

# Complete diagonalization studies of doped Heisenberg spin rings

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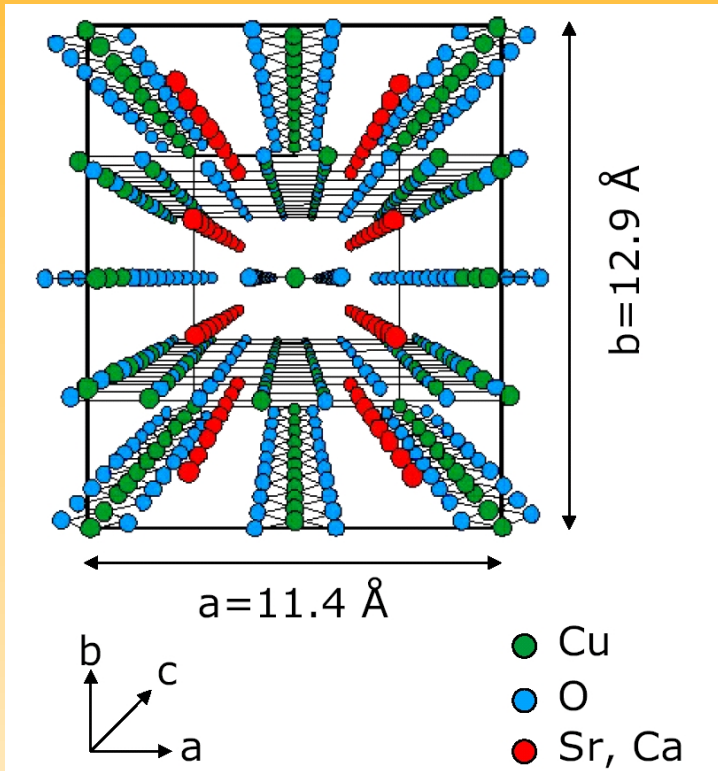
# Sorry, I am a bloody beginner on cuprates



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



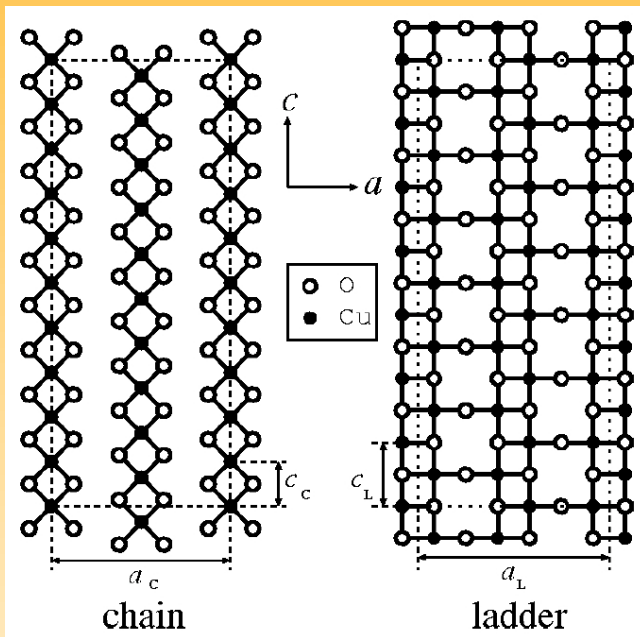
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$\text{Sr}_{14-x}\text{Ca}_x\text{Cu}_{24}\text{O}_{41}$ ,  
 Tomislav Ivek, Zagreb

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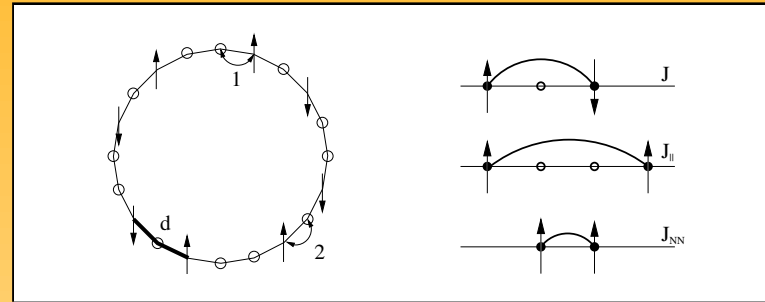
# Introduction



