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Impurity effects in quasi-one-dimensional $S=\frac{1}{2}$ antiferromagnetic chain $KCuF_3$ studied by muon spin rotation

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Abstract

The local magnetic susceptibility χ_{loc} around a positive muon in quasi-one-dimensional spin $\frac{1}{2}$ antiferromagnetic chain compounds dichlorobis $KCuF_3$ has been investigated using muon spin rotation/relaxation (μ^+SR). We compare χ_{loc} with the bulk magnetic susceptibility χ measured in a SQUID magnetometer. In all cases there is a dramatic difference between χ_{loc} and χ, as predicted by theory.

Keywords: Low dimensionality; Strongly correlated insulators; Correlation in quantum systems

Novel Kondo-like effects are predicted for a non-magnetic impurity in a one-dimensional (1D) spin $\frac{1}{2}$ antiferromagnetic chain [1–3]. In particular, at low T the local magnetic susceptibility χ_{loc} in the region of a perturbed link is expected to differ dramatically from the uniform bulk susceptibility χ. Fig. 1 shows an impurity effect for a single straightened link. Notice the shift of the unperturbed maximum to lower T with increasing perturbation and the overall increase in amplitude of χ_{loc}. When the perturbation is strong enough the maximum vanishes completely and the overall behaviour is Curie-like. A μSR experiment is an ideal way to test such predictions since the muon acts as both the impurity and the probe of the local magnetic susceptibility. We anticipate that the positively charged muon will distort the crystal lattice, thereby altering the exchange coupling J between the magnetic ions in the vicinity of the muon. The resulting modification of the local susceptibility will be reflected in the muon frequency shift.

$KCuF_3$ has a tetragonal crystal structure (I4/mcm space group) with lattice parameters $c = 7.8487(8)$ Å and $a = b = 5.8569(6)$ Å. The single crystal used in this experiment was polytype a with $T_N = 39.3$ K.

All the measurements were performed at the M20 beamline at TRIUMF which delivers nearly 100% spin polarized positive muons. Fig. 2 shows frequency spectra at 100 K obtained by fast Fourier transforming the muon spin precession signal $AP_x(t)$. The muon frequency shifts shown in Fig. 3 are both positive and originate from the local dipolar field from the four nearest-neighbour Cu moments plus the contact interaction term. The bulk susceptibility in $KCuF_3$ peaks at around J and decreases at lower T due to short-range AF correlations [5]. This is clearly not the case for f_2 where the magnitude of the shift increases dramatically below 200 K. The T dependence of f_1 is somewhat weaker, but still does not follow the bulk susceptibility at all. This indicates a strong perturbation of the local coupling parameters. Similar behaviour has also been recently observed in $CuCl_2 \cdot 2NC_5H_5$ (CPC) [6] and

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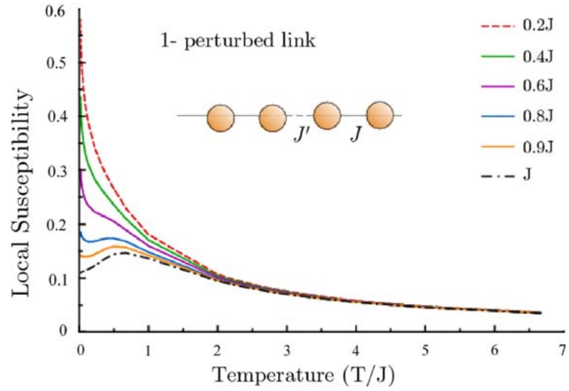

Fig. 1. Theoretically predicted impurity susceptibility for one perturbed link as a function of T [3]. The case of $J' = J$ corresponds to the unperturbed chain.

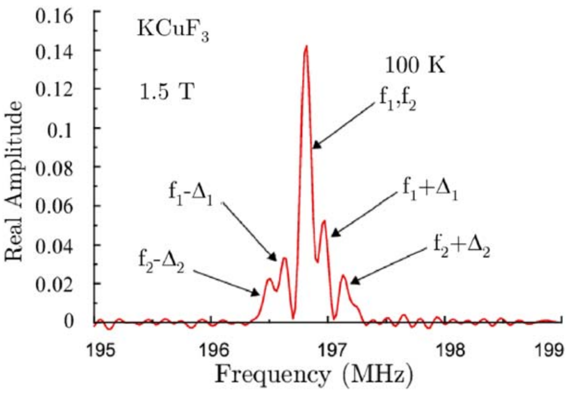

Fig. 2. Fast Fourier transforms of the μSR time spectra in a field of 1.5 T applied along the c-axis at $T = 100$ K. Additional lines imply two magnetically inequivalent FμF centres labelled as f_1 and f_3 [5].

$KCuCl_3$ [7]. The solid lines in Fig. 3 show a quantitative comparison with the theoretical calculations assuming a completely broken link (site 1) and two completely broken links (site 2), respectively. The overall agreement

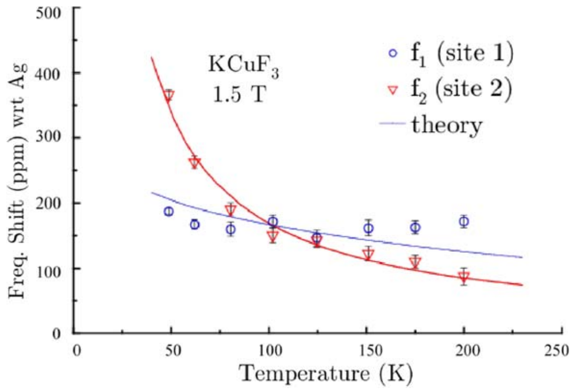

Fig. 3. Temperature dependence of the muon frequency shifts at two interstitial sites in a magnetic field $H = 1.5$ T. Note that the frequency shifts are corrected by subtracting the dipolar fields from all Cu^{2+} moments other than the four nearest neighbours.

is rather good, but some deviations should be expected since we have assumed earlier that all Cu ions contribution is the same, which is a simplification for a 1-d systems [1–3,8].

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