Anisotropic Heisenberg antiferromagnets in two dimensions

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XXZ model

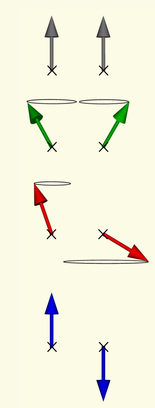
$$\mathcal{H}_{\mathrm{XXZ}} = J \sum_{\langle i,j \rangle} \left[\Delta (S_i^x S_j^x + S_i^y S_j^y) + S_i^z S_j^z \right] - H \sum_i S_i^z$$

nearest-neighbour pairs	$\langle i,j \rangle$
coupling strength	$J > 0$
easy-axis anisotropy	$\Delta < 1$
field in z-direction	H

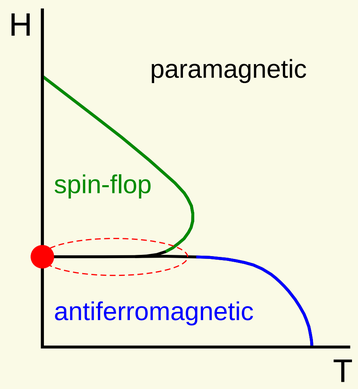
quantum: spin-operators $S_i^x,\ S_i^y,\ S_i^z;\quad S = \frac{1}{2}$

classical: spin-vectors $\vec{S}_i = (S_i^x, S_i^y, S_i^z);\quad |\vec{S}_i| = 1$

classical ground states



Structures



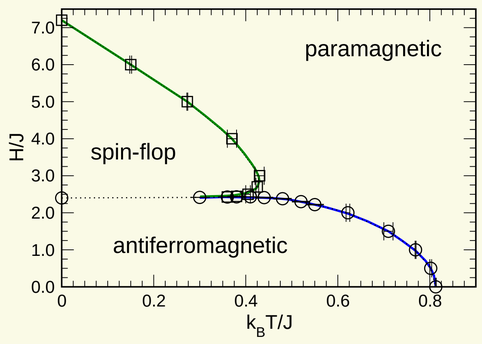
- spin-flop (SF) phase
  - 2D-XY-phase, algebraic order
  - large magnetization
- antiferromagnetic (AF) phase
  - long range order, large staggered magnetization
  - small magnetization
- ground state degeneracy:
  - antiferromagnetic, spin-flop, and biconical structures

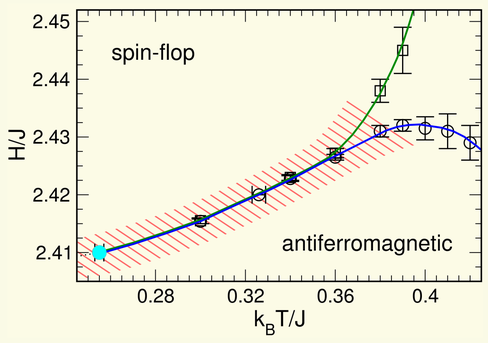
Classical model

Monte Carlo simulations:

- Metropolis updates
- Wang-Landau sampling

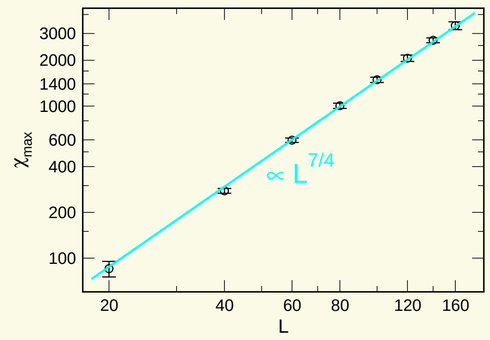
Phase diagram $(\Delta = 4/5)$





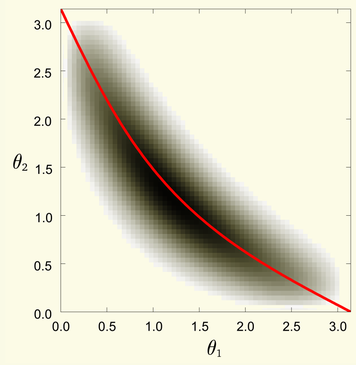
Staggered susceptibility

$H/J = 2.41$



finite-size behaviour suggests Ising transition, similar findings for specific heat

