Revisiting the magnetism of hole-doped CuO_2 spin chains in $Sr_{14-x}Ca_xCu_{24}O_{41}$

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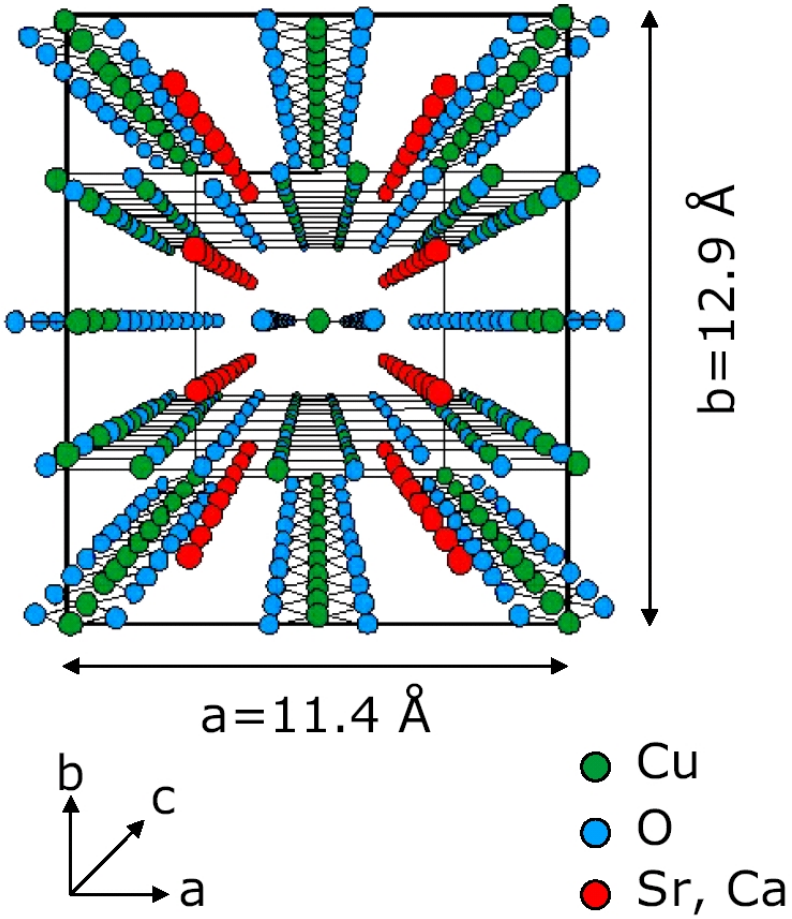

$Sr_{14-x}Ca_xCu_{24}O_{41}$

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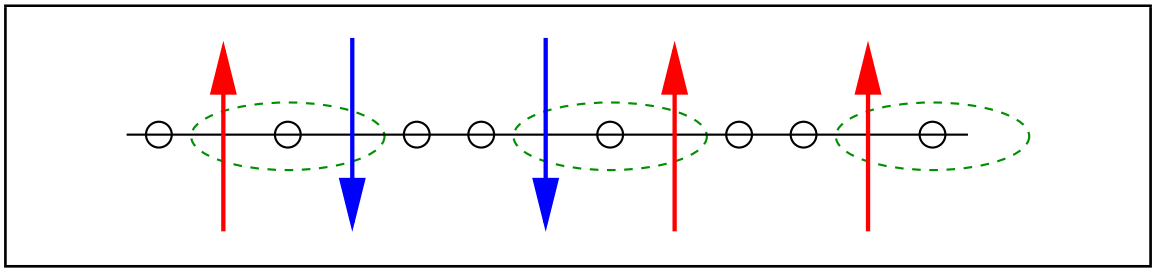
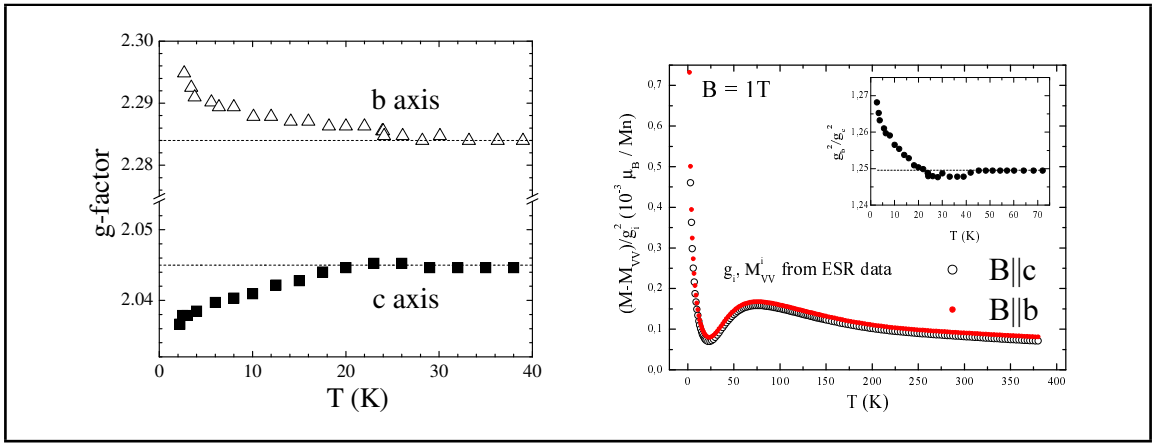
$Sr_{14}Cu_{24}O_{41}$ – Folklore



