Complete diagonalization studies of doped Heisenberg spin rings

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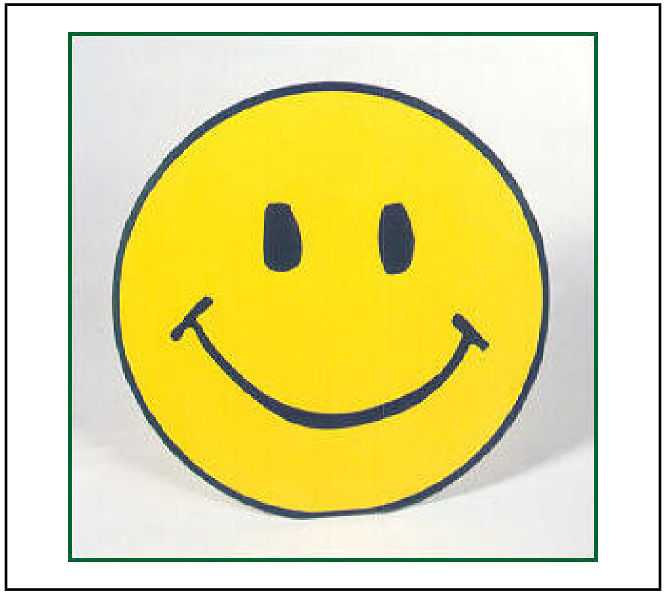
IFW, Dresden, July 2, 2004

Sorry, I am a bloody beginner on cuprates

A good strategy for a beginner certainly is to ignore everything that was done before!



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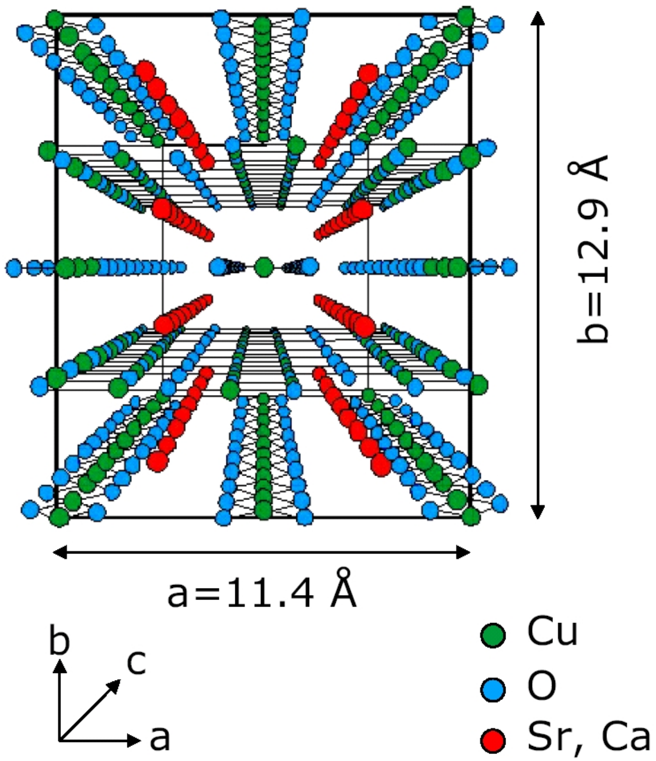

