Anisotropic three-dimensional Heisenberg antiferromagnets in a field

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XXZ model on a cubic lattice

$$\mathcal{H} \;=\; J \sum_{\langle i,j \rangle} \left[\Delta (S_i^x S_j^x + S_i^y S_j^y) + S_i^z S_j^z \right] \;-\; H \sum_i S_i^z$$

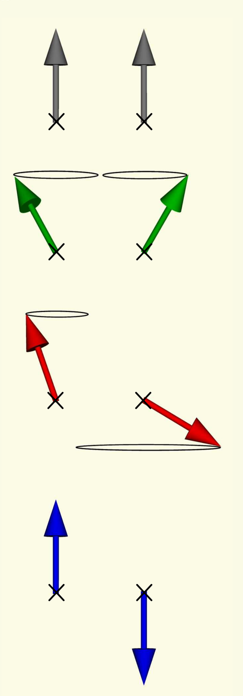
nearest-neighbour pairs	$\langle i,j \rangle$
coupling strength	$J > 0$
easy-axis anisotropy	$\Delta < 1$
field in z-direction	H
classical spin-vectors	$\vec{S}_i = (S_i^x, S_i^y, S_i^z);\quad \lvert\vec{S}_i\rvert = 1$

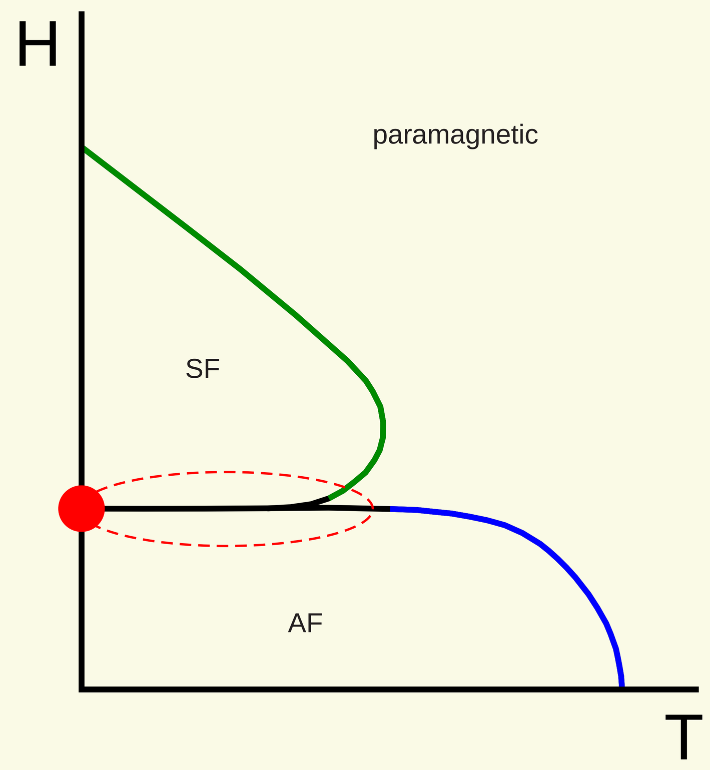
Methods

- Monte-Carlo simulations
- Ground state considerations

Structures

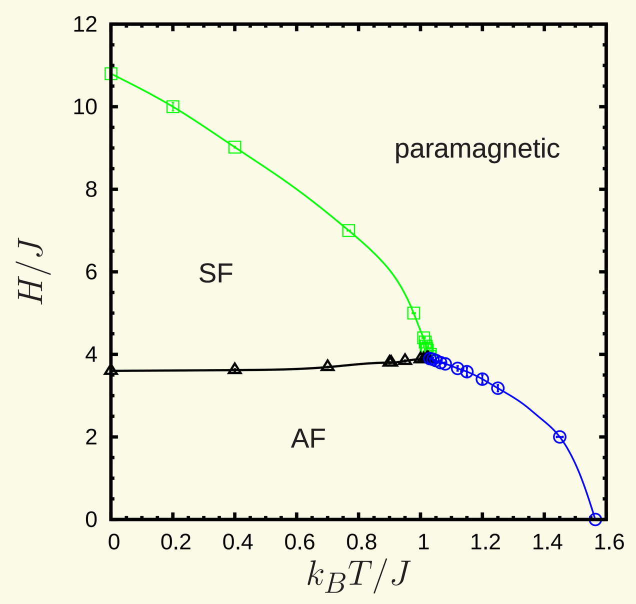