- Contains weekly coupled chains and ladders; is intrinsically doped with 6 holes per f.u.. At room temperatures all(?) holes reside on the chain (1).
- The ladder has a large singlet-triplet gap, therefore below ≈ 200 K only the chains contribute to magnetization (1).
- 60 % holes on the chain suggest dimer-configuration (figure); recent DFT calculations suggest irregular structure (2).

(1) N. Nücker *et al.*,Phys. Rev. B **62**, 14384 (2000)
(2) A. Gelle & M.B. Lepetit, Phys. Rev. Lett. **92**, 236402 (2004)

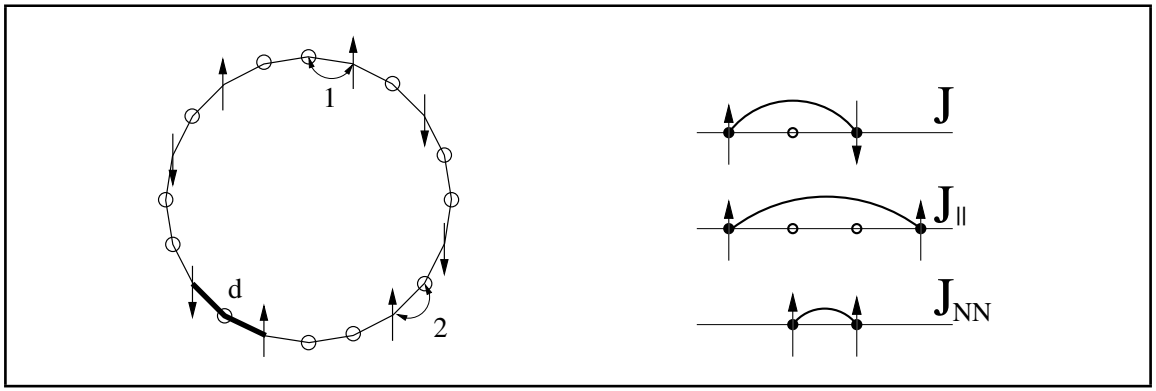
$Sr_{14}Cu_{24}O_{41}$ – Recent experimental results



- EPR of single-crystal $Sr_{14}Cu_{24}O_{41}$ at low temperature (1) shows that Cu "impurities" have almost the same g-tensor as Cu ions in dimers, i. e. impurities reside on intact chains!
- Deviation of g at $T \lessapprox 20$ K due to single Cu spins; rather small therefore "free" Cu ions very likely have the same chemical environment as the chain Cu ions.
- Scaled magnetization measurements lead to the same conclusion.

