Complete diagonalization studies of doped Heisenberg spin rings

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DPG Frühjahrstagung

Berlin, March 8th 2005

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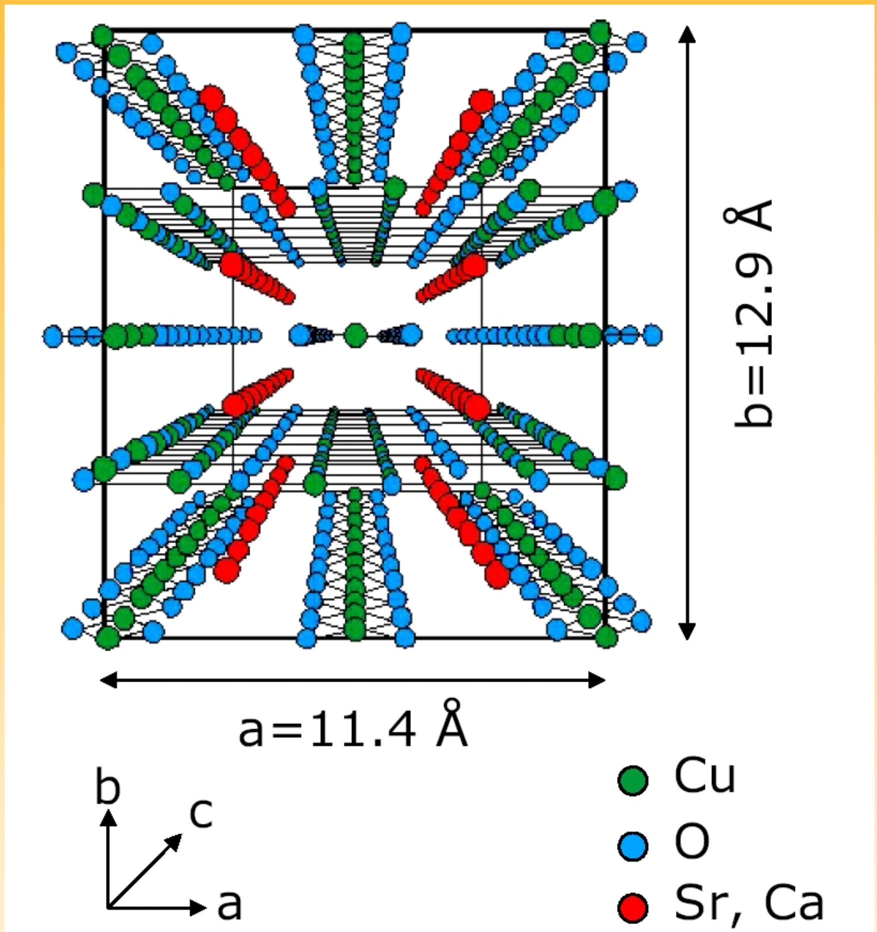

