Modern aspects in magnetic structure and dynamics

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Modern Aspects in Nuclear Structure and Reactions
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Universität Bielefeld
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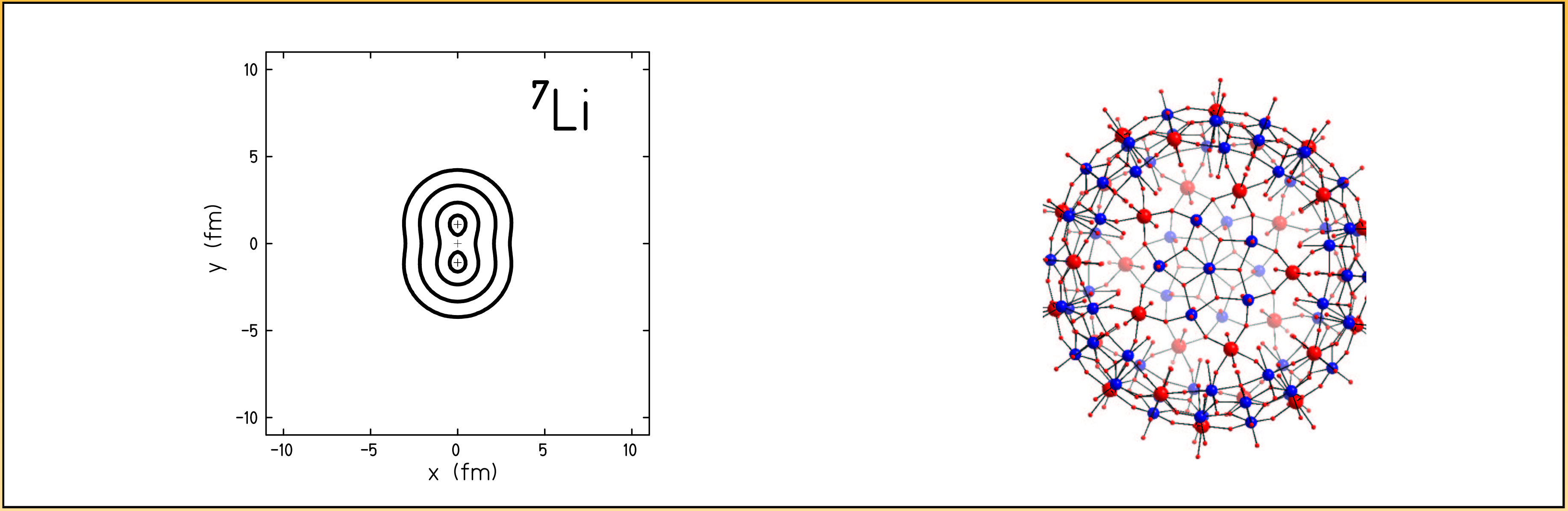
From today’s perspective:

nuclei and magnetic molecules share many interesting properties

Today’s perspective I – finite quantum systems



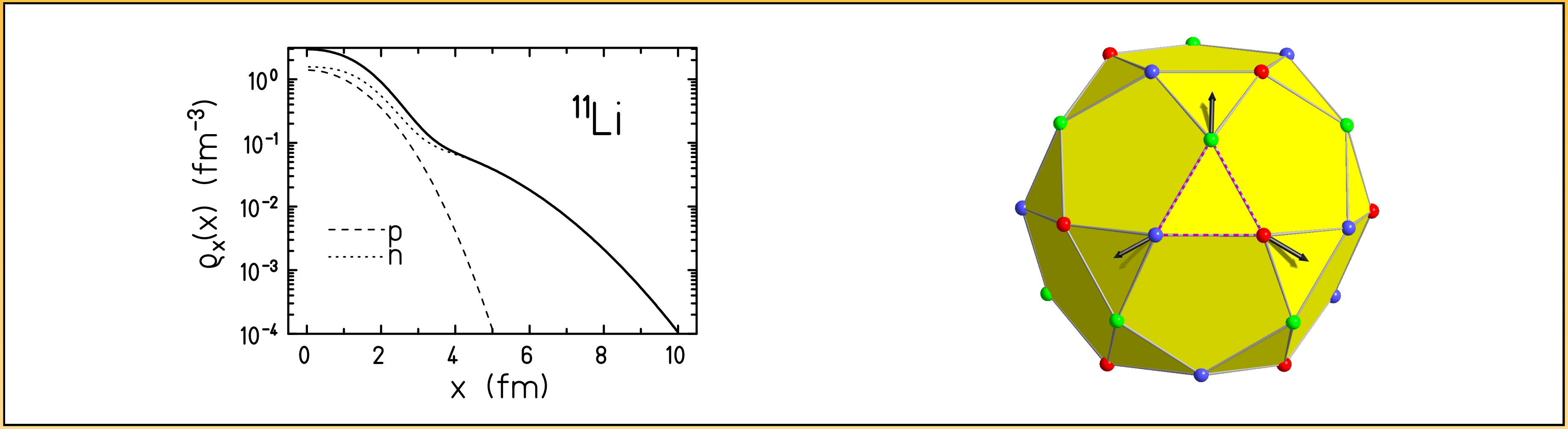
- nuclei built of nucleons
- coordinates, spins, isospins

