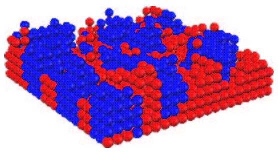

Quantum disorder due to singlet formation: The Plaquette lattice

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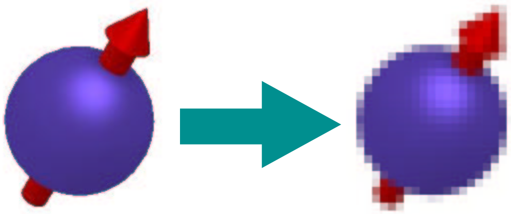
Introduction

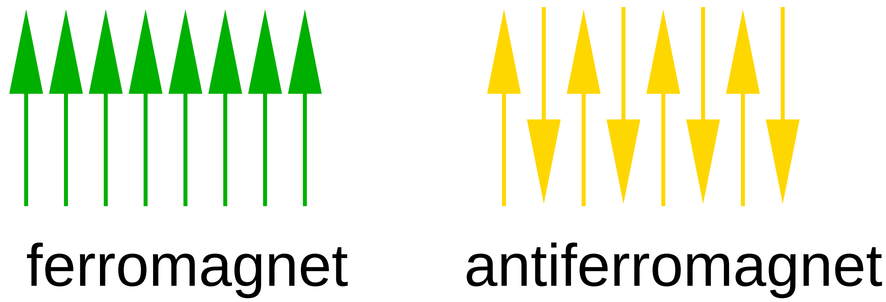
- quantum spin systems = quantum many-body systems
- basic element = magnetic moment of particles = spin
- spin - quantum object with ,,fluctuation"



- interaction = exchange between spins $\hat{\mathbf{s}}_\mathbf{i} \leftrightarrow \hat{\mathbf{s}}_\mathbf{j}$
  - isotropic Heisenberg exchange J

$$\mathsf{J}(\hat{\mathbf{s}}_\mathbf{i}\hat{\mathbf{s}}_\mathbf{j}) = \mathsf{J}(\hat{\mathbf{s}}_\mathbf{i}^\mathbf{x}\hat{\mathbf{s}}_\mathbf{j}^\mathbf{x} + \hat{\mathbf{s}}_\mathbf{i}^\mathbf{y}\hat{\mathbf{s}}_\mathbf{j}^\mathbf{y} + \hat{\mathbf{s}}_\mathbf{i}^\mathbf{z}\hat{\mathbf{s}}_\mathbf{j}^\mathbf{z})$$

- different kinds of magnetic order



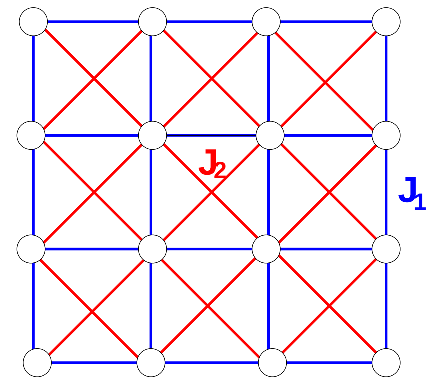
- parameters which influences the magnetic order

f ... frustration, T ... temperature, J_s ... singlet formation

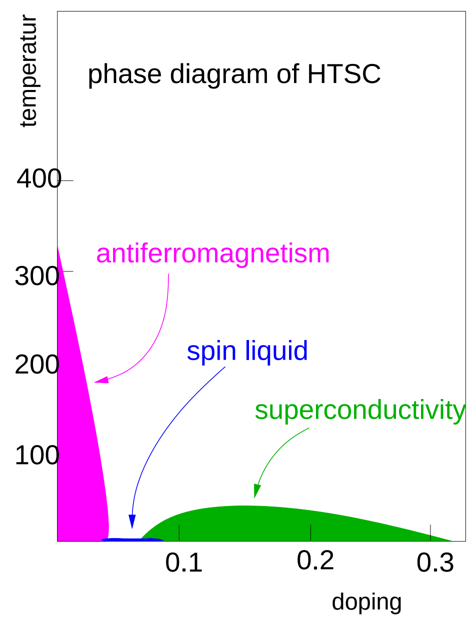
d ... dimension,z ... coordination number, S ... spin quantum number