(1) R. Klingeler, B. Büchner, K.-Y. Choi, V. Kataev, U. Ammerahl, A. Revcolevschi, J. Schnack, Phys. Rev. B **73**, 014426 (2006)

$Sr_{14}Cu_{24}O_{41}$ – Effective spin model I



Effective Heisenberg Hamiltonian depends on spin-hole configuration $\vec{c}$

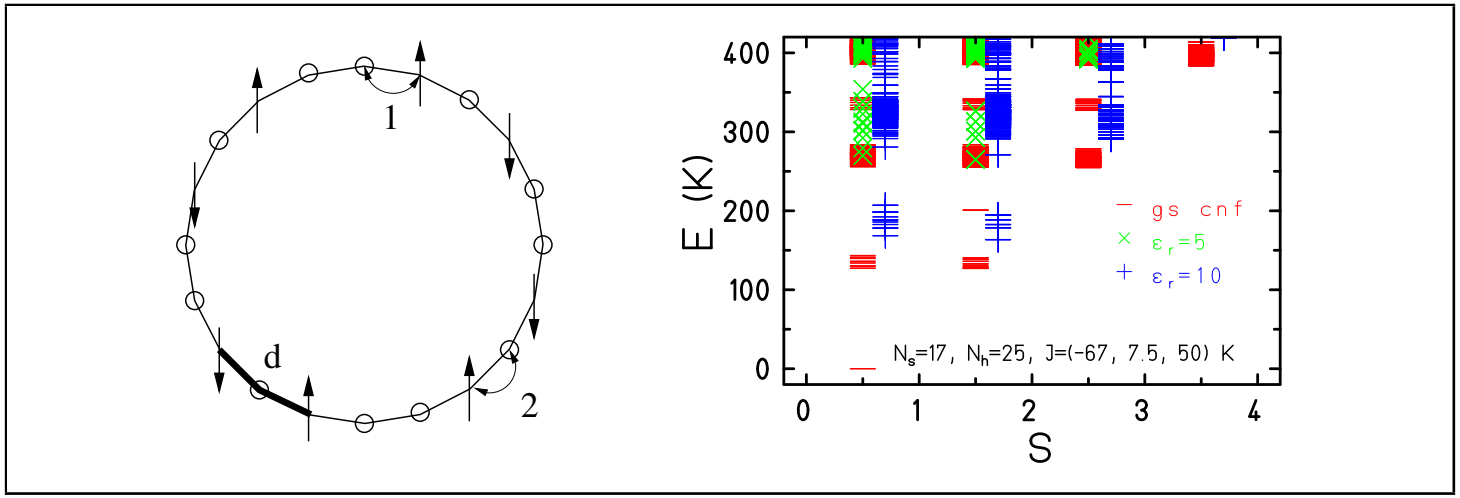
$$\underset{\sim}{H} = \sum_{\vec{c}} \left(\underset{\sim}{H}(\vec{c}) + V(\vec{c}) \right) \quad , \quad \underset{\sim}{H}(\vec{c}) = -\sum_{u,v} J_{uv}(\vec{c})\ \underset{\sim}{\vec{s}}(u) \cdot \underset{\sim}{\vec{s}}(v)$$

$J_{uv}(\vec{c}) : J = -67$ K, $J_{\|} = 7.5$ K, $J_{NN} = 50$ K

Alternative: Transformation from Hubbard to spin-only model (1).

(1) J.-Y.P. Delannoy, M.J.P. Gingras, P.C.W. Holdsworth, A.-M.S. Tremblay, Phys. Rev. B **72**, 115114 (2005)