ground states



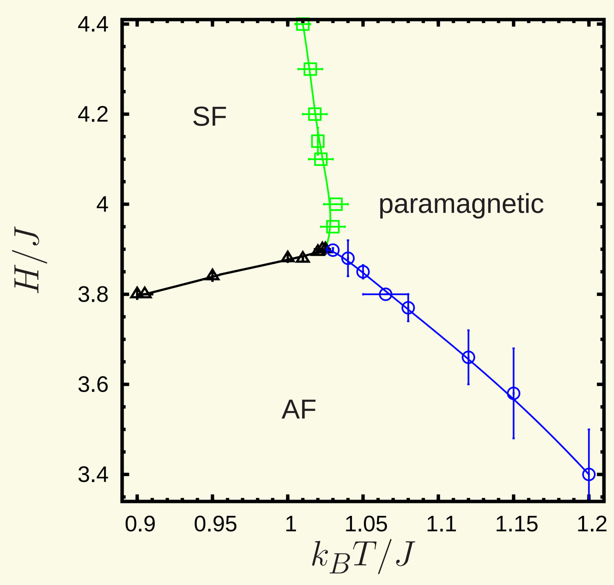


- spin-flop (SF) phase
  - XY-like phase
  - large magnetization
- antiferromagnetic (AF) phase
  - Ising-like phase
  - small magnetization
- ground state degeneracy:
  - AF, SF, and biconical (BC) structures

Phase diagram ($\Delta = 0.8$)



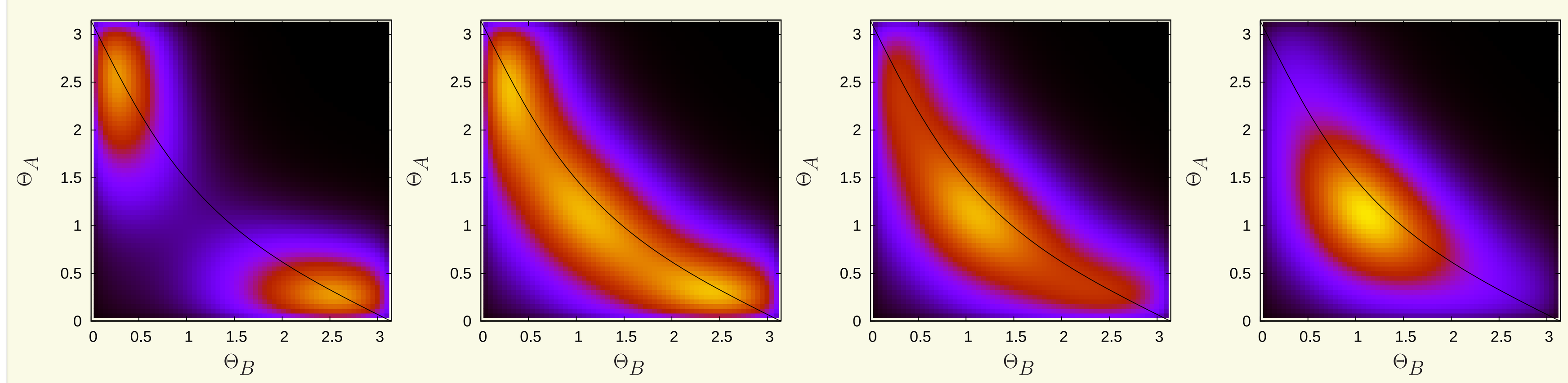
Global phase diagram



Vicinity of triple point

At low temperatures:

first order transition, biconical fluctuations



$H/J = 3.691$ $\quad H/J = 3.6925$ $\quad H/J = 3.693$ $\quad H/J = 3.694$

probability of tilt angles θ_A and θ_B at neighbouring sites for $k_BT/J = 0.7$

relation of tilt angles θ_A, θ_B in degenerate ground state (see solid black line)

