

TT 22: CE: Low-dimensional Systems - Materials 2

Time: Tuesday 10:30–13:00

Location: HSZ 304

TT 22.1 Tue 10:30 HSZ 304

Peculiar high-field quantum magnetism in the frustrated $s = 1/2$ spin chain cuprate linarite — ●M. SCHÄPERS¹, A. U. B. WOLTER¹, S.-L. DRECHSLER¹, S. NISHIMOTO¹, Y. SKOURSKI², M. UHLARZ², M. SCHMITT³, H. ROSNER³, K. C. RULE⁴, S. SÜLLOW⁵, G. HEIDE⁶, and B. BÜCHNER¹ — ¹Leibniz-Institut IFW Dresden, Dresden, Germany — ²Dresden High Magnetic Field Laboratory, Dresden, Germany — ³MPI-CPfS, Dresden, Germany — ⁴HZB für Materialien und Energie, Berlin, Germany — ⁵IPKM, TU Braunschweig, Braunschweig, Germany — ⁶TU Bergakademie Freiberg, Freiberg, Germany

We present an experimental and theoretical study of the quasi-one-dimensional $s = 1/2$ Heisenberg magnet linarite $\text{PbCuSO}_4(\text{OH})_2$, with competing ferromagnetic nearest-neighbor and antiferromagnetic next-nearest-neighbor exchange interactions. It includes magnetization and NMR studies as well as theoretical simulations for the determination of the leading exchange couplings, which are about an order of magnitude higher as determined previously.[1] Furthermore, a manifold of field-induced phases are probed, from which we draw a preliminary phase diagram. Notably, spin-lattice relaxation investigations indicate that linarite might undergo a magnetic quadrupolar spin liquid phase transition as recently predicted for such materials.[2]

[1] M. Baran, et al., Phys. Stat. Sol. (c) 3, 220 (2006).

[2] M. Sato, T. Momoi, A. Furusaki, Phys. Rev. B 79, 060406(R) (2009).

TT 22.2 Tue 10:45 HSZ 304

Magnetism in the Diamond Spin Chain Azurite — ●MATHIAS KRAKEN¹, JOSEFIN ENGELKE¹, STEFAN SÜLLOW¹, JOCHEN LITTERST¹, ANJA WOLTER², BERND WOLF³, MICHAEL LANG³, CHRIS BAINES⁴, and HUBERTUS LUETKENS⁴ — ¹IPKM, TU Braunschweig, D-38106 Braunschweig, Germany — ²Institute for Solid State Research, IFW, D-01069 Dresden, Germany — ³Physikalisches Institut, J.W. Goethe Universität, D-60438 Frankfurt (Main), Germany — ⁴ μ S, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland

Azurite is a mineral, which has been proposed as a model substance for a 1D spin- $\frac{1}{2}$ -Heisenberg-diamond-chain. Specific heat [1] indicated a magnetic phase transition at 1.8K, where the coupling between the 1D Cu-chains sets in. At 0.5K indications of another phase transition, with yet unknown nature, were observed [3]. Due to the small magnetic moments and the complex structure of azurite, the magnetic ground state is yet not well understood.

We performed μ SR measurements at PSI on a single crystal and a powdered sample, in extension of already published μ SR-data [4]. Our measurements revealed a critical behaviour of the transversal damping approaching T_c as well as clear evidence of static magnetic order below T_c . The phase transition at 0.5K is observable as well, and can be related to an alteration in the local environment of the Cu^{2+} monomers.

[1] H. Kikuchi et al., Phys. Rev. Lett. 94, 227201 (2005).

[2] B. Gu and G. Su, Phys. Rev. Lett. 97, 089701 (2006).

[3] P.T. Cong et al., J. Phys.: Conf. Ser. 200, (2010).

[4] M.C.R. Gibson et al., Phys. Rev. B 81, 140406 (2010).

TT 22.3 Tue 11:00 HSZ 304

Magnetic coupling and dynamics in the 1D quantum magnet azurite $\text{Cu}_3(\text{CO}_3)_2(\text{OH})_2$ as determined from inelastic neutron scattering. — ●KIRRILY RULE¹, ALAN TENNANT^{1,2}, MARK TELLING³, SEBASTIAN GERISCHER¹, STEFAN SÜLLOW⁴, and MICHAEL LANG⁵ — ¹Helmholtz-Zentrum Berlin, Berlin, Germany — ²Institut fuer Festkoerperphysik, TU Berlin, Berlin, Germany — ³ISIS, Rutherford Appleton Laboratories, Chilton, UK — ⁴Institut fuer Physik der Kondensierten Materie, TU Braunschweig, Braunschweig, Germany — ⁵Goethe Universitat, Frankfurt(M), SFB/TR 49, Germany

