Magneto-thermal properties of highly frustrated Heisenberg spin clusters: the approach to the classical limit

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Heisenberg antiferromagnets: classical limit of thermodynamic quantities

Heisenberg model

$$H = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j - h \sum_i S_i^z$$

- $\vec{S}_i$: *quantum* spin-s operators
- $J > 0$: exchange constant
- $\langle i,j \rangle$: nearest neighbor sites
- h: external magnetic field

Adiabatic cooling rate at fixed entropy S

$$\Gamma_h = \frac{1}{T} \left. \frac{\mathrm{d}T}{\mathrm{d}h} \right|_S = -\frac{1}{C} \left. \frac{\mathrm{d}M}{\mathrm{d}T} \right|_h .$$

Classical limit

$s \to \infty$ at fixed

$$J_{\mathrm{cl}} = s^2 J\,, \quad h_{\mathrm{cl}} = s\,h$$

⇒ $\vec{S}_i$: unit vectors

⇒ scaling of thermodynamic quantity $\mathcal{Q}_s$ with s:

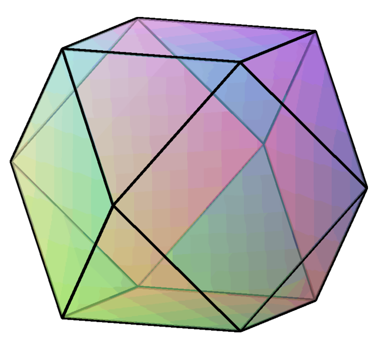
$$s^{\alpha_{\mathcal{Q}}} \mathcal{Q}_s \left(\frac{T}{s^2 J}, \frac{h}{s\,J} \right) \underset{s \to \infty}{\longrightarrow} \mathcal{Q}_{\mathrm{cl.}} \left(\frac{T}{J_{\mathrm{cl}}}, \frac{h_{\mathrm{cl}}}{J_{\mathrm{cl}}} \right) \qquad (\star)$$