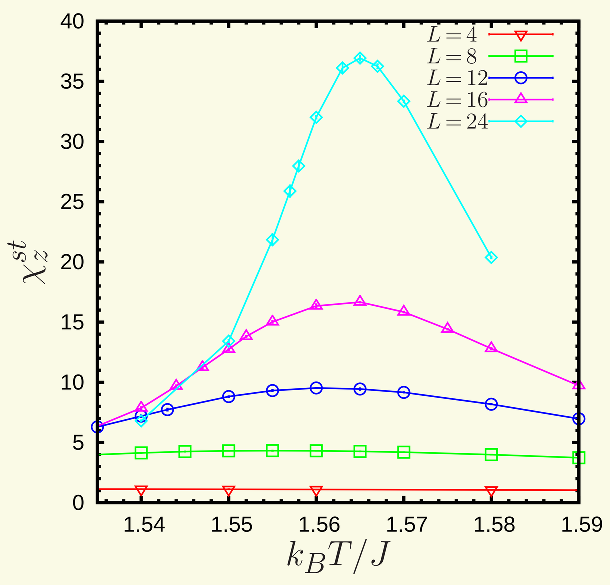
$$\theta_B \;=\; \arccos\left(\frac{\sqrt{1-\Delta^2} \;-\; \cos\theta_A}{1 \;-\; \sqrt{1-\Delta^2}\,\cos\theta_A} \right)$$

Evidence for coexistence of AF and SF phases at $H/J = 3.6925$,
i.e. first order transitions (in agreement with analyses of critical exponents)

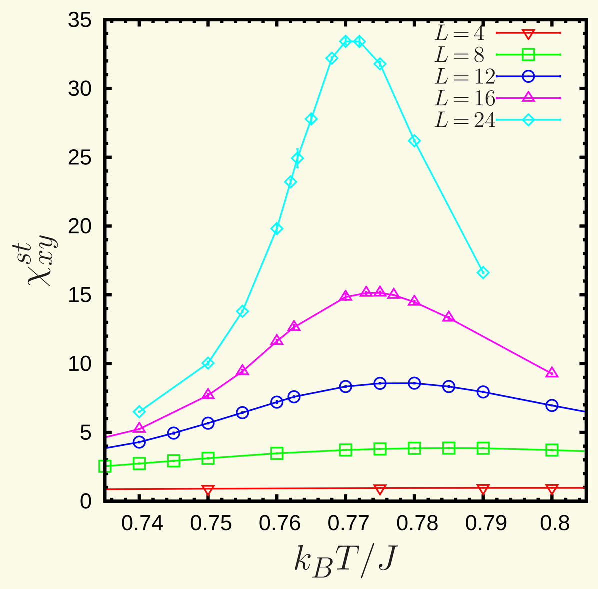
Critical properties of AF and SF phase boundaries

Example: Finite size behaviour of the staggered susceptibilities at selected fields

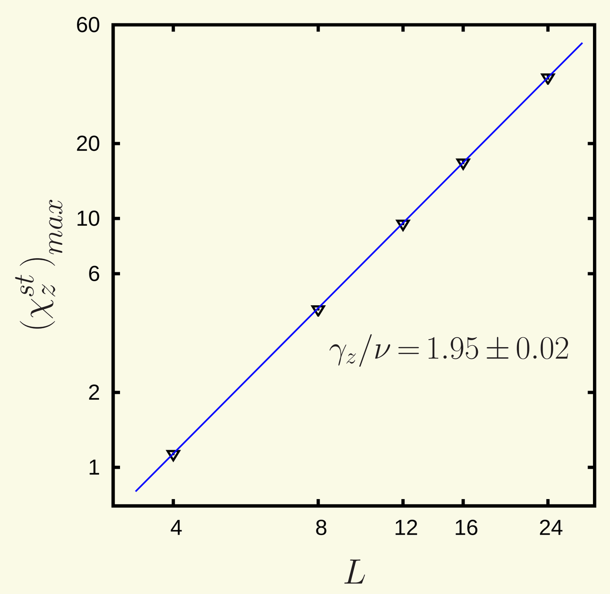
AF phase boundary ($H/J = 0$)