H. Feldmeier, J. Schnack, Rev. Mod. Phys. **72**, 655 (2000)

- magnetic molecules containing paramagnetic ions
- spins, phonons

J. Schnack, in Lecture Notes in Physics **645**, 155 (2004)

Today's perspective II – correlated eigenstates



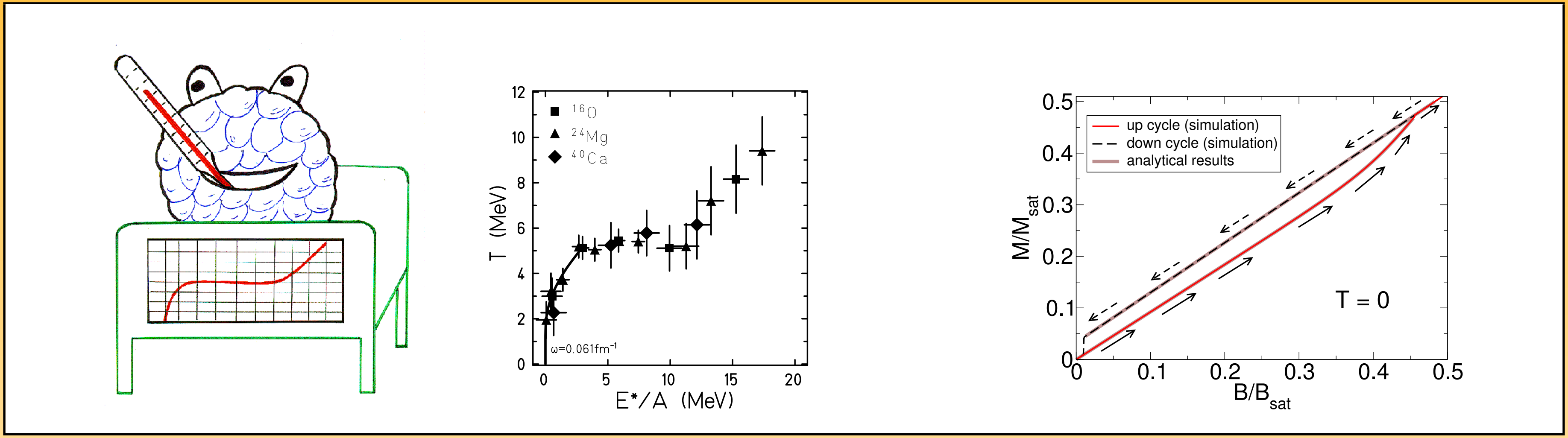
- many-body effects
- short-range correlations

H. Feldmeier, T. Neff, R. Roth, J. Schnack, Nucl. Phys. A **632**, 61 (1998)

- many-body effects
- geometric frustration

J. Schulenburg, A. Honecker, J. Schnack, J. Richter, H.-J. Schmidt, Phys. Rev. Lett. **88**, 167207 (2002)

Today’s perspective III – phase transitions



- nuclear caloric curve
- first order phase transition (boiling)

J. Schnack, H. Feldmeier, Phys. Lett. B **409**, 6 (1997)

- metamagnetic $(T = 0)$ phase transition
- first order, hysteresis

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

But at the beginning:

the start was a bit problematic

Problematic start I – Trabant against Mercedes

- At the very day of my arrival in September 1991: annual works outing (Betriebsausflug) to Kloster Lorsch; did not know the way, could not follow on the Autobahn!

...

Problematic start II – attraction won

- Crashed a chair in the restaurant! Got drunk at the wine tasting! Drove back trough dark night, crossing the Rhine with a ferry, . . .
- Had to redo my exams in Theoretical and Experimental Physics![1]
- It all proves the attraction of Hans Feldmeier’s group!

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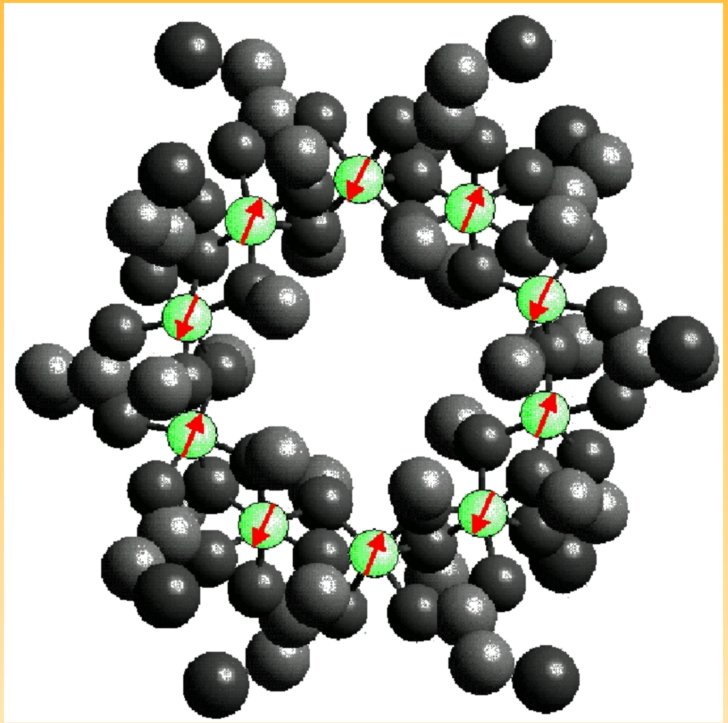
[1] Has nothing to do with the points above!