Motivation

- theoretical interest in magnetic phase transition
- plaquette state $\longrightarrow$ possible ground state in the strong frustrated region of the J_1-J_2 model

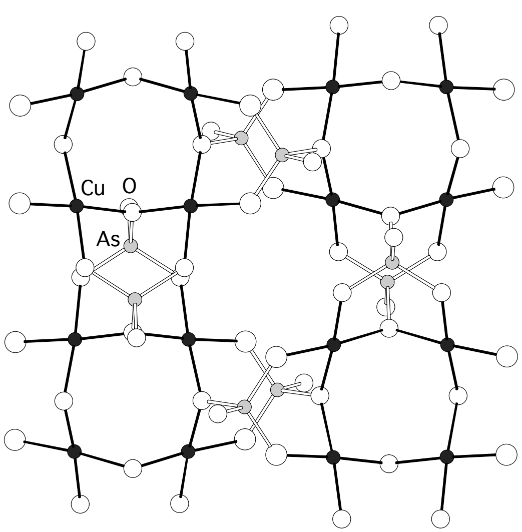


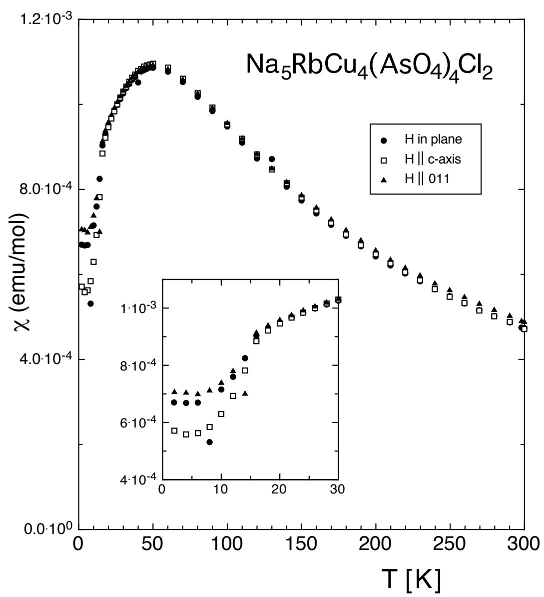
- high–T_c superconductors: theoretical explanation still missing $\longrightarrow$ antiferromagnetic correlations important
- doping of cuprates: change in nearest neighbor interaction $\longrightarrow$ Plaquette lattice

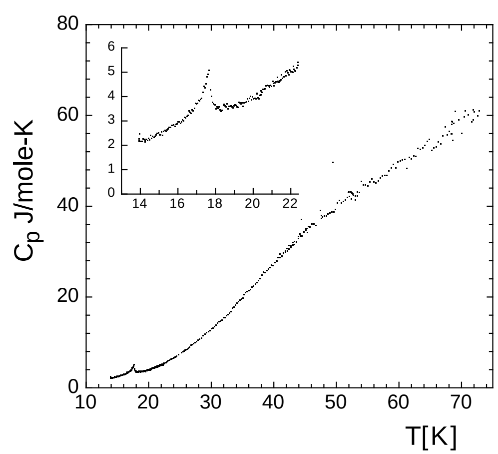


Experimental Motivation: $Na_5RbCu_4(AsO_4)_4Cl_2$

- nearly tetragonal insulating magnetic material
- two-dimensional, layered compound with square-planar arrangement of copper and oxygen
- magnetic transition at T=17K: susceptibility, heat capacity



