Metamagnetic phase transition of the af Heisenberg icosahedron

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Novel theoretical aspects of frustrated spin systems

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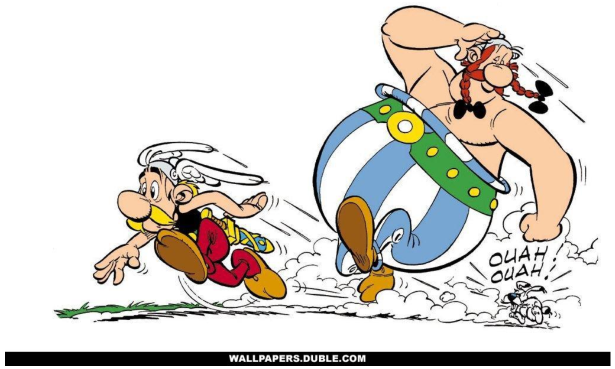
History of Frustration in Osnabrück

"Quintilius Varus, give me back my legions."

Augustus

Strong frustration in France 50 B.C.



Nous sommes en 50 avant Jésus-Christ. Toute la Gaule est occupée par les Romains... Toute? Non! Un village peuplé d'irréductibles Gaulois résiste encore et toujours à l'envahisseur. Et la vie n'est pas facile pour les garnisons de légionnaires romains des camps retranchés de Babaorum, Aquarium, Laudanum et Petitbonum...

(The year is 50 B.C. Gaul is entirely occupied by the Romans. Well not entirely! One small village of indomitable Gauls still holds out against the invaders. And life is not easy for the Roman legionaries who garrison the fortified camps of Totorum, Aquarium, Laudanum and Compendium...)

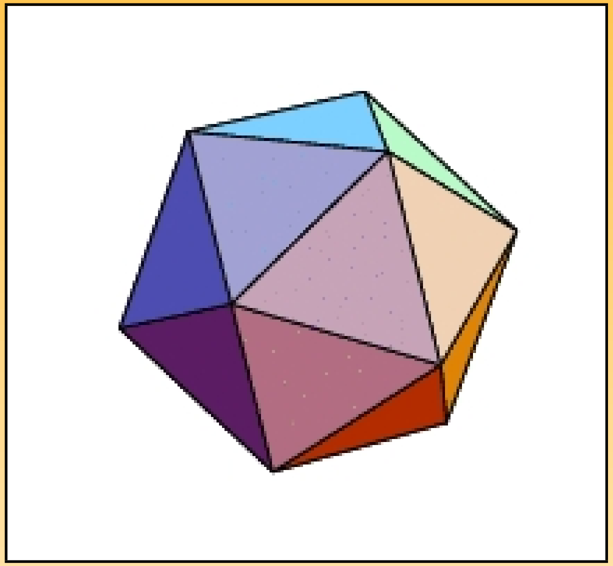
Strong frustration in Germany 9 AD


- Varus battle (9 AD) in *Kalkriese* close to Osnabrück, over 20.000 Romans killed;
- Proven due to coins from LUGDUNUM (Lyon), only coins before 9 AD found;
- Osnabrück remained barbarian: $\Rightarrow$ University founded not until 1974!

Today’s frustration in Osnabrück

1. Extension of Lieb, Schultz, and Mattis: k–rule for odd rings (poster)
2. $\{\text{Mo}_{72}\text{Fe}_{30}\}$ – a molecular brother of the kagome lattice (DMRG, poster)
3. Giant magnetization jumps in frustrated antiferromagnets
4. Magnetization plateaus and susceptibility minima in magnetic polytopes
5. Enhanced magnetocaloric effect
6. Hysteresis without anisotropy