Contents for you today

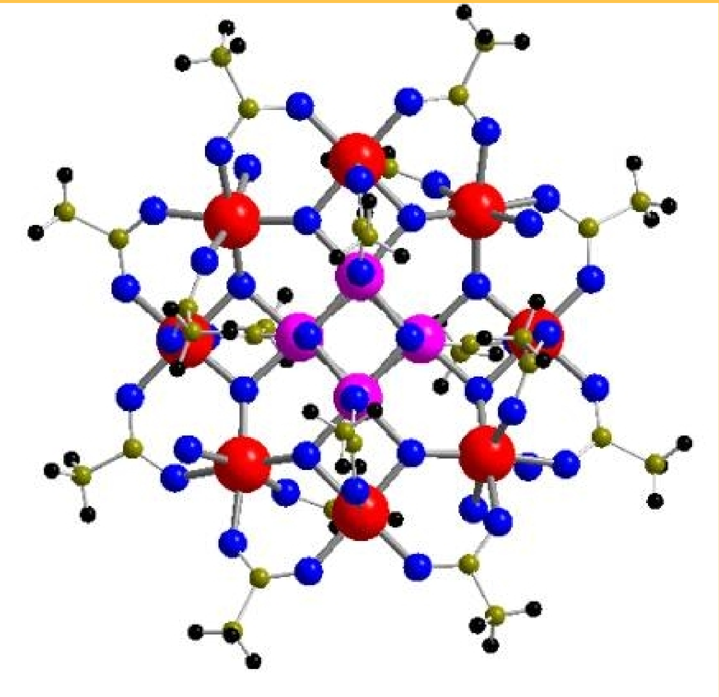


Fe$_{10}$

1. The suspects: magnetic molecules
2. Independent magnons on frustrated antiferromagnets
3. Metamagnetic phase transitions

Magnetic Molecules

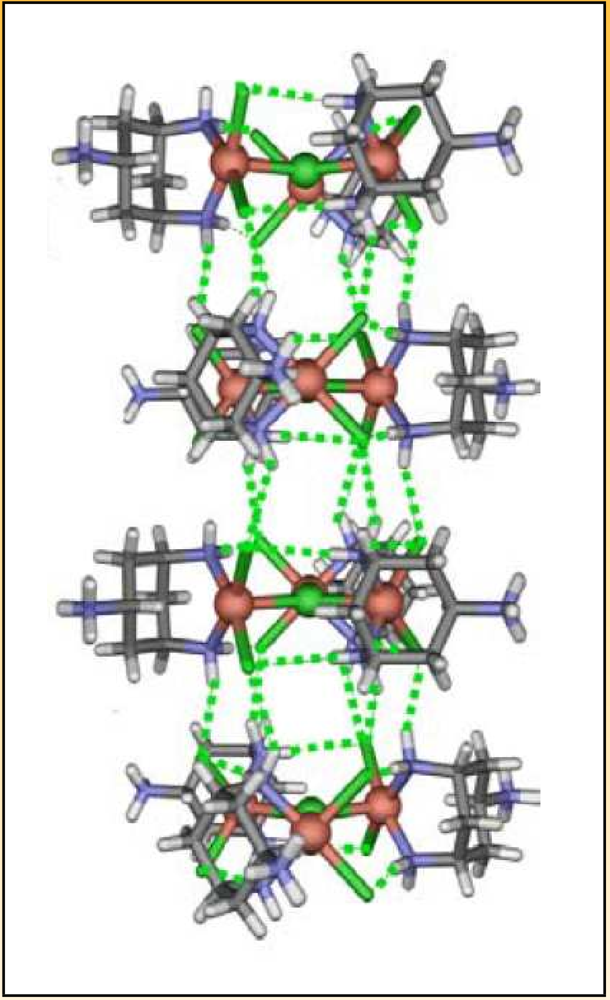
The beauty of magnetic molecules I



Mn$_{12}$

- Inorganic or organic macro molecules, where paramagnetic ions such as Iron (Fe), Chromium (Cr), Copper (Cu), Nickel (Ni), Vanadium (V), Manganese (Mn), or rare earth ions are embedded in a host matrix;
- Pure organic magnetic molecules: magnetic coupling between high spin units (e.g. free radicals);
- Speculative applications: magnetic storage devices, magnets in biological systems, light-induced nano switches, displays, catalysts, transparent magnets, qubits for quantum computers.