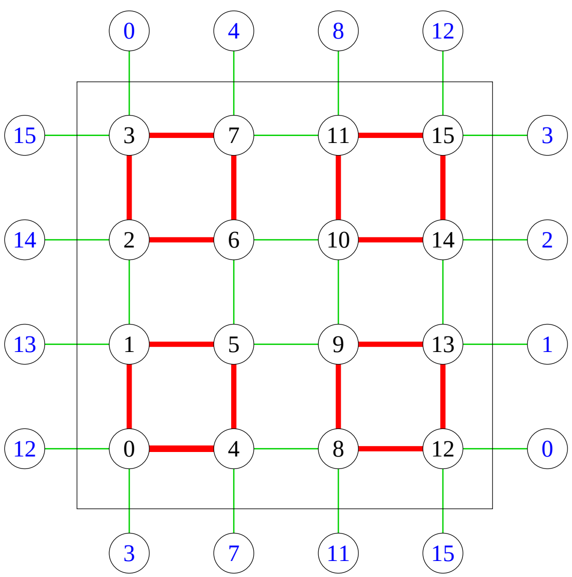




The Plaquette–lattice

- spin system on square lattice with two different interactions

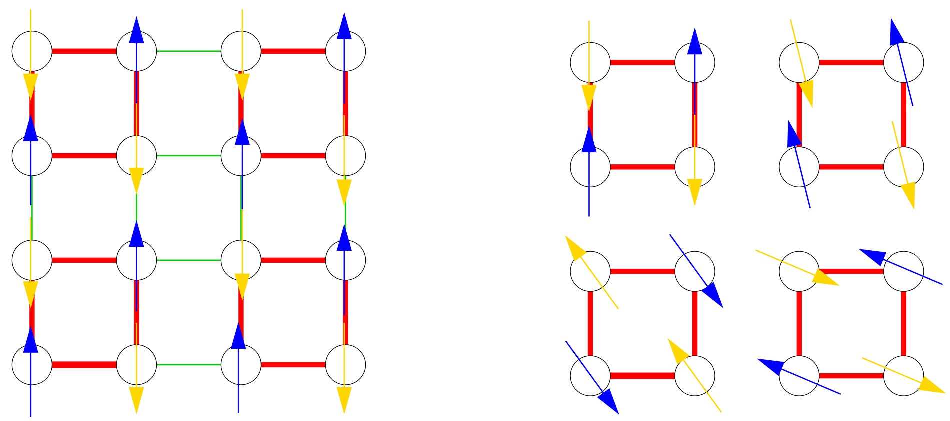
$$H = J_p \sum_{inter} \hat{s}_i \hat{s}_j + J_n \sum_{intra} \hat{s}_i \hat{s}_j$$



- J_p,J_n antiferromagnetic $\longrightarrow$ no frustration
- $J_n = 0$: plaquette in Singlet-state (total spin $\mathbf{S} = \mathbf{0}$)
- $J_n = 1$: simple square lattice with LRO
- symmetric solution if $J_n \rightarrow 0$ or $J_n \rightarrow \infty$

The classical ground state

- J_p,J_n antiferromagnetic $\longrightarrow$ no frustration
- $J_n > 0$: Neél state is always the ground state
- $J_n = 0$: Neél state one possible ground state
- $J_n = 0$: ground state degeneracy due to free rotation of the plaquettes respectively to each other



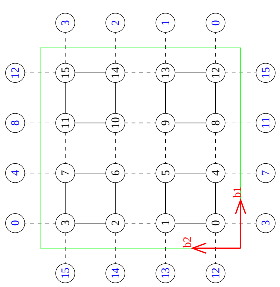
$J_n > 0$ $\qquad\qquad$ $J_n = 0$

What happens, if quantum fluctuations come into play?

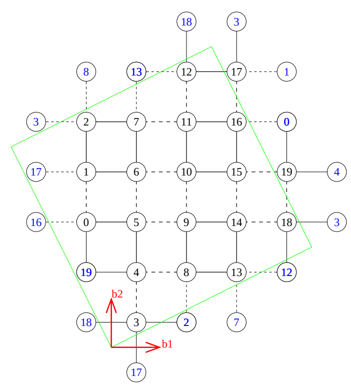
Numerical results

- Method: exact diagonalization of finite systems with Lanczos method $\longrightarrow$ ground state and low energy states
- computational effort for N=36 using all symmetries: $\approx$ 65 million vector entries $\longrightarrow$ 1GByte memory (using 2 vectors)
- finite lattices with periodic boundary conditions