Introduction

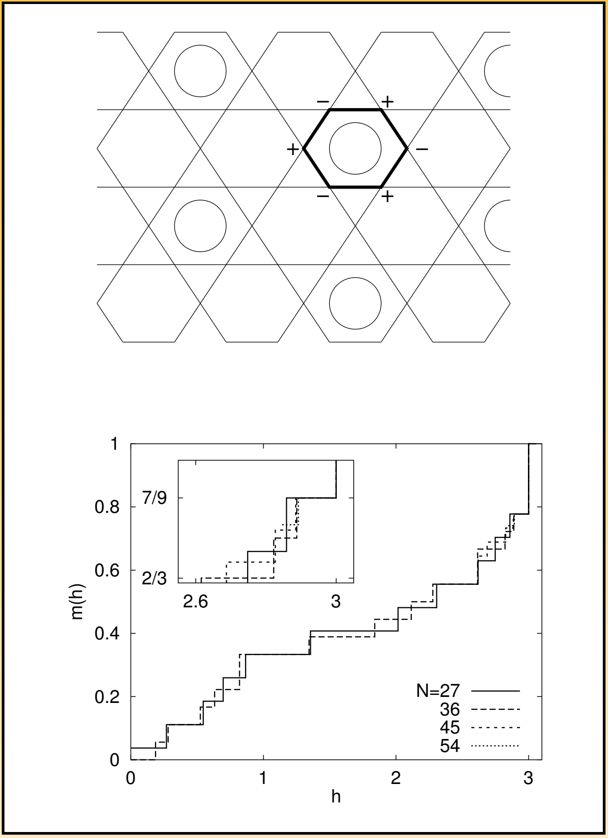


- Investigate antiferromagnetically coupled spins mounted on the vertices of an icosahedron.
- Isotropic Heisenberg exchange + applied magnetic field.
- Classical realization: magnetization jump, 1st order phase transition, hysteresis, metastability.
- Quantum realization: with increasing s unusual jumps of the magnetization.

Classical First Order $(T = 0)$ Phase Transition

C. Schröder, H.-J. Schmidt, J. Schnack, M. Luban, Phys. Rev. Lett. **94**, 207203 (2005)

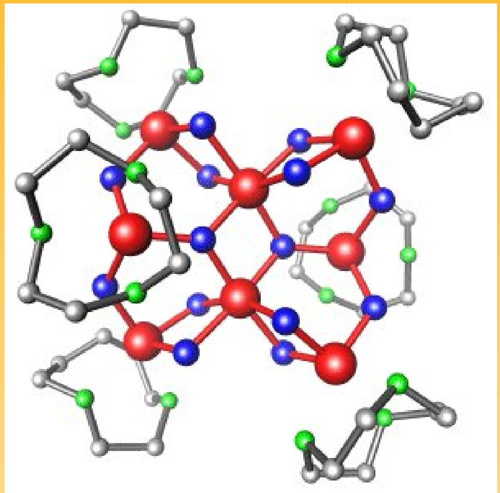
Magnetization jumps due to independent magnons

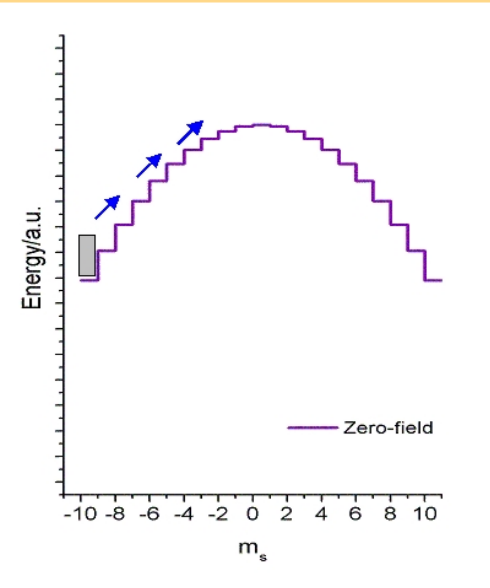


- Non-interacting one-magnon states can be placed on various lattices (Fe_{30}, kagome, pyrochlore, . . .).
- Each state of n independent magnons is the ground state in the Hilbert subspace with $M = Ns - n$.
- Linear dependence of E_{min} on M (non-convex) $\Rightarrow$ magnetization jump;
- Maximal number of independent magnons for the kagome: N/9;
- Jump is a macroscopic quantum effect!

J. Schulenburg, A. Honecker, J. Schnack, J. Richter, H.-J. Schmidt, Phys. Rev. Lett. **88**, 167207 (2002)
J. Richter, J. Schulenburg, A. Honecker, J. Schnack, H.-J. Schmidt, J. Phys.: Condens. Matter **16**, S779 (2004)

Hysteresis in molecular magnets





- Single Molecule Magnets (SMM): magnetic molecules with large ground state moment;

- Example: $S = 10$ for Mn_{12} or Fe_8;

- Anisotropy dominates approximate single-spin Hamiltonian:

$$\underset{\sim}{H} = -D\underset{\sim}{S}_z^2 + \underset{\sim}{H}', \qquad \left[\underset{\sim}{S}_z, \underset{\sim}{H}'\right] \neq 0$$

- Molecular Magnets show metastable magnetization and hysteresis due to anisotropy.

  Compare extensive work of R. Sessoli, W. Wernsdorfer, D. Gatteschi, I. Chiorescu, and many others.

