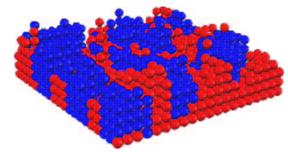

Anisotropic spin exchange in the Plaquette lattice

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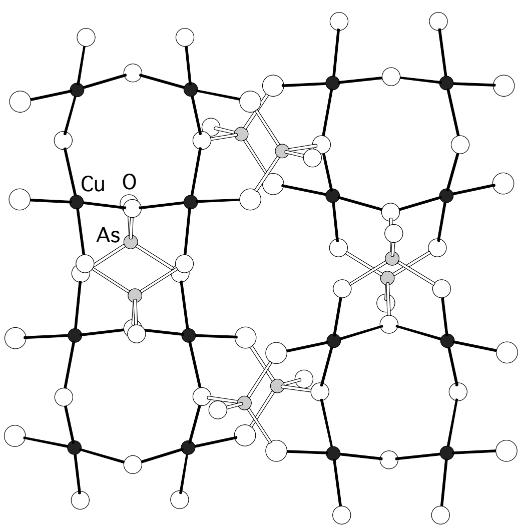
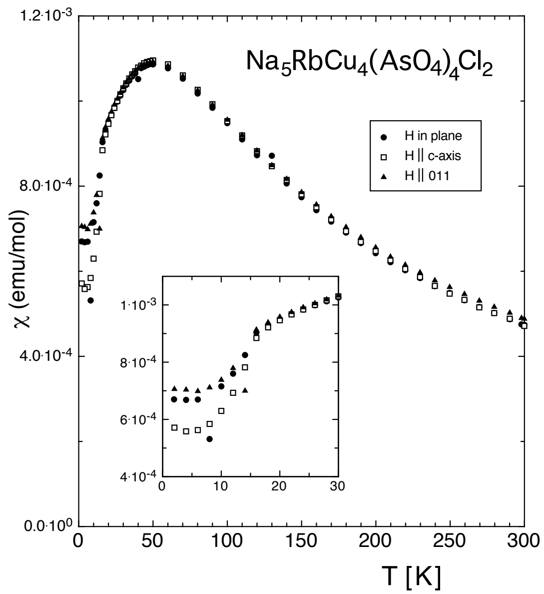
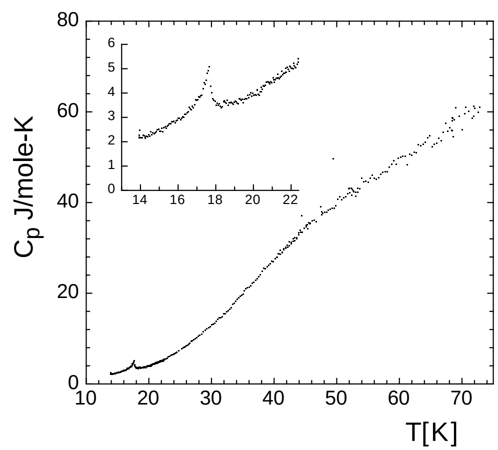
Experimental Motivation:

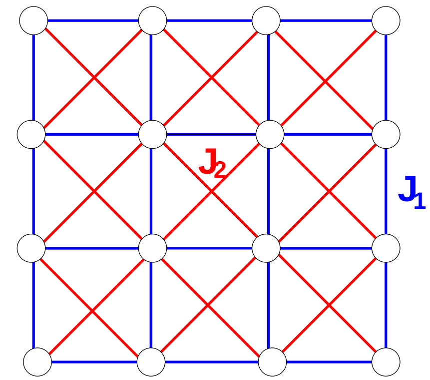
- nearly tetragonal insulating magnetic material
- two-dimensional, layered compound with square-planar arrangement of copper and oxygen
- susceptibility, heat capacity → low temperature magnetic transition at T=17K (non Néel like?)