Low dimensional magnetic systems, in particular, copper oxides are interesting subjects of study due to the novel physics that can arise in such systems at low temperatures. Both a natural mineral and quantum magnet, $\text{Cu}_3(\text{CO}_3)_2(\text{OH})_2$ is a candidate model of the so-called Distorted Diamond Chain system. Early studies of this material imply the presence of an ordered antiferromagnetic phase below $T_N \sim 1.9$ K while magnetization measurements have revealed a $1/3$ magnetization plateau. Most recently the interactions and magnetic exchange couplings have been hotly debated. We will present our analysis of the inelastic neutron scattering data, highlighting the temperature and

field dependence of the low energy spin chain excitations. We will also reveal information about the as yet unseen higher energy magnetic excitations. Finally we would like to consolidate this data by presenting a model to describe this intriguing 1D quantum magnet.

TT 22.4 Tue 11:15 HSZ 304

Distinct magnetic regimes through site-selective atom substitution in the frustrated quantum antiferromagnet $\text{Cs}_2\text{CuCl}_{4-x}\text{Br}_x$ — ●BERND WOLF¹, PHAM THANG CONG¹, MARIANO DE SOUZA¹, NATALIE KRÜGER¹, AMIR HAGHIGHIRAD¹, FRANZ RITTER¹, WOLF ASSMUS¹, INGO OPAHLE², KATARYNA FOYEVTSOVA², ROSER VALENTI², HARALD JESCHKE², LEONORE WIEHL³, and MICHAEL LANG¹ — ¹Physikalisches Institut, Goethe Universität Frankfurt — ²Institut für theoretische Physik, Goethe Universität Frankfurt — ³Institut für Geowissenschaften, Goethe Universität Frankfurt

We report on a systematic study of the magnetic properties on single crystals of the solid solution $\text{Cs}_2\text{CuCl}_{4-x}\text{Br}_x$ ($0 \leq x \leq 4$), which include the two known end-member compounds Cs_2CuCl_4 and Cs_2CuBr_4 , classified as quasi-two-dimensional quantum antiferromagnets with different degrees of magnetic frustration. By comparative measurements of the magnetic susceptibility $\chi(T)$ on as many as eighteen different Br concentrations, we found that the in-plane and out-of-plane magnetic correlations do not show a smooth variation with x . Rather three distinct concentration regimes can be identified, which are separated by critical concentrations $x_{c1} = 1$ and $x_{c1} = 2$. This unusual magnetic behavior can be explained by considering the structural peculiarities of the materials, especially the distorted Cu-halide tetrahedra, which support a site-selective replacement of Cl^- by Br^- ions.

TT 22.5 Tue 11:30 HSZ 304

Ultrasonic investigation in the vicinity of the quantum-critical point in Cs_2CuCl_4 — ●P. T. CONG, B. WOLF, S. BELZ, N. KRÜGER, F. RITTER, W. ASSMUS, and M. LANG — Physikalisches Institut, Goethe Universität-Frankfurt, SFB/TR 49, D-60438 Frankfurt(M)

The insulator Cs_2CuCl_4 is a quasi-two-dimensional triangular lattice (bc plane) spin- $1/2$ antiferromagnet (AFM) with a weak interlayer coupling. This material has been considered as one of the prime example for studying the phenomenon of Bose-Einstein condensation (BEC) of magnetic excitations [1]. The long-range antiferromagnetic order ($T_N = 0.6$ K at $B = 0$) can be suppressed to $T_N = 0$ in a magnetic field $B_c \sim 8.5$ T ($B||a$), which constitutes a quantum-critical point (QCP). Anomalous physical properties at finite temperature are expected to be observed at B_c due to quantum-critical fluctuations. Here we present a detailed investigation of the elastic constants c_{11} , c_{22} and c_{33} together with the ultrasonic attenuation near the B-induced QCP. Distinct anomalies were found at $B_c \sim 8.5$ T, which are particularly strongly pronounced in the ultrasonic attenuation. At low temperature and around B_c , the ultrasonic attenuation of the all three modes exhibits a pronounced double peak structures, indicating two anomalies of different origin. While one of them is very sharp, strongly temperature dependent and coinciding with $T_N(B)$, the other one is distinctly broader and located at slightly higher fields. Upon cooling both features merge and extrapolate to $B_c \sim 8.5$ T for $T \rightarrow 0$.

[1] T. Radu *et al.*, Phys. Rev. Lett. **95**, 127202 (2005).

