Physics of a new copper-based triangular chain

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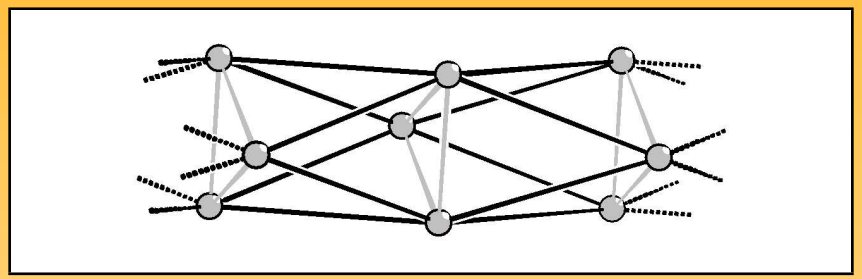
Preliminary results



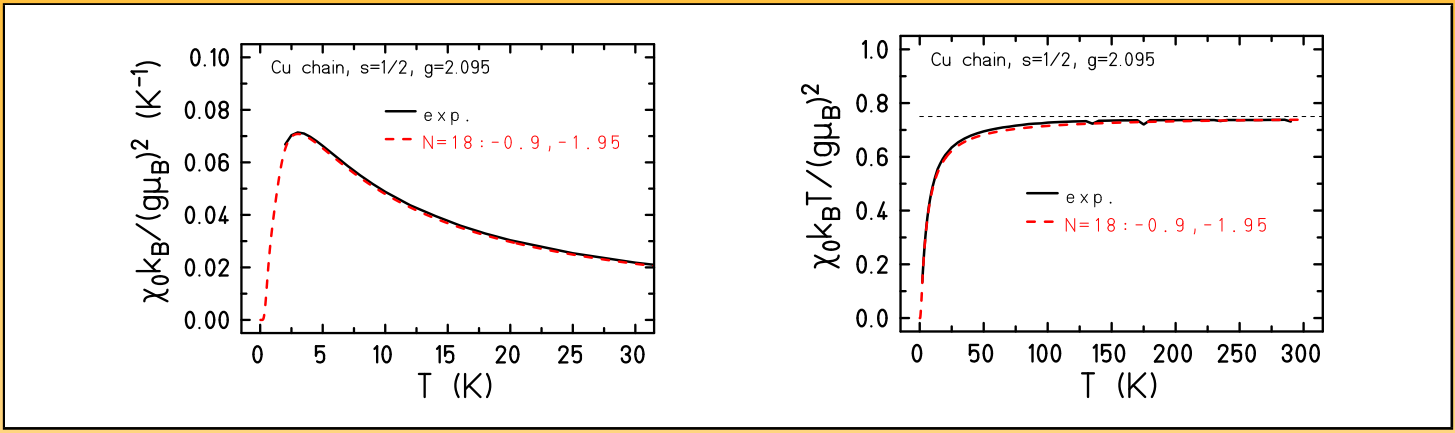
- New cluster compound $[(CuCl_2tachH)_3Cl]Cl$,
  tach $=$ *cis,trans*-1,3,5-triamino-cyclohexane (1,2)

- One-dimensional stack of antiprisms of antiferromagnetically coupled equilateral copper(II) triangles; system is a Heisenberg three-leg ladder with frustrated rung boundary condition.

- Intra-triangle couplings (J_1) are drawn by grey lines, inter-triangle couplings (J_2) are given by black lines.

(1) Georg Seeber, Paul Kögerler, Benson M. Kariuki, and Leroy Cronin, submitted
(2) G. Seeber, A. Pickering, D. Long, L. Cronin, Chem. Commun., 2002, 2003

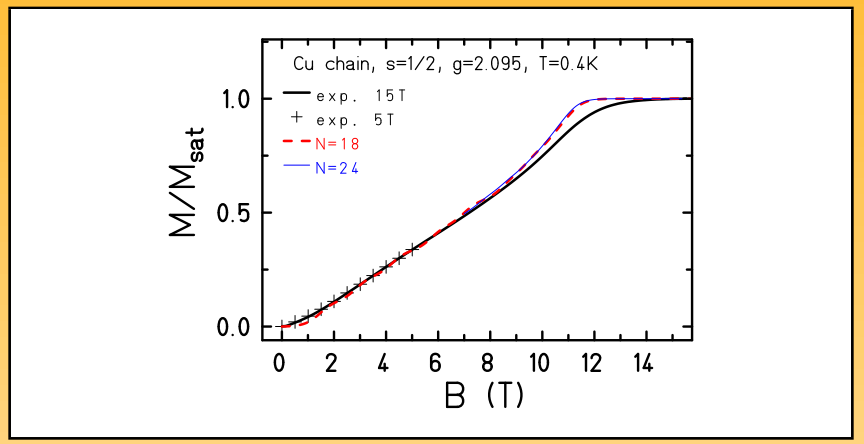
Susceptibility



- Intra-triangle exchange: bridging chloro ligand and hydrogen bonds; Cu-Cu distance is 4.46 Å.
- Inter-triangle exchange: hydrogen-bonded Cu-Cl$\cdots$H-N-Cu super-exchange; Cu-Cu distance is 6.82 Å.
- Conjecture: weakly coupled triangles, i. e. $|J_2| \ll |J_1|$
  $\Rightarrow$ independent triangles at high T; effective spin-$1/2$ chain at low T.