$Sr_{14-x}Ca_xCu_{24}O_{41}$

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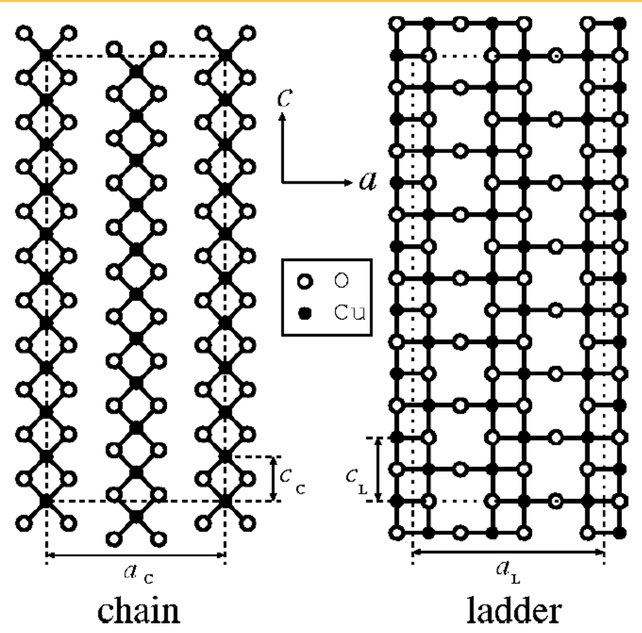
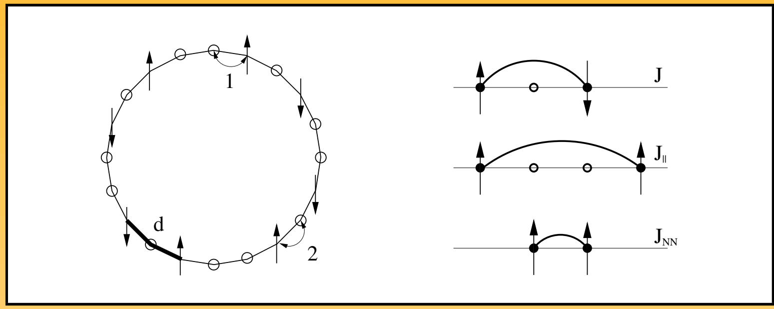
Introduction



Fukuda, Mizuki, Matsuda

- Aim: Understand thermodynamic properties of $Sr_{14-x}Ca_xCu_{24}O_{41}$ 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 $\vec{c}$

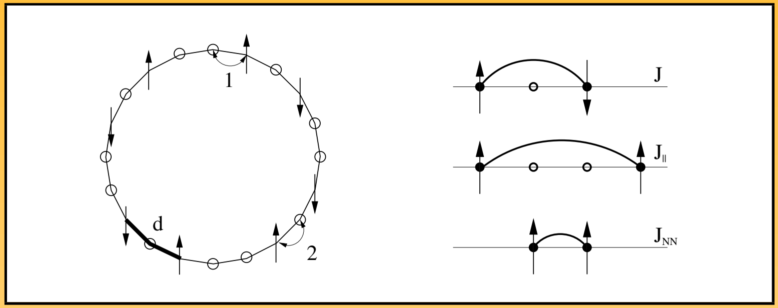
$$\underset{\sim}{H} = \sum_{\vec{c}} \left(\underset{\sim}{H}(\vec{c}) + V(\vec{c}) \right) \quad , \quad \underset{\sim}{H}(\vec{c}) = -\sum_{u,v} J_{uv}(\vec{c})\ \underset{\sim}{\vec{s}}(u) \cdot \underset{\sim}{\vec{s}}(v)$$

