B1 Interacting magnetic excitations in quantum spin systems - Thermodynamic investigations

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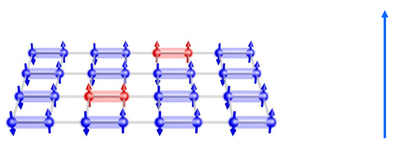
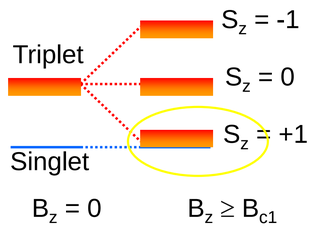
Introduction

Exploring the collective behaviour of magnetic excitations in quantum-spin systems, e.g., arrays of coupled (S = ½) dimers in magnetic fields





Main objectives

i) Spin-phonon interaction and quantum criticality

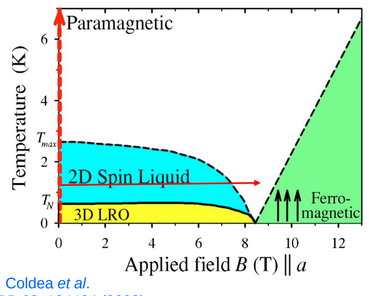
ii) *B*-induced order in coupled-dimer systems

iii) Magnetocaloric effect around a quantum-critical point

i) Magnetic and thermodynamic properties near a *B*-induced quantum-critical point

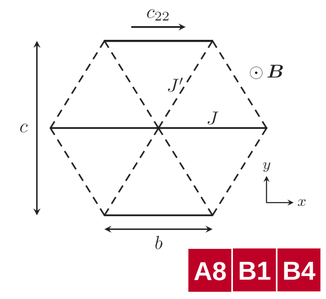
Achievements

Cs_2CuCl_4: 2D triangular-lattice antiferromagnet



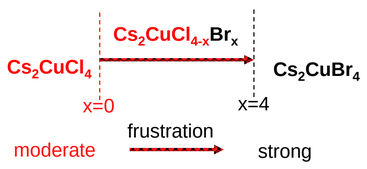
R. Coldea *et al.*
PRB **68**, 134424 (2003)

- coupling constants
  J = 4.35 K
  J' = 0.34 J
  J'', D = 0.05 J
- magnetic excitations dominant along ***b*** axis
  ⇒ dimensional reduction; description in terms of Heisenberg chain



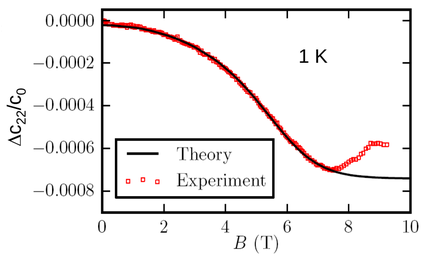
A8 B1 B4

Streib *et al.*, PRB **91**, 041108(R) (2015), joint publication



- $Cs_2CuCl_{4-x}Br_x$: well-suited for investigating the interplay of
  - strong quantum fluctuations in reduced dimensions
  - the effects of geometrical frustration
  - spin-lattice interaction

- novel microscopic description of the magnetoelastic coupling in the spin-liquid regime
- model not applicable close to the QCP



Goals and work programme

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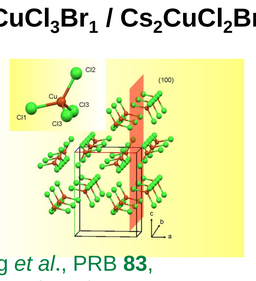
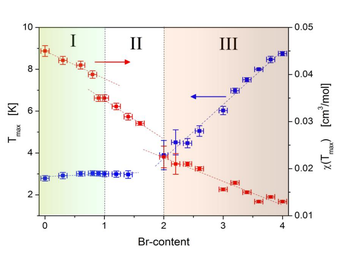
Novel mixed Cu-halides discovered in the SFB/TR 49: $Cs_2CuCl_3Br_1$ / $Cs_2CuCl_2Br_2$



Cong *et al.*, PRB **83**, 064425 (2011)

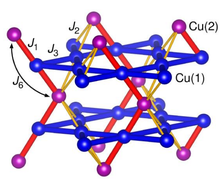


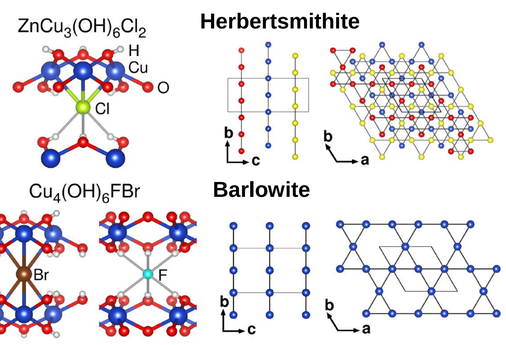
- influence of different degrees of frustration
  - on the magnetoelastic coupling
  - on the spin liquid properties
- experimental and theoretical investigations of the magnetoelastic behaviour near QCP

B1 B4 B2 B3

new kagome systems

based on novel design strategy: ⇒ variations in kagome stacking pattern and terms (such as DM) in the spin Hamiltonian