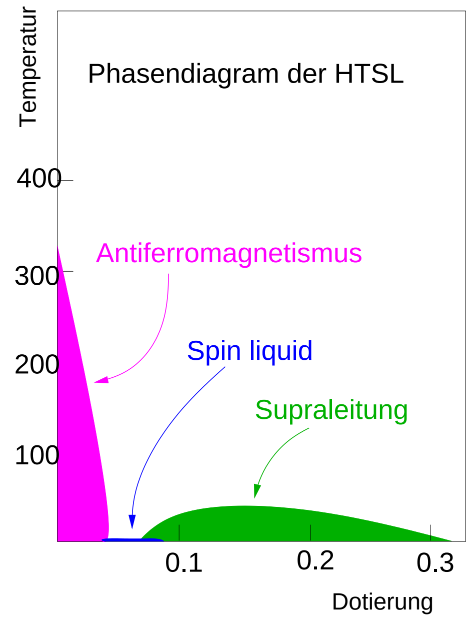




- theoretical interest in magnetic phase transition
- plaquette state $\longrightarrow$ possible ground state in the strong frustrated region of the J_1-J_2 model



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



Isotropic Heisenberg exchange

- isotropic spin exchange with ,,fluctuation" - Heisenberg J

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

- often rewritten in spin-raising $\hat{\mathbf{s}}_{\mathbf{i}}^{+}$ and lowering operators $\hat{\mathbf{s}}_{\mathbf{i}}^{-}$

$$\hat{\mathbf{s}}_{\mathbf{i}}^{+}|\uparrow> = |\downarrow>, \ \hat{\mathbf{s}}_{\mathbf{i}}^{-}|\downarrow> = |\uparrow>$$

$$\hat{\mathbf{s}}_{\mathbf{i}}^{\mathbf{z}}|\uparrow> = +\frac{1}{2}|\uparrow>, \ \hat{\mathbf{s}}_{\mathbf{i}}^{\mathbf{z}}|\downarrow> = -\frac{1}{2}|\downarrow>$$

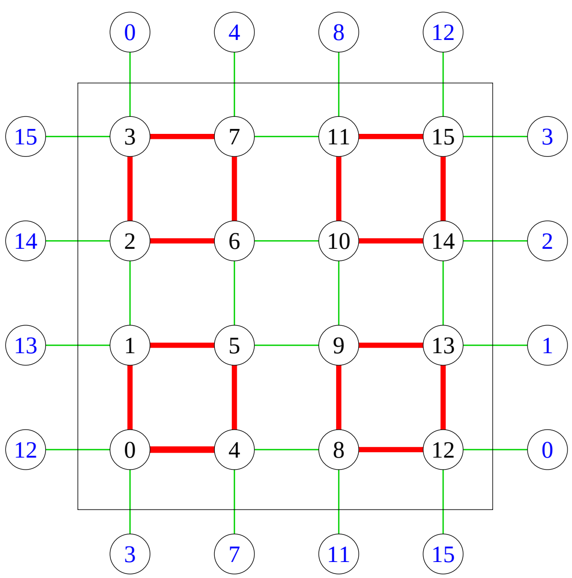
$$\mathsf{J}(\hat{\mathbf{s}}_{\mathbf{i}}\hat{\mathbf{s}}_{\mathbf{j}}) = \mathsf{J}[\frac{1}{2}(\hat{\mathbf{s}}_{\mathbf{i}}^{+}\hat{\mathbf{s}}_{\mathbf{j}}^{-} + \hat{\mathbf{s}}_{\mathbf{i}}^{-}\hat{\mathbf{s}}_{\mathbf{j}}^{+}) + \hat{\mathbf{s}}_{\mathbf{i}}^{\mathbf{z}}\hat{\mathbf{s}}_{\mathbf{j}}^{\mathbf{z}}]$$

- non-diagonal terms $\hat{\mathbf{s}}_{\mathbf{i}}^{+}\hat{\mathbf{s}}_{\mathbf{i}}^{-}$ create all the numerical difficulties, but total S^z is still conserved

