Quantum Magnetization Steps in $Cr_{12}Cu_2$ Magnetic Molecule

S. Yeninas, M. Luban, M. Tanatar, R. Prozorov (Iowa State Univ./Ames Laboratory), J. S. Brooks (FSU/NHMFL)

Introduction

$Cr_{12}Cu_2$ ($[N(C_2H_5)C_3H_8)_2]_2$ $[Cr_{12}Cu_2F_{16}(O_2CCMe_3)_{26}]$), shown in **Figure 1**, has a predicted saturation magnetic field H_{sat} = 80.7 T offering a model single molecular magnet system allowing for experimental verification of Quantum Monte Carlo (QMC) predictions. Tunnel – diode spectroscopy of $Cr_{12}Cu_2$ in the dilution refrigerator in fields up to 14 T yielded great agreement with QMC [1]. Higher fields were necessary to explore the whole magnetic field range.

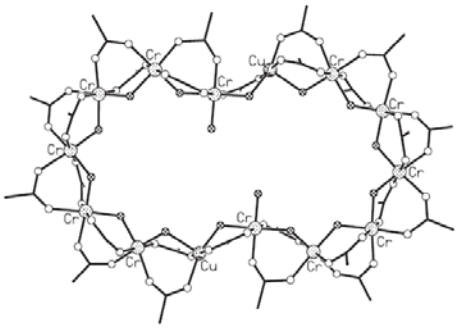

FIG. 1. Chemical structure of the $Cr_{12}Cu_2$ magnetic molecule. Cr^{3+} ions are shown as dotted circles and Cu^{2+} ions as heavily shaded circles. The compound has inversion symmetry and the metal centers within the molecule lie within a plane. The metal–metal edges are bridged by fluoride (crossed circles) and carboxylate ligands (oxygen open circles and carbon as lines). There are two ethyl-di-*iso*-propylammonium cations at the centers of each lobe of the hour glass which are not shown.

Experimental

The real component of the dynamic magnetic susceptibility was probed using a tunnel-diode resonator (TDR). The measurements were carried at 0.6 K in a ^{3}He cryostat in a 65 T short pulse magnet at NHMFL LANL. Two counter wound coils were used to reduce background from the pulse. Powder samples were packed directly in to the coils to increase the filling factor and signal intensity.

Results and Discussion

The magnetic molecule $Cr_{12}Cu_2$ (Cr^{3+}, S_{Cr} = 3/2; Cu^{2+}, S_{Cu} = ½) has an S = 1 ground state in zero magnetic field as determined by DC SQUID measurements. In applied fields, Zeeman splitting produces level crossings between the spin states. Using QMC, three nearest neighbor inter-ion exchange constants were derived from the DC magnetic susceptibility using an isotropic exchange model: $J_{Cr\text{-}Cr}$ = 15.6 K, $J_{Cr\text{-}Cu}$ = 57.2 K, and $J_{Cr\text{-}Cu}$ = - 20.8 K (ferromagnetic). Ground state energy crossings were predicted at: **8.15, 11.9, 16.2, 19.8, 24.1, 27.6, 31.7, 35.15, 39.3, 42.6, 47.1, 50.1, 55.2, 57.65**, 64.3, 65.5, and 80.7 T. Values in bold have been observed in pulsed fields at *T* = 0.6 K as shown in **Figure 2** after subtracting a constant background. **Figure 3** plots the field value for each level crossing versus the peak number for the experimentally determined values from the down sweep data, and the theoretically predicted values. The agreement is very good and provides a firm support to QMC predictions.

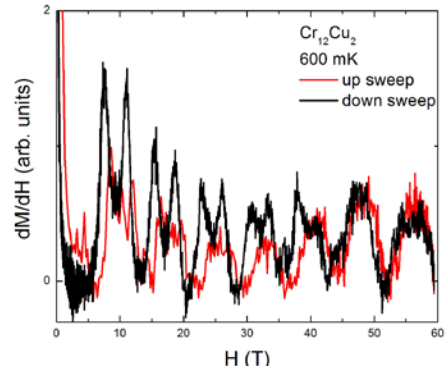

Figure 2. Plot of dM/dH for up and down sweeps after subtracting background.

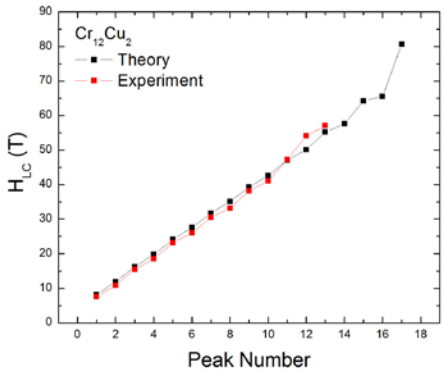

Figure 3. Field values for level crossings.

Conclusions

We demonstrated that the experimental setup at LANL is suitable for detecting level crossings in $Cr_{12}Cu_2$ for fields up to 65 T. We are currently awaiting time on the 100 T multi-shot magnet to verify all QMC predicted level crossings in fields exceeding 81 T.

Acknowledgements

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References

[1] C. Martin, *et al.,* Phys. Rev. B **80,** 100407 (2009).