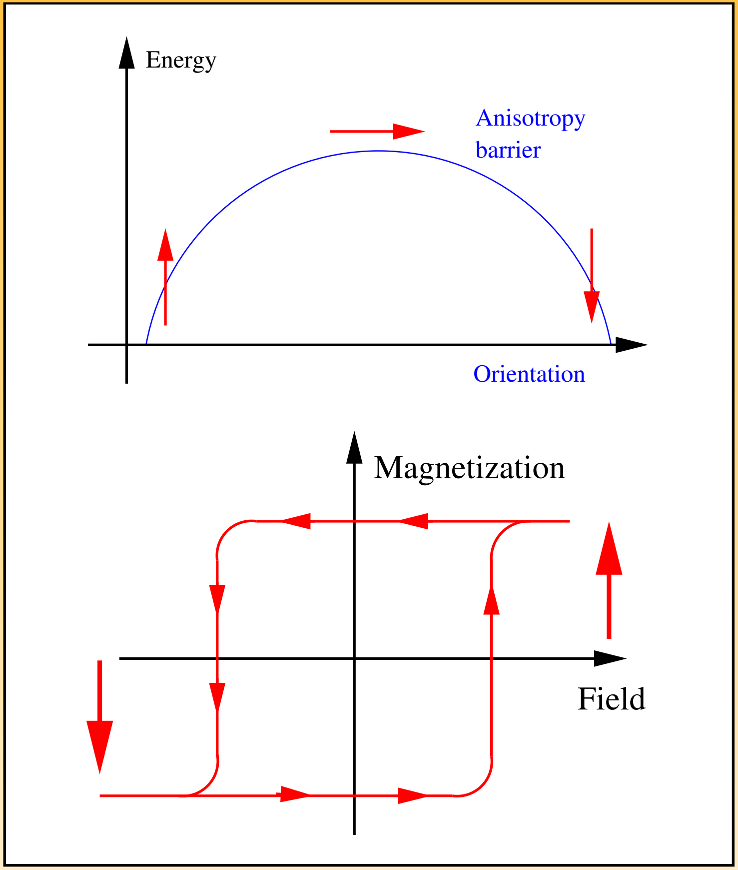
The beauty of magnetic molecules II



- Dimers (Fe_2), tetrahedra (Cr_4), cubes (Cr_8);
- Rings, especially iron and chromium rings
- Complex structures (Mn_{12}) – drosophila of molecular magnetism;
- “Soccer balls”, more precisely icosidodecahedra (Fe_{30}) and other macro molecules;
- Chain like and planar structures of interlinked magnetic molecules, e.g. triangular Cu chain:

  J. Schnack, H. Nojiri, P. Kögerler, G. J. T. Cooper, L. Cronin, Phys. Rev. B 70, 174420 (2004); Sato, Sakai, Läuchli, Mila, . . .

The beauty of magnetic molecules III



- Single Molecule Magnets (SMM): magnetic molecules with large ground state moment; e.g. $S = 10$ for Mn_{12} or Fe_8
- Anisotropy barrier dominates behavior (as in your hard drive);
- Single molecule is a magnet and shows metastable magnetization and hysteresis; but also magnetization tunneling.
- Today's major efforts: improve stability of magnetization; investigate on surfaces.

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

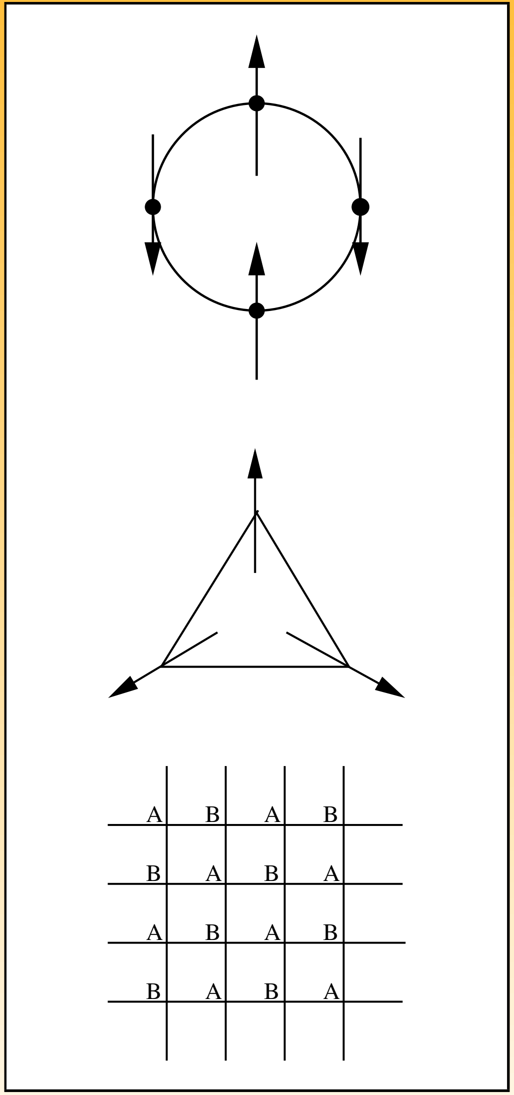
Very often anisotropic terms are utterly negligible, then . . .

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

Heisenberg Zeeman

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

Definition of frustration



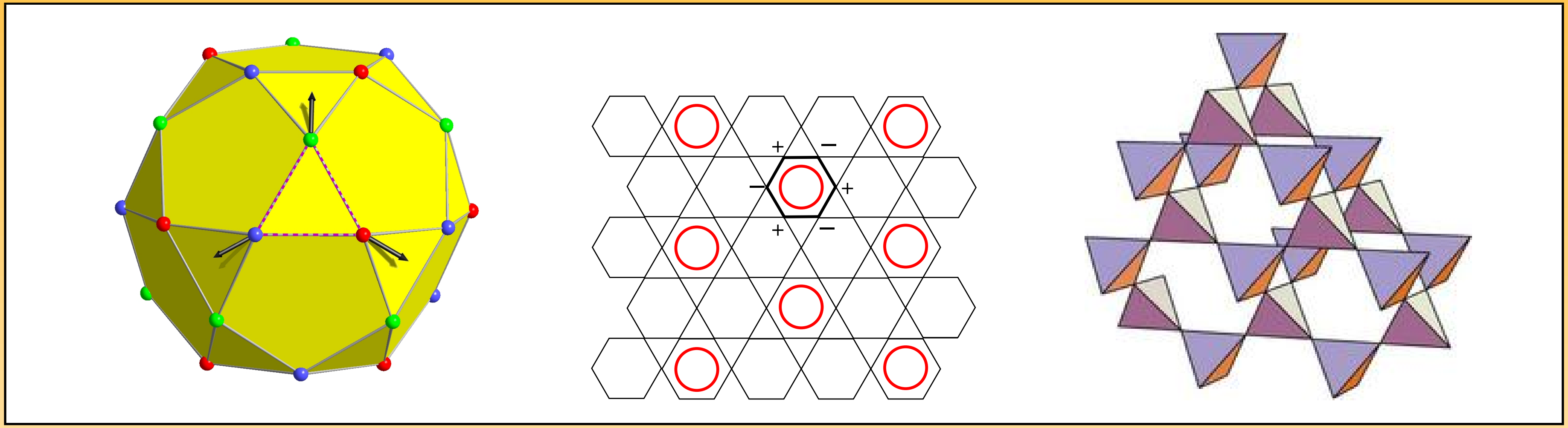
- Simple: An antiferromagnet is frustrated if in the ground state of the corresponding classical spin system not all interactions can be minimized simultaneously.

