

Complete diagonalization studies of doped Heisenberg spin rings

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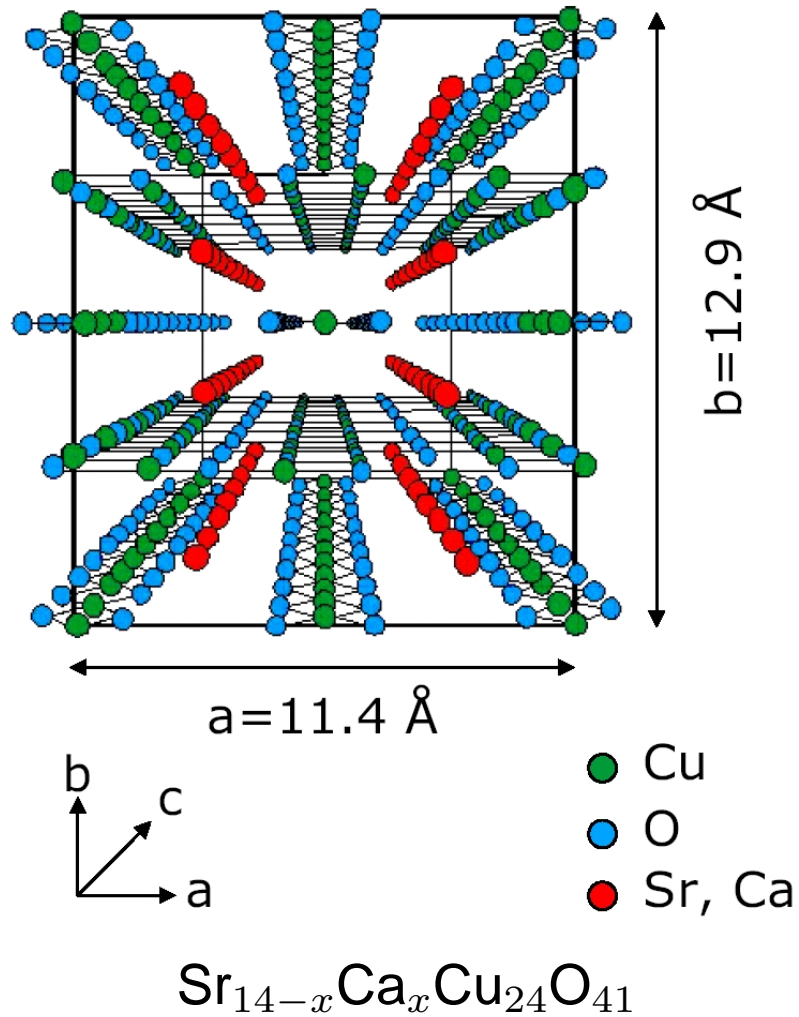
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DPG Frühjahrstagung

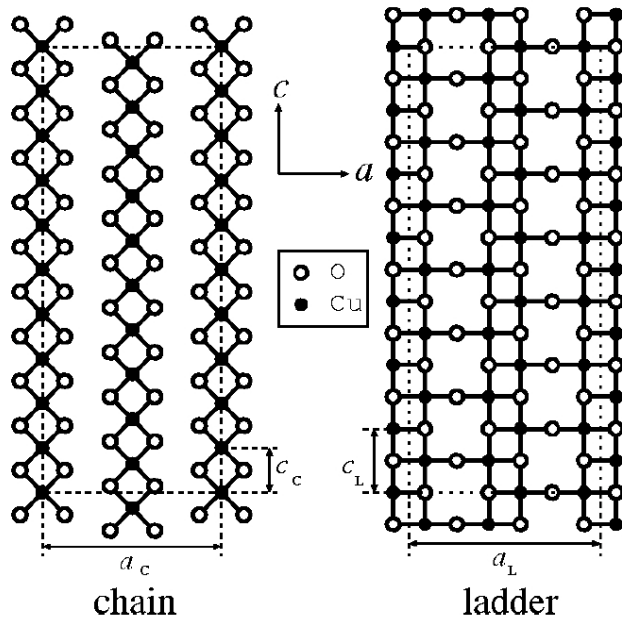
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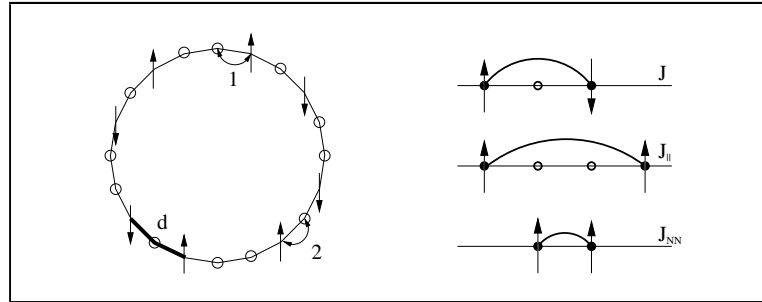
Introduction