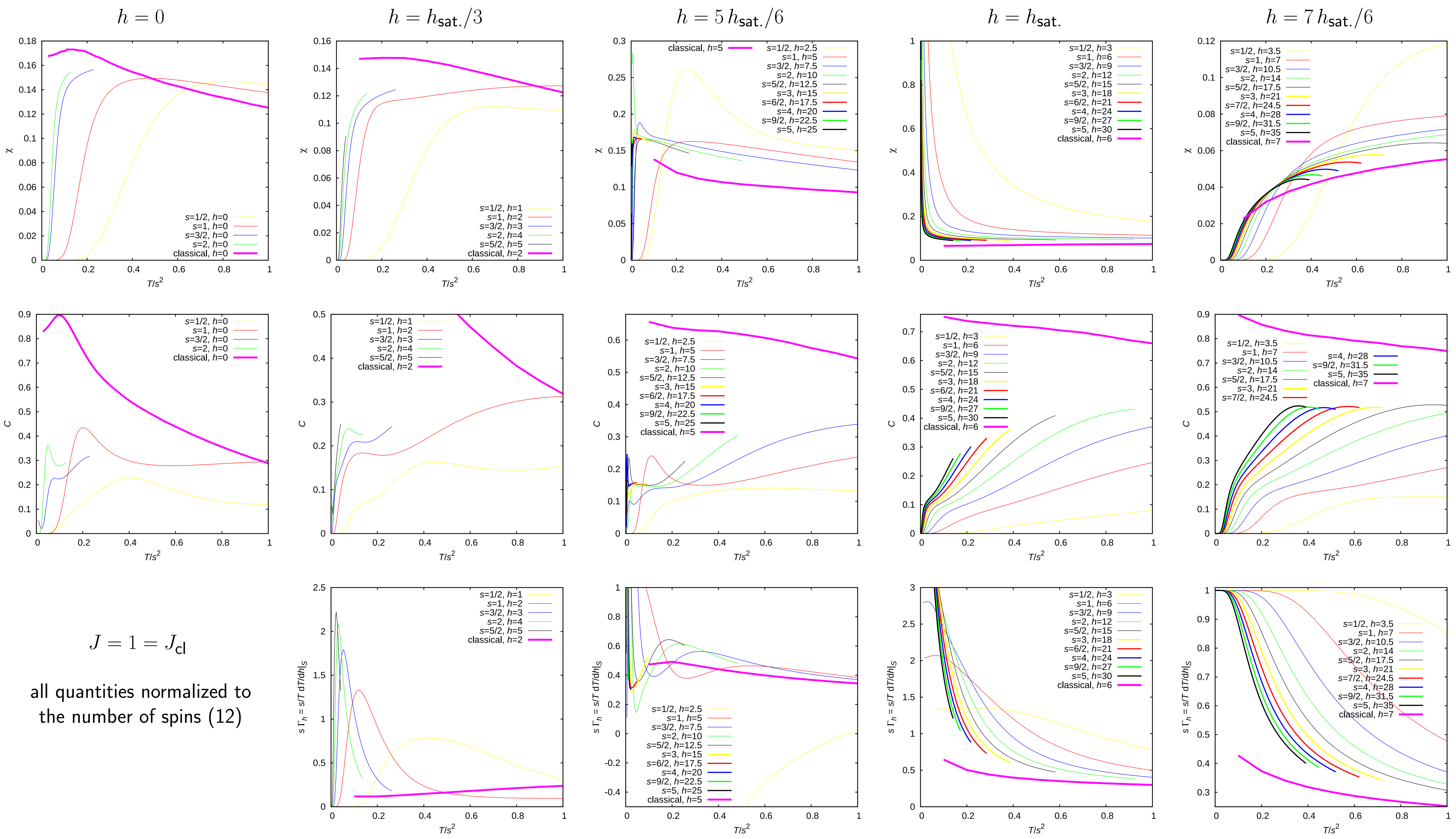
- magnetic susceptibility: $\alpha_\chi = 0$
- cooling rate: $\alpha_{\Gamma_h} = 1$
- specific heat: $\alpha_C = 0$
- magnetization: $\alpha_M = -1$

Motivation / Questions

- Application efficient low-temperature cooling by adiabatic demagnetization [1–5]
- Computations for frustrated quantum magnets restricted to low s and/or low dimensions [3–6]
- Good agreement of some experiments with classical simulations [1,2]
- How good is the approximation of a spin-s system by a classical system in terms of ($\star$) ?
- $T \le c\,J\,s$: level spacing visible ⇒ deviation from classical behavior
  - What is the prefactor c ?
  - Is c small for frustrated magnets ?

Cuboctahedron





- Supports localized magnons [7,8]
  - ⇒ degeneracy at saturation field $h_{\mathrm{sat.}} = 6\,J\,s$
  - ⇒ enhanced magnetocaloric effect
- Used as a model system, see also [9–11]

- Full diagonalization for $s = 1/2$ and 1
- Truncation to low energies for $s > 1$
  Spectrum complete until E_{c}: restrict to

$$T \le E_{\mathrm{c}}/10$$

- Classical spins: Metropolis Monte Carlo with over-relaxation

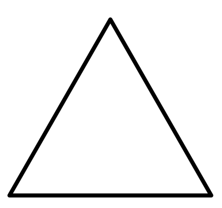
$$J = 1 = J_{\mathrm{cl}}$$

all quantities normalized to the number of spins (12)

Results for $T \lesssim J\,s^2$:

- Trend of convergence towards classical limit
- Substantial quantitative deviations, even for $s = 5$