Fukuda, Mizuki, Matsuda

- “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;

# Model



Heisenberg Hamiltonian depends on spin-hole configuration

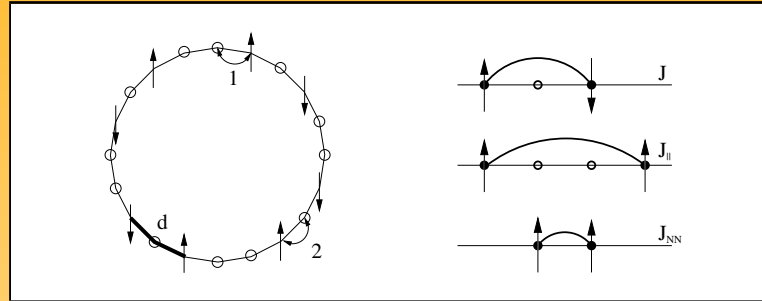
$$\tilde{H}(\vec{c}) = - \sum_{u,v} J_{uv}(\vec{c}) \vec{s}(u) \cdot \vec{s}(v)$$

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

screened electrostatic hole-hole repulsion

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

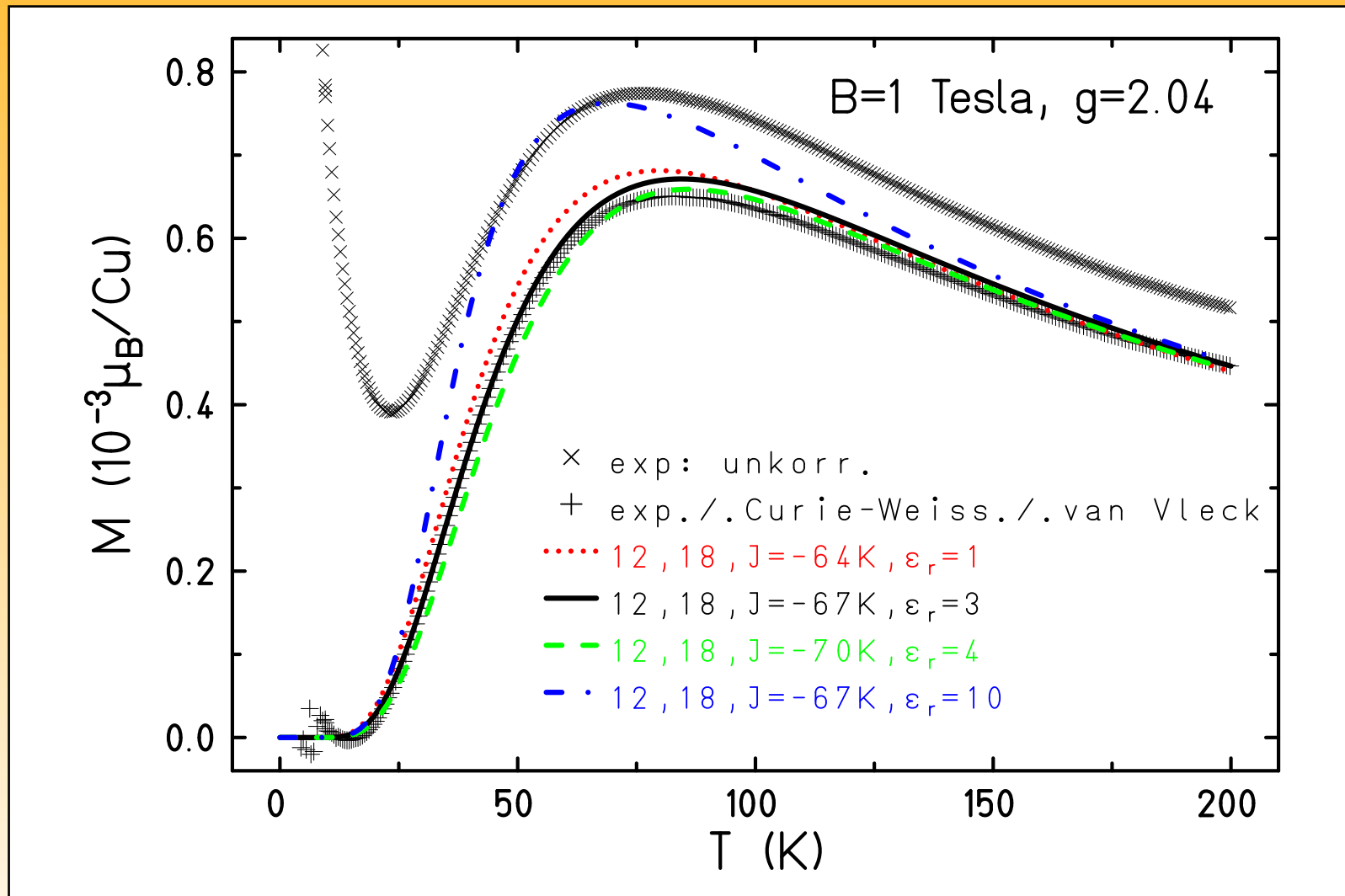
# Discussion of the model



- 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:  

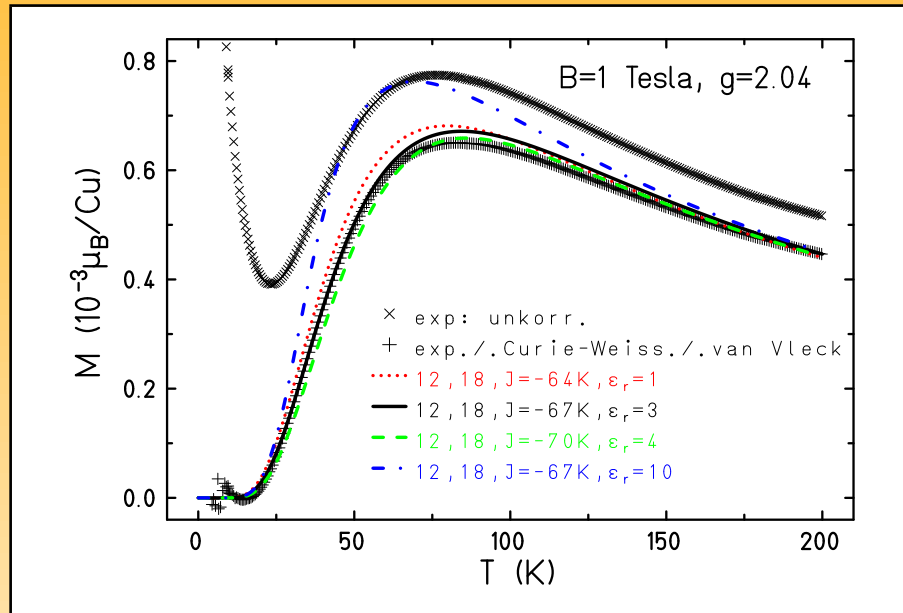
$$E_\nu(\vec{c}) = E_\nu^{\text{Heisenberg}}(\vec{c}) + V(\vec{c});$$
- All thermodynamic quantities can be evaluated without further approximation. Various spin-hole configuration may contribute according to the Boltzmann weight of their energy levels.

