Revisiting the magnetism of hole-doped CuO$_2$ spin chains in Sr$_{14-x}$Ca$_x$Cu$_{24}$O$_{41}$

Jürgen Schnack$^1$, Rüdiger Klingeler$^2$, Vladik Kataev$^2$, and Bernd Büchner$^2$

$^1$Universität Osnabrück, $^2$IFW Dresden
http://obelix.physik.uni-osnabrueck.de/~schnack/

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Jürgen Schnack, Revisiting the magnetism of hole-doped CuO\(_2\) spin chains in \( \text{Sr}_{14-x}\text{Ca}_x\text{Cu}_{24}\text{O}_{41} \)
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 $\approx 200$ K only the chains contribute to magnetization (1).

- 60 % holes on the chain suggest dimer-configuration (figure); recent DFT calculations suggest irregular structure (2).

**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 $T \lesssim 20$ 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.

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

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

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

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

Different configurations should have a different energy offset (Coulomb, interaction with chain environment, . . .).

In-medium hole-hole Coulomb interaction:

\[
V(\vec{c}) = \frac{e^2}{4\pi \varepsilon_0 \varepsilon_r r_0} \frac{1}{2} \sum_{u \neq v} \frac{1}{|u - v|}
\]

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:
  $\bar{c}_{17,26} = sdddddddddd \ (\rho_h = 60.4 \%)$, $\bar{c}_{17,25} = tddddddd \ (\rho_h = 59.5 \%)$.

Chemical pressure due to Ca doping leads to partial charge transfer to the ladders (1). How many holes are transferred? 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 \( x \)!

Strange magnetization

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

- Origin of this contribution unknown!

$\text{Sr}_{14-x}\text{Ca}_x\text{Cu}_{24}\text{O}_{41}$ – Simulations with effective Hamiltonian I

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Sr$_{14-x}$Ca$_x$Cu$_{24}$O$_{41}$ – Simulations with effective Hamiltonian II

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**Sr$_{14-x}$Ca$_x$Cu$_{24}$O$_{41}$ – Open problems**

- Sr$_{14-x}$Ca$_x$Cu$_{24}$O$_{41}$ shows relatively large magnetization at $\approx 100$ 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 $\rho_h$ and others with smaller $\rho_h$. 

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Thank you very much for your attention.

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