Fukuda, Mizuki, Matsuda

- **Aim:** Understand thermodynamic properties of $\text{Sr}_{14-x}\text{Ca}_x\text{Cu}_{24}\text{O}_{41}$ as function of T and B .
- **Needed:** Excitations involving charge motion.
 \Rightarrow Screened electrostatic hole-hole repulsion has to be taken into account.
- **Means:** Complete diagonalization of effective Heisenberg Hamiltonian that depends parametrically on hole positions;
- **Conditions:** For $T < 200$ K only chain magnetically active.

Model



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

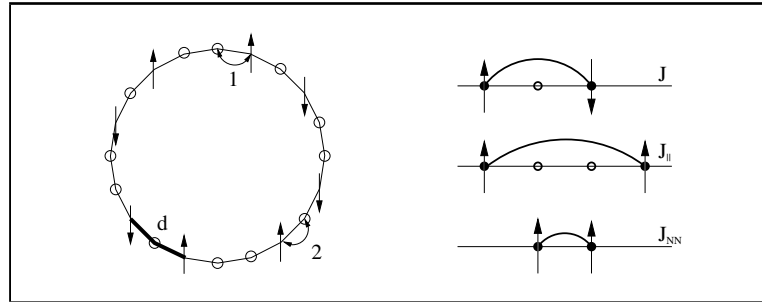
$$\tilde{H} = \sum_{\vec{c}} \left(\tilde{H}(\vec{c}) + V(\vec{c}) \right) \quad , \quad \tilde{H}(\vec{c}) = - \sum_{u,v} J_{uv}(\vec{c}) \vec{s}(u) \cdot \vec{s}(v)$$