- Advanced: A non-bipartite antiferromagnet is frustrated. A bipartite spin system can be decomposed into two sublattices A and B such that for all exchange couplings:
  $J(x_A, y_B) \leq g^2$, $J(x_A, y_A) \geq g^2$, $J(x_B, y_B) \geq g^2$,
  cmp. (1,2).

(1) E.H. Lieb, T.D. Schultz, and D.C. Mattis, Ann. Phys. (N.Y.) **16**, 407 (1961)
(2) E.H. Lieb and D.C. Mattis, J. Math. Phys. **3**, 749 (1962)

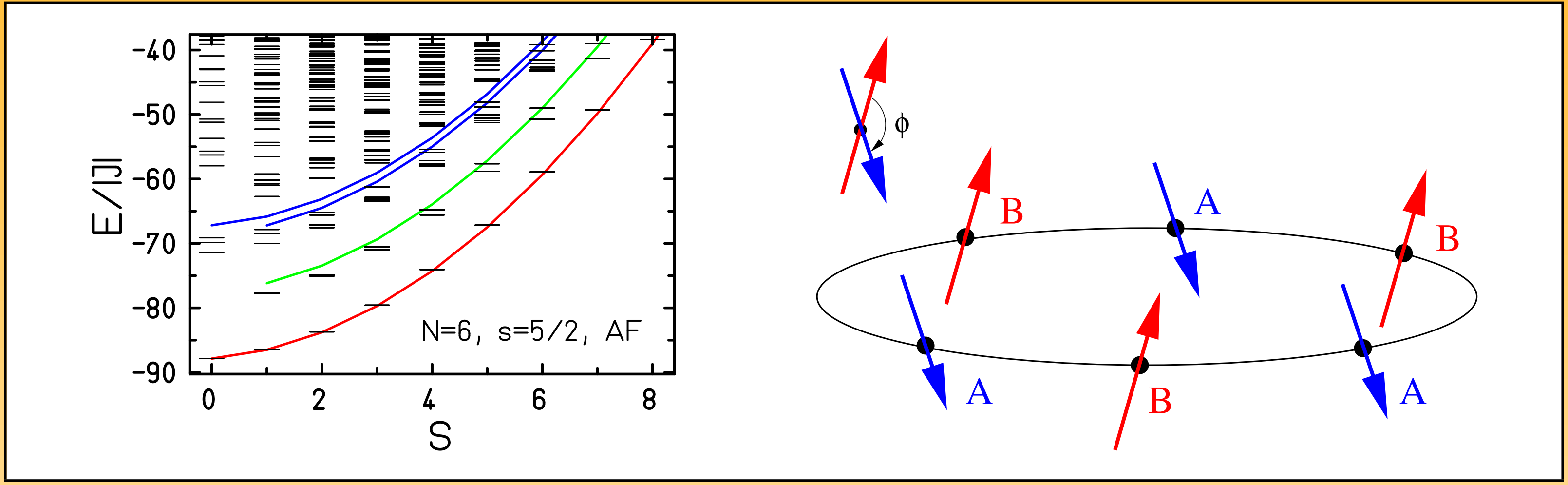
Independent magnons on frustrated antiferromagnets

Fe$_{30}$ and friends
Corner sharing triangles and tetrahedra



- Several frustrated antiferromagnets show an unusual magnetization behavior, e.g. plateaus and jumps.
- Example systems: icosidodecahedron, kagome lattice, pyrochlore lattice.

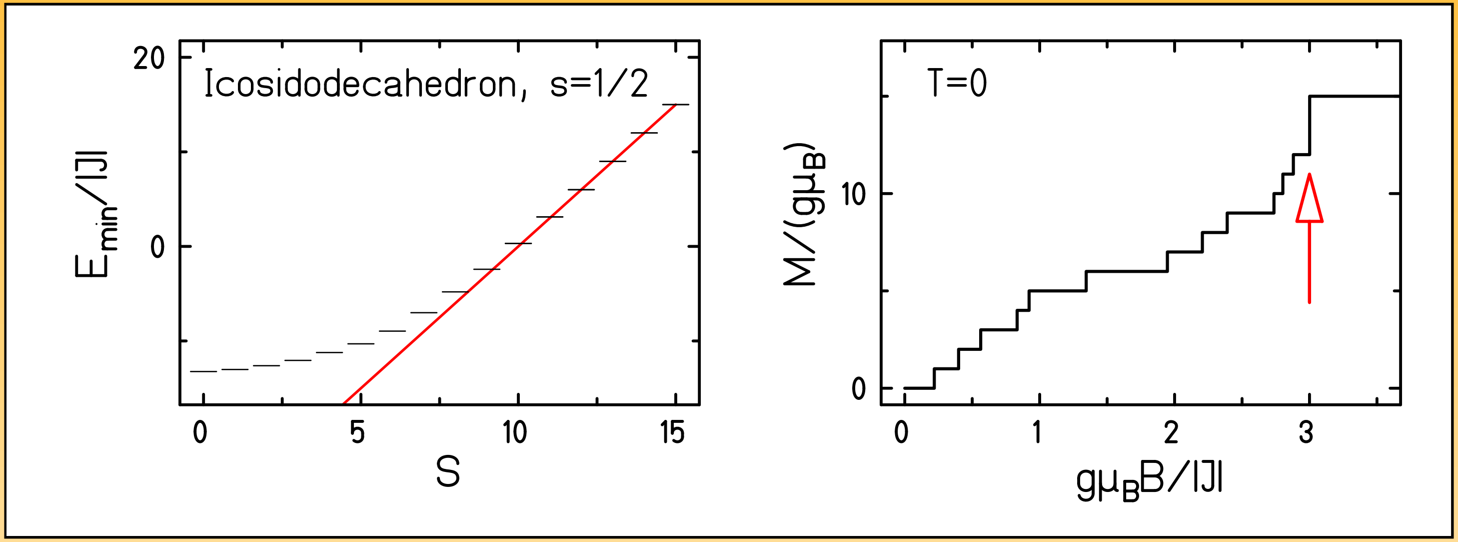
Rotational bands in non-frustrated antiferromagnets