$Sr_{14}Cu_{24}O_{41}$ – Effective spin model II

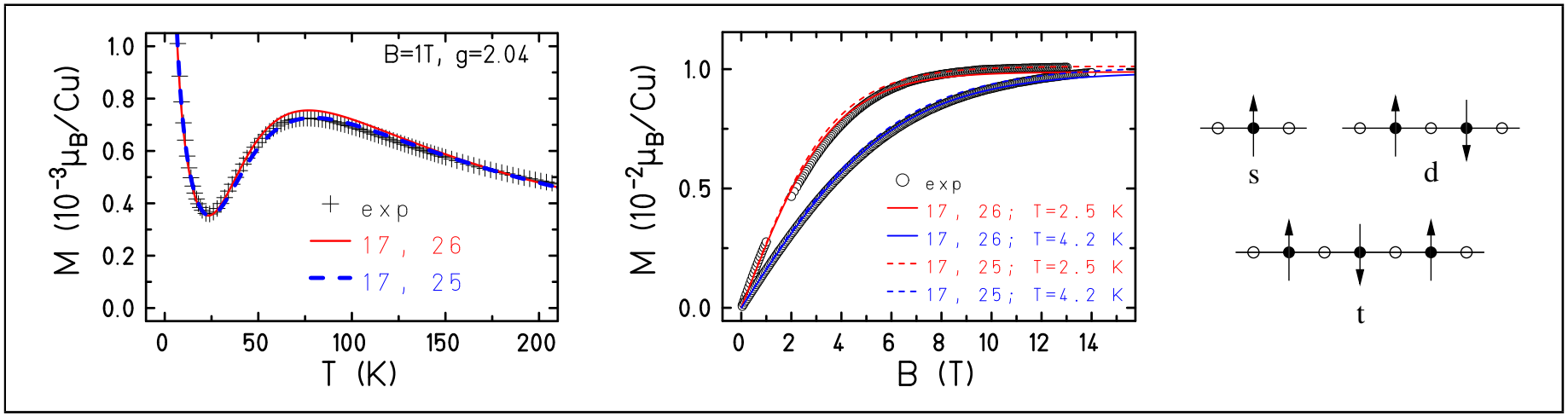


Different configurations should have a different energy offset (Coulomb, interaction with chain environment, . . .).
In-medium hole-hole Coulomb interaction:

$$V(\vec{c}) = \frac{e^2}{4\pi\epsilon_0\,\epsilon_r\,r_0}\frac{1}{2}\sum_{u\neq v}\frac{1}{|u-v|}$$

J. Schnack, Eur. Phys. J. B **45**, 311 (2005)

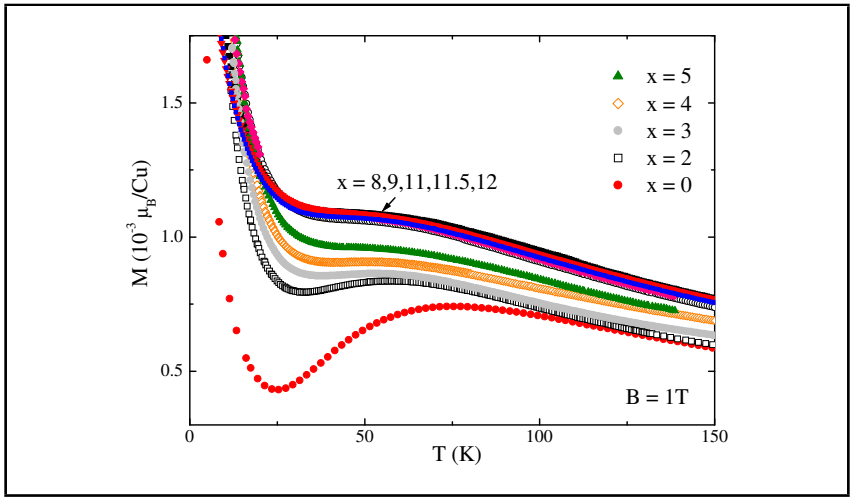
$Sr_{14}Cu_{24}O_{41}$ – Results



- Perfect agreement between theory and experiment (1).
- Up to $\epsilon_r \approx 5$ only ground state configuration contributes:
  $\vec{c}_{17,26} = sddddddd$ ($\rho_h = 60.4$ %), $\vec{c}_{17,25} = tddddddd$ ($\rho_h = 59.5$ %).

