Experimental report

28/08/2021

Proposal: 5-32-907 **Council:** 4/2020

Title: Magnetic correlations in a quantumcritical S = 1/2 spin ladder system

Research area: Physics

This proposal is a new proposal

Main proposer: Edmund CUSSEN

Experimental team: Lucile MANGIN-THRO
Otto MUSTONEN

Local contacts: Lucile MANGIN-THRO

Samples: Ba2CuTe0.9W0.1O6
Ba2CuTe0.95W0.05O6

Instrument	Requested days	Allocated days	From	To
D7	5	5	09/02/2021	14/02/2021

Abstract:

Spin ladders are excellent model systems for studying quantum phase transitions, as they exhibit a quantum critical point between non-magnetic spin singlet dimers to Néel magnetic order as inter-ladder exchange is increased. Ba2CuTeO6 is a Cu2+ S = 1/2 two-leg spin ladder system, that is close to the quantum critical point on the Néel ordered side. By replacing Te with W in a Ba2CuTe1-xWxO6 solid solution, we have managed to tune the system to quantum criticality with a potential spin liquid state. We will use polarised neutron diffraction with XYZ analysis to study magnetic correlations in these compositionally tuned samples. This will allow us to study how this affects correlations within the ladders and between them, and to better understand the possible spin liquid state.

Magnetic correlations in a quantum critical S = 1/2 spin ladder system

Proposal no: 5-32-907
Instrument: D7, 5 days of beamtime
Experiment team: Edmund Cussen, Otto Mustonen, Helen Walker, Charlotte Pughe, Alex Gibbs
Local contact: Lucile Mangin-Thro

Ba_2CuTeO_6 is a Cu^{2+} S = 1/2 spin ladder compound with a hexagonal perovskite-type structure [1–3]. Ba_2CuTeO_6 is magnetically ordered with T_N = 14 K and a Néel type antiferromagnetic structure. It is known to be close to a quantum critical point between Néel order and a spin singlet ground state [3]. In the Ba_2CuTeO_6 structure, the spin ladders are formed by corner-sharing CuO_6 octahedrons linked by TeO_6 octahedrons. The ladders are linked by an interladder exchange along a facesharing Cu-Te-Cu trimer. We have previously established that substituting $4d^{10}$ Te^{6+} with $5d^0$ W^{6+} has a significant effect on the magnetic interactions in the related compound $Sr_2CuTe_{1-x}W_xO_6$, which consists entirely out of corner-sharing CuO_6 octahedrons linked by TeO_6 octahedrons [4,5].

In the case of Ba_2CuTeO_6, just 5% W^{6+} doping is enough to completely suppress magnetic order as revealed by muon measurements. However, inelastic neutron scattering measurements showed that the doped $Ba_2CuTe_{1-x}W_xO_6$ samples do not have a singlet-triplet gap, and therefore are not in the singlet state expected of the *S* = 1/2 spin ladder model. Our main objective for this D7 experiment was to investigate the nature of the dynamic low-temperature magnetic state in these materials. We measured 20g samples of $Ba_2CuTe_{1-x}W_xO_6$ powder with *x* = 0.05, 0.1 and 0.3 at on the cryostat at 1.5 K. The diffuse magnetic scattering was extracted using xyz polarisation analysis, and we fitted the data using Spinvert [6] in order to obtain the spin-spin correlations. The experiment was quite difficult due to the small Cu^{2+} *S* = 1/2 even with the large sample sizes. We were able to observe differences in the diffuse magnetic scattering between samples and in the spin-spin correlations. A more thorough analysis using Spinvert is ongoing.

