Thermodynamics of quantum magnets at large S

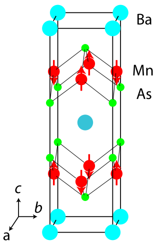
GEORG-AUGUST-UNIVERSITÄT GÖTTINGEN

Andreas Honecker[1], Mike Zhitomirsky[2], Johannes Richter[3], Moritz Härtel[3]

[1] *Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany*
[2] *Commissariat à l'Energie Atomique, DSM/INAC/SPSMS, Grenoble, France*
[3] *Institut für Theoretische Physik, Otto-von-Guericke-Universität Magdeburg, Germany*

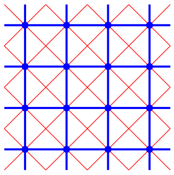
The challenge: example $BaMn_2As_2$

Crystal structure

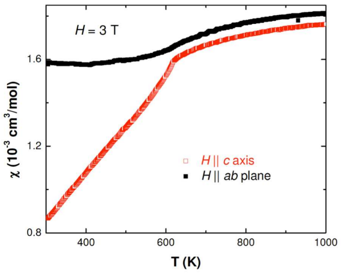


Heisenberg Hamiltonian

$$\mathcal{H} = \sum_{\langle i,j \rangle} J_{i,j}\, \vec{S}_i \cdot \vec{S}_j$$



Magnetic susceptibility [1]



Numerical methods

- **exact (full) diagonalization (ED):** restricted to $N \leq 10$ sites for $S = 2, 5/2$
- **Classical Monte Carlo: (MC)** no quantum corrections – accuracy unclear
- **Quantum Monte Carlo (QMC):** sign problem for J_1, $J_2 > 0$

  ALPS 1.3 directed loop application in stochastic series expansion framework

ALPS Applications and Libraries for Physics Simulations

http://alps.comp-phys.org/

☞ Probably a frustrated square lattice with exchange constants J_1, J_2 and spin $S = 2$ or $5/2$

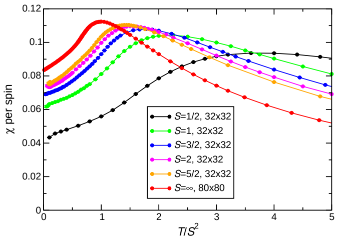
☞ **Goal:** Compute thermodynamic quantities (susceptibility χ) around the maximum and at higher temperatures

Scaling with spin S: MC + QMC for simple square-lattice antiferromagnet

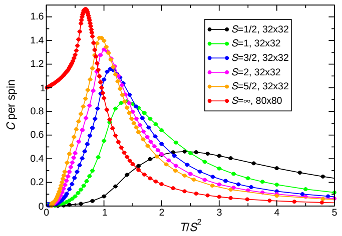
$J_1 = 1,\ J_2 = 0,\ H = 0$

Scaling with S^2 (scaling analysis of Hamiltonian in a magnetic field H) [2]

Susceptibility

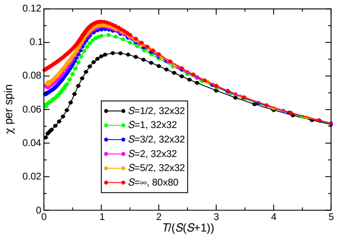


Specific heat

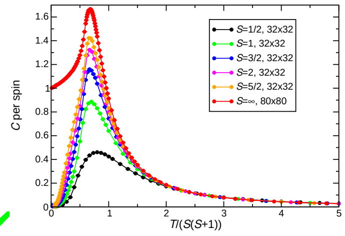


Scaling with $S\,(S+1)$ [3, 4] (leading term of high-T expansion at $H = 0$)

Susceptibility



Specific heat



Cumulant expansion

☞ **Spin-coherent states [5]**

$$\mathcal{C}_S \int \mathrm{d}\vec{n}\, |\vec{n}\rangle\langle\vec{n}| = \mathbb{I}\,, \qquad \mathrm{Tr} A = \mathcal{C}_S \int \mathrm{d}\vec{n}\, \langle\vec{n}|A|\vec{n}\rangle$$

☞ partition function

$$Z = \mathrm{Tr}\mathrm{e}^{-\beta\mathcal{H}} = \mathcal{C}_S^N \int \prod_{i=1}^N \mathrm{d}\vec{n}_i\, \langle\vec{n}|\mathrm{e}^{-\beta\mathcal{H}}|\vec{n}\rangle =: \mathcal{C}_S^N \int \prod_{i=1}^N \mathrm{d}\vec{n}_i\, \mathrm{e}^{-\beta\tilde{\mathcal{H}}}$$

with temperature-dependent **classical** Hamiltonian

$$\begin{aligned}\tilde{\mathcal{H}} &= -\frac{1}{\beta}\ln\langle\vec{n}|\mathrm{e}^{-\beta\mathcal{H}}|\vec{n}\rangle = -\frac{1}{\beta}\langle\vec{n}|\mathrm{e}^{-\beta\mathcal{H}} - 1|\vec{n}\rangle_c \\ &= \sum_{k=1}^{\infty}\frac{(-\beta)^{k-1}}{k!}\langle\vec{n}|\mathcal{H}^k|\vec{n}\rangle_c =: \sum_{k=1}^{\infty}\frac{(-\beta)^{k-1}}{k!}\tilde{\mathcal{H}}_k\end{aligned}$$

and **cumulants [6]:** $\ln\langle\vec{n}|\mathrm{e}^{\lambda\mathcal{H}}|\vec{n}\rangle = \langle\vec{n}|\mathrm{e}^{\lambda\mathcal{H}} - 1|\vec{n}\rangle_c$

