Complete diagonalization studies of doped Heisenberg spin rings

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\[ \text{Sr}_{14-x}\text{Ca}_x\text{Cu}_{24}\text{O}_{41} \]
Introduction

- **Aim:** Understand thermodynamic properties of Sr$_{14-x}$Ca$_x$Cu$_{24}$O$_{41}$ as function of $T$ and $B$.

- **Needed:** Excitations involving charge motion. 
  ⇒ Screened electrostatic hole-hole repulsion has to be taken into account.

- **Means:** Complete diagonalization of effective Heisenberg Hamiltonian that depends parameterically on hole positions;

- **Conditions:** For $T < 200$ K only chain magnetically active.
Heisenberg Hamiltonian depends on spin-hole configuration $\vec{c}$

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

$J = (-64, -67, -70) \; \text{K}, \; J_\parallel = 5.8 \; \text{K}, \; J_{NN} = 8.7 \; \text{K}$

Debye-screened electrostatic hole-hole repulsion ($\lambda_D = \infty$ in the following)

$$V(\vec{c}) = \frac{e^2}{4\pi\epsilon_0 \epsilon_r \lambda_D} \sum_{u \neq v} \frac{1}{2} \text{exp} \left\{ -r_0 |u - v| / \lambda_D \right\}$$
Discussion of the model

- Ansatz is similar to a simple Born-Oppenheimer description where the electronic Hamiltonian (here spin Hamiltonian) depends parametrically on the positions of the classical nuclei (here hole positions);

- Heisenberg Hamiltonian can be diagonalized for each spin-hole configuration;

- Screened electrostatic potential energy is the additional energy offset:
  \[ E_\nu(\vec{c}) = E_\nu^{\text{Heisenberg}}(\vec{c}) + V(\vec{c}); \]

- All thermodynamic quantities can be evaluated without further approximation. Various spin-hole configuration may contribute according to the Boltzmann weight of their energy levels.
60% holes on the ring

\[ B=1 \text{ Tesla, } g=2.04 \]

\[ M \left( 10^{-3} \mu_B/Cu \right) \]

- \( \times \) exp: unkorr.
- \( + \) exp./.Curie-Weiss./.van Vleck
- \( \cdots \) 12,18, \( J=-64K, \varepsilon_r=1 \)
- \( - \) 12,18, \( J=-67K, \varepsilon_r=3 \)
- \( - \) 12,18, \( J=-70K, \varepsilon_r=4 \)
- \( - \) 12,18, \( J=-67K, \varepsilon_r=10 \)
60 % holes on the ring – discussion

- Ground state indeed dimer-configuration; nearest-neighbor Coulomb repulsion wouldn’t be sufficient;

- Magnetization curve strongly dependent on $J$ and $\epsilon_r$;

- For $\epsilon_r = 1$ only the dimer configuration contributes; for $\epsilon_r \gtrsim 3$ several hole configurations contribute with their respective magnetic spectra.

- It seems that $\epsilon_r \approx 3$, which is in good agreement with a dielectric constant of 3.3 found in Ref. [1];

Coulomb effects – levels

\[ \lambda_D = \infty, \text{ dielectric constant } \epsilon_r \text{ is the only free parameter.} \]
The high degeneracy of excited hole configurations plays an important role, since they substantially contribute to observables at low temperature although lying rather high in energy.
Rough sketch of the lowest transitions observable with inelastic neutron scattering. The arrow marks the singlet-triplet transition at about 135 K.
Outlook

- Model depends on four parameters \((J, J_{||}, J_{NN}, \epsilon_r)\);
- Refine model using the wealth of accumulated magnetization data;
- A direct measurement of the energy needed to excite hole movements would be very valuable since it would put additional restrictions on the range of the dielectric constant \(\epsilon_r\) – INS?
- Intermodel comparison with Hubbard and \(t-J\) model (Fatiha Ouchni). First results show that a strong Coulomb repulsion indeed leads to localized holes on the chain.
Thank you very much for your attention.

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