The Plaquette–lattice

- spin system on square lattice with two different interactions

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

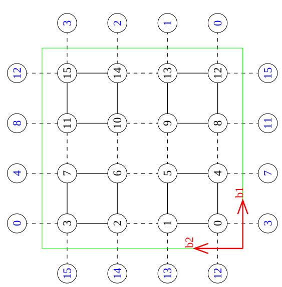


- J_p,J_n antiferromagnetic $\rightarrow$ no frustration
- $J_n = 0$: plaquette in Singlet-state (total spin $\mathbf{S} = \mathbf{0}$)
- $J_n = 1$: simple square lattice with LRO
- symmetric solution if $J_n \rightarrow 0$ or $J_n \rightarrow \infty$

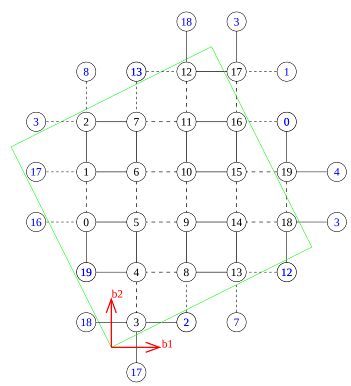
Numerical results

- 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

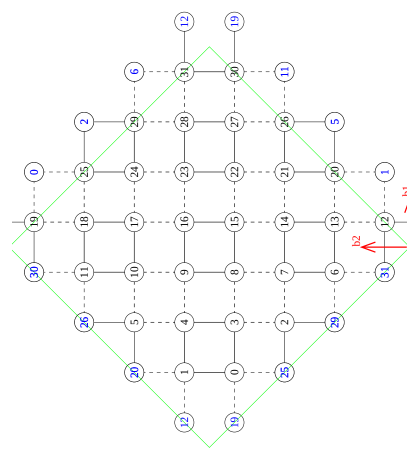
N=16



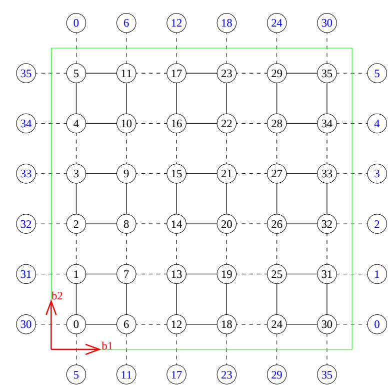
N=20



N=32

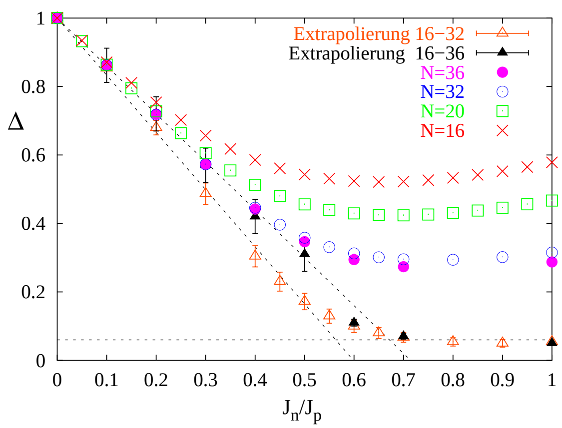


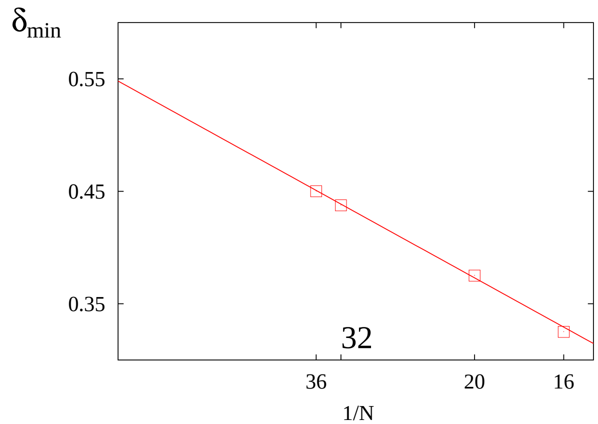
N=36



Results for the isotropic Heisenberg exchange