- Often minimal energies $E_{min}(S)$ form a rotational band: Landé interval rule (1);
- For bipartite systems (2,3): $\underset{\sim}{H}^{\text{eff}} = -2\, J_{\text{eff}}\, \underset{\sim}{\vec{S}}_A \cdot \underset{\sim}{\vec{S}}_B$;
- Lowest band – rotation of Néel vector, second band – spin wave excitations (4).

(1) A. Caneschi *et al.*, Chem. Eur. J. **2**, 1379 (1996), G. L. Abbati *et al.*, Inorg. Chim. Acta **297**, 291 (2000)
(2) J. Schnack and M. Luban, Phys. Rev. B **63**, 014418 (2001)
(3) O. Waldmann, Phys. Rev. B **65**, 024424 (2002)
(4) P.W. Anderson, Phys. Rev. B **86**, 694 (1952), O. Waldmann *et al.*, Phys. Rev. Lett. **91**, 237202 (2003).

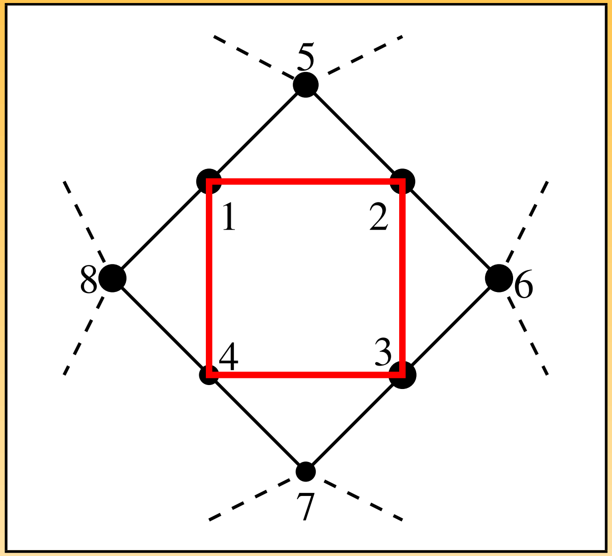
Giant magnetization jumps in frustrated antiferromagnets I
$\{\textbf{Mo}_{72}\textbf{Fe}_{30}\}$



- Close look: $E_{\text{min}}(S)$ linear in S for high S instead of being quadratic (1);
- Heisenberg model: property depends only on the structure but not on s (2);
- Alternative formulation: independent localized magnons (3);

(1) J. Schnack, H.-J. Schmidt, J. Richter, J. Schulenburg, Eur. Phys. J. B **24**, 475 (2001)
(2) H.-J. Schmidt, J. Phys. A: Math. Gen. **35**, 6545 (2002)
(3) J. Schulenburg, A. Honecker, J. Schnack, J. Richter, H.-J. Schmidt, Phys. Rev. Lett. **88**, 167207 (2002)

Giant magnetization jumps in frustrated antiferromagnets II
Localized Magnons

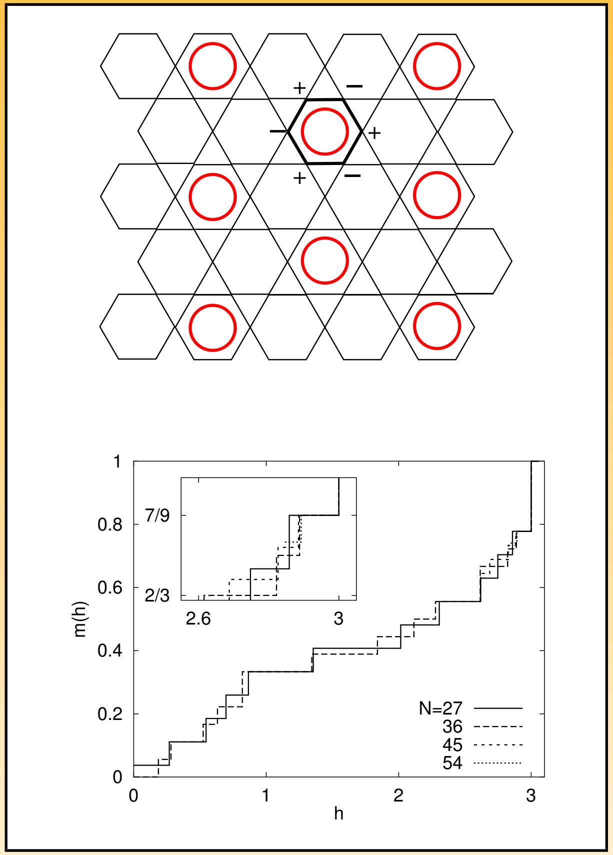


- $\mid$localized magnon$\,\rangle = \frac{1}{2}\left(\mid 1\,\rangle - \mid 2\,\rangle + \mid 3\,\rangle - \mid 4\,\rangle\right)$
- $\mid 1\,\rangle = \underset{\sim}{s}^{-}(1)\mid\uparrow\uparrow\uparrow\ldots\rangle$ etc.
- $\underset{\sim}{H}\mid$localized magnon$\,\rangle \propto \mid$localized magnon$\,\rangle$
- Localized magnon is state of lowest energy (1,2).