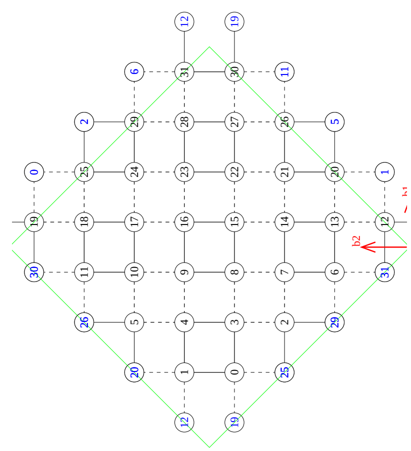
N=16



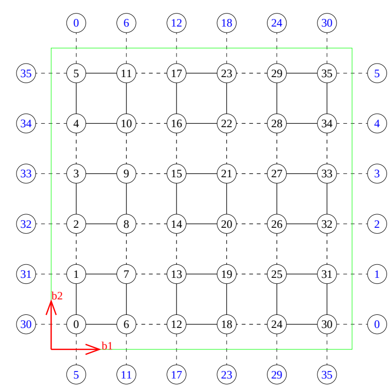
N=20



N=32

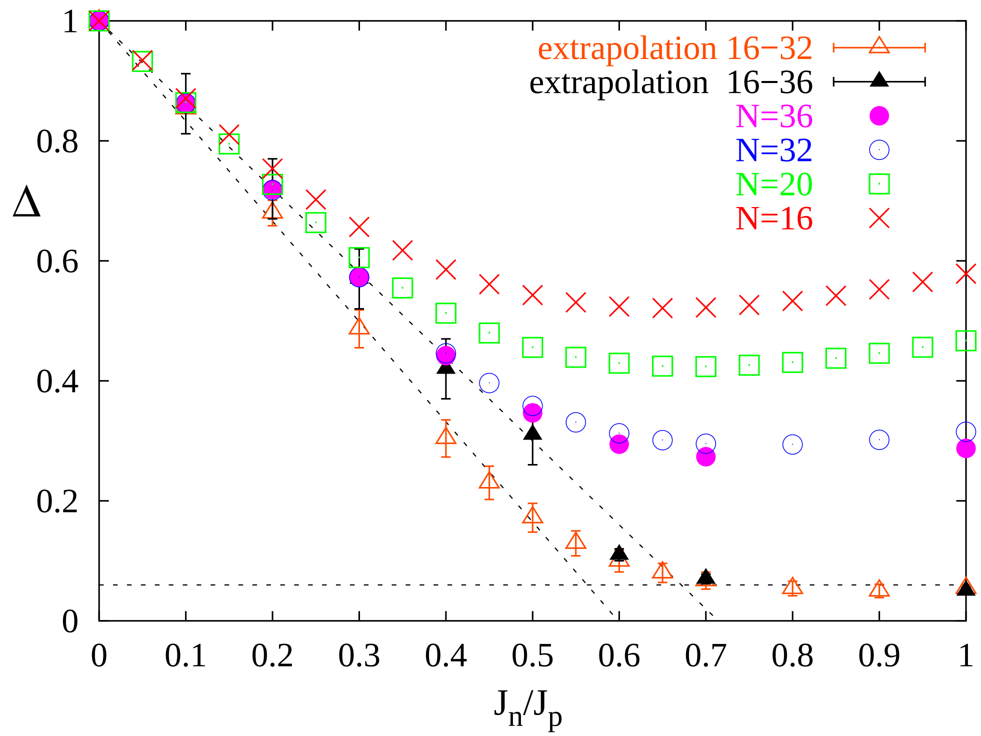


N=36



The spin gap Δ

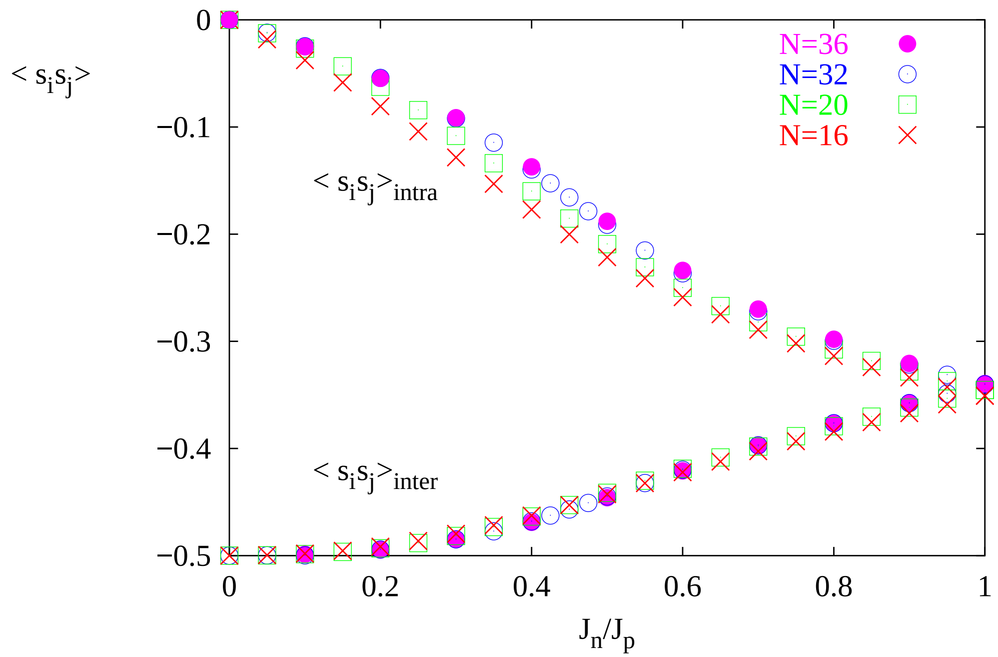
- disordered spin systems show a spin gap:
  $\Delta = E_{min}(S_{min}+1) - E_{min}(S_{min})$



- finite size extrapolation $\Delta \propto N^{-1}$
  - works well for $J_n/J_p \geq 0.6$ (small errorbars)