Model Hamiltonian – Heisenberg-Model

$$\underset{\sim}{H} = \sum_{i,j} \underset{\sim}{\vec{s}}(i) \cdot \mathbf{J}_{ij} \cdot \underset{\sim}{\vec{s}}(j) + \sum_{i,j} \vec{D}_{ij} \cdot \left[\underset{\sim}{\vec{s}}(i) \times \underset{\sim}{\vec{s}}(j) \right] + \mu_B \, B \sum_{i}^{N} g_i \, \underset{\sim}{s}_z(i)$$

Exchange/Anisotropy   Dzyaloshinskii-Moriya   Zeeman

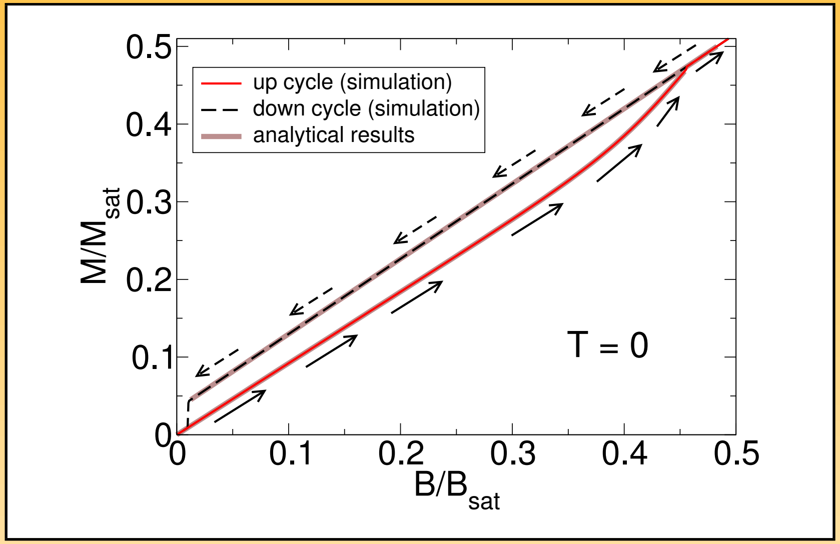
Very often anisotropic terms are utterly negligible, then . . .

$$\underset{\sim}{H} = -\sum_{i,j} J_{ij} \, \underset{\sim}{\vec{s}}(i) \cdot \underset{\sim}{\vec{s}}(j) + g \, \mu_B \, B \sum_{i}^{N} \underset{\sim}{s}_z(i)$$

Heisenberg   Zeeman

The Heisenberg Hamilton operator together with a Zeeman term are used for the following considerations; $J < 0$: antiferromagnetic coupling.

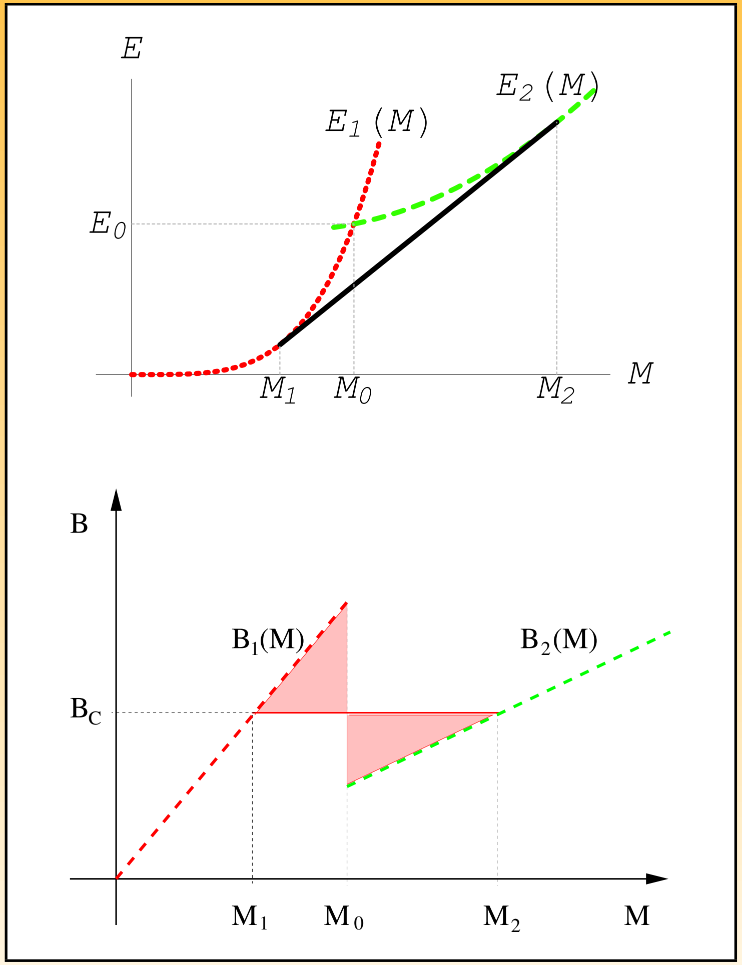
Metamagnetic phase transition I
Hyteresis without anisotropy



- Hysteresis behavior of the classical icosa-hedron in an applied magnetic field.
- Classical spin dynamics simulations (thick lines).
- Analytical stability analysis (grey lines).