# 60 % holes on the ring





## 60 % holes on the ring – discussion

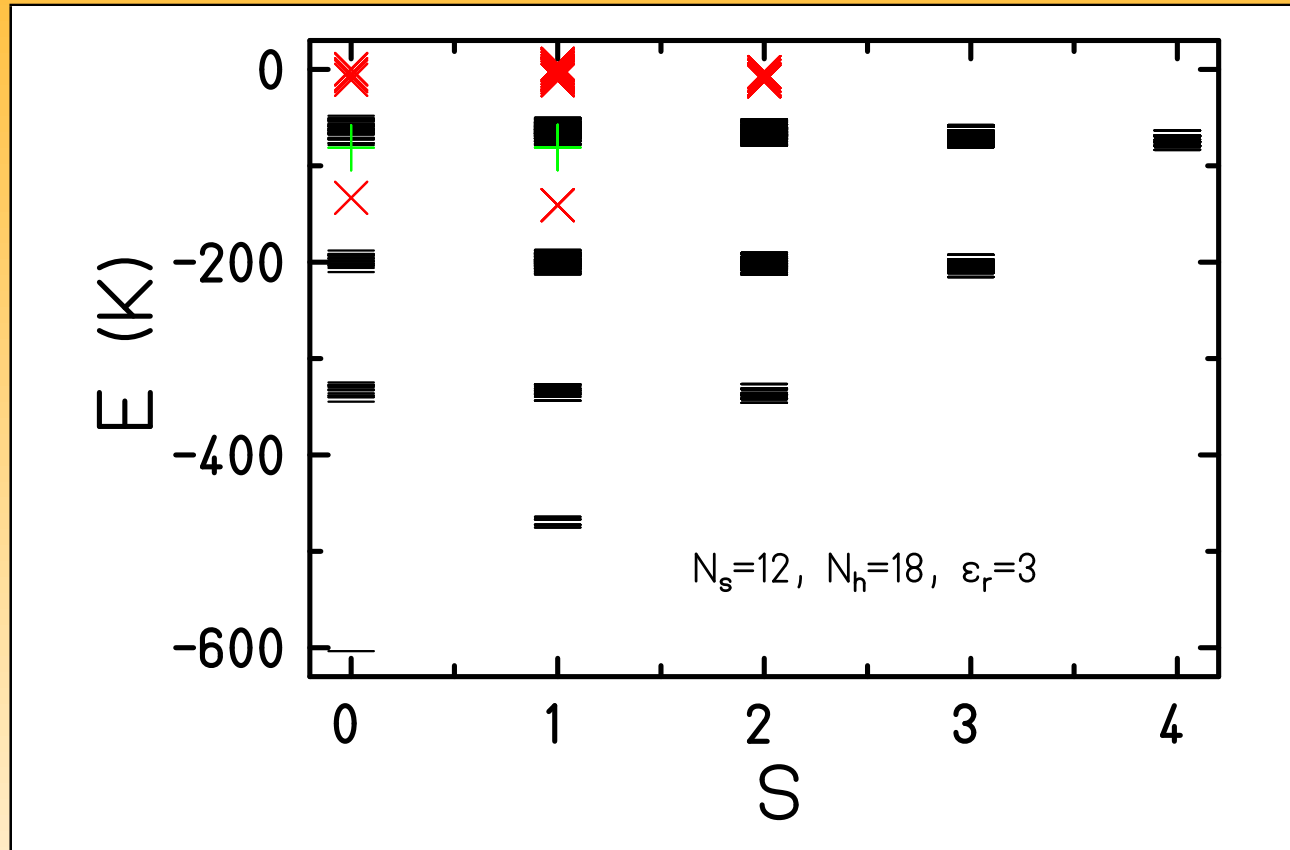


- Ground state indeed dimer-configuration; nearest-neighbor Coulomb repulsion wouldn't be sufficient;
- Magnetization curve strongly dependent on  $J$  and  $\epsilon_r$ ;
- For  $\epsilon_r = 1$  only the dimer configuration contributes; for  $\epsilon_r \gtrsim 3$  several hole configurations contribute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