$Sr_{14-x}Ca_xCu_{24}O_{41}$,
Tomislav Ivek, Zagreb

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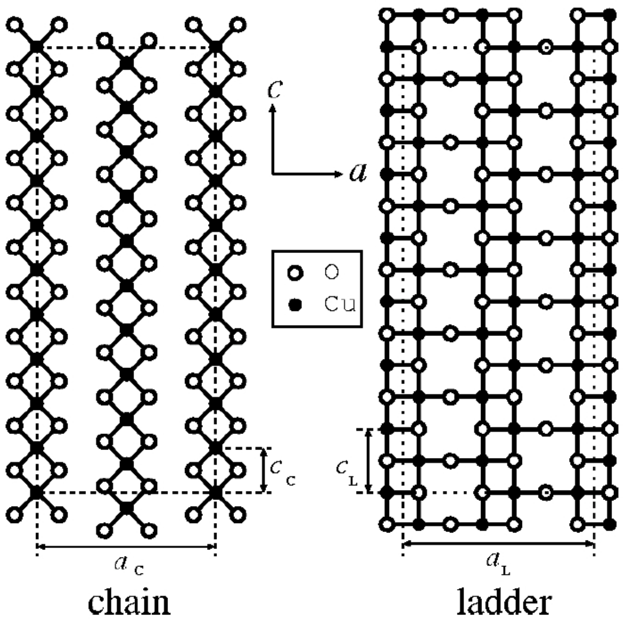
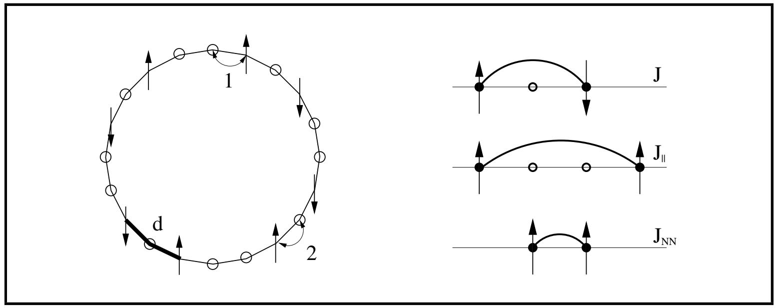
Introduction



Fukuda, Mizuki, Matsuda

- "telephone number compound" $Sr_{14}Cu_{24}O_{41}$ 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;

Model



Heisenberg Hamiltonian depends on spin-hole configuration

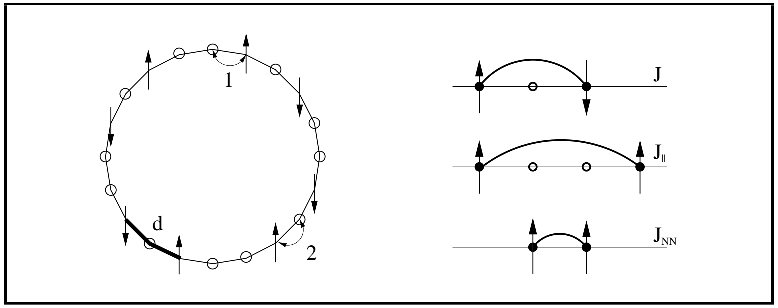
$$\underset{\sim}{H}(\vec{c}) \quad = \quad -\sum_{u,v} J_{uv}(\vec{c})\ \underset{\sim}{\vec{s}}(u) \cdot \underset{\sim}{\vec{s}}(v)$$