  - less appropriate for $J_n/J_p \leq 0.5$ (larger errorbars)
- crossing of fit lines: $J_n/J_p{}^{crit} \approx 0.63 \pm 0.05 \rightarrow$ phase transition point

Inter– and Intra–Plaquette spin–spin correlation

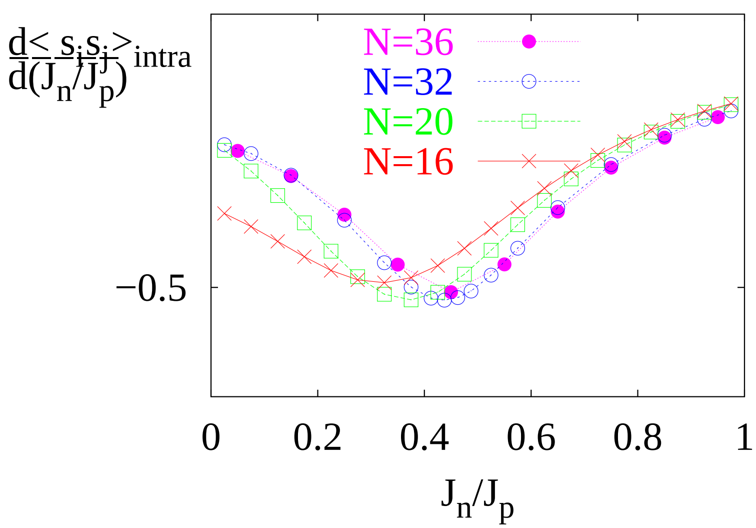
- $\langle \hat{s}_i \hat{s}_j \rangle_{intra}$:
  correlation on a J_n bond
- $\langle \hat{s}_i \hat{s}_j \rangle_{inter}$:
  correlation on a J_p bond