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

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

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

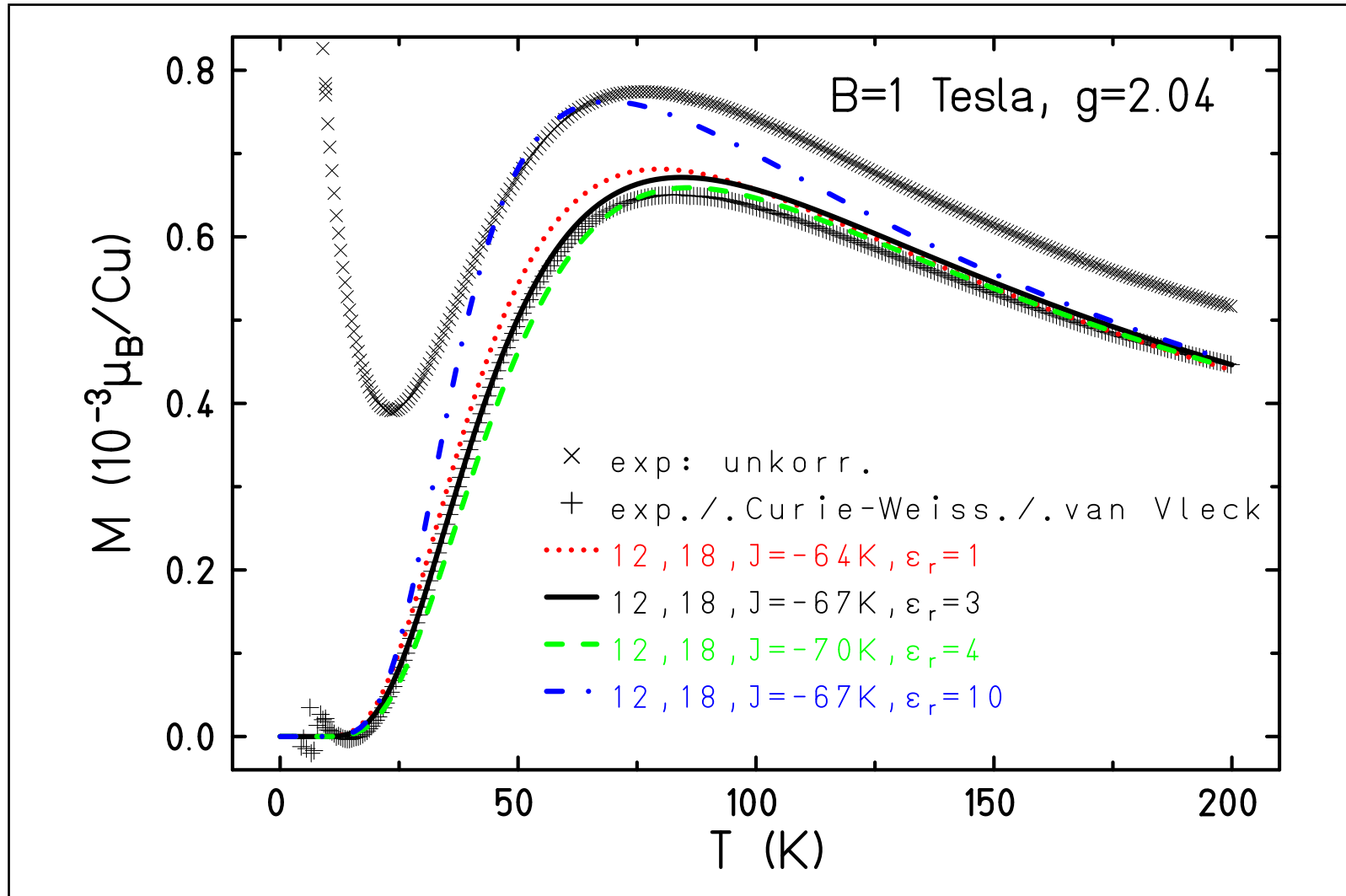
Discussion of the model



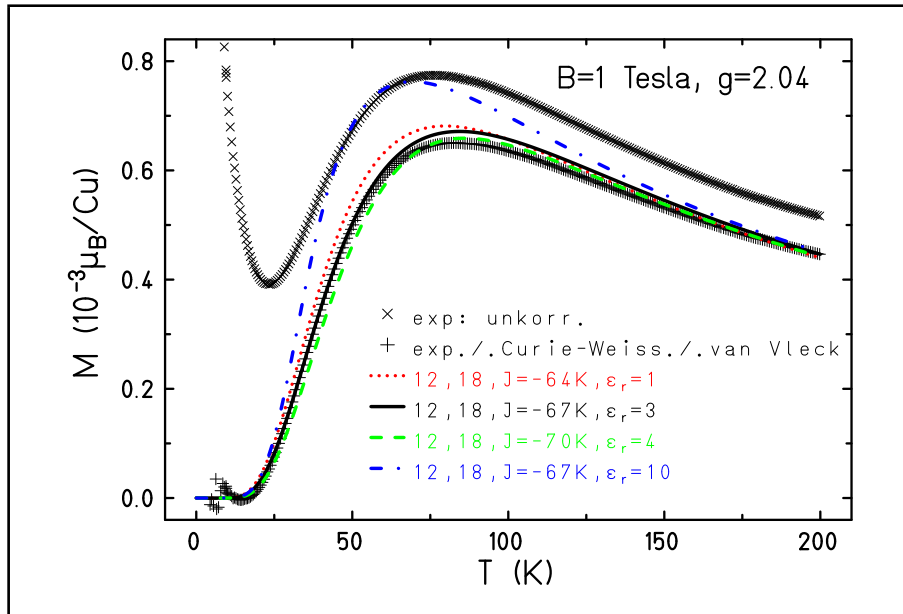
- Ansatz is similar to a simple Born-Oppenheimer description where the electronic Hamiltonian (here spin Hamiltonian) depends parametrically on the positions of the classical nuclei (here hole positions);
- Heisenberg Hamiltonian can be diagonalized for each spin-hole configuration;
- Screened electrostatic 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