- Triangles trap the localized magnon, amplitudes cancel at outer vertices.

(1) J. Schnack, H.-J. Schmidt, J. Richter, J. Schulenburg, Eur. Phys. J. B **24**, 475 (2001)
(2) H.-J. Schmidt, J. Phys. A: Math. Gen. **35**, 6545 (2002)

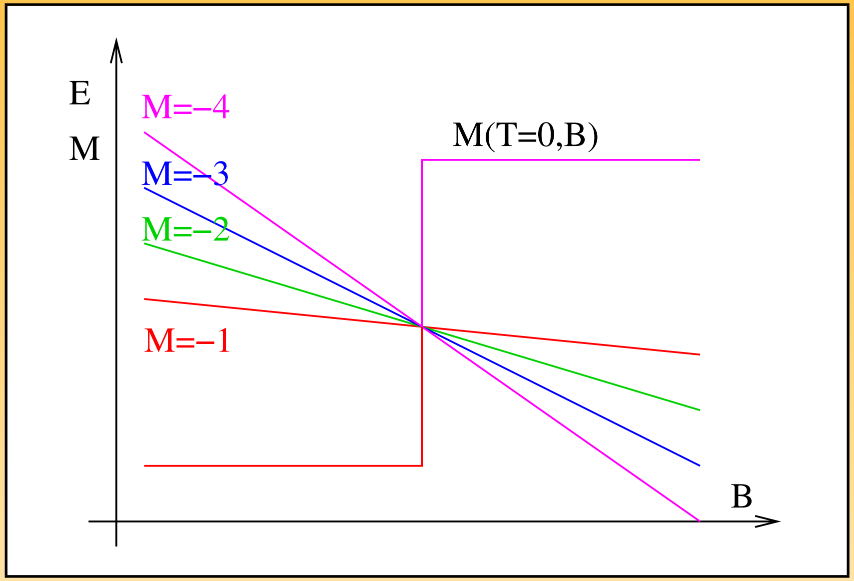
Giant magnetization jumps in frustrated antiferromagnets
Kagome Lattice



- Non-interacting one-magnon states can be placed on various lattices, e. g. kagome or pyrochlore;
- Each state of n independent magnons is the ground state in the Hilbert subspace with $M = Ns - n$; Kagome: max. number of indep. magnons is N/9;
- Linear dependence of E_{min} on M $\Rightarrow \quad (T=0)$ magnetization jump;
- Jump is a macroscopic quantum effect!
- A rare example of analytically known many-body states!

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)

Magnetocaloric effect I
Giant jumps to saturation



- Many Zeeman levels cross at one and the same magnetic field.
- High degeneracy of ground state levels $\Rightarrow$ large residual entropy at $T = 0$.
- $$\left(\frac{\partial T}{\partial B}\right)_S = -\frac{T}{C}\left(\frac{\partial S}{\partial B}\right)_T$$

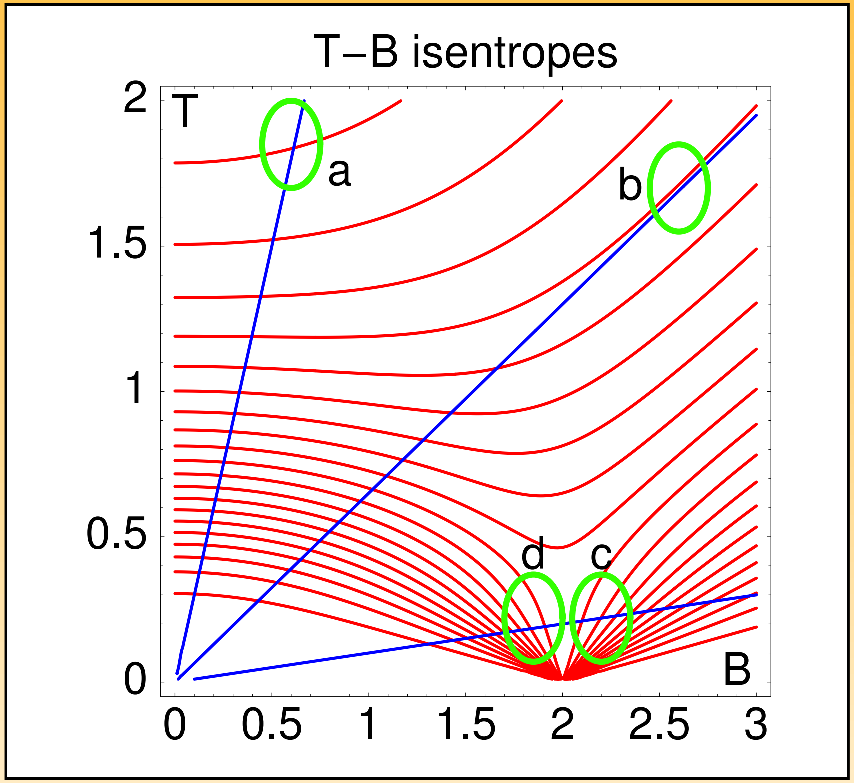
J. Schulenburg, A. Honecker, J. Schnack, J. Richter, H.-J. Schmidt, Phys. Rev. Lett. **88**, 167207 (2002)

