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Quantum criticality in the frustrated Laves phase compound $NbFe_2$

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Abstract

Geometric frustration in nearly magnetic metals provides a promising and relatively little explored path to obtaining high electronic densities of states—the hatching condition of novel quantum order. Various geometrically frustrated compounds close to the border of magnetism can be found amongst the intermetallic C14 and C15 Laves phases and we have selected $NbFe_2$ as one of the more interesting examples. We report on measurements of the DC magnetisation, AC magnetic susceptibility, specific heat capacity and electrical resistivity in off-stoichiometric $Nb_{1-y}Fe_{2+y}$ ($y \simeq -0.04$). Our sample is classified as a strongly enhanced Pauli paramagnet with anomalous resistivity power-law behaviour: the low-temperature electrical resistivity follows the form $\rho = \rho_0 + AT^{\alpha}$ with $1 < \alpha < 1.5$ over a wide range and returns to the quadratic temperature dependence expected from Fermi Liquid theory in its simplest form only below 500 mK. The absolute magnitude of the measured low-temperature heat capacity is inconsistent with a model based solely on proximity to ferromagnetism and suggests a significant contribution from antiferromagnetic fluctuations.

Keywords: Non-Fermi liquid behaviour; Quantum criticality

The threshold of magnetism represents a crucial base point for seeking novel electronic states. Geometric frustration provides a promising and largely unexplored path for obtaining a high electronic density of states. The abundance of nearly degenerate spin configurations in a frustrated structure translates into enhanced magnetic fluctuations over large regions in reciprocal space. A considerable number of intermetallic compounds close to the border of magnetism can be found among the C14 and C15 Laves phases. We selected the C14 compound $NbFe_2$, a delicate system susceptible to both ferro- and antiferromagnetic order, falling into one or another depending on small variations of quantum control parameters, such as pressure, magnetic field or composition [1–4].

Our primary control parameters in this initial study are temperature, T, and magnetic field, B. The sample was produced by RF heating the

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elements on a water-cooled copper hearth. No phase other than C14 $Nb_{1-y}Fe_{2+y}$ was detected by X-ray diffraction, but the lattice parameters ($a = 4.844$ Å, $b = 4.844$ Å, $c = 7.903$ Å) indicate that the sample is far off stoichiometry ($y = -0.04$) [4], in a region of the phase diagram which has so far not been subjected to detailed study.

Resistivity, heat capacity and magnetic susceptibility measurements have been carried out in the range $1.8\,\mathrm{K} < T < 300\,\mathrm{K}$ on a physical properties measurement system (PPMS), and an adiabatic demagnetization refrigerator (CMR) has been used for resistivity measurements down to the 50 mK range.

An Arrott plot analysis of the DC magnetisation (Fig. 1a) shows nearly parallel straight lines at all temperatures and over a wide range of magnetic field, extrapolating to small but positive inverse susceptibilities H/M for $M^2 \to 0$. This behaviour differs from observations on the stoichiometric compound, which has been classified as antiferromagnetic below about 20 K [1–4], indicating the absence of both ferro- and anti-ferromagnetic order at least down to 2 K. At very low fields and low temperatures, the Arrott plot data turn sharply towards the left, towards very small inverse susceptibilities.

This upturn in the magnetic susceptibility at low T and small B is reflected in measurements of the AC susceptibility (Fig. 1b). It might signal a propensity to some very weak form of ferromagnetic order, but we suspect rather it is due to small inclusions or clusters of ferromagnetic impurities, such as iron.

The dominant phase, $Nb_{1.04}Fe_{1.96}$ is expected to determine electronic transport and heat capacity (Fig. 2). Over a wide range in temperature and magnetic field, the resistivity data deviate strongly from the quadratic exponent normally associated with a Fermi liquid. A thorough analysis of the critical exponent indicates a quadratic behaviour only at temperatures lower than 500 mK in zero field (main part of Fig. 2).