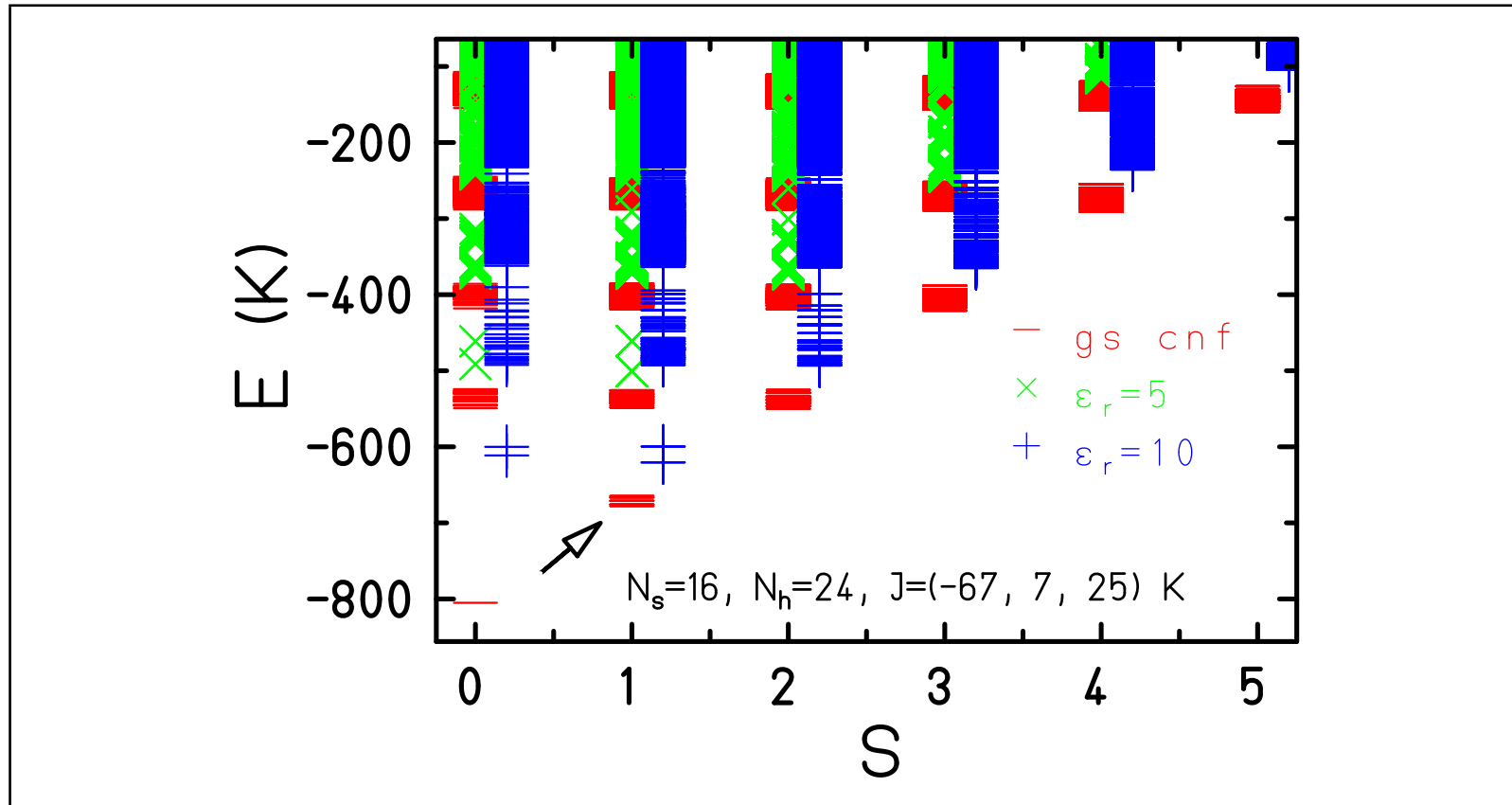


- Ground state indeed dimer-configuration; nearest-neighbor Coulomb repulsion wouldn't be sufficient;
- Magnetization curve strongly dependent on J and ϵ_r ;
- For $\epsilon_r = 1$ only the dimer configuration contributes; for $\epsilon_r \gtrsim 3$ several hole configurations contribute with their respective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

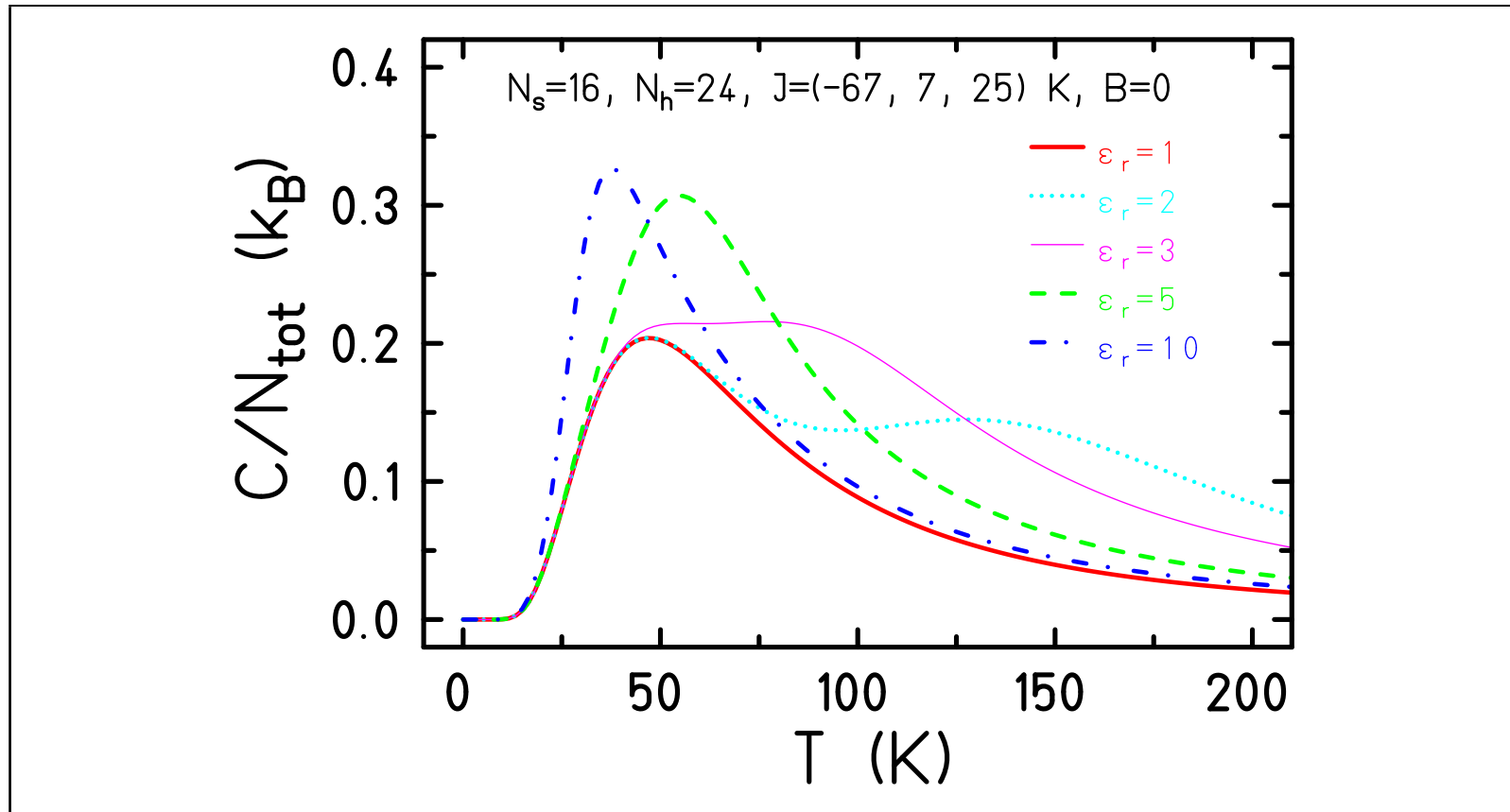
[1] Y. Mizuno, T. Tohyama, and S. Maekawa, Phys. Rev. B **58** (1998) 14713

