Complete diagonalization studies of doped Heisenberg spin rings

Jürgen Schnack

Department of Physics - University of Osnabrück
http://obelix.physik.uni-osnabrueck.de/~schnack/

Seminar, Osnabrück, October 26, 2004
Sorry, I am a bloody beginner on cuprates
A good strategy for a beginner certainly is to ignore everything that was done before!
Contents

- Introduction
- Model
- 60% holes on the ring
- Doped rings
- Coulomb effects
- Outlook

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

“telephone number compound” $\text{Sr}_{14}\text{Cu}_{24}\text{O}_{41}$ contains two magnetic one-dimensional structures, chains and ladders;

at low $T$ ladder subsystems magnetically inactive due to a large spin gap;

investigate magnetic properties of the chain subsystems with the help of a Heisenberg Hamiltonian that depends parametrically on hole positions;

screened electrostatic hole-hole repulsion is taken into account;

assume 60 % holes in the chain for the undoped compound;
Heisenberg Hamiltonian depends on spin-hole configuration $\vec{c}$

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

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

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

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

\begin{figure}
\centering
\includegraphics[width=\textwidth]{unilogo-m-rot.jpg}
\end{figure}

Jürgen Schnack, Complete diagonalization studies of doped Heisenberg spin rings
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];

Low-lying excited hole configurations

black dashes – dimer configuration, red x-symbols – one hole moved, green crosses – two holes moved

$E$ (K)

$N_g=12$, $N_h=18$, $\epsilon_r=3$
50 % – 60 % holes

\[ \frac{M}{B} \frac{k_B}{(g\mu_B)^2/N_{\text{tot}}} (10^{-3}/K) \]

\[ B=1 \text{ Tesla} \]

Jürgen Schnack, Complete diagonalization studies of doped Heisenberg spin rings
\[ \lambda_D = \infty, \text{ dielectric constant } \epsilon_r \text{ is the only free parameter.} \]
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.

Special thanks to

- Dr. Rüdiger Klingeler for endless discussions and for providing magnetization data;
- Prof. Dr. Bernd Büchner for valuable discussions;
- Fatiha Ouchni for drawing my attention to the existing literature and for challenging my ideas.