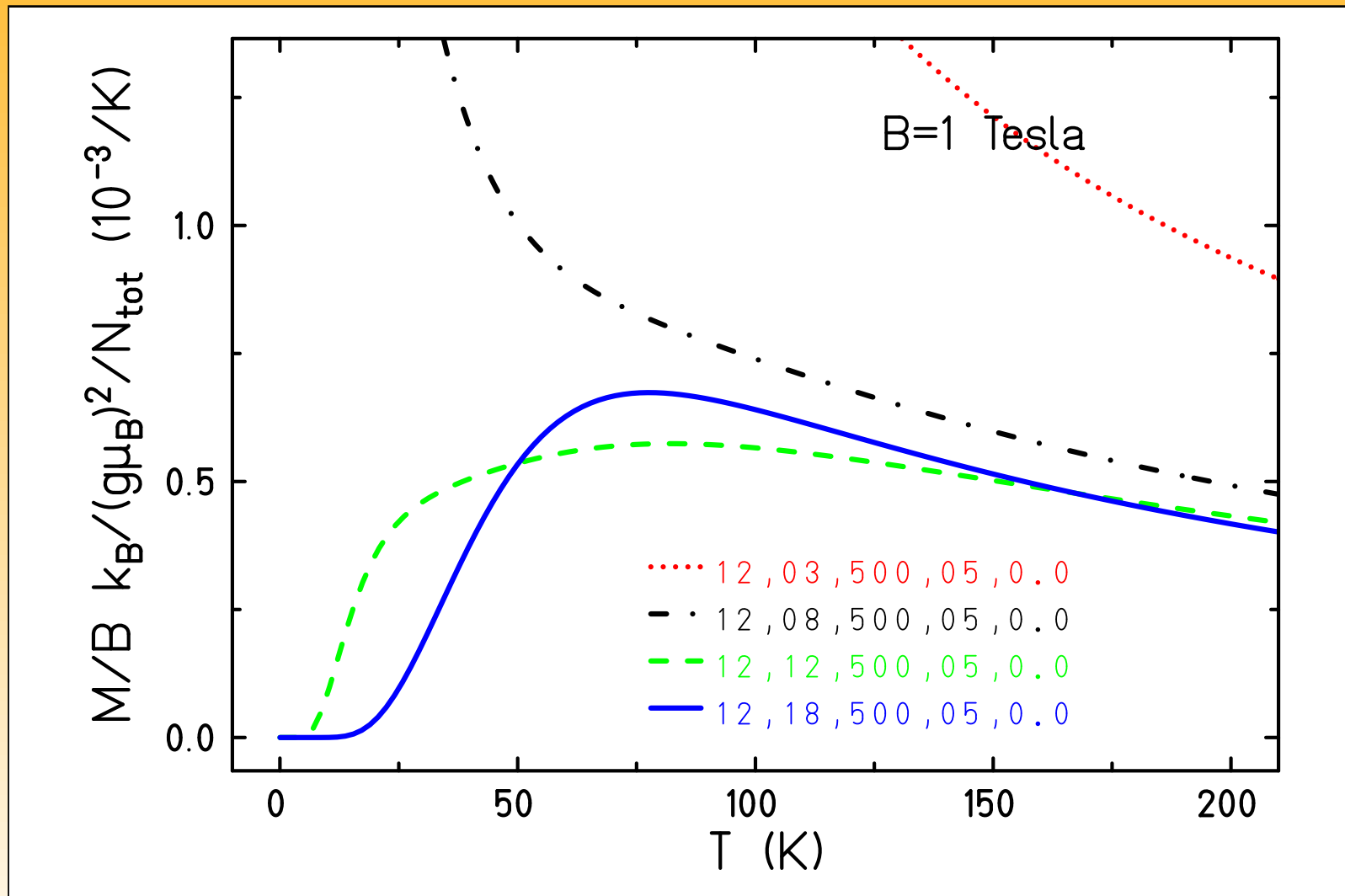
[1] Y. Mizuno, T. Tohyama, and S. Maekawa, Phys. Rev. B **58** (1998) 14713