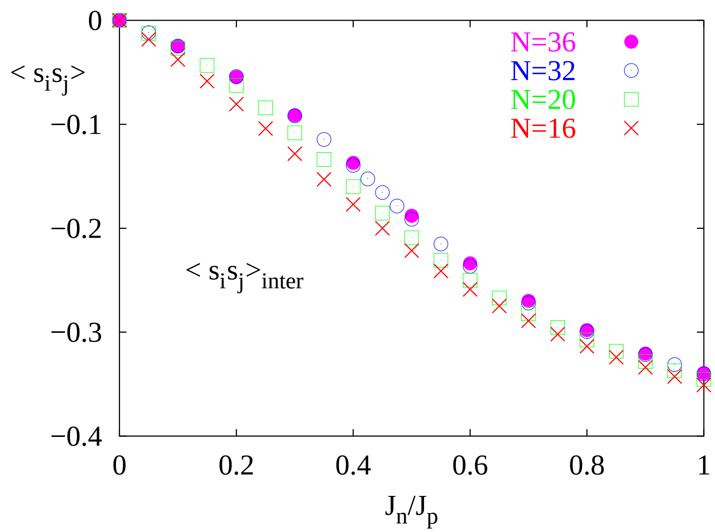
- left: spin gap – $\Delta = E_{min}(S_{min}+1) - E_{min}(S_{min})$
- right: extrema of the differential inter spin-spin correlation $\frac{\partial \langle \hat{s}_i \hat{s}_j \rangle_{inter}}{\partial (J_n/J_p)}$

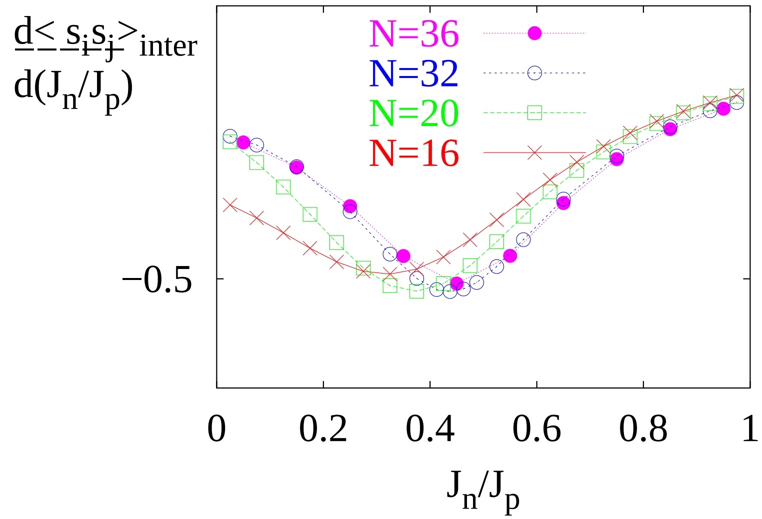




- spin gap extrapolation: ${J_n/J_p}^{crit} \approx 0.63 \pm 0.05 \longrightarrow$ phase transition point
- scaling of correlation change: δ_{min} vs. $1/N \longrightarrow$ phase transition point at ${J_n/J_p}^{crit} \approx 0.55 \pm 0.05$
- compares well with other results: 4th order plaquette expansion: ${J_n/J_p}^{crit} \approx 0.54$, Ising series expansion: ${J_n/J_p}^{crit} \approx 0.55$, quantum Monte-Carlo calculation: ${J_n/J_p}^{crit} \approx 0.55$