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

screened electrostatic hole-hole repulsion

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

Discussion of the model



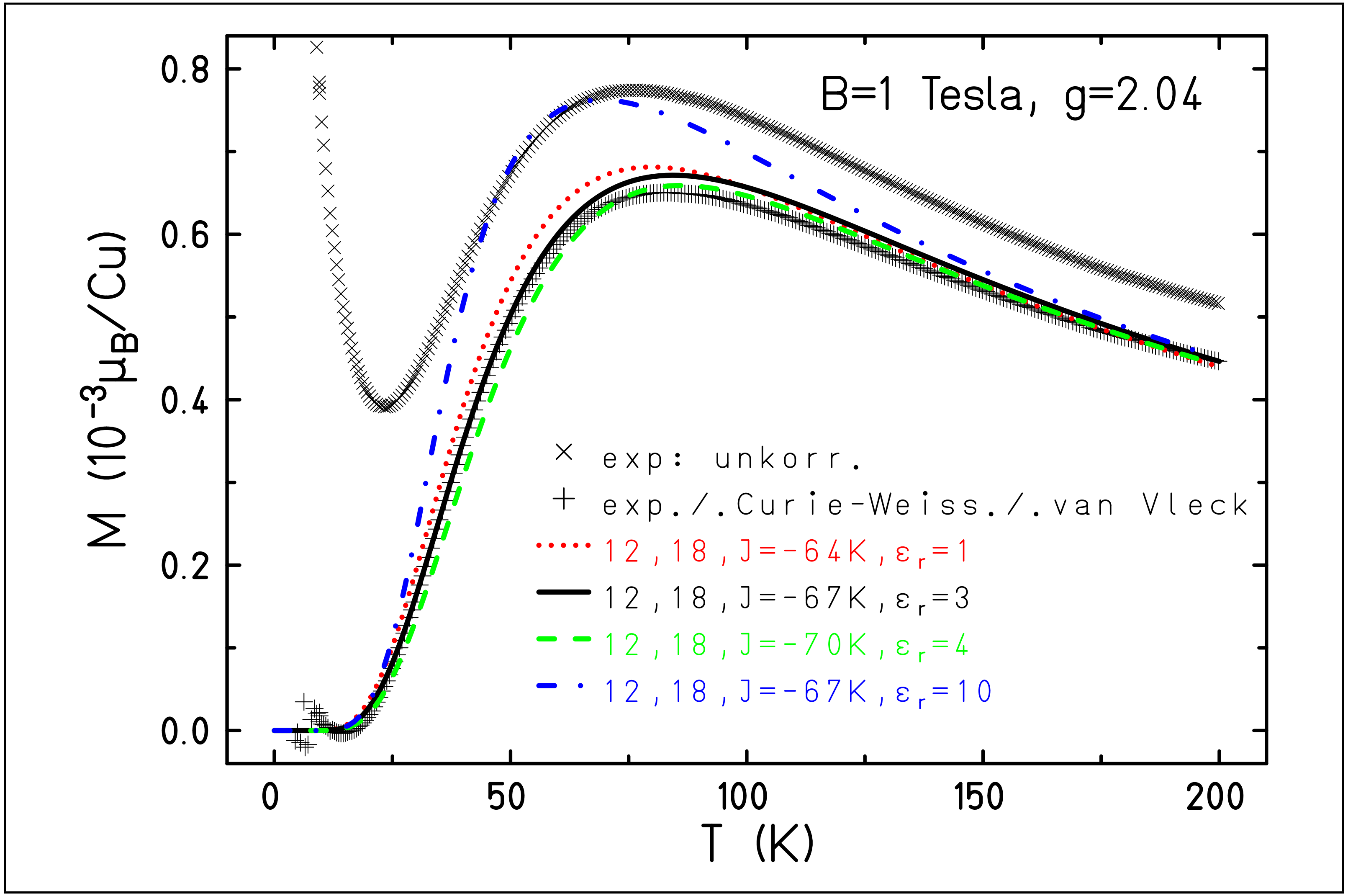
- Ansatz is similar to a simple Born-Oppenheimer description where the electronic Hamiltonian (here spin Hamiltonian) depends parametrically on the positions of the classical nuclei (here hole positions);

