldsymbol{q}_{\mathrm{SDW}}$ in $Nb_{1-y}Fe_{2+y}$ across the critical field near the suspected QMCP.

3. Experimental set up

At ThALES we investigated the almost stoichiometric sample $Nb_{1-y}Fe_{2+y}$ with y=0.003 (Sample A) with $\boldsymbol{q}_{\mathrm{FM}}$=(0 0 2) and $\boldsymbol{q}_{\mathrm{SDW}}$ =(0 0 2.156) that was clamped into an Al holder and aligned such that a^*-c^* of the reciprocal lattice of the hexagonal C14 Laves phase crystal structure formed the horizontal scattering plane. The sample holder was placed inside a 10T cryomagnet. The vertical field was pointing along the a axis, i.e. providing a transverse field with respect to the c axis, which is the magnetic easy axis. All measurements were done at 2K and using neutrons with k_F=1.5Å^{-1}.

4. Experimental results

After cooldown and sample alignment the transverse field dependence of the SDW Bragg peak strength at (1 0 0.0844) was measured to determine the critical field for the transition from the SDW phase to the field polarized state. (Fig. 1b) The critical field was found to be at H_c = 3.34 T. The bulk of the beamtime was used for low-E scans in the $\boldsymbol{q}$ region from (0 0 2.0) to (0 0 2.4). Data at 0 T was taken to create an overlap with and cross check of previous measurements and shows quasielastic scattering with a strong $\boldsymbol{q}$ dependence (Fig. 1c). Of particular interest was then the transverse-field dependence of the signal at (0 0 2.2) near the SDW ordering wave vector. We collected E scans at 0.00, 2.00, 2.80, 3.34, 5.00, 6.00, 7.50, and 9.00 T. A plot with a selection of those scans (fig 1d) shows quasielastic scattering with a linewidth that decreases from 0 T to the critical field and which then gives way to weak broad inelastic scattering. The $\boldsymbol{q}$ dependence of the low-E spectra was also determined at the critical field. Here the quasielastic scattering is characterized by a narrow linewidth from (0 0 2.0) to (0 0 2.2) before it collapses at (0 0 2.3) and beyond (Fig. 2a). The $\boldsymbol{q}$ dependence of the low-E spectra was finally determined at 9 T (Fig. 2b). The inelastic scattering is seen in a substantial $\boldsymbol{q}$ range with changing width, which is smallest at (0 0 2.0). The excitation energy of approx. 1.1 meV could be explained by a more conventional spin-flip excitation in the field polarized state and the observed field dependence of this excitation (not shown) represents a further indication of this scenario.

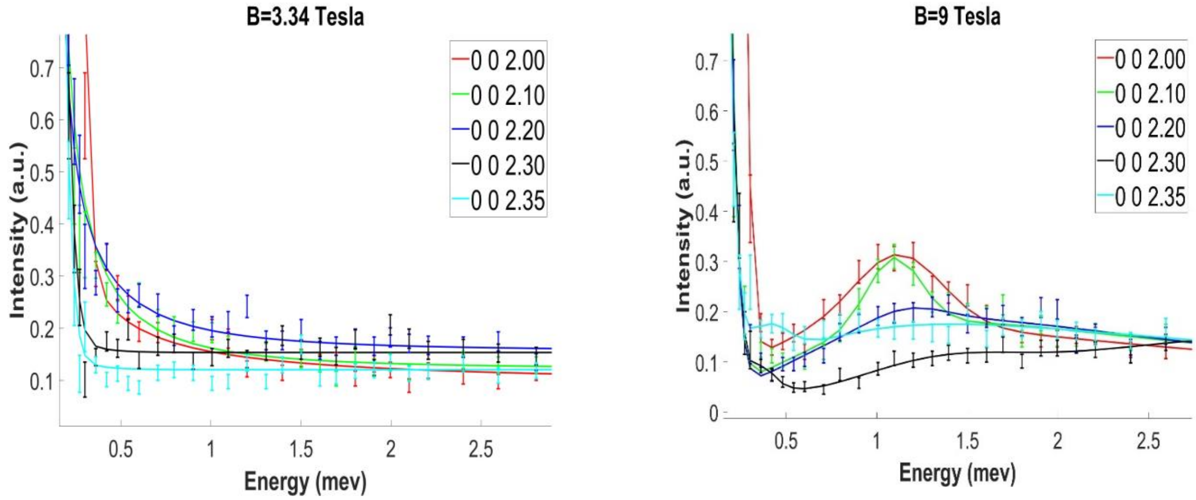

Fig 2: I dependence across $\boldsymbol{q}_{\mathrm{FM}}$ and $\boldsymbol{q}_{\mathrm{SDW}}$ of the low-E spectra in Sample A at low T (a) at H_c and (b) at 9 T.

5. Conclusions and outlook

Using ThALES we fully achieved the aims of this experiment by collecting a comprehensive set of low-energy spectra of nearly-stoichiometric $NbFe_2$ in a transverse magnetic field at 2K. While a quantitative analysis of the results is ongoing the qualitative features of the observed data include quasielastic scattering that appears to become soft in a wide $\boldsymbol{q}$ range at the critical field for the suppression of the SDW phase in the vicinity of the FM phase and that gives way to inelastic excitations in the field-polarised state. It is envisaged to complete this data set in the future with equivalent E scans that follow the phase transition line in the field-temperature phase diagram and that also map the temperature dependence at the critical field.

References

[1] M. Brando et al., Phys. Rev. Lett. 101, 026401 (2008), D. Rauch et al., Phys. Rev. B 91, (2015). [2] G. Abdul-Jabbar et al, Nat Phys 11, 321 (2015). [3] e.g. M. Brando, D. Belitz, F. M. Grosche, T. R. Kirkpatrick, Rev. Mod. Phys 88, 025006 (2016), T. Vojta et al., Ann. Phys. (Leipzig) 8, 593 (1999). [4] P. G. Niklowitz et al., Phys. Rev. Lett. **123**, 247203 (2019).