# Low-lying excited hole configurations

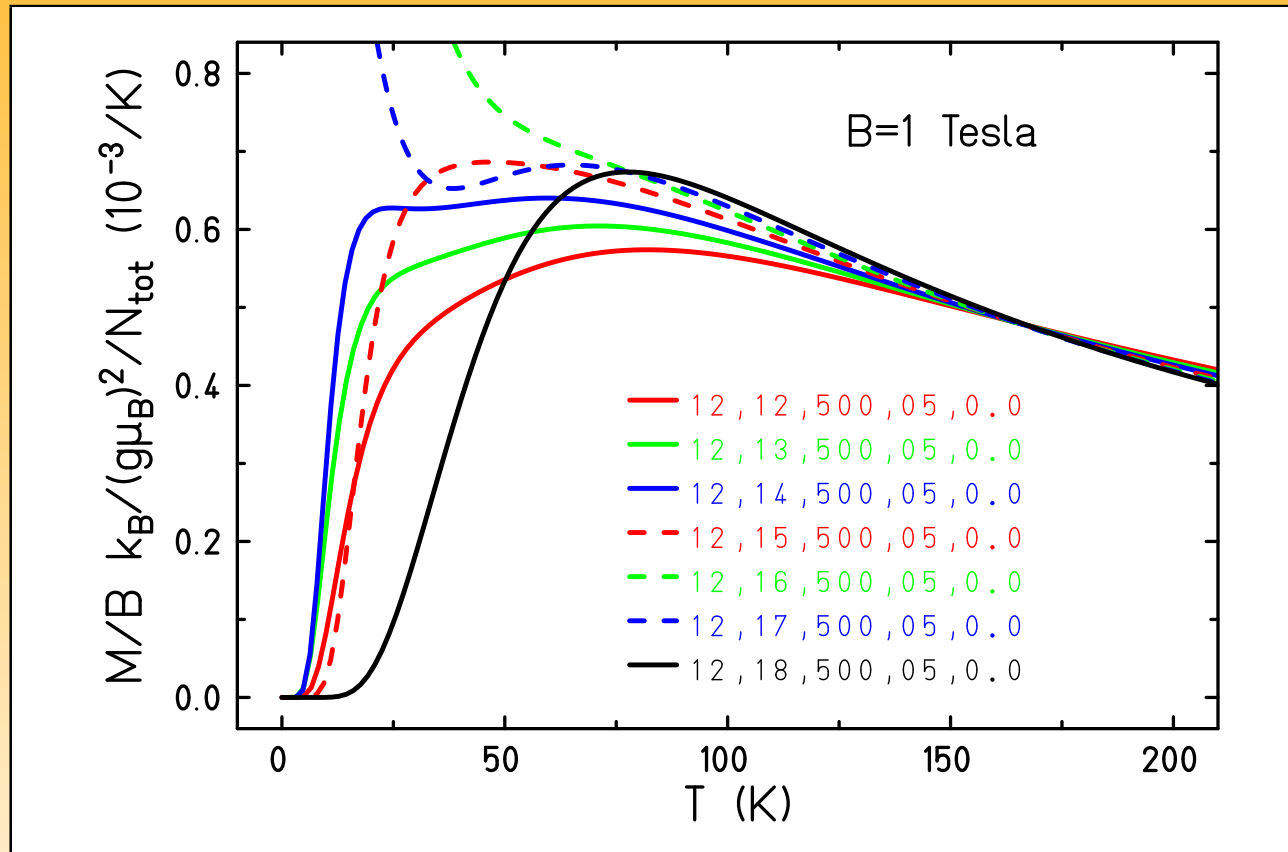


black dashes – dimer configuration, red x-symbols – one hole moved, green crosses – two holes moved