The resistivity power-law exponent is roughly consistent with scattering expected from ferromagnetic fluctuations, as calculated within a spin fluctuation approach (e.g. [5]), with the inverse susceptibility obtained from the Arrott plot and

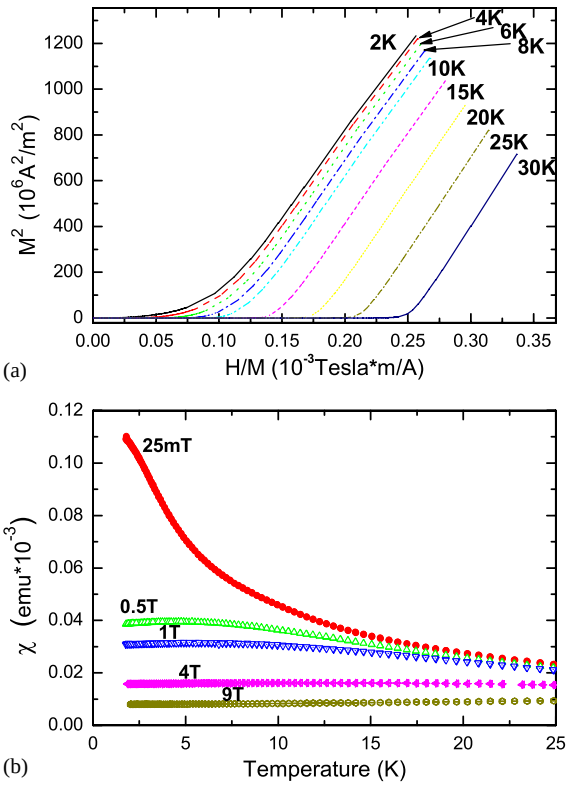

Fig. 1. Magnetic properties of $Nb_{1.04}Fe_{1.96}$. (a) Arrot plot analysis of the DC magnetisation, indicating the absence of magnetic order down to 2 K. (b) AC magnetic susceptibility, exhibiting a strong upturn at low fields and low temperatures, possibly attributable to ferromagnetic inclusions.

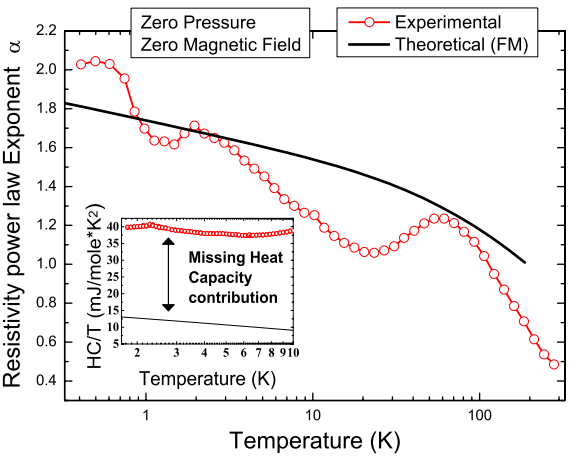

Fig. 2. Electric resistivity (main figure, circles) and heat capacity (inset, circles) of $Nb_{1.04}Fe_{1.96}$, compared to a ferromagnetic spin fluctuation calculation (solid lines).

other parameters taken from the comparable d-metal compound $ZrZn_2$. However, comparing experimental heat capacity with theoretical calculations for only ferromagnetic fluctuations, a large contribution to $C(T)$ is missing (inset of Fig. 2).

Off-stoichiometric $Nb_{1.04}Fe_{1.96}$ shows anomalously low-power-law exponents in $\rho(T)$ over a wide temperature range, returning to a quadratic behaviour only at temperatures below 500 mK. While the resistivity behaviour is broadly consistent with a model based on scattering from ferromagnetic fluctuations, the heat capacity of this material is more than double the value expected from ferromagnetic fluctuations alone. The proximity of this system to both ferromagnetism and antiferromagnetism, as reported in the literature, suggests that soft antiferromagnetic fluctuations spread over a wide range in reciprocal space may play an important role and contribute significantly to the specific heat capacity.

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