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

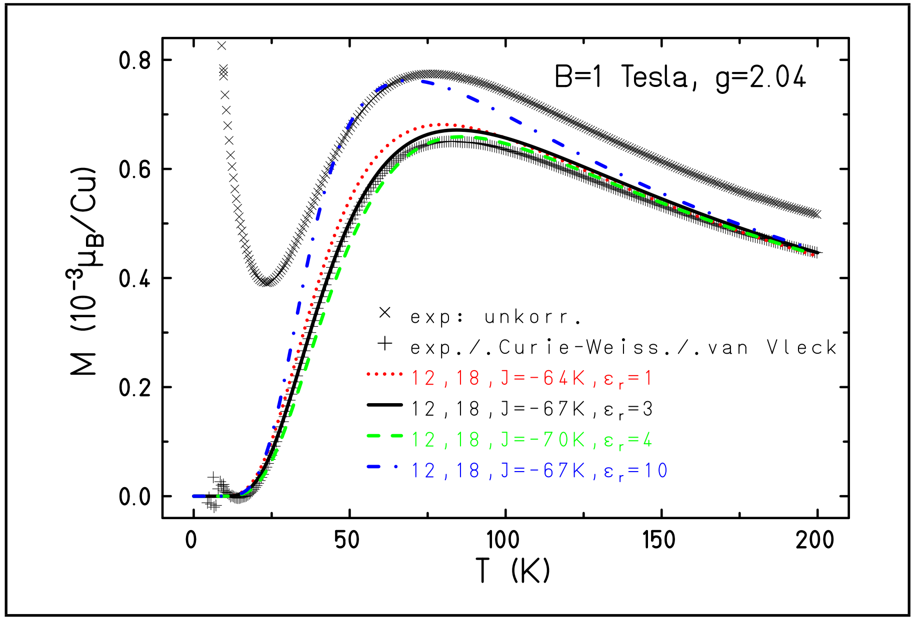
- Screened electrostatic potential energy is the additional energy offset: $E_\nu(\vec{c}) = E_\nu^{\text{Heisenberg}}(\vec{c}) + V(\vec{c})$;