15 min. break

TT 22.6 Tue 12:00 HSZ 304

Spin-spin correlation of the spin- $1/2$ Heisenberg-chain compound CuPzN measured by magnetostriction — ●JENS ROHRKAMP¹, MARKUS GARST², MATT D. PHILLIPS³, MARK M. TURNBULL³, and THOMAS LORENZ¹ — ¹II. Physikalisches Institut, Universität zu Köln, Germany — ²Institut für theoretische Physik, Universität zu Köln, Germany — ³Carlson School of Chemistry and Biochemistry, Clark University, USA

The spin- $1/2$ Heisenberg chain is one of the rare examples of quantum-spin Hamiltonians, which can be solved analytically exact. An experimental realization of this Hamiltonian is found in copper pyrazine dinitrate $\text{Cu}(\text{C}_4\text{H}_4\text{N}_2)(\text{NO}_3)_2$ (or CuPzN). The weak coupling con-

stant $J \approx 10$ K in this compound leads to a critical magnetic field of about 14 T, which is accessible in typical superconducting laboratory magnets. At this field the system undergoes a quantum phase transition from the gapless Luttinger-liquid state to the fully saturated state with a finite excitation gap. As recently shown in [1] the field- and temperature-induced length changes are proportional to the spin-spin correlation function $\langle S_i S_j \rangle$. We present high-resolution measurements of thermal expansion and magnetostriction and compare these to calculations performed via Bethe ansatz.

[1] Anfuso *et al.* PRB **77**, 235113 (2008)

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TT 22.7 Tue 12:15 HSZ 304

Competing ground states in a novel Ni based hybrid $S = 1$ chain investigated with Electron spin resonance spectroscopy

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A new hybrid material that comprises arrays of one dimensional (1D) chains of NiCl₆ octahedra separated by a framework of organic molecules is investigated with different methods. The Ni²⁺(3d⁸) ions in the NiCl₆ chain possess an integer spin $S = 1$. The temperature dependence of the static susceptibility shows a broad maximum suggesting an AFM coupling with a nearest neighbour exchange constant around 25 K. The ESR signal consists of a single lorentzian line at a g -factor of 2.2 typical for Ni²⁺. The ESR spectrum is isotropic proofing the absence of a single ion anisotropy. This indicates a good realization of the Haldane conjecture which predicts a non-magnetic ground state for an isotropic AFM Heisenberg $S = 1$ chain and a gapped spin excitation spectrum. In contrast to this, a magnetic ordering is observed at temperatures below 10 K with ESR and μ sr. In the low temperature regime the static susceptibility and ESR measurements reveal an anisotropic behaviour for the magnetic field applied along and perpendicular to the chain. We discuss a possible ground state and spin dynamics of the studied compound.

TT 22.8 Tue 12:30 HSZ 304

Nature of electronic correlations in strongly doped Na_xCoO₂

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With the combination of the rotationally invariant slave-boson mean-field theory (RISB) [1,2] and the local-density approximation (LDA) to density functional theory, the phase diagram of layered sodium cobaltate Na_xCoO₂ is investigated in the high-doping regime close to zero temperature [3]. This system represents one of the rare natural examples of a doped strongly correlated triangular lattice. Utilizing a tailored realistic single-band approach in a cellular-cluster framework, we investigate the effect of electronic correlations with doping until the band-insulating ($x=1$) limit. The experimentally verified [4] in-plane crossover from antiferromagnetic tendencies at low x towards ferromagnetic order for $x > 0.75$ is revealed with an on-site Hubbard interaction. Relevant charge-ordering physics in the system is modelled via an additional inter-site Coulomb interaction V on an effective kagomé lattice, as observed in experiment [5].

[1] T. Li *et al.*, PRB **40**, 6817 (1989).

[2] F. Lechermann *et al.*, PRB **76**, 155102 (2007).

[3] C. Piefke *et al.*, PRB **82**, 165118 (2010).

[4] G. Lang *et al.*, PRB **78**, 155116 (2008).

[5] H. Alloul *et al.*, EPL **85**, 47006 (2009).

TT 22.9 Tue 12:45 HSZ 304

Implications of Choosing the Local Coordinate Frame for the Understanding of Magnetism in Highly Anisotropic Co^{II} Clusters

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Molecular nanomagnets containing Co^{II} ions are currently of much interest, because they provide large magnetic anisotropy and hence potentially superior magnetic properties. However, only relatively few examples can be found in the literature, which might be due to the complications in describing the magnetic properties of such clusters.

Here we report our studies of the magnetic properties in a polynuclear Co₂^{III}Co₆^{II} complex. An effective low-temperature model reproduces excellently our magnetic data at the lowest temperatures and the general trend at higher temperatures. However, the derived exchange parameters are maximally anisotropic, while the energy spectrum is typical for the strong exchange limit, in which anisotropy is weak. This will be explained by noting the implications of the freedom to choose the local coordinate frame at will. The consequences thereof, which are potentially of general interest, will be discussed.