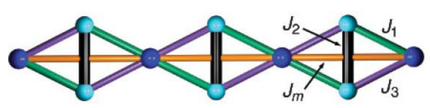
- investigation of the spin-liquid properties
- study the interplay between the tuning parameter and spin-liquid states

Jeschke *et al.*,arXiv 1412.4668 (2014) joint publication

Achievements

azurite: distorted frustrated diamond chain;

- natural mineral; model system for distorted frustrated diamond chain

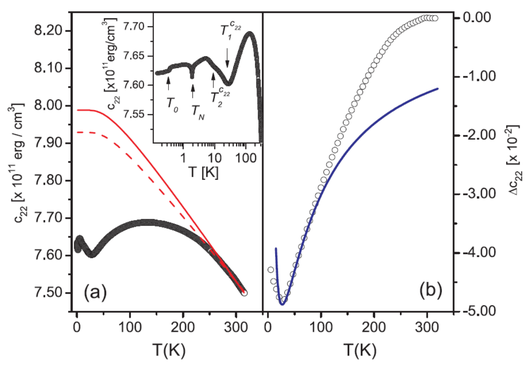


- effective S = ½ model
  ⇒ explanation for experimental findings

Jeschke *et al.*, PRL **106**, 217201 (2011)

- model description does not include magnetoelastic couplings

B1 B2



Cong *et al.*, PRB **89**, 174427 (2014)

- exceptionally large magnetoelastic coupling constant: $G = \partial J_2/\partial \varepsilon_b \gg 1$
  ⇒ anomalous magnetoelastic coupling indicating structural pecularities

Goals and work programme

- perturbation theory-based calculations ⇒ origin of the huge magnetoelastic coupling

B1 B13N

ii) Exploring the *B*-induced order in 2D coupled-dimer systems

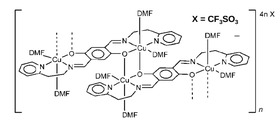
Achievements

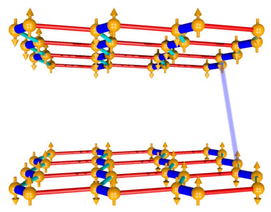
B1 B2 B5

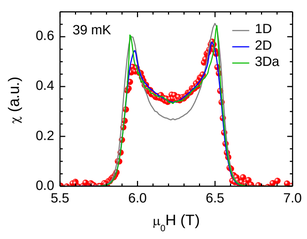
Cu-coordination polymer TK 91: 2D-coupled-dimer system

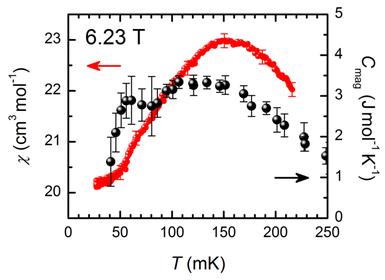
Tutsch *et al.*, Nature Commun. **5**, 5169 (2014) joint publication

- TK 91 ($C_{36}H_{48}Cu_2F_6N_8O_{12}S_2$), characterized by $\chi(T,B)$ and $C(T,B)$
  ⇒ Field-induced "ordered state"
  ⇒ no long-range order for $T \geq 27$mK



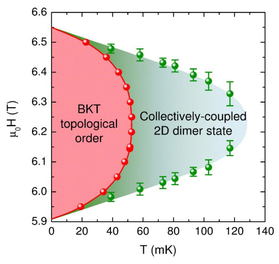




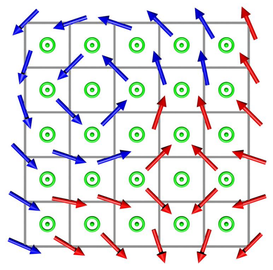


- *ab initio* calculations and quantum Monte Carlo simulations
  ⇒ excitations reveal a distinctly 2D character
  ⇒ Berezinskii-Kosterlitz-Thouless scenario

- broad maximum in specific heat at 120 mK is consistent with a 2D-Heisenberg model



⇒ occurrence of vortex and antivortex excitations in the collectively-coupled dimer state

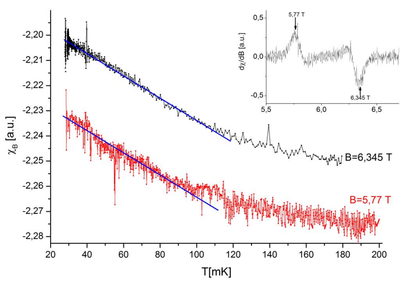


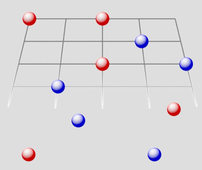
- For 2D systems:
  quantum Monte Carlo simulations predict an in-T linear change of magnetization at the critical fields
  ⇒ observed in *ac*-susceptibility measurements

$$\chi = \frac{\partial M}{\partial H} \xrightarrow{H = \text{const.}} \chi_B \propto M$$

Straßel *et al.*, arXiv: 1412.0266

χ at the critical fields for TK 91





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