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

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

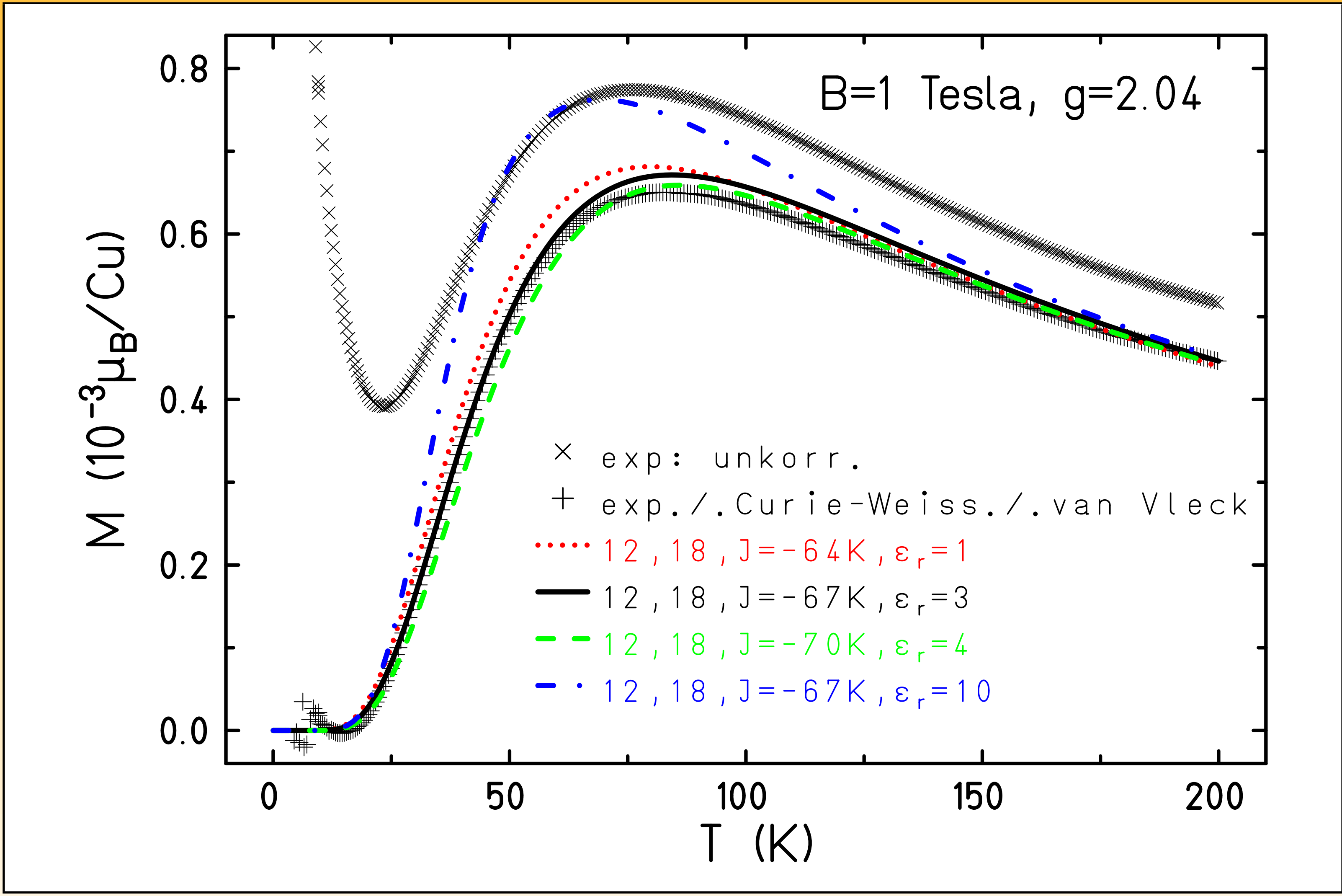
$$V(\vec{c}) \quad = \quad \frac{e^2}{4\pi\epsilon_0\,\epsilon_r\,r_0}\frac{1}{2}\sum_{u\neq v}\frac{\exp\left\{-r_0|u-v|/\lambda_D\right\}}{|u-v|}$$