(1) R. Klingeler, B. Büchner, K.-Y. Choi, V. Kataev, U. Ammerahl, A. Revcolevschi, J. Schnack, Phys. Rev. B **73**, 014426 (2006)

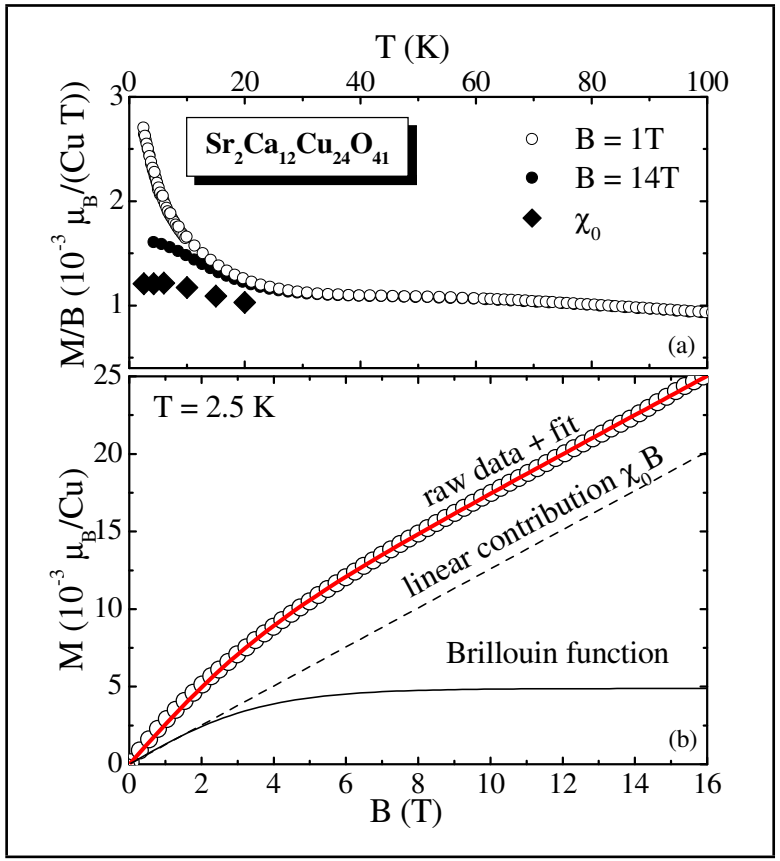
$Sr_{14-x}Ca_xCu_{24}O_{41}$ – Common belief



- Chemical pressure due to Ca doping leads to partial charge transfer to the ladders (1). How many holes are transfered? By Ca doping max. 1/f.u. (2).
- Magnetization (3) is attributed to the chains only due to the large gap in the ladder subsystem for all x!

(1) N. Nücker *et al.*,Phys. Rev. B **62**, 14384 (2000); (2) V. Kataev, V., K.Y. Choi, M. Grüninger, U. Ammerahl, B. Büchner, A. Freimuth, A. Revcolevschi, Phys. Rev. B **64**, 104422 (2001); (3) R. Klingeler, N. Tristan, B. Büchner, M. Hücker, U. Ammerahl, A. Revcolevschi, Phys. Rev. B **72**, 184406 (2005)