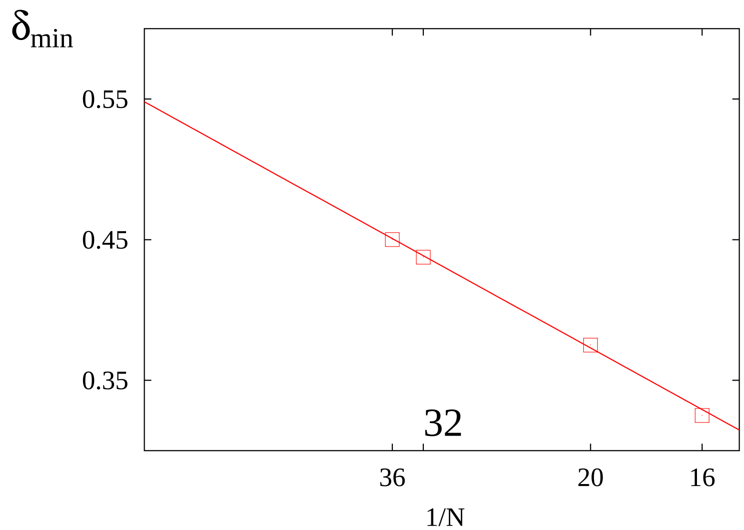


- $J_n = 0$
  - $\langle \hat{s}_i \hat{s}_j \rangle_{intra} = 0 \longrightarrow$ decoupled plaquettes without LRO
  - $\langle \hat{s}_i \hat{s}_j \rangle_{inter} = -0.5 \longrightarrow$ singlet plaquette ground state
- $J_n = 1$
  - $\langle \hat{s}_i \hat{s}_j \rangle_{intra} = \langle \hat{s}_i \hat{s}_j \rangle_{inter} \longrightarrow$ simple square lattice with LRO
- inflection point at the phase transition?

Differential Intra–Plaquette spin–spin correlation

- left figure: inflection point $\longrightarrow$ numerical differentiation: $\frac{\partial \langle \hat{s}_i \hat{s}_j \rangle_{intra}}{\partial (J_n/J_p)}$
- right figure: scaling of the peak position with system size N





- a delta-like peak seems to develop $\longrightarrow$ phase transition point
- scaling of the peak δ_{min} vs. $1/N$ $\longrightarrow$ phase transition point at $J_n/J_p{}^{crit} \approx 0.55 \pm 0.05$

Discussion

Comparison with other methods

- non-linear σ model approach: failed to predict a phase transition [Koga, *J.Phys.Soc.Jpn.* **68**(2), p.642, 1999]
- spin wave calculation: ${J_n/J_p}^{crit} \approx 0.11 \longrightarrow$ can be ruled out [Koga, *ibid*]
- 4th order plaquette expansion : ${J_n/J_p}^{crit} \approx 0.54 \longrightarrow$ close to our result [Koga, *J.Phys.Soc.Jpn.* **68**(7), p.2373, 1999]
- Ising series expansion : ${J_n/J_p}^{crit} \approx 0.55 \longrightarrow$ compares well with our result [Singh,*PRB* **60**(10), p.7278, 1999]
- quantum Monte-Carlo calculation : ${J_n/J_p}^{crit} \approx 0.55 \longrightarrow$ compares well with our result [Wessel, *private communication*]

Exact diagonalization

- valuable tool for studying quantum spin systems
- verification and validation of others methods
- can be a starting point for the evaluation of a phase diagram
- should be combined with other approaches
- finite size scaling needs to be addressed

Outlook

First or second order phase transition?

- spin correlation with developing delta-peak points to first order
- more detailed study $\rightarrow$ quantum Monte-Carlo calculation by Wessel under way

Exotic phases possible?

- several plaquettes building larger structure $\rightarrow$ super–plaquettes?
- plaquette breaking $\rightarrow$ dimerization?

Magnetic transition in $Na_5RbCu_4(AsO_4)_4Cl_2$

- pure Heisenberg antiferromagnet in d=2 $\rightarrow$ no non-zero phase transition possible (Mermin-Wagner theorem)
- include additional interaction like Dzyaloshinskii-Moriya
- include small interaction between 2D–planes

Acknowledgement

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