Discussion of the model

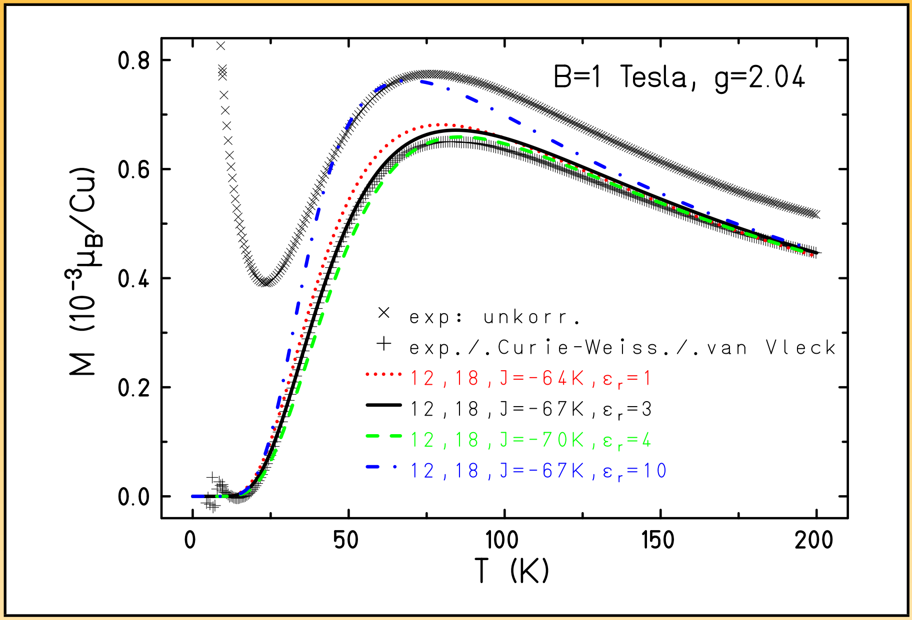


- Ansatz is similar to a simple Born-Oppenheimer description where the electronic Hamiltonian (here spin Hamiltonian) depends parametrically on the positions of the classical nuclei (here hole positions);
- Heisenberg Hamiltonian can be diagonalized for each spin-hole configuration;
- Screened electrostatic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