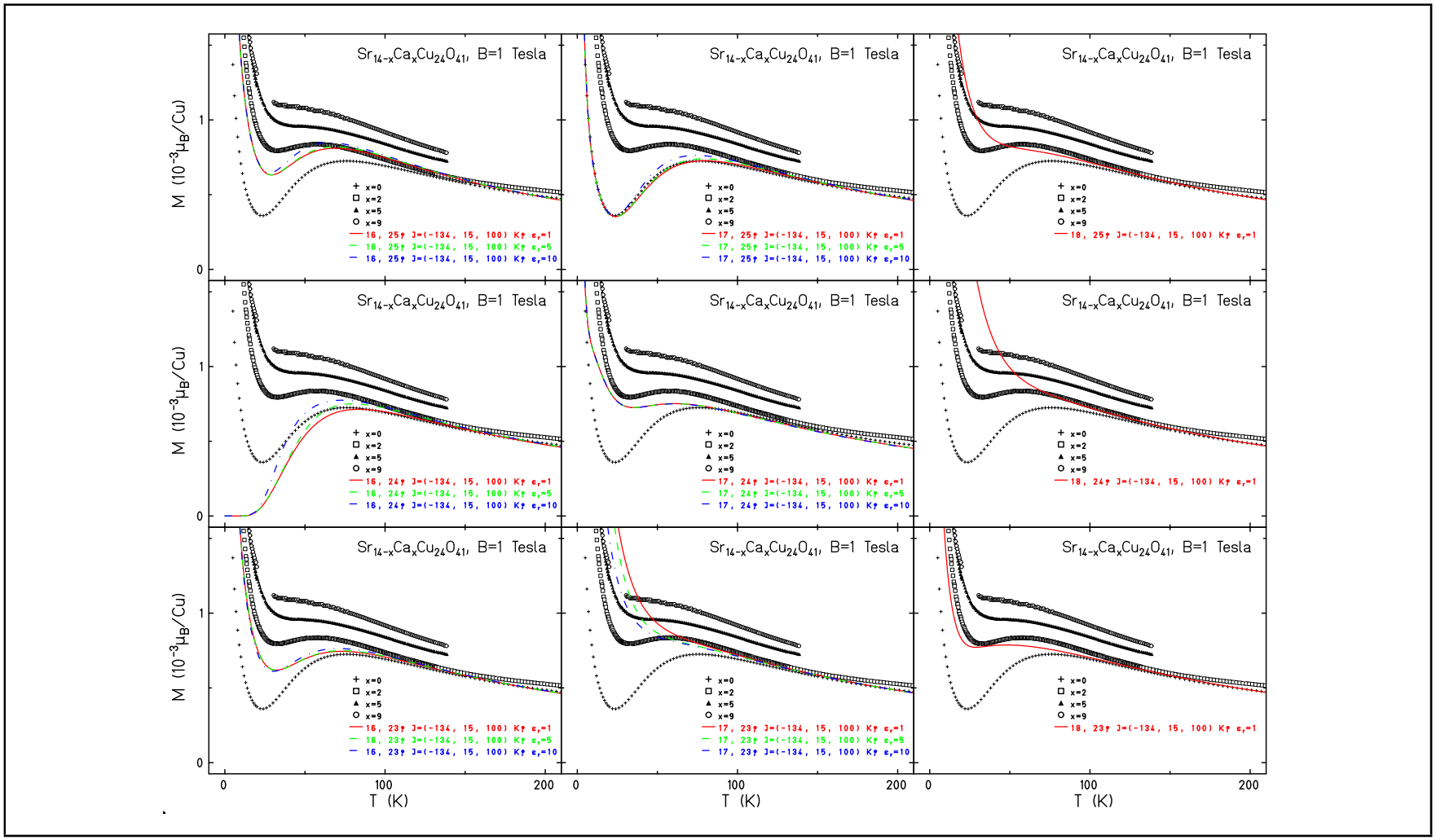
$Sr_{14-x}Ca_xCu_{24}O_{41}$ – Strange magnetization