- 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



60 % holes on the ring – discussion

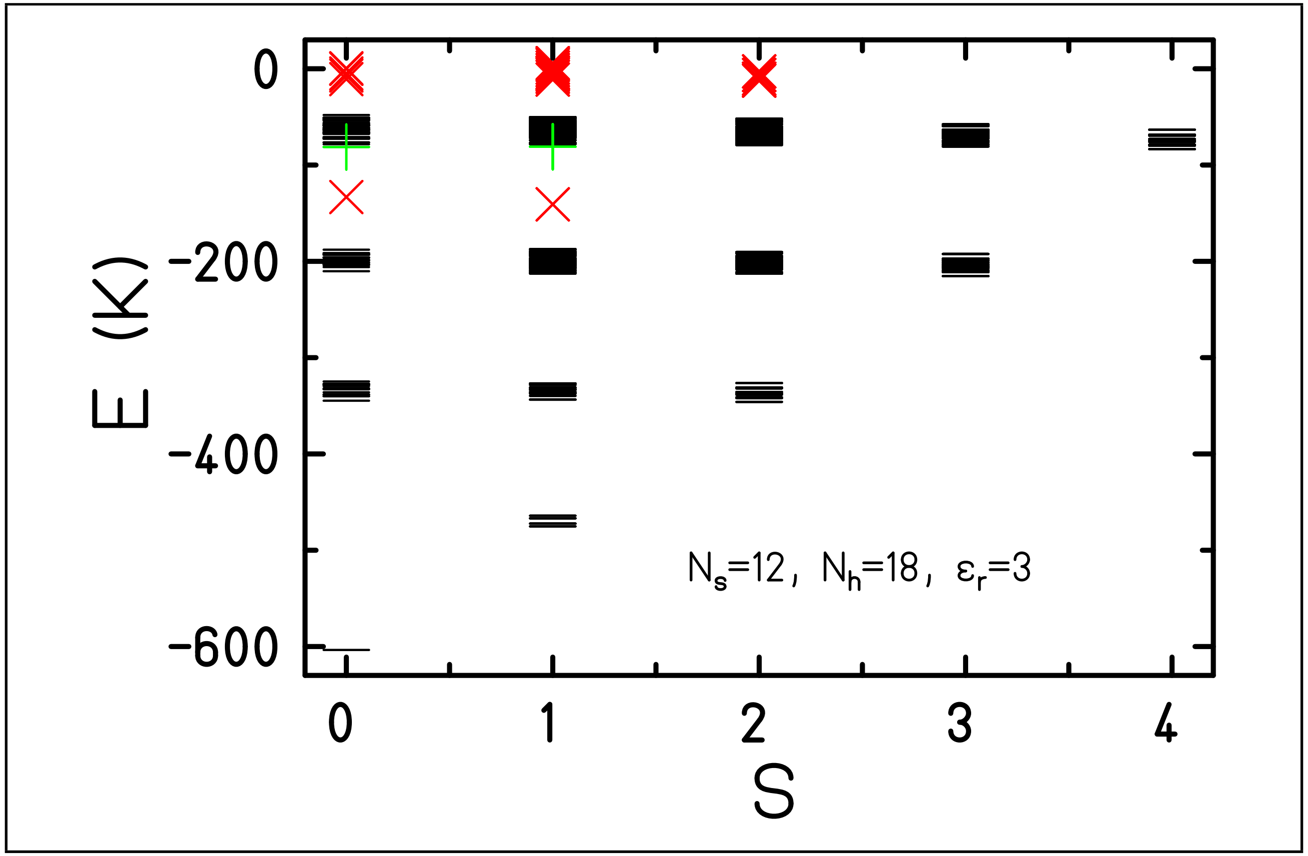


- Ground state indeed dimer-configuration; nearest-neighbor Coulomb repulsion wouldn't be sufficient;
- Magnetization curve strongly dependent on J and ϵ_r;