Differential inter spin–spin correlation explained





- $J_n = 0$: $\langle \hat{s}_i \hat{s}_j \rangle_{inter} = 0 \longrightarrow$ decoupled plaquettes without LRO
- inflection point at the phase transition $\longrightarrow$ numerical differentiation: $\frac{\partial \langle \hat{s}_i \hat{s}_j \rangle_{intra}}{\partial (J_n / J_p)}$
- scaling of the peak position with system size $N \longrightarrow$ phase transition point

Anisotropic spin exchange

- band structure calculation for $Na_5RbCu_4(AsO_4)_4Cl_2$ $\longrightarrow$ anisotropic spin exchange probably not small
- two types are discussed:
  1. Dzyaloshinskii-Moriya exchange: $\vec{D}_{ij}$
  2. 4-spin exchange: $\vec{P}_{ij}$
- we study in more detail the Dzyaloshinskii-Moriya exchange

$$\vec{D}_{ij}(\hat{s}_i \times \hat{s}_j) = \begin{bmatrix} d_{ij}^x & d_{ij}^y & d_{ij}^z \\ \hat{s}_i^x & \hat{s}_i^y & \hat{s}_i^z \\ \hat{s}_j^x & \hat{s}_j^y & \hat{s}_j^z \end{bmatrix}$$

Symmetry considerations

- $\vec{D}_{ij}$ is site dependent and defined by symmetries:
  1. $\vec{D}_{ij} = -\vec{D}_{ji}$
  2. no z-component of $\vec{D}_{ij} = (d_1, d_2, 0)$
  3. $\vec{D}_{12} = -\vec{D}_{43}$
  4. $\vec{D}_{12} = (d_1, d_2, 0) \rightarrow \vec{D}_{14} = (-d_2, -d_1, 0)$
- and by the lattice structure of $Na_5RbCu_4(AsO_4)_4Cl_2$
  1. $\vec{D}_{ij} \neq 0$ only on J_p bonds
  2. simplification: $|d_1| = |d_2| = d$
- calculation becomes more complicated

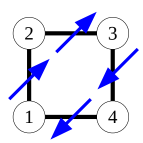
$$\vec{D}_{ij}(\hat{\mathbf{s}}_\mathbf{i} \times \hat{\mathbf{s}}_\mathbf{j}) = d_1[(\hat{\mathbf{s}}_\mathbf{i}^\mathbf{y}\hat{\mathbf{s}}_\mathbf{j}^\mathbf{z} - \hat{\mathbf{s}}_\mathbf{i}^\mathbf{z}\hat{\mathbf{s}}_\mathbf{j}^\mathbf{y}) - d_2[(\hat{\mathbf{s}}_\mathbf{i}^\mathbf{x}\hat{\mathbf{s}}_\mathbf{j}^\mathbf{z} - \hat{\mathbf{s}}_\mathbf{i}^\mathbf{z}\hat{\mathbf{s}}_\mathbf{j}^\mathbf{x})$$

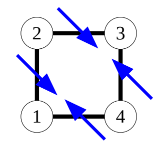
- cross terms mix S^z subspaces

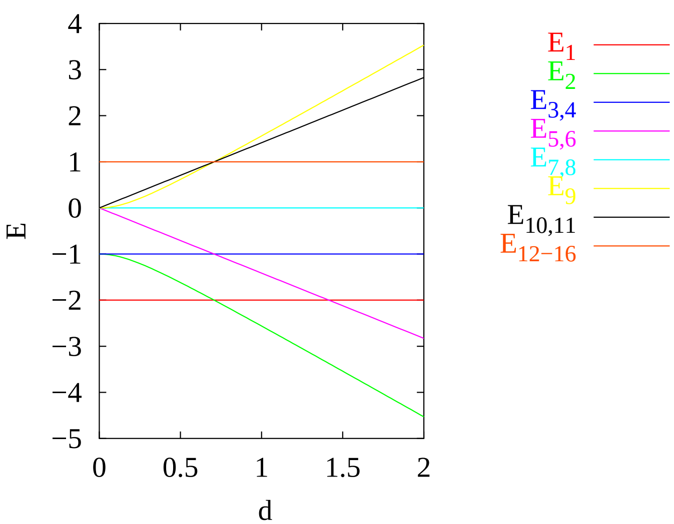
$$\hat{\mathbf{s}}_\mathbf{i}^\mathbf{y}\hat{\mathbf{s}}_\mathbf{j}^\mathbf{z} = -\frac{1}{2}\mathrm{i}(\hat{\mathbf{s}}_\mathbf{i}^+ - \hat{\mathbf{s}}_\mathbf{i}^-)\hat{\mathbf{s}}_\mathbf{j}^\mathbf{z}$$