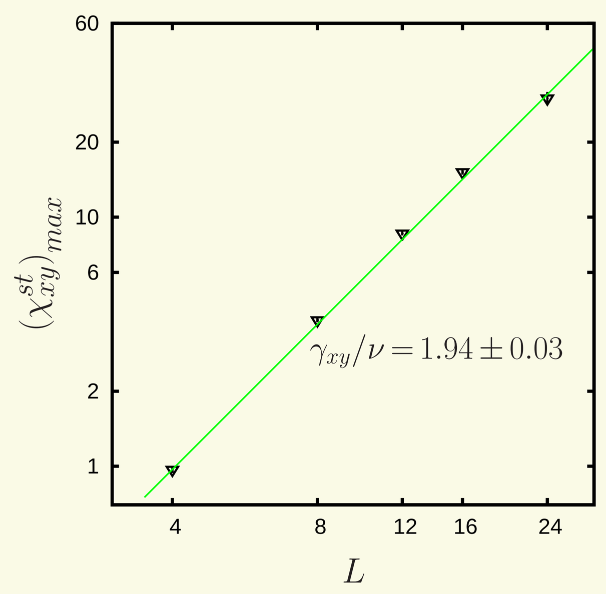


SF phase boundary ($H/J = 7$)



$(\chi_z^{st})_{max} \sim L^{\frac{\gamma_z}{\nu}}$ $\qquad (\chi_{xy}^{st})_{max} \sim L^{\frac{\gamma_{xy}}{\nu}}$





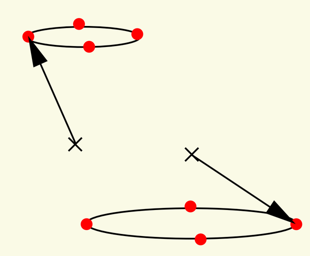
$\gamma_z/\nu = 1.95 \pm 0.01$ in agreement with Ising universality ($\gamma/\nu = 1.9635\ldots$)

$\gamma_{xy}/\nu = 1.94 \pm 0.03$ in agreement with XY universality ($\gamma/\nu = 1.9613...$)

Confirmed by analyses of specific heat, Binder cumulant, ... for various cases

Extension: XXZ antiferromagnet + cubic symmetry

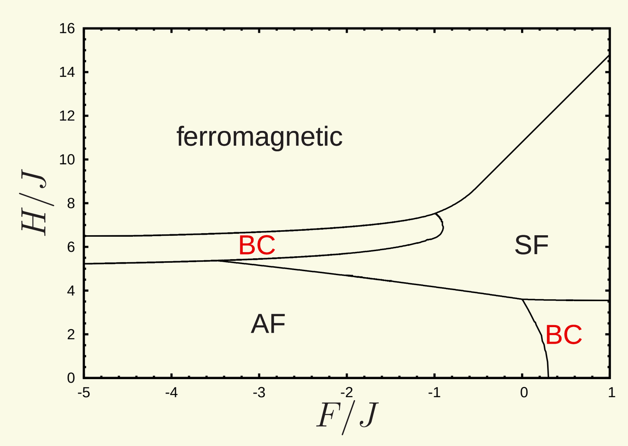
$$\mathcal{H} \;=\; \mathcal{H}_{xxz} \;-\; F \sum_i \left((S_i^x)^4 + (S_i^y)^4 + (S_i^z)^4 \right)$$



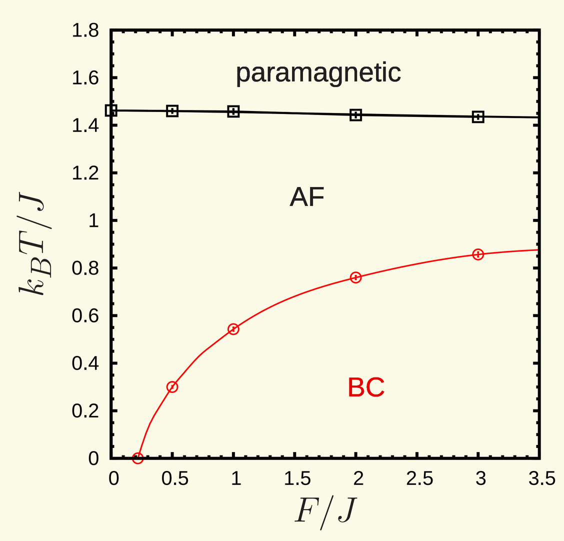
fourfold degenerate BC structure

$F > 0$:	Spins tend to align in direction of x-,y- and z-axis
$F < 0$:	Spins tend to align along the diagonals of cubic lattice