Coulomb effects – levels



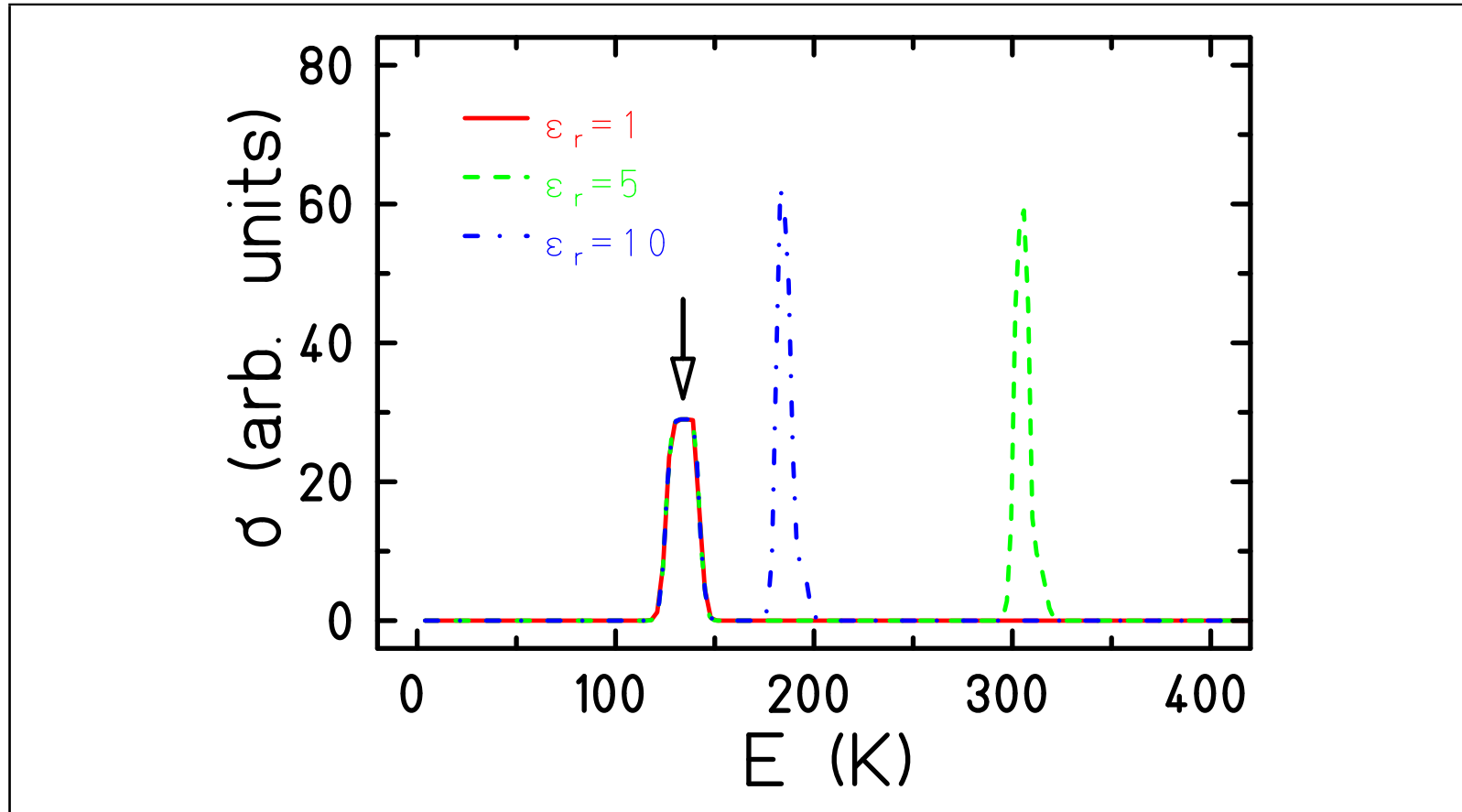
$\lambda_D = \infty$, dielectric constant ϵ_r is the only free parameter.