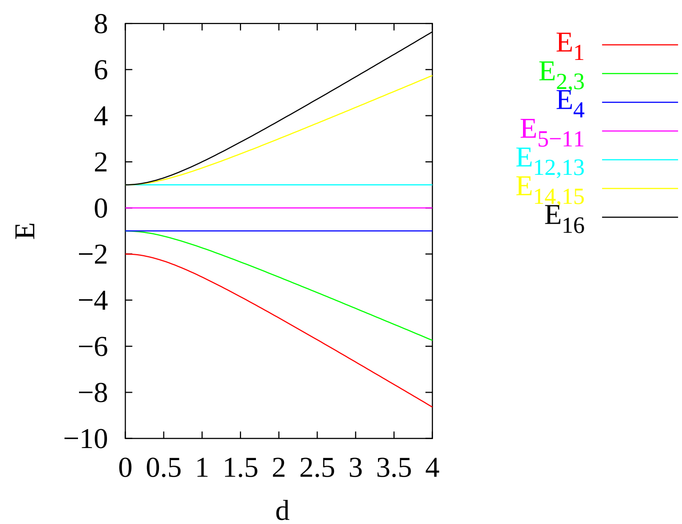
Single Plaquette results

- first study of single plaquette: N=4
- completely solvable → examine energy spectrum
- two cases interesting: $d_1 = +d_2$ or $d_1 = -d_2$