Ground state

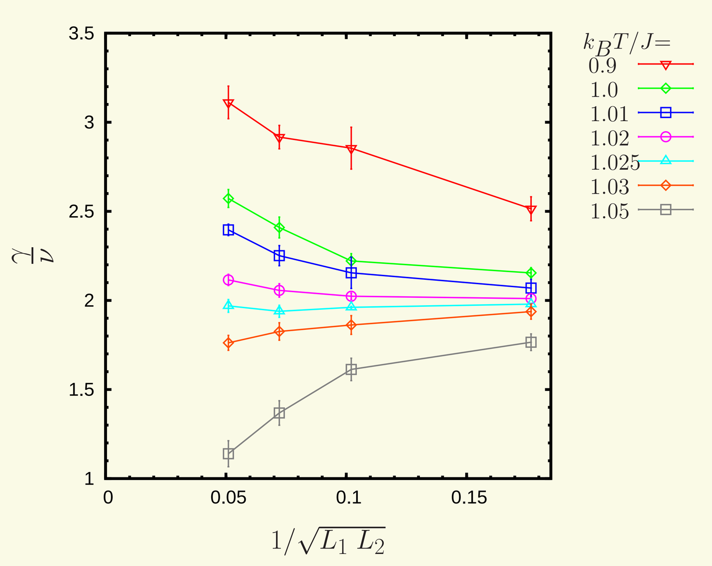


$H/J = 1.8$

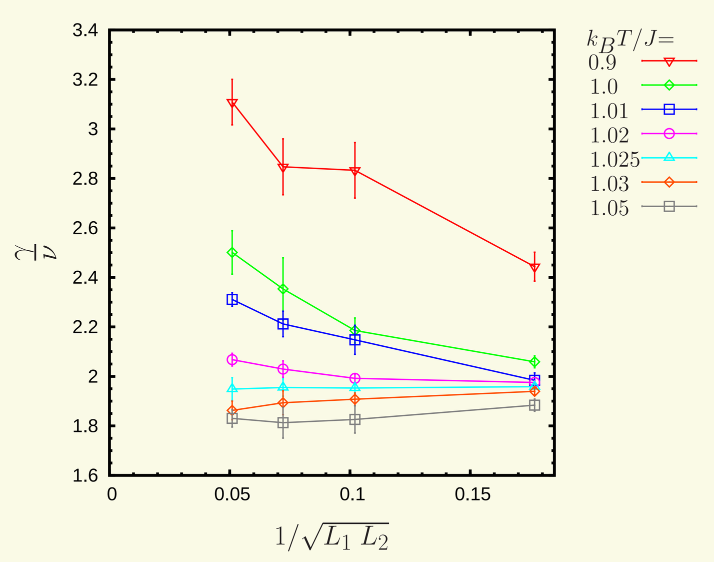


Locating the triple point $k_BT_{tp}/J,\ H_{tp}/J$

effective exponents for χ_{xy}^{st}



effective exponents for χ_z^{st}



Location: $\quad k_BT_{tp}/J \;=\; 1.025 \pm 0.015$, $\quad H_{tp}/J \;=\; 3.90 \;\pm 0.03$

For comparison:
D. P. Landau, K. Binder, PRB (1978)

See also:
R. Folk, Yu Holovatch, G. Moser, PRE (2008); P. Calabrese, A. Pelissetto, E. Vicari, PRB (2003)

Conclusions

- At low temperatures, XXZ model in $d = 3$ displays a first order phase transition between AF and SF phases, in contrast to $2d$ version; BC fluctuations are observed.
- Triple point, at which AF, SF, and disordered phases meet, has been accurately located.
- Introducing a cubic symmetry term, discretized BC phases and structures are stabilized.

WS, M.Holtschneider, R. Leidl, S. Wessel, and GB, Computer Simulations Studies in Condensed Matter Physics XXI (2008)

Outlook, in progress

- Quantum-Heisenberg antiferromagnets with spin-liquid (spin-flop) and supersolid (biconical) phases, found using DMRG calculations.