60 % holes on the ring – discussion

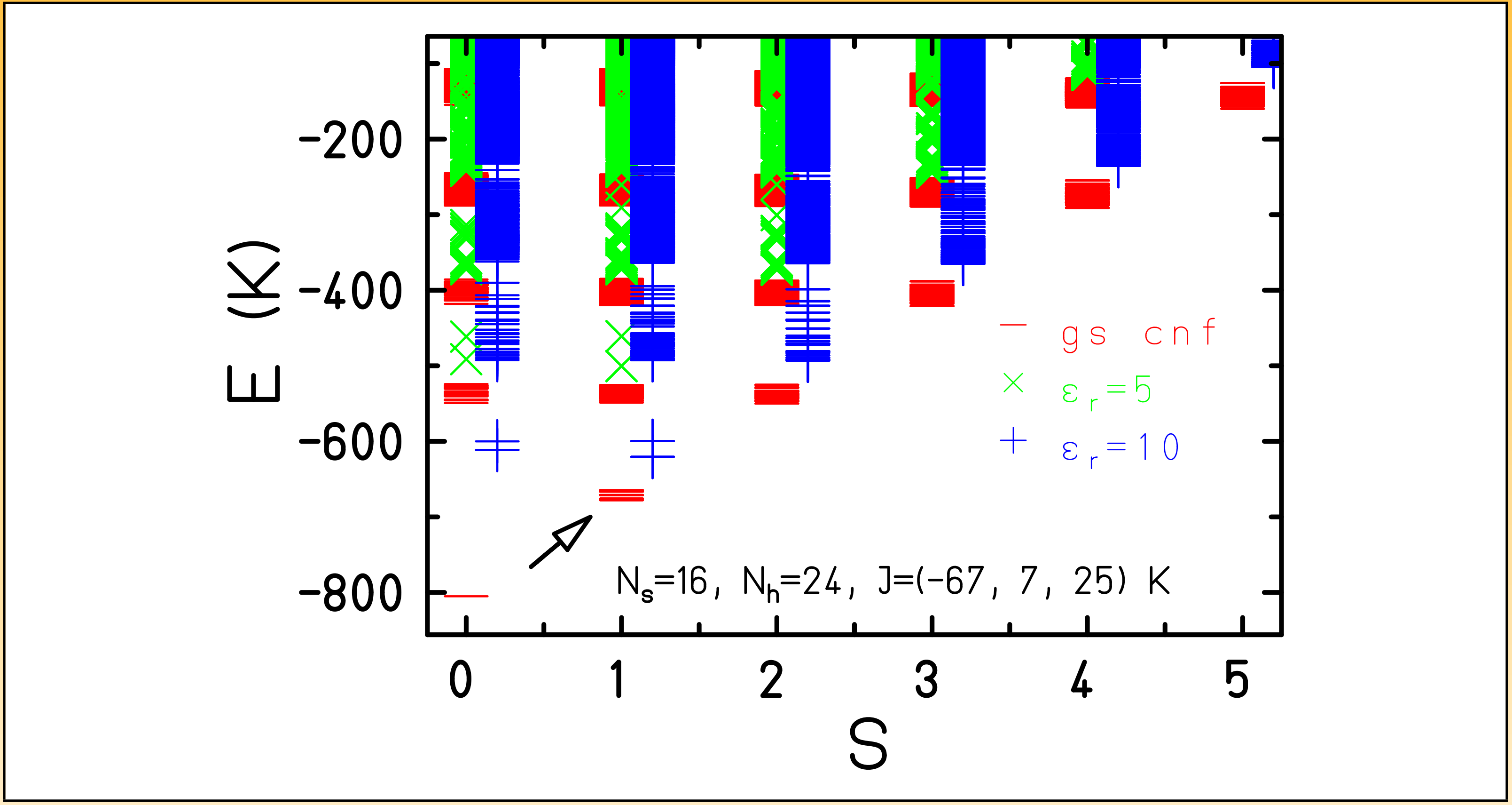


- Ground state indeed dimer-configuration; nearest-neighbor Coulomb repulsion wouldn't be sufficient;
- Magnetization curve strongly dependent on J and ϵ_r;
- For $\epsilon_r = 1$ only the dimer configuration contributes; for $\epsilon_r \gtrsim 3$ several hole configurations contribute with their respective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

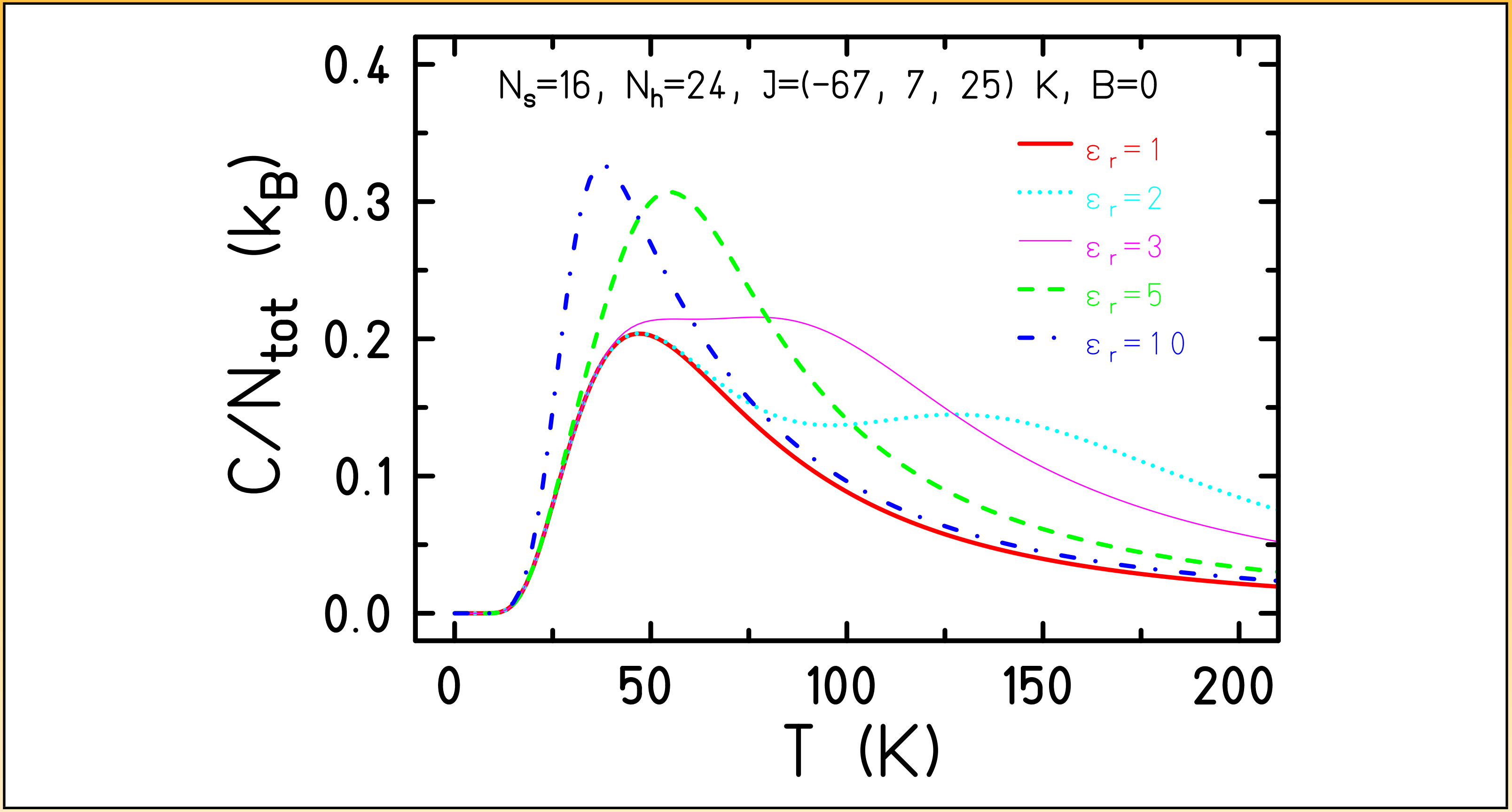
[1] Y. Mizuno, T. Tohyama, and S. Maekawa, Phys. Rev. B **58** (1998) 14713