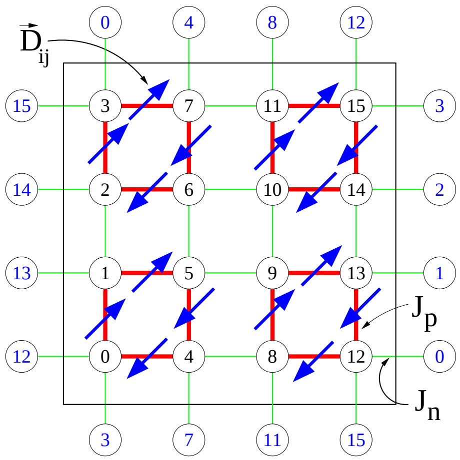








Coupled plaquettes: The new phase diagram

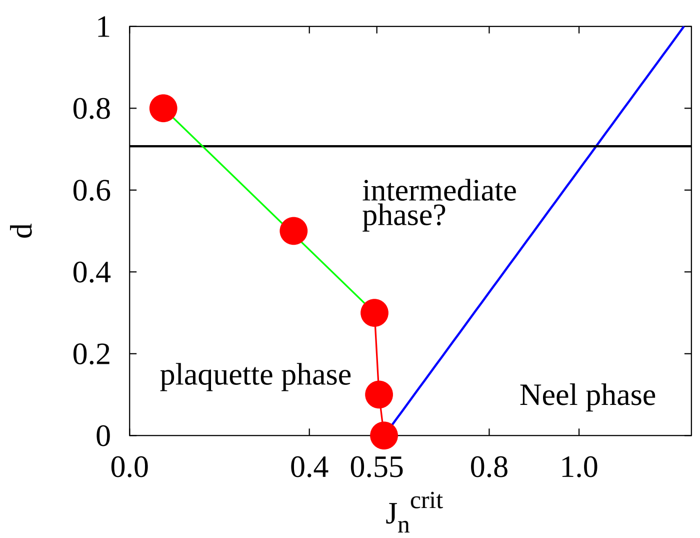


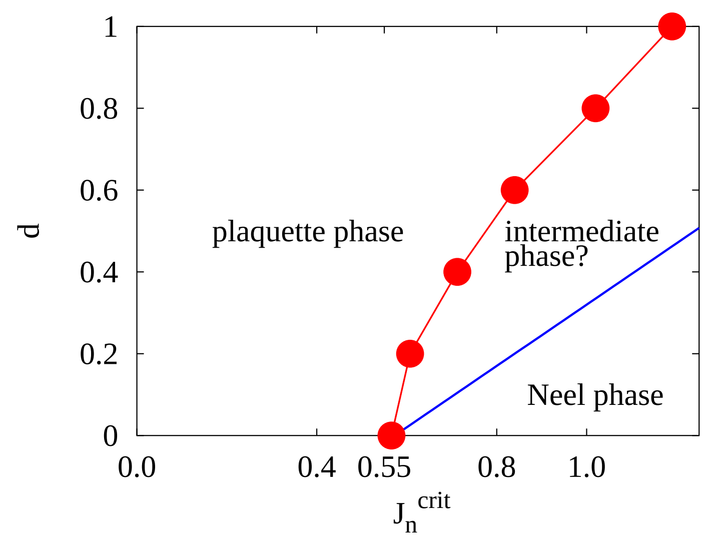
$$\hat{H} = \hat{H}_{J_p, J_n} + \sum_{intra} \vec{D}_{ij}(\hat{s}_i \times \hat{s}_j)$$

- study of spin-spin correlations (now anisotropic!): $\langle \hat{s}_i^\alpha \hat{s}_j^\alpha \rangle$ with $\alpha = x, y, z$
- due to symmetric $\vec{D}_{ij} \rightarrow \langle \hat{s}_i^x \hat{s}_j^x \rangle_{inter} = \langle \hat{s}_i^y \hat{s}_j^y \rangle_{inter} \neq \langle \hat{s}_i^z \hat{s}_j^z \rangle_{inter}$
- study of differential inter spin-spin correlation: $\frac{\partial \langle \hat{s}_i \hat{s}_j \rangle_{inter}}{\partial (J_n/J_p)}$
- phase transition point $\equiv$ extrema: weak dependence on $\alpha \rightarrow$ display $\alpha = x$

The two cases

$d_1 = +d_2$ and $d_1 = -d_2$





- almost no change of phase transition point (remember N=4 spectra)
- additional phase for $d > \frac{1}{\sqrt{2}}$? or stabilization of Néel order?
- strong shift of phase transition to larger J_n/J_p $\longrightarrow$ de-stabilization of Néel order
- some intermediate phase possible?
- very similar to J_1-J_2+DM (Voigt, Richter: *JPC* **8**, p.5059, 1996)

Summary and Outlook

Dzyaloshinskii-Moriya exchange influences phase transition point

- stabilizes or destabilizes Néel order
- may explain low temperature magnetic transition in $Na_5RbCu_4(AsO_4)_4Cl_2$

First or second order phase transition?

- spin correlation with developing delta-peak points to first order
- more detailed study necessary $\longrightarrow$ variational wave function and Monte-Carlo

Exotic phases possible?

- detailed study of phase space
- dimerization, super–plaquettes, stripes?

4-Spin exchange

- induces frustration $\longrightarrow$ destabilization of Néel order?
- may enhance plaquette building $\longrightarrow$ similar to observed behavior for triangular lattice

Danksagung

A big *thanks to all the people in the Center for Simulational Physics, the Department of Physics and Astronomy, the University and Athens which helped me to gain a lot of experience, to increase my knowledge about the world of physics and far beyond and simply to have a really good time here in Athens.*

And because I did not get any cookies in time at least the pizza is on me today!

I especially want to mention (and now this list in alphabetical order, because none of them should be last in any list of importance):

- Tom Barnello (who help out with keys at several occasions ;)
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