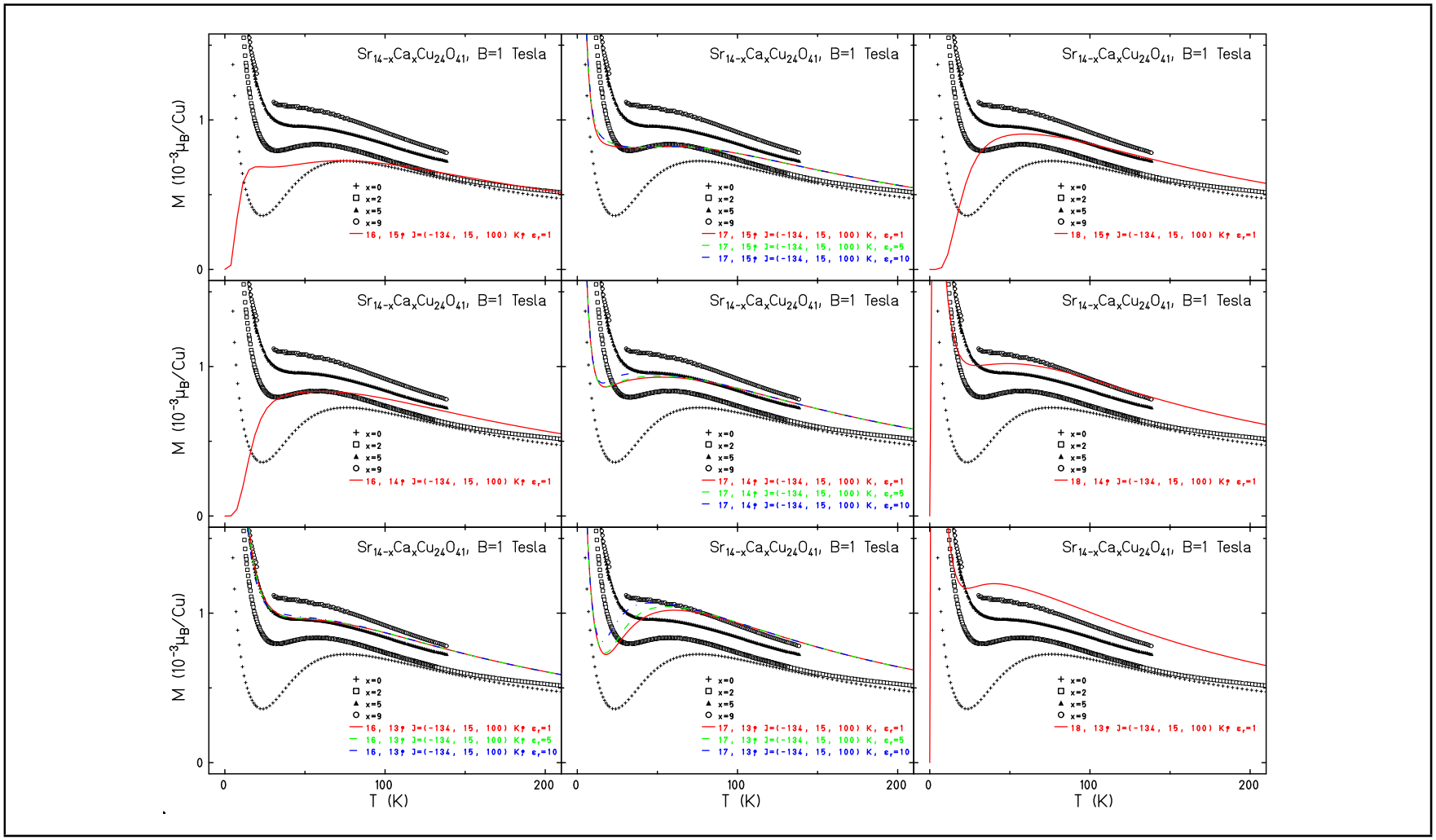
- Interesting feature: for $x > 0$ susceptibility $\mathcal{M}/B$ acquires a constant contribution (1)!
- Origin of this contribution unknown!

(1) R. Klingeler, N. Tristan, B. Büchner, M. Hücker, U. Ammerahl, A. Revcolevschi, Phys. Rev. B **72**, 184406 (2005)

$Sr_{14-x}Ca_xCu_{24}O_{41}$ – Simulations with effective Hamiltonian I



$Sr_{14-x}Ca_xCu_{24}O_{41}$ – Simulations with effective Hamiltonian II



$Sr_{14-x}Ca_xCu_{24}O_{41}$ – Open problems

- $Sr_{14-x}Ca_xCu_{24}O_{41}$ shows relativly large magnetization at ≈ 100 K and as function of field. Effective Hamiltonian does not yield such high magnetization with $\rho_h \gtrsim 0.5$!

- Possible solutions:
  - Contribution of the ladder subsystem to magnetization. Gap?!
    INS experiments suggest a small gap in $Sr_{2.5}Ca_{11.5}Cu_{24}O_{41}$ (A. Tennant).
  - Hole content decreases to smaller values than previously assumed.
    Christian Hess will solve this issue soon. 
  - Effective Hamiltonian for $x > 0$ too simple. Implicit assumption of charge localization no longer valid.
  - Real system not homogeneous, e.g. parts with larger ρ_h and others with smaller ρ_h.

Thank you very much for your attention.

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