C. Schröder, H.-J. Schmidt, J. Schnack, M. Luban, Phys. Rev. Lett. **94**, 207203 (2005)

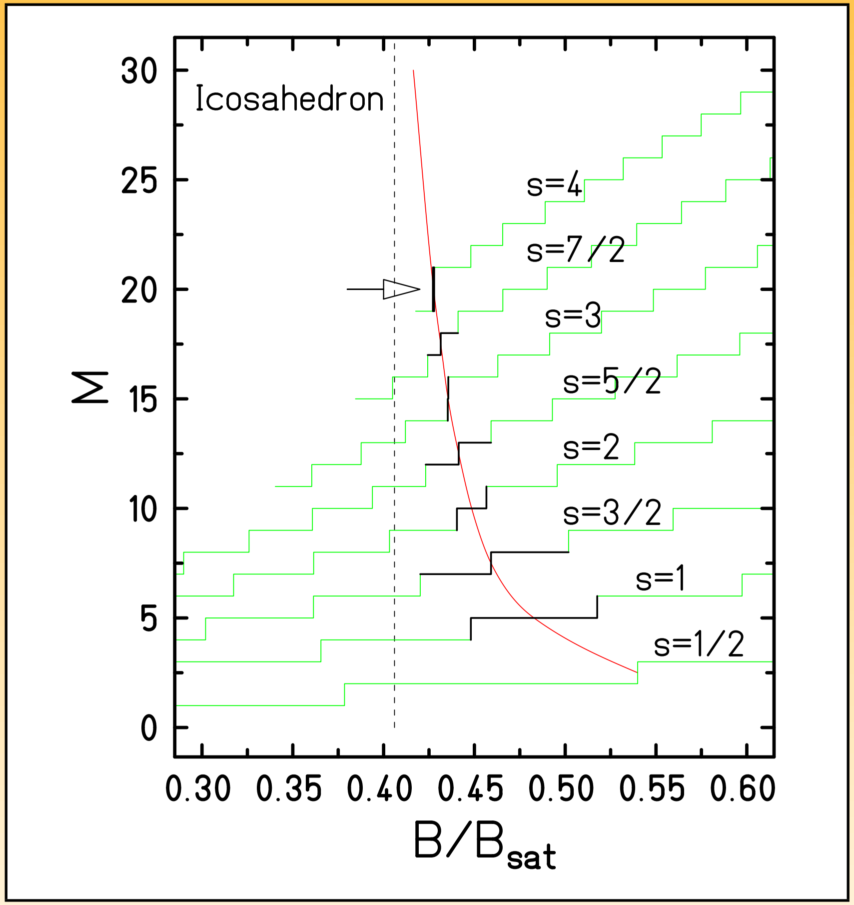
Metamagnetic phase transition II
Non-convex minimal energy



- Minimal energies realized by two families of spin configurations (1): $E_1(M)$ – "4-θ-family", $E_2(M)$ – "decagon family"
- Overall minimal energy curve is not convex.
- Maxwell construction yields ($T = 0$) 1st order phase transition at B_c (1,2,3)
- ($T = 0$)–magnetization dynamics extends into metastable region.