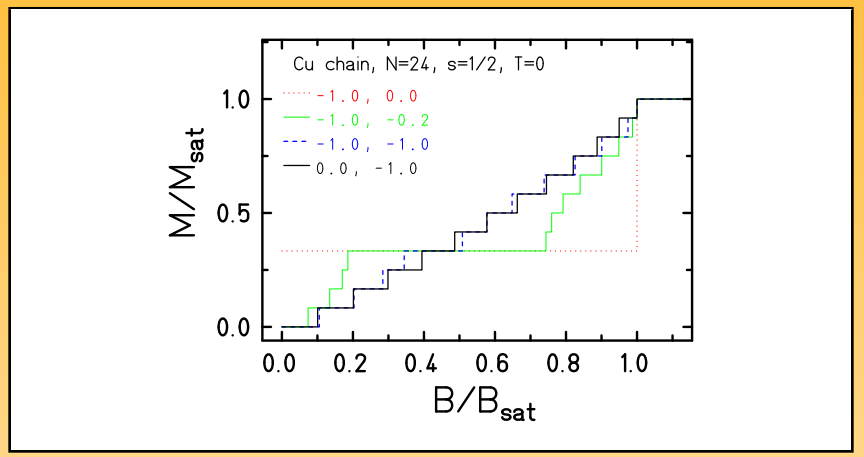
(1) Jürgen Schnack, Hiroyuki Nojiri, Paul Kögerler, Geoffrey J. T. Cooper, Leroy Cronin, to be submitted to Phys. Rev. B

Magnetization



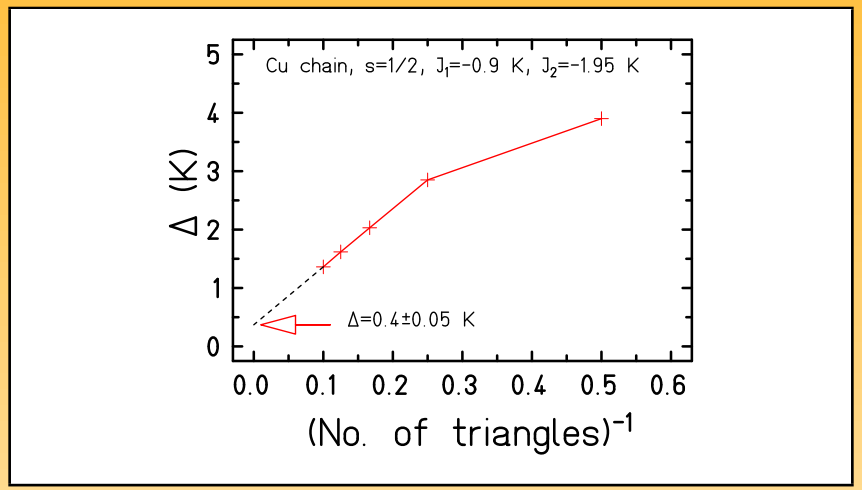
- Weakly coupled triangles would result in pronounced plateau at $1/3$ of the saturation magnetization.
- High-field magnetization measurement show, however, no plateau.
- Solution: isotropic Heisenberg model with antiferromagnetic exchange parameters $J_1 = -0.9$ K and $J_2 = -1.95$ K and $g = 2.095$ (average of small g-anisotropy).
- Deviations at high field: g-anisotropy and staggered field; deviations at low field: singlet-triplet gap overestimated in finite systems.

General considerations



- $J_1 = 0, J_2 < 0$: system is bipartite, classical ground state shows collinear Néel order; quantal square lattice on a torus, $S = 0$ non-degenerate (LSM).
- $J_1 < 0, J_2 = 0$: system is three-colorable, classical ground state has coplanar $120°$ order; quantal independent triangles, only two levels, one jump to saturation.
- $J_1 = J_2 < 0$: system is three-colorable, classical ground state has coplanar $120°$ order; quantal triangular lattice on a torus, order?

Zero-temperature properties



- Finite size diagonalizations for [($CuCl_2$tachH)$_3$Cl]Cl result in a ground state spin $S = 0$.
- Finite size extrapolation with up to 10 triangles shows that the ground state with $S = 0$ is separated from the triplet by $\Delta \approx 0.4 \pm 0.05$ K.

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