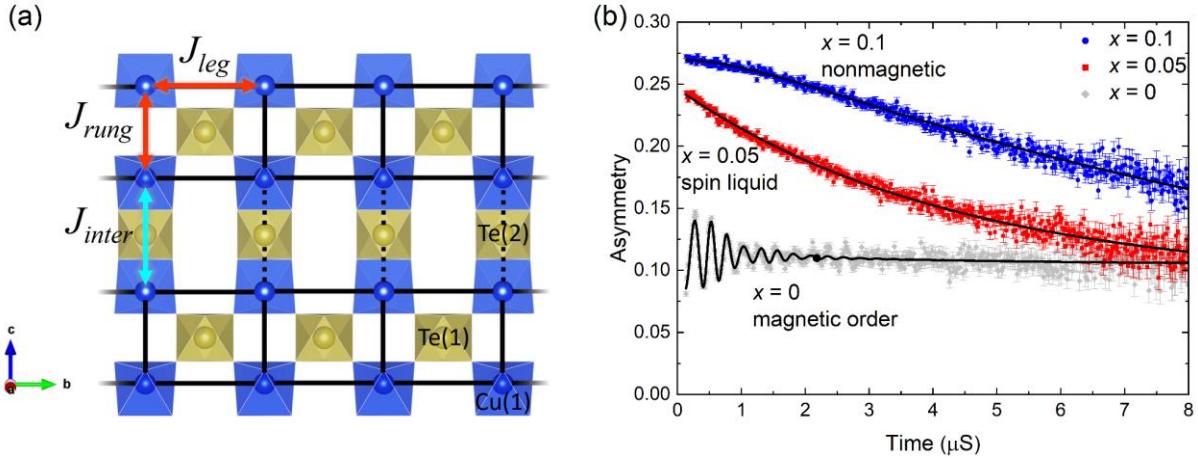

Figure 1. (a) The spin ladder structure of $Ba_2CuTe_{1-x}W_xO_6$. The W^{6+} cations are substituted onto the corner-sharing Te(I) site allowing the direct tuning of interactions in the ladder. (b) Muon spin rotation and relaxation measurements on *x* = 0.05 and *x* = 0.1, which reveal the lack of magnetic ordering.