# Doped rings with less than 60 % holes

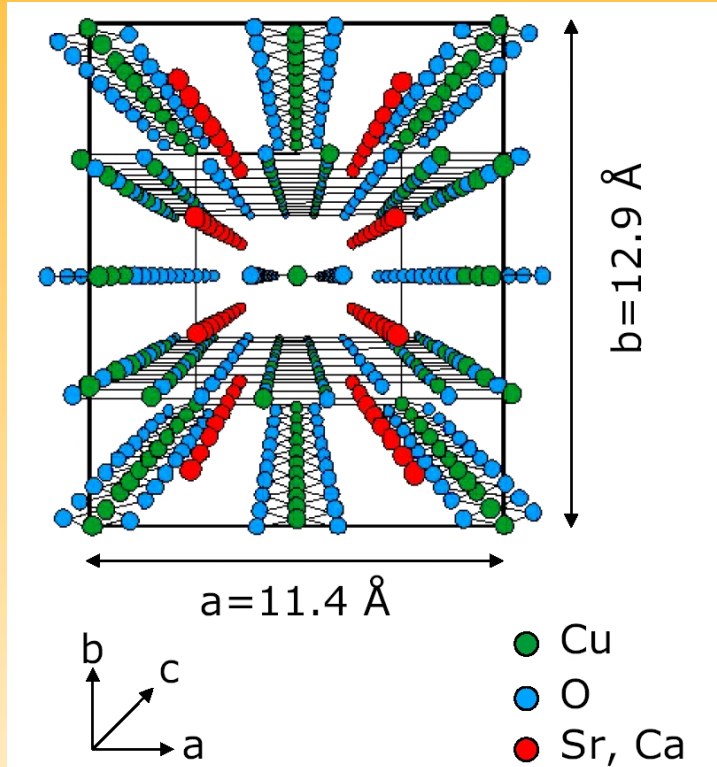


# 50 % – 60 % holes



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

# Outlook



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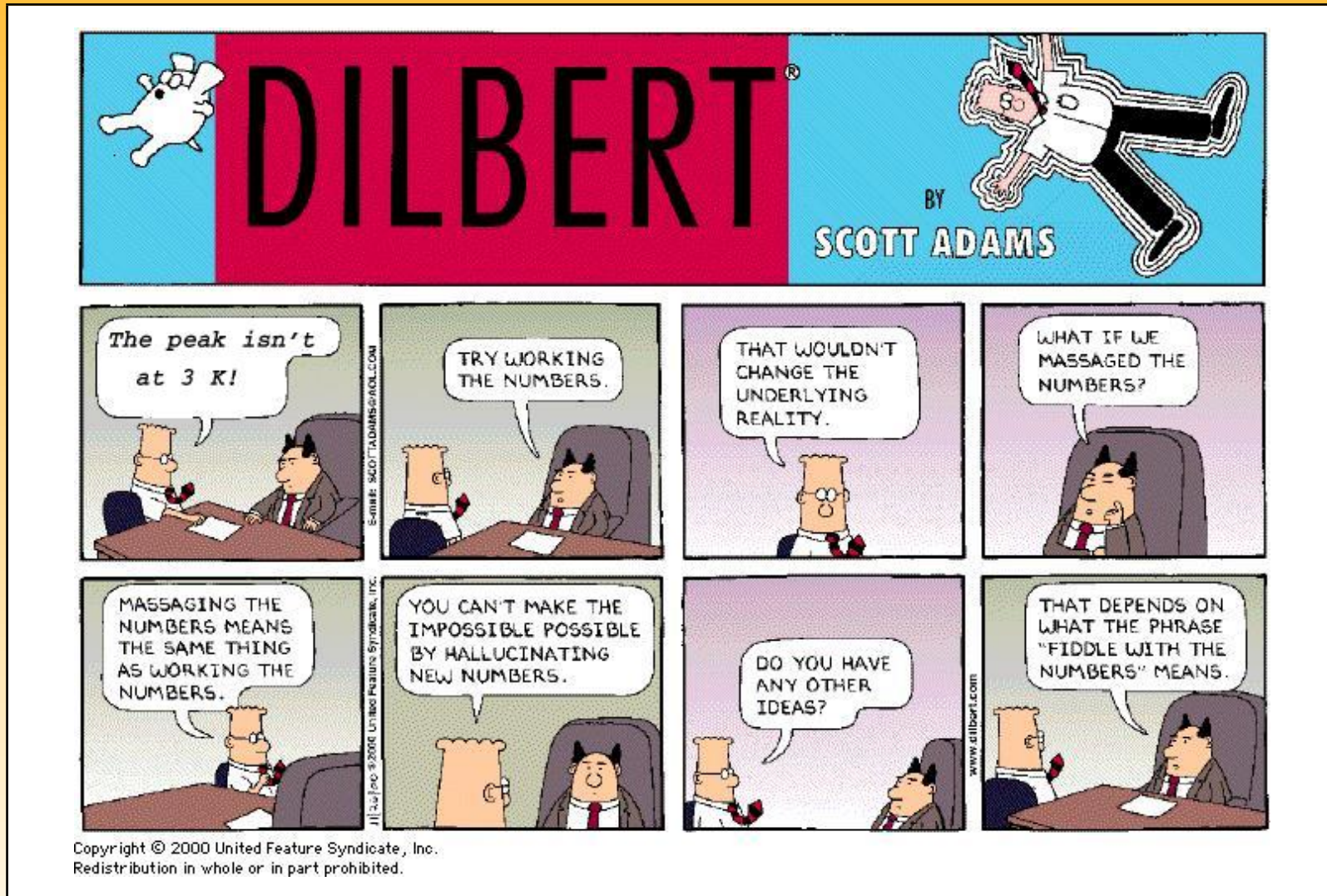
- Model depends on four parameters ( $J, J_{\parallel}, J_{NN}, \epsilon_r$ );
- Refine model using the wealth of accumulated magnetization data;
- A direct measurement of the energy needed to excite hole movements would be very valuable since it would put additional restrictions on the range of the dielectric constant  $\epsilon_r$ ;
- 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?



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# Open questions

1. Is it possible that  $J_{\parallel}$  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 subtracted 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.