Biconical fluctuations



joint probability (higher = darker) of tilt angles at neighbouring sites

$H/J = 2.41 \quad k_BT/J = 0.255 \quad L = 80$

in biconical ground state:

$$\theta_2 = \arccos\left(\frac{\sqrt{1-\Delta^2} - \cos\theta_1}{1 - \sqrt{1-\Delta^2}\cos\theta_1} \right)$$

Conclusions

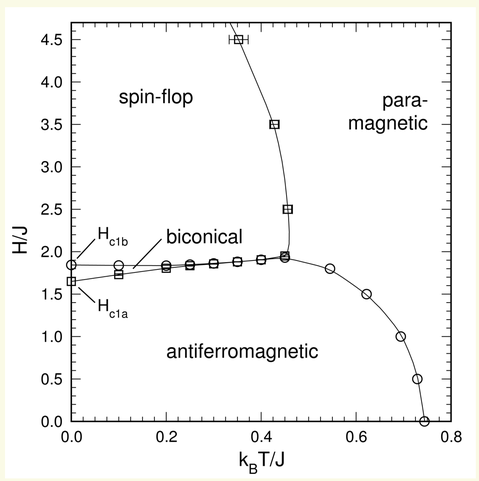
- AF phase boundary of Ising type down to lowest temperatures studied
- narrow intermediate phase with biconical fluctuations between AF and SF phases

Liu and Fisher, J. Low Temp. Phys. 10 (1973) 655
Landau and Binder, Phys. Rev. B 24 (1981) 1391
Holtschneider, W.S., and Leidl, Phys. Rev. B 72 (2005) 064443
Zhou, Landau, and Schulthess, Phys. Rev. B 74 (2006) 064407
Holtschneider, Weßel, and W.S., Phys. Rev. B 75 (2007) 224417
Pelissetto and Vicari, Phys. Rev. B (in print)

XXZ model with single-ion anisotropy

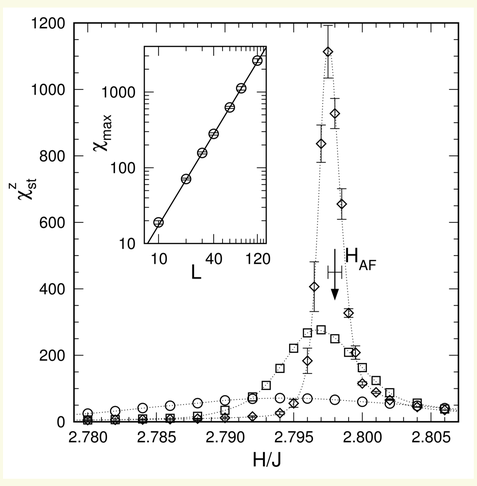
$$\mathcal{H} = \mathcal{H}_{\mathrm{XXZ}} + D \sum_i (S_i^z)^2$$

$D > 0$



stable biconical phase

$D < 0$



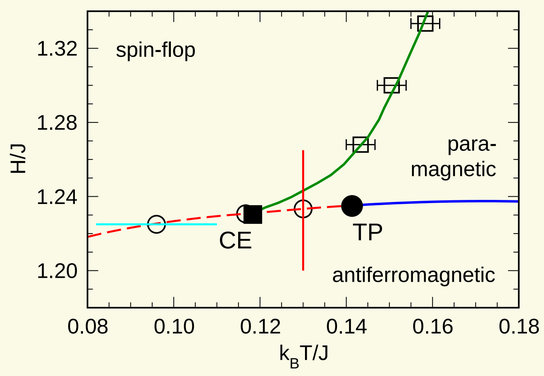
first order transition (AF ↔ SF) at low T

Quantum model

Quantum Monte Carlo simulations:

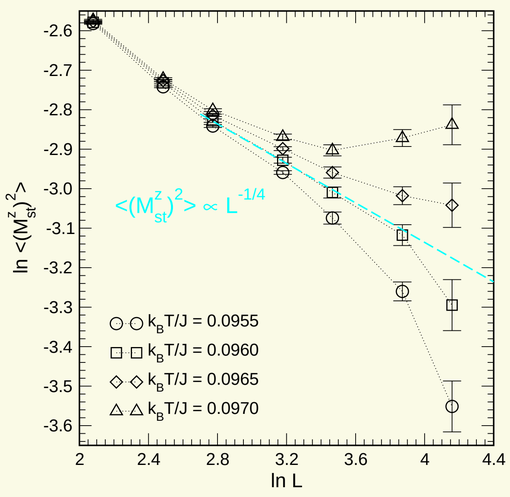
- stochastic series expansion
- directed loops
- parallel tempering