☞ Lowest order: **classical** Heisenberg model

$$\tilde{\mathcal{H}}_1 = \tilde{J}\sum_{\langle i,j\rangle}\vec{n}_i\cdot\vec{n}_j \qquad \text{with } \tilde{J} = S^2\,J$$

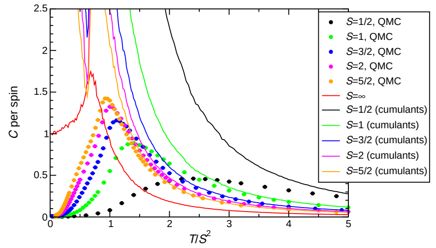
☞ perturbative $1/S$ expansion for free energy
⇒ first correction to specific heat

$$\begin{aligned}\Delta C_1 = \frac{\beta^2}{S}\Big\{&\langle U_2\rangle - 2\beta\left[\langle U_2\tilde{\mathcal{H}}_1\rangle - \langle U_2\rangle\langle\tilde{\mathcal{H}}_1\rangle\right] \\ &+\frac{\beta^2}{2}\left[\langle U_2\tilde{\mathcal{H}}_1^2\rangle - 2\langle U_2\tilde{\mathcal{H}}_1\rangle\langle\tilde{\mathcal{H}}_1\rangle - \langle U_2\rangle\langle\tilde{\mathcal{H}}_1^2\rangle + 2\langle U_2\rangle\langle\tilde{\mathcal{H}}_1\rangle^2\right]\Big\}\end{aligned}$$

with

$$\begin{aligned}U_2 = -\frac{2S}{\beta}\tilde{\mathcal{H}}_2 = \tilde{J}^2\sum_{\langle i,j\rangle}&\left\{1 - (\vec{n}_i\cdot\vec{n}_j)^2 + \frac{1}{4S}\left[1 - \vec{n}_i\cdot\vec{n}_j\right]^2\right\} \\ &-\frac{\tilde{J}^2}{2}\sum_i\sum_{j\neq k}\left\{(\vec{n}_i\cdot\vec{n}_j)\,(\vec{n}_i\cdot\vec{n}_k) - (\vec{n}_j\cdot\vec{n}_k)\right\}\end{aligned}$$

Specific heat for 32×32 square lattice

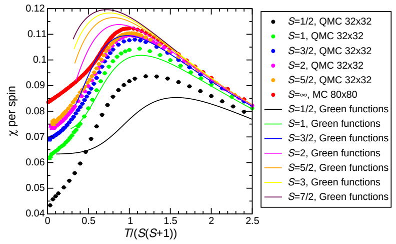


Automatically correct scaling with S at high T

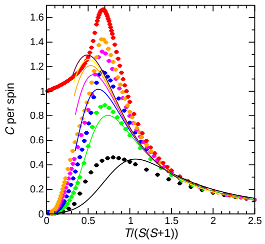
Green-function theory: higher-order $SU(2)$-invariant mean-field theory

$J_1 = 1,\ J_2 = 0,\ H = 0$

Susceptibility



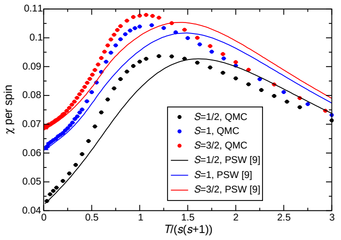
Specific heat



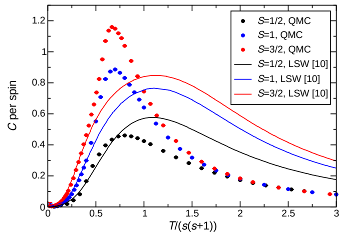
for the technique compare [7] and references therein

Linearized spin-wave (LSW) and perturbative spin-wave (PSW) theory in the spirit of Takahashi [8]

Susceptibility



Specific heat



Restricted to low temperatures

References

[1] Y. Singh, B. Lake, D. Johnston *et al.*, unpublished

[2] A. Honecker, M.E. Zhitomirsky, J. Phys.: Conf. Ser. **145** (2009) 012082

[3] Y.J. Kim, M. Greven, U.-J. Wiese, R.J. Birgeneau, Eur. Phys. J. B **4** (1998) 291

[4] L. Engelhardt, M. Luban, C. Schröder, Phys. Rev. B **74** (2006) 054413

[5] E.H. Lieb, Comm. Math. Phys. **31** (1973) 327

[6] K. Kladko, P. Fulde, D.A. Garanin, Europhys. Lett. **46** (1999) 425

[7] I. Juhász Junger, D. Ihle, J. Richter, Phys. Rev. B **80** (2009) 064425

[8] M. Takahashi, Phys. Rev. B **40** (1989) 2494

[9] Y.H. Su, M.M. Liang, G.M. Zhang, arXiv:0912.3859

[10] M.M. Liang, Y.H. Su, arXiv:0912.4965

Acknowledgments

Heisenberg-Programm
Deutsche Forschungsgemeinschaft
SFB 602

Korrelationstage 2011