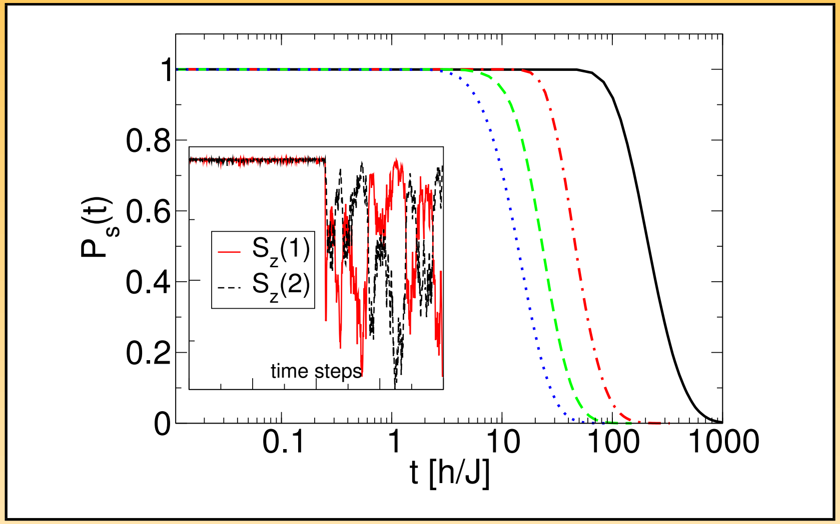
(1) C. Schröder, H.-J. Schmidt, J. Schnack, M. Luban, Phys. Rev. Lett. **94**, 207203 (2005)
(2) D. Coffey and S.A. Trugman, Phys. Rev. Lett. **69**, 176 (1992)
(3) C. Lhuillier and G. Misguich, in *High Magnetic Fields*, Eds. C. Berthier, L. Levy, and G. Martinez, Springer (2002) 161-190

Metamagnetic phase transition III
Quantum icosahedron



- Quantum analog:
  Non-convex minimal energy levels
  $\Rightarrow$ magnetization jump of $\Delta M > 1$.
- Lanczos diagonalization for various s.
- True jump of $\Delta M = 2$ for $s = 4$.
- Polynomial fit in $1/s$ yields the classically observed transition field.

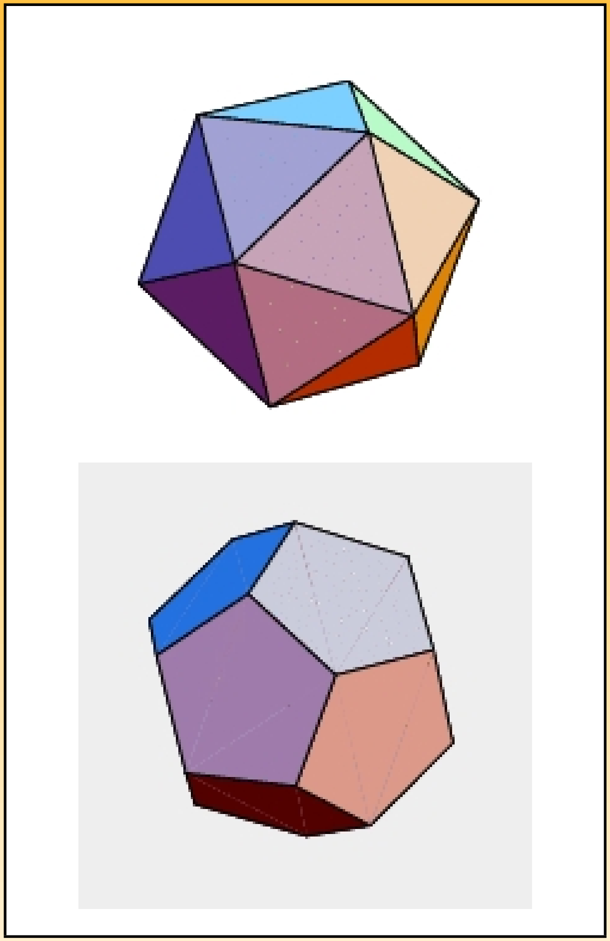
Metamagnetic phase transition IV
Metastability



- Classical spin dynamics simulations (Christian Schröder).
- Survival probability $P_{\mathrm{s}}(t)$ for the metastable decagon phase subject to an external field $B/B_{\mathrm{sat}} = 0.27$ for temperatures $k_B T/J = 0.025, 0.015, 0.005, 0.0005$ (left to right).
- Inset: Example trajectory of the system's time evolution at finite temperature.

C. Schröder, H.-J. Schmidt, J. Schnack, M. Luban, Phys. Rev. Lett. **94**, 207203 (2005)

Similar transitions



- First noticed in the context of the Buckminster fullerenes C_{20} and C_{60} (1).
- This phase transition exists in the edge-sharing icosahedron and the dodecahedron.
- It seems to be important that the ground state is not coplanar and spins do not fold umbrella-like in field. The symmetry of low-field and high-field ground states needs to be different;
Counter examples: $\{Mo_{72}Fe_{30}\}$, kagome lattice.

(1) D. Coffey and S.A. Trugman, Phys. Rev. Lett. **69**, 176 (1992).

Summary

Frustration can lead to exotic behavior.

And, the end is not in sight, . . .

. . . , however, this talk is at its end!

Thank you very much for your attention.

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