- For $\epsilon_r = 1$ only the dimer configuration contributes; for $\epsilon_r \gtrsim 3$ several hole configurations contribute with their respective 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];

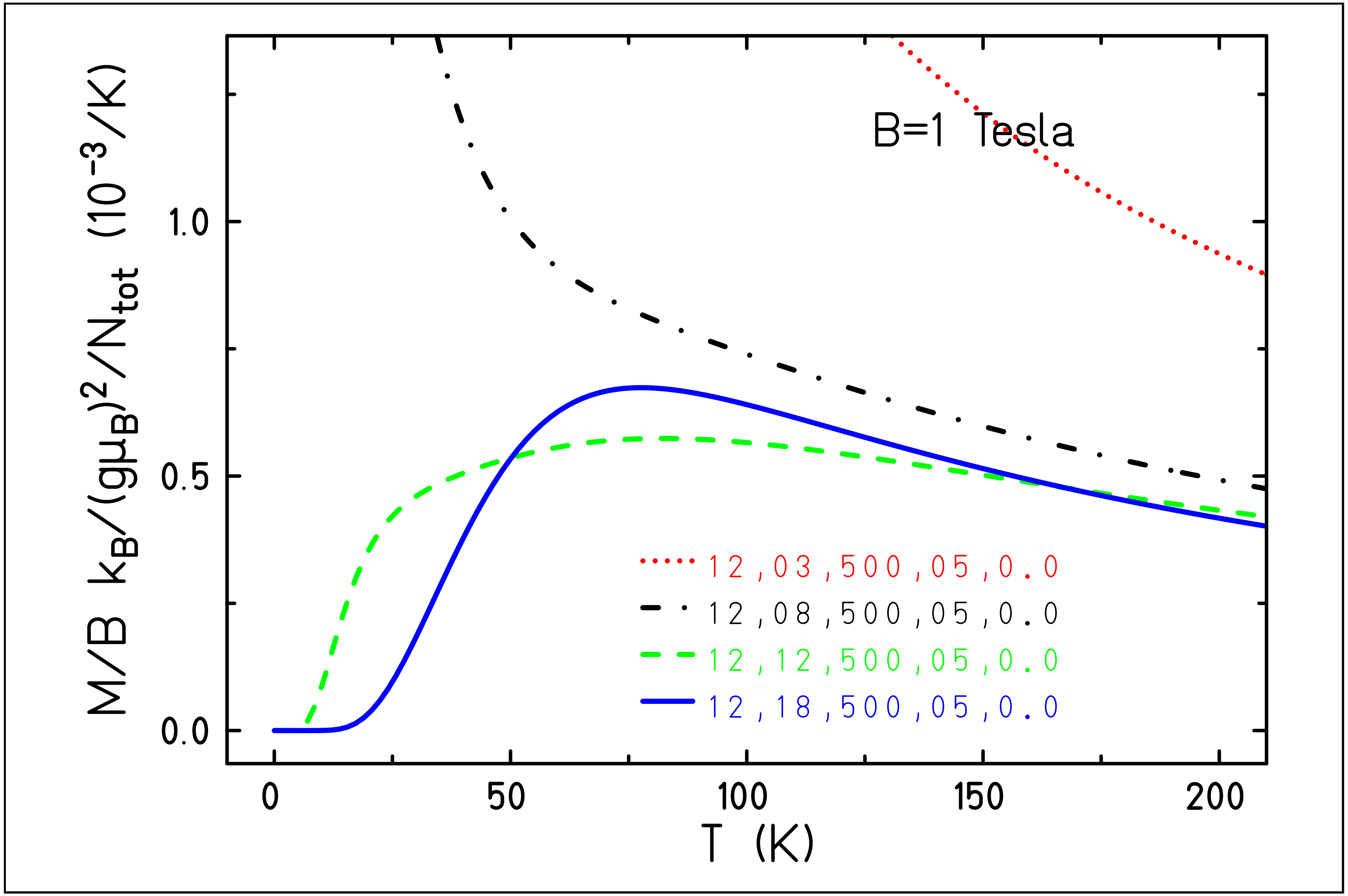
[1] Y. Mizuno, T. Tohyama, and S. Maekawa, Phys. Rev. B **58** (1998) 14713