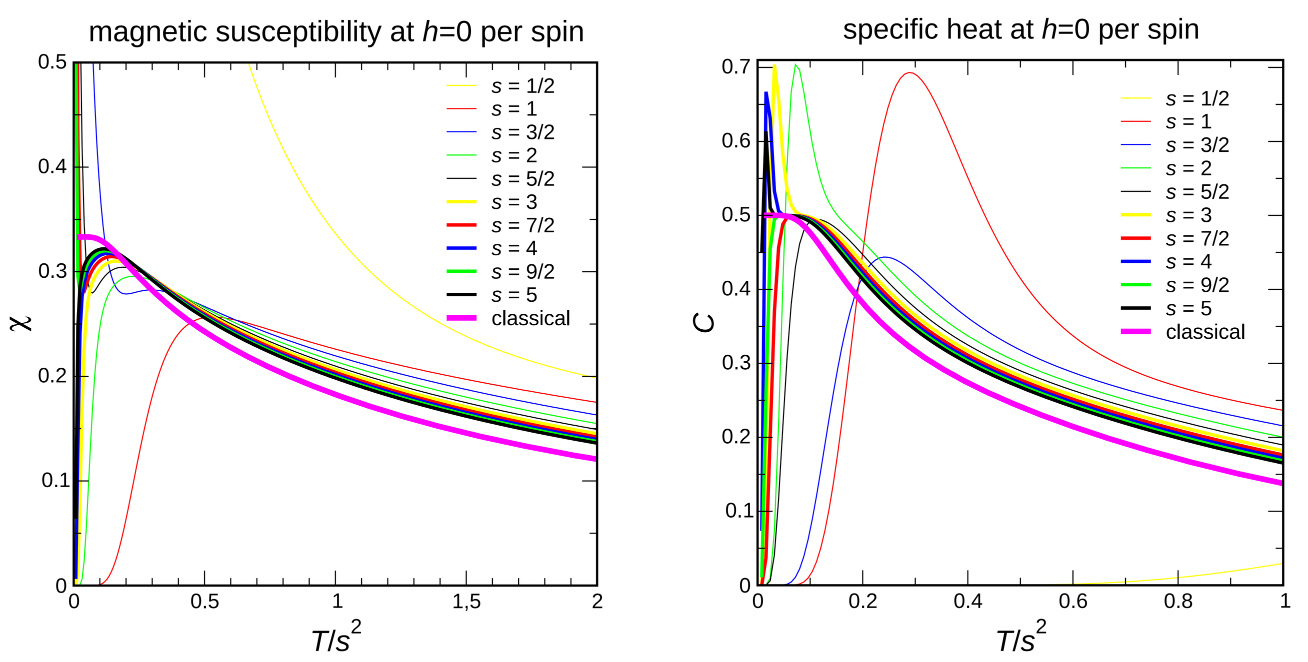
Triangle



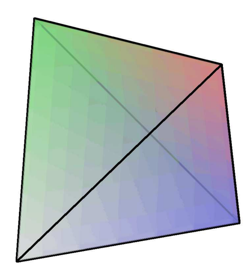
$$H = \frac{J}{2} \vec{S}_{\mathrm{tot.}}^2 - h S_{\mathrm{tot.}}^z - 3\,s\,(s+1)/2$$