Phase diagram $(\Delta = 2/3)$



based on: Schmid, Todo, Troyer, and Dorneich, Phys. Rev. Lett. 88 (2002) 167208

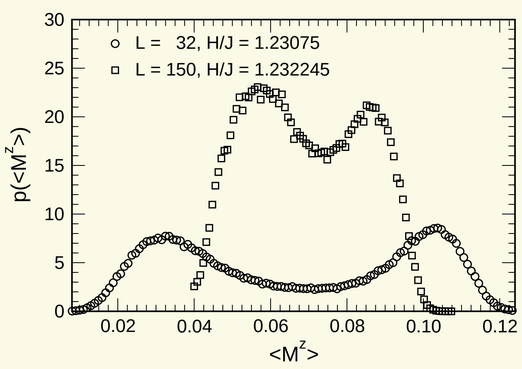
Order parameter: staggered magnetization



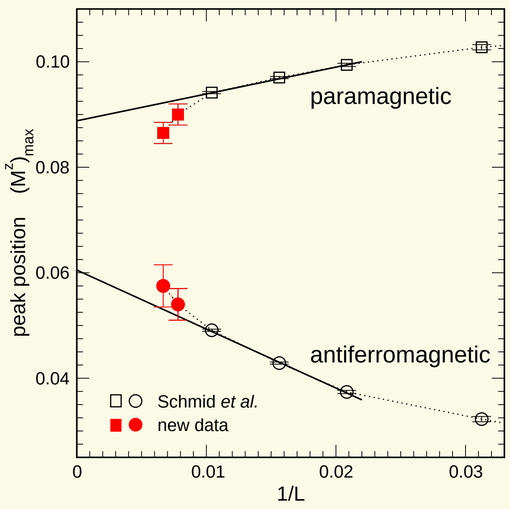
$H/J = 1.225$

finite-size behaviour is consistent with Ising transition

Magnetization histograms



$k_BT/J = 0.13$

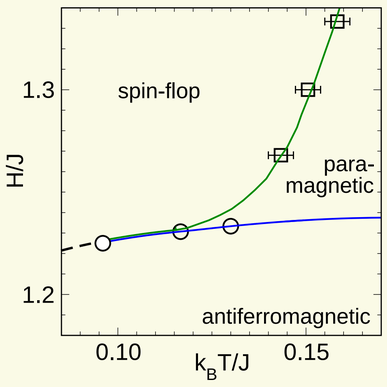


data for larger lattices deviate from previous extrapolation of peak positions

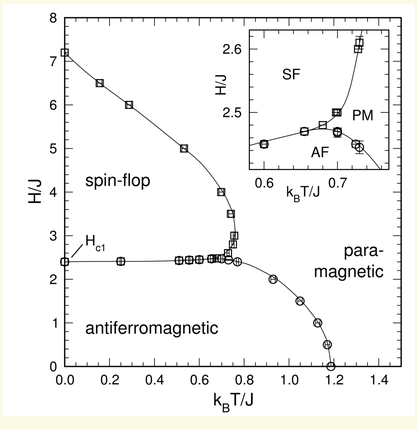
and suggest a second order AF to paramagnetic transition

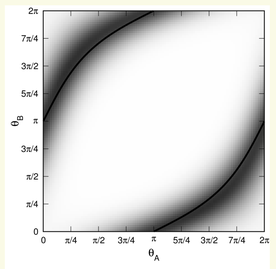
Conclusions

- AF to SF transition (for at least $k_BT/J > 0.0965$):
  - AF phase boundary is of Ising type
  - SF phase boundary consistent with KT transition
- TP and CE shift to lower temperatures or, possibly, different scenario realised
- biconical structures?



Anisotropic XY model





grey scale representation of joint probability of tilt angles at neighbouring sites

$H/J = 2.44 \quad k_BT/J = 0.558$

evidence for narrow disordered bidirectional phase between AF and SF phases

Holtschneider and W. S., Phys. Rev. B (in print, Rapid Comm.)