Low-lying excited hole configurations

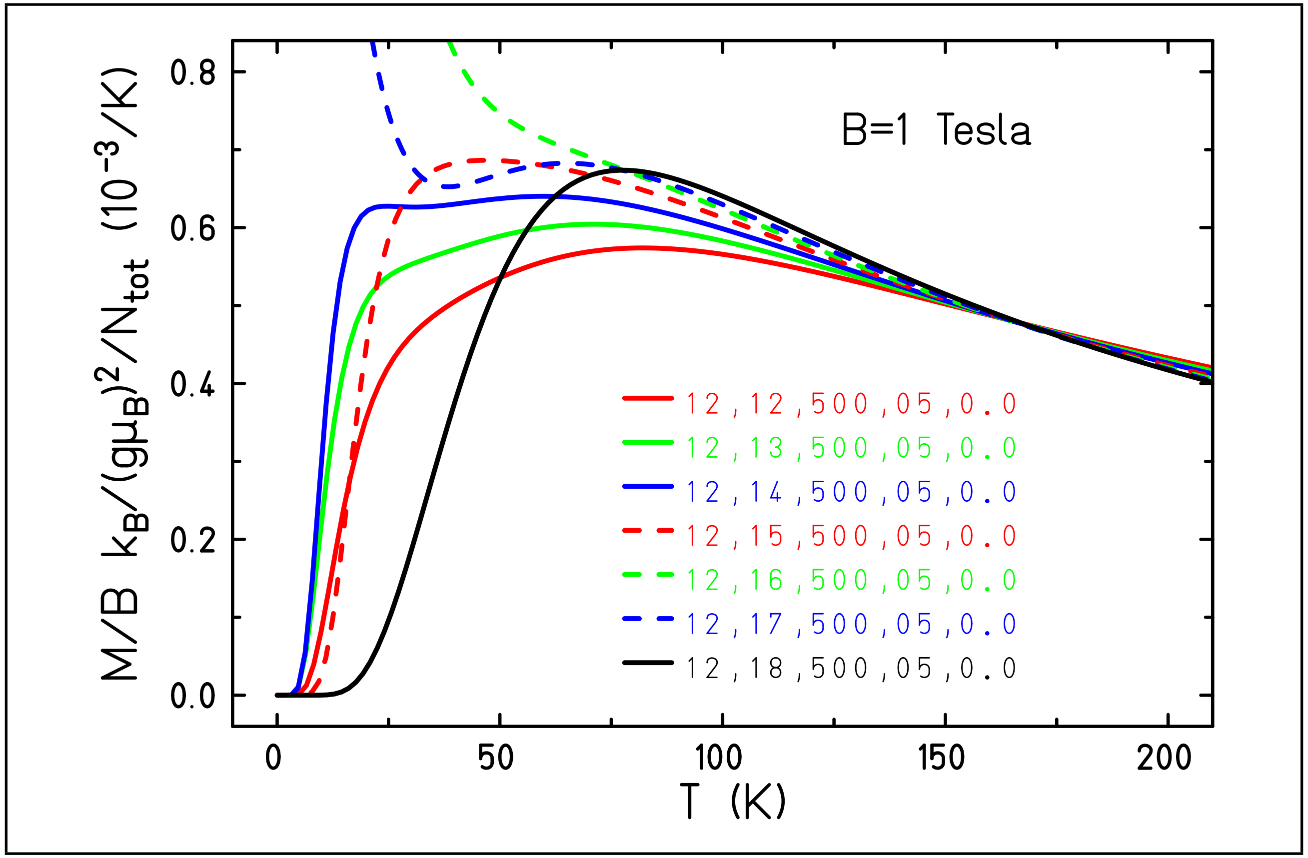


black dashes – dimer configuration, red x-symbols – one hole moved, green crosses – two holes moved

Doped rings with less than 60 % holes

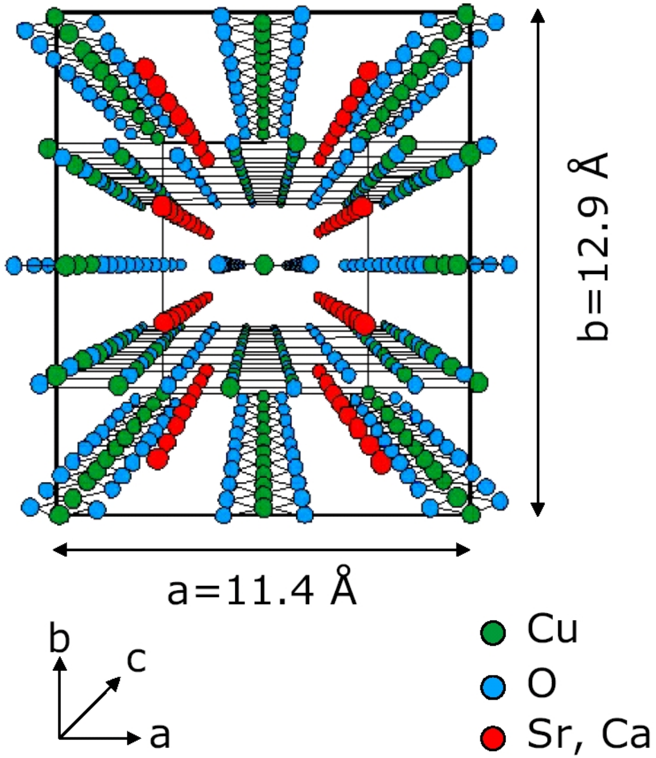


50 % – 60 % holes



Very preliminary! Strong finite size effects are possible for these hole fractions due to the very unregular struture.