with $\vec{S}_{\mathrm{tot.}} = \sum_{i=1}^{3} \vec{S}_i$

⇒ analytic results



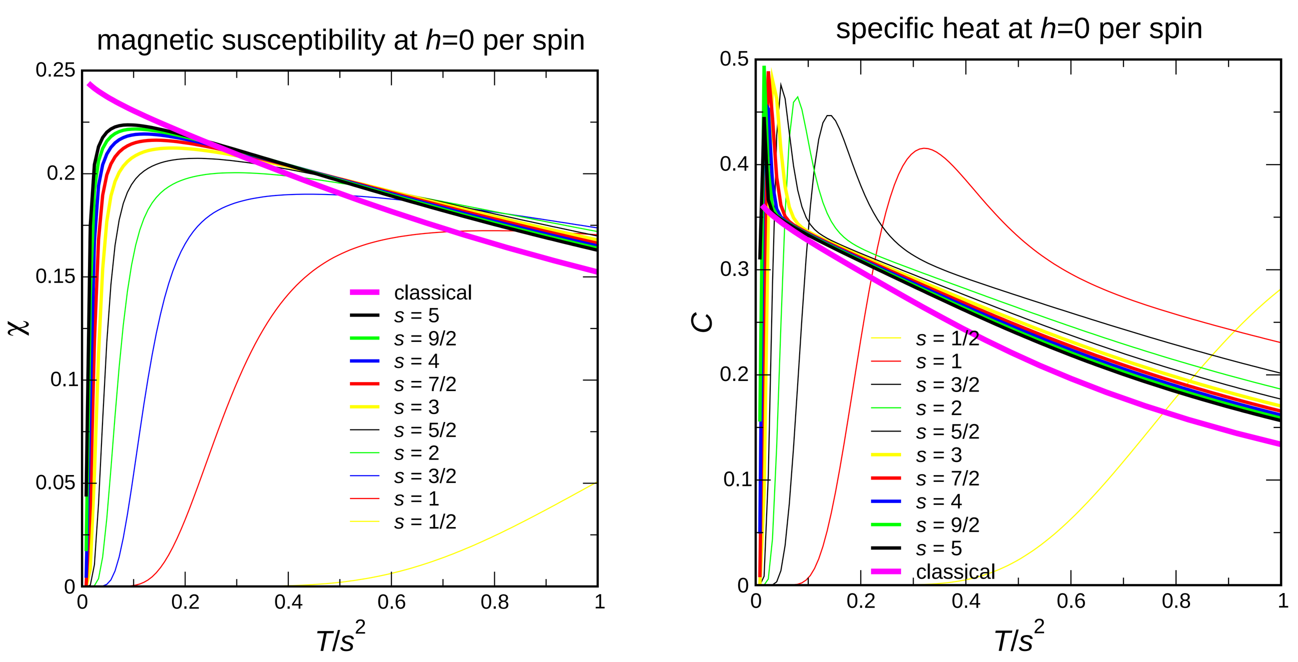
Tetrahedron



$$H = \frac{J}{2} \vec{S}_{\mathrm{tot.}}^2 - h S_{\mathrm{tot.}}^z - 2\,s\,(s+1)$$

with $\vec{S}_{\mathrm{tot.}} = \sum_{i=1}^{4} \vec{S}_i$

⇒ analytic results



Conclusion

Be careful when using a classical model for a quantitative description of a "large-spin" Heisenberg antiferromagnet in the low-temperature region $T \lesssim J\,s^2$

(compare also [12,13])

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References

[1] Zhitomirsky M E 2003 *Phys. Rev. B* **67** 104421

[2] Sosin S S, Prozorova L A, Smirnov A I, Golov A I, Berkutov I B, Petrenko O A, Balakrishnan G, Zhitomirsky M E 2005 *Phys. Rev. B* **71** 094413

[3] Zhitomirsky M E, Honecker A 2004 *J. Stat. Mech.: Theor. Exp.* P07012

[4] Honecker A, Wessel S 2006 *Physica B* **378-380** 1098

[5] Schmidt B, Thalmeier P, Shannon N 2007 *Phys. Rev. B* **76** 125113

[6] Boyarchenkov A S, Bostrem I G, Ovchinnikov A S 2007 *Phys. Rev. B* **76** 224410

[7] Schnack J, Schmidt H-J, Richter J, Schulenburg J 2001 *Eur. Phys. J. B* **24** 475

[8] Schulenburg J, Honecker A, Schnack J, Richter J, Schmidt H-J 2002 *Phys. Rev. Lett.* **88** 167207

[9] Schmidt R, Richter J, Schnack J 2005 *J. Magn. Magn. Mater.* **295** 164

[10] Schnack J, Richter J, Schmidt R 2007 *Phys. Rev. B* **76** 054413

[11] Rousochatzakis I, Läuchli A M, Mila F 2008 *Phys. Rev. B* **77** 094420.

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

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

[14] Honecker A, Zhitomirsky M E 2008 *submitted to the proceedings*