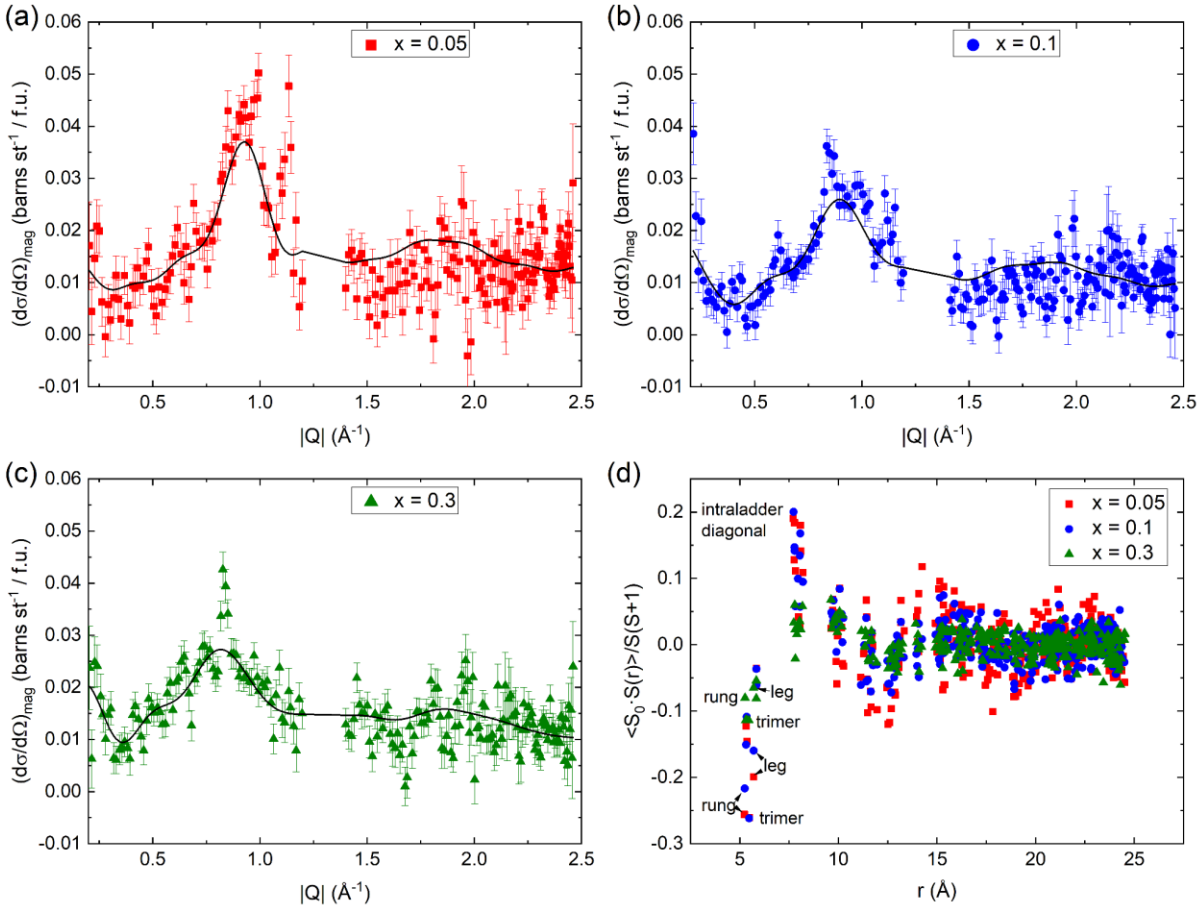

Figure 2. The measured diffuse magnetic scattering of $Ba_2CuTe_{1-x}W_xO_6$ samples and corresponding Spinvert fits (black line) for x = 0.05 (a), x = 0.1 (b) and x = 0.3 (c). (d) The spin-spin correlations obtained from reverse Monte Carlo fits to the diffuse magnetic scattering using Spinvert.

Figure 2 shows the measured diffuse magnetic scattering at 1.5 K for $Ba_2CuTe_{1-x}W_xO_6$ samples with x = 0.05, 0.1 and 0.3. The magnitude of diffuse magnetic scattering is very low due to the small Cu^{2+} moment. For x = 0.05 in panel (a), we observe a broad peak at about $|Q|$ = 0.85 Å-1. This occurs at the same position as the main magnetic Bragg peak in the magnetically ordered x = 0 parent phase. This suggests that the dynamic magnetic state in x = 0.05 is closely related to the magnetic order in x = 0. There is also a sharp feature around $|Q|$ = 1.13 $Å^{-1}$, that is being fit very poorly by Spinvert. The origin of this feature is unclear, and it is does not appear to be related to the parent phase nor is it an artifact due to positions of nuclear Bragg peaks. The diffuse scattering for x = 0.1 in panel (b) is similar to x = 0.05, although the main feature at $|Q|$ = 0.85 $Å^{-1}$ is broader and less intense. The diffuse scattering for x = 0.3 is similar, but the feature at $|Q|$ = 0.85 $Å^{-1}$ is very broad.

The spin-spin correlations obtained from Spinvert fits are shown in panel (d). The correlations along the main spin-ladder interactions along the leg and rung are strongly antiferromagnetic as expected. Similarly, the diagonal intraladder correlations are also strongly ferromagnetic as expected. Surprisingly, the correlations along the Cu-Te-Cu trimer are also quite

strong and antiferromagnetic. As x is increased, all spin-spin correlations become weaker. We do not see a change in sign for any of the spin-spin correlations upon doping, which is different from our previous results on $Sr_2CuTe_{1-x}W_xO_6$.

We conclude, that fundamentally the dynamic magnetic state observed in doped $Ba_2CuTe_{1-x}W_xO_6$ compounds is similar for the full range of x = 0.05 – 0.3 with the spin-spin correlations simply getting weaker with increasing x. This dynamic magnetic state appears to be related to the magnetic order observed in the x = 0 parent compound. We also observe an additional feature at $|Q|$ = 1.13 $Å^{-1}$ that is currently poorly understood. This experiment will form an important part of our publication on the ground state of the S = 1/2 spin ladder system $Ba_2CuTe_{1-x}W_xO_6$.

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