Coulomb effects – levels



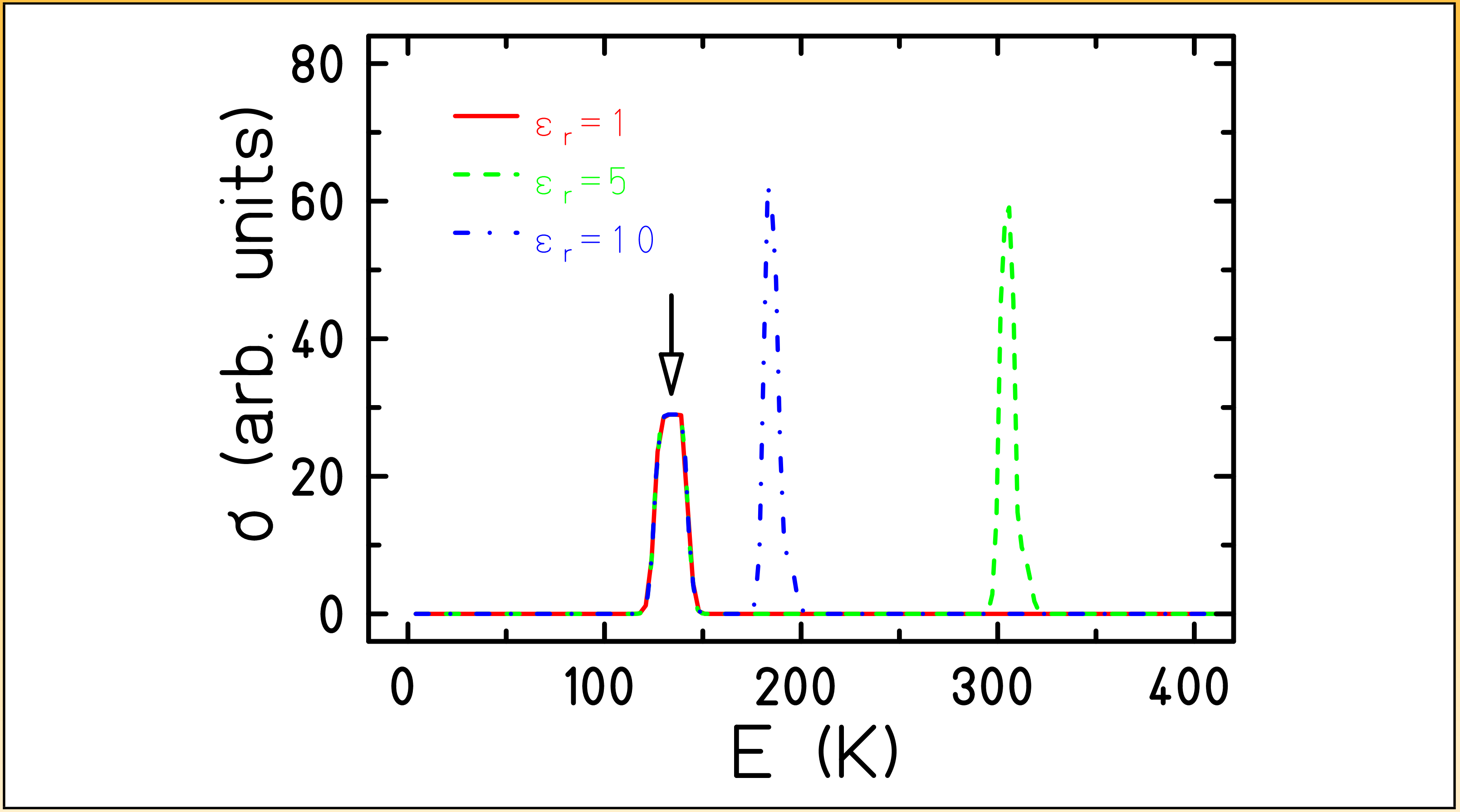
$\lambda_D = \infty$, dielectric constant ϵ_r is the only free parameter.

