Anisotropic Heisenberg Antiferromagnets

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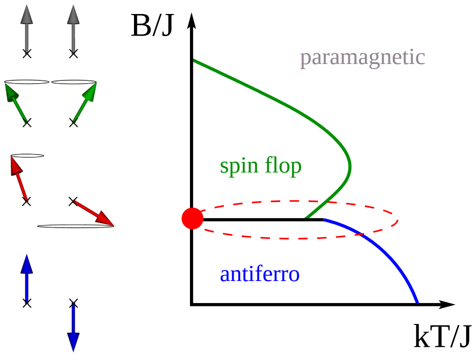
Supported by JARA-SIM

D.P. , I.P. McCulloch, W. Selke, Phys. Rev. B **79**, 132406 (2009)
W. Selke, G. Bannasch, M. Holtschneider, D.P., S. Wessel, Condensed Matter Physics **12**, 547 (2009)
D.P., I.P. McCulloch, W. Selke, Journal of Physics: Conf. Ser. **200**, 022046 (2010)

The uniaxial XXZ antiferromagnet

$$\mathcal{H}_{XXZ} = J\sum_{\langle ij\rangle}(S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z) - B\sum_i S_i^z$$



- uniaxial: $\Delta > 1$
- classical spins
- degenerate biconical (BC) configurations in the groundstate

Generic model for spin flop phase and multicritical phenomena (numerous experiments)

Lifting degeneracy and stabilizing BC-structures by single ion anisotropy :

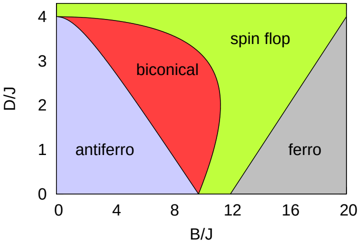
$$\mathcal{H} = \mathcal{H}_{\text{XXZ}}(\Delta, B) + D \sum_i (S_i^z)^2$$

Groundstate phase diagrams for chains

(a) $\Delta = 5$

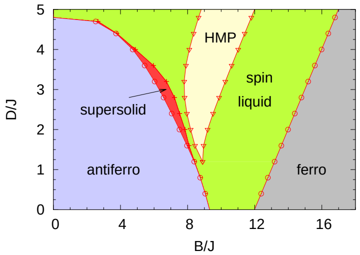
Classical spins

Energy minimization[1]



Quantum spins, $S = 1$

DMRG[1,2]



spin flop → spin liquid (SL)

biconical → supersolid (SS)

HMP = half magnetization plateau

[1] D.P., I.P. McCulloch, W. Selke,
Journal of Physics: Conf. Ser. **200**, 022046 (2010)

[2] T. Tonegawa, et al. PTP Suppl. **159** 77 (2005)

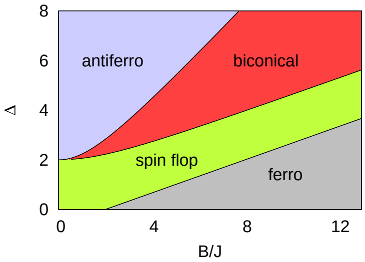
(b) $J\Delta/D = 2$

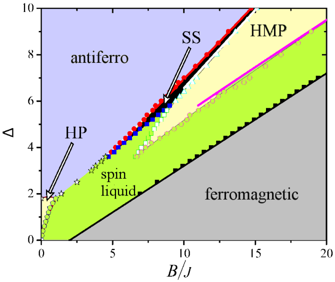
Classical spins

Energy minimization

Quantum spins, $S = 1$

QMC[1] confirmed by DMRG[2]



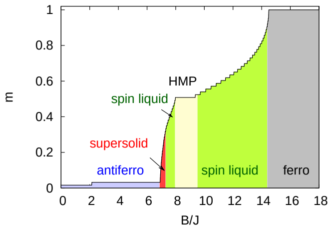


Additional new phase: HP=Haldane phase

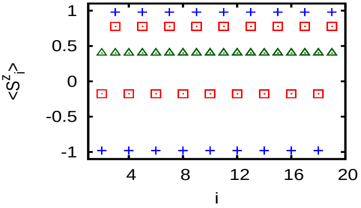
[1] P. Sengupta and C. D. Batista, Phys. Rev. Lett. **98**, 227201 (2007)

[2] D.P. , I.P. McCulloch, W. Selke, Phys. Rev. B **79**, 132406 (2009)

Identification of quantum phases using density matrix renormalization group (DMRG)



- phase borders: discontinuities and turning points in $m(B)$, the total magnetization
- finite chain of 63 spins with open boundary condition
- $\Delta = 2D/J = 5$



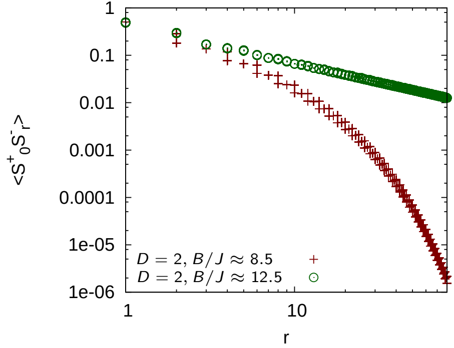
Parts of magnetization profiles from infinite DMRG:

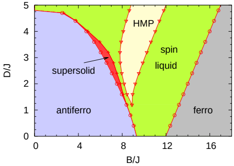
- antiferro, supersolid: different sublattice magnetizations in contrast to spin liquid phase
- $\Delta = 2D/J = 5$, $B/J = 6.9 \ldots 7.7$

Identification of the quantum phases by correlation functions

Transverse correlation function

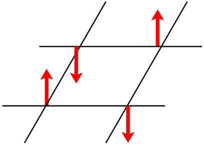
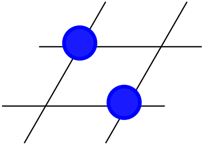
$\Delta = 5$





- Clear distinction between algebraic decay (spin liquid) and exponential decay (HMP)

Mapping Heisenberg antiferromagnets to quantum lattice gases

Quantum spin model		Quantum lattice gas
		
$s_i = 1/2, -1/2$		$n_i = 0, 1$
anisotropic exchange (J, Δ)	$\longleftrightarrow$	hopping t, interaction U
field B in z direction	$\longleftrightarrow$	chemical potential

T. Matsubara, H. Matsuda (1956)

Correspondence between spin and lattice gas phases

Based on this mapping[1]:

Spin model	**Quantum lattice gas**
antiferromagnet	solid
biconical	supersolid
spin flop	superfluid
ferromagnet	normal liquid

[1] H. Matsuda, T. Tsuneto (1970), K.S. Liu, M.E. Fisher (1973)

Note: At present, renewed interest in supersolid phases in ^{4}He and magnets

e.g. Z. Nussinov (2008), S. Balibar (2009)

Summary and outlook

- Quantum (and classical) groundstate phase diagrams of XXZ, plus single ion anisotropy, spin chains using infinite DMRG, exact diagonalization and Monte Carlo simulations: identification of antiferromagnetic, spin liquid (spin flop), supersolid (biconical), HMP and ferromagnetic phases.
- Further characterization of spin liquid (commensurate or incommensurate correlations) and transitions between various phases.