Coulomb effects – specific heat



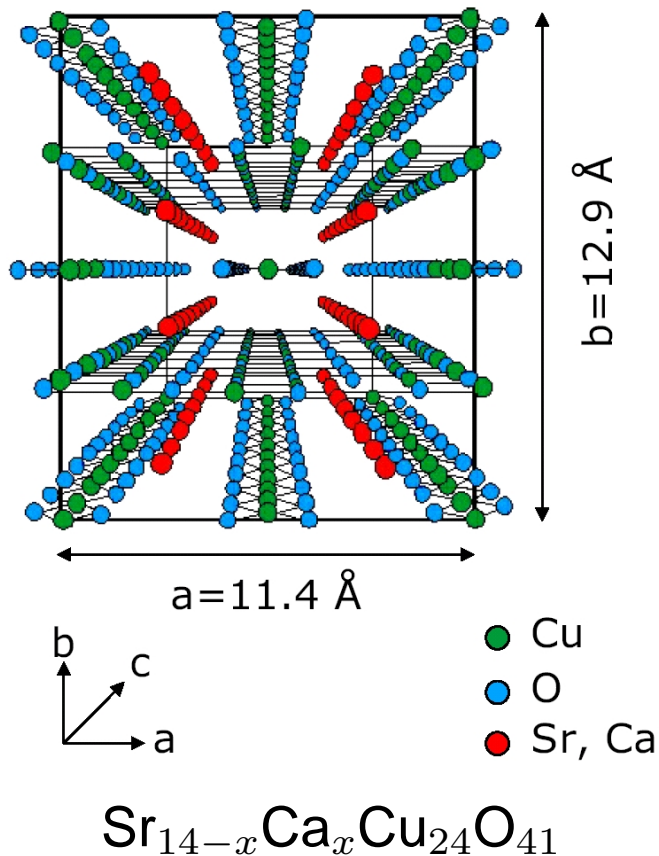
The high degeneracy of excited hole configurations plays an important role, since they substantially contribute to observables at low temperature although lying rather high in energy.

Coulomb effects – inelastic neutron scattering



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 ($J, J_{\parallel}, J_{NN}, \epsilon_r$);
- 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 ϵ_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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