Coulomb effects – specific heat



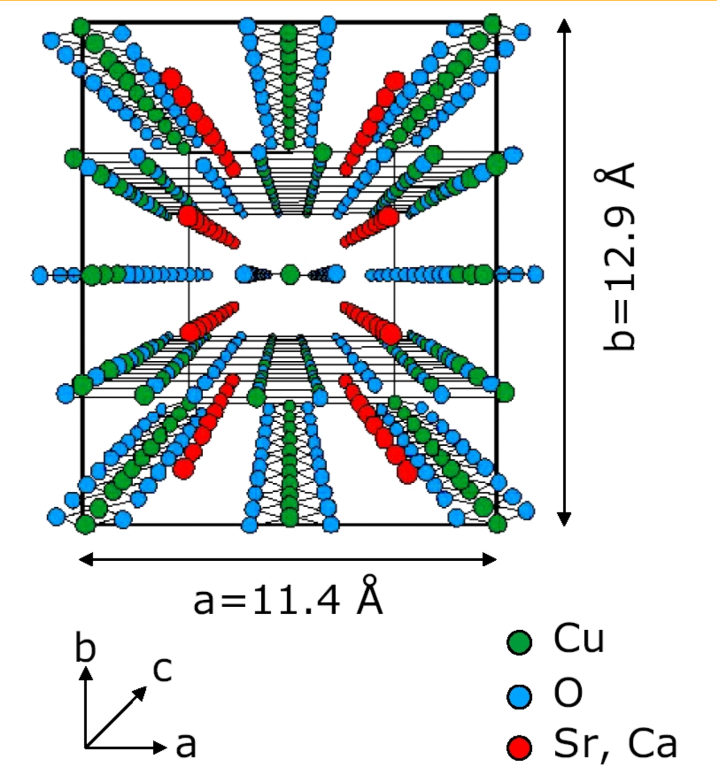
The high degeneracy of excited hole configurations plays an important role, since they substantially contribute to observables at low temperature although lying rather high in energy.

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



$Sr_{14-x}Ca_xCu_{24}O_{41}$

- 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 – 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.