Outlook



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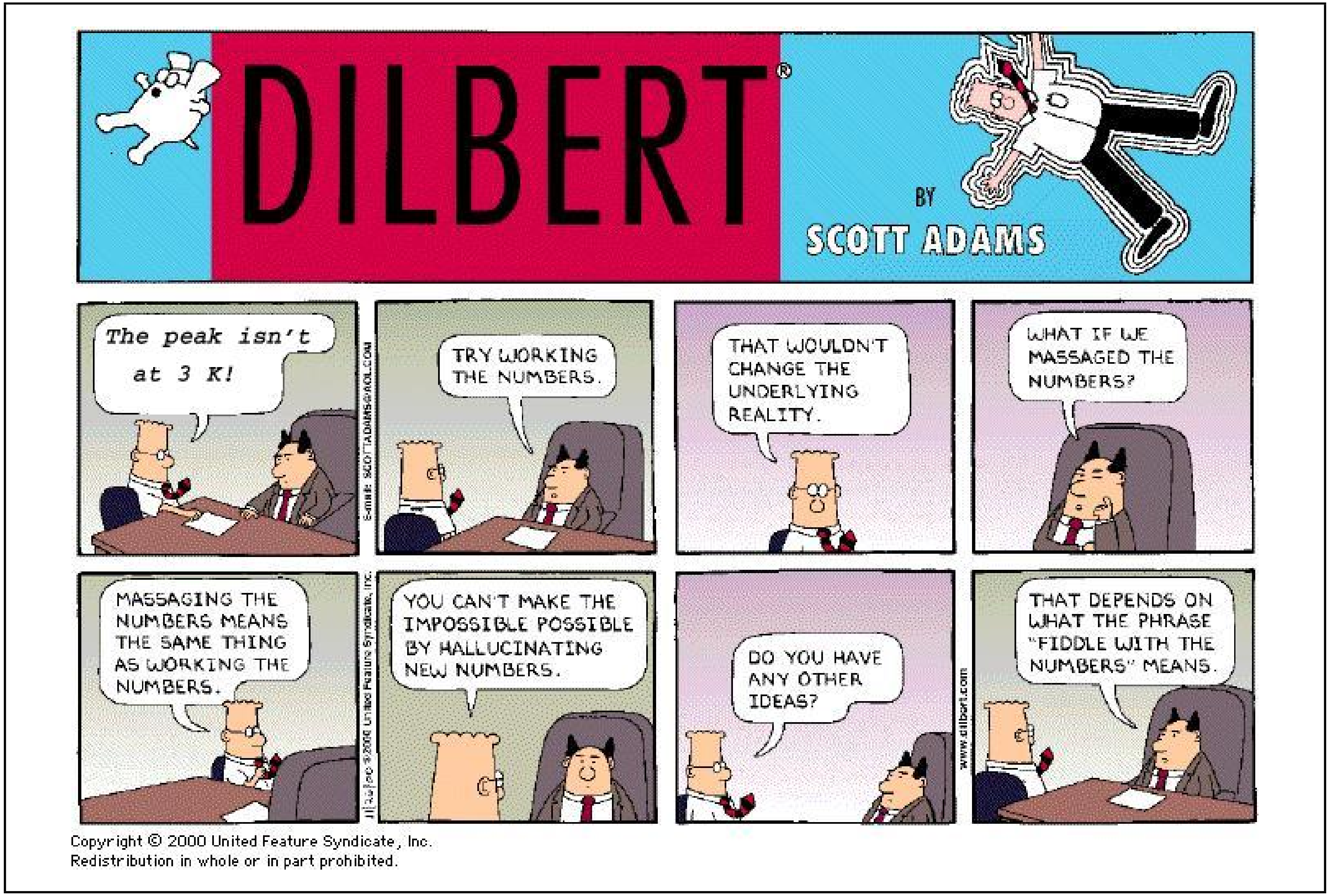
- Model depends on four parameters $(J, J_{\|}, J_{NN}, \epsilon_r)$;
- Refine model using the wealth of accumulated magnetization data;
- A direct measurement of the energy needed to excite hole movements would be very valuable since it would put additional restrictions on the range of the dielectric constant ϵ_r;
- It is our hope that a refined model will allow more insight into the interplay of charge order and magnetism.

Thank you very much for your attention.

Special thanks

- Dr. Rüdiger Klingeler for endless discussions and for providing magnetization data;
- Prof. Dr. Bernd Büchner for valuable discussions (will qualify for *endless* later today).

Guess, who is Rüdiger who is Jürgen?



Open questions

1. Is it possible that $J_{||}$ is antiferromagnetic?

2. Why is $N_D = 0.0777$ and not $N_D = 2/24 = 0.08333$?

3. Could it be that too much is substracted from the original magnetization data? How strict are the Curie-Weiss and van Vleck corrections of the experimental data?

4. Any ideas about the gap to one-hole movements?

5.