A. Honecker, J. Richter, Condensed Matter Physics **8**, 813 (2005)

H.-J. Schmidt, Johannes Richter, Roderich Moessner, J. Phys. A: Math. Gen. **39**, 10673 (2006)

O. Derzhko, J. Richter, A. Honecker, H.-J. Schmidt, Low Temp. Phys. **33**, 745 (2007)

Magnetocaloric effect II
Isentrops of af $s = 1/2$ dimer



blue lines: ideal paramagnet, red curves: af dimer

Magnetocaloric effect:

(a) reduced,

(b) the same,

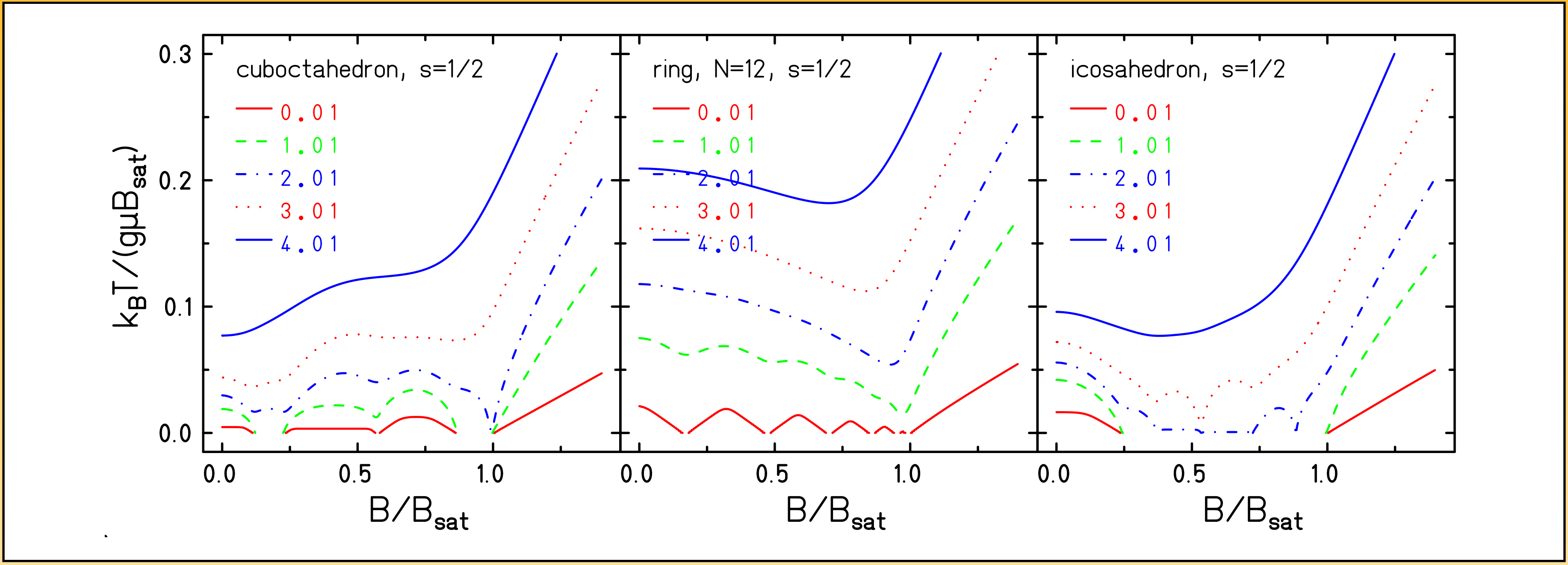
(c) enhanced,

(d) opposite

when compared to an ideal paramagnet.

Case (d) does not occur for a paramagnet.

Magnetocaloric effect III – Molecular systems

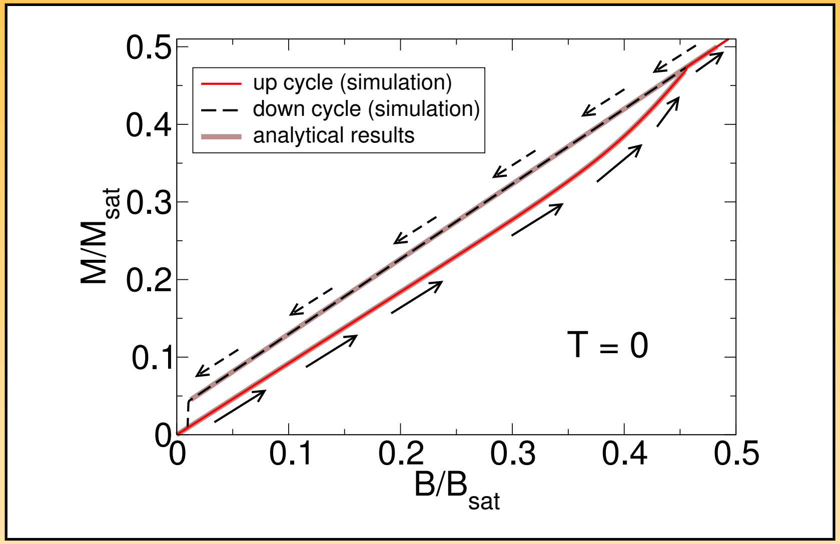


- Cuboctahedron: high cooling rate due to independent magnons;
- Ring: normal level crossing, normal jump;
- Icosahedron: unusual behavior due to edge-sharing triangles, high degeneracies all over the spectrum; high cooling rate.

J. Schnack, R. Schmidt, J. Richter, Phys. Rev. B **76**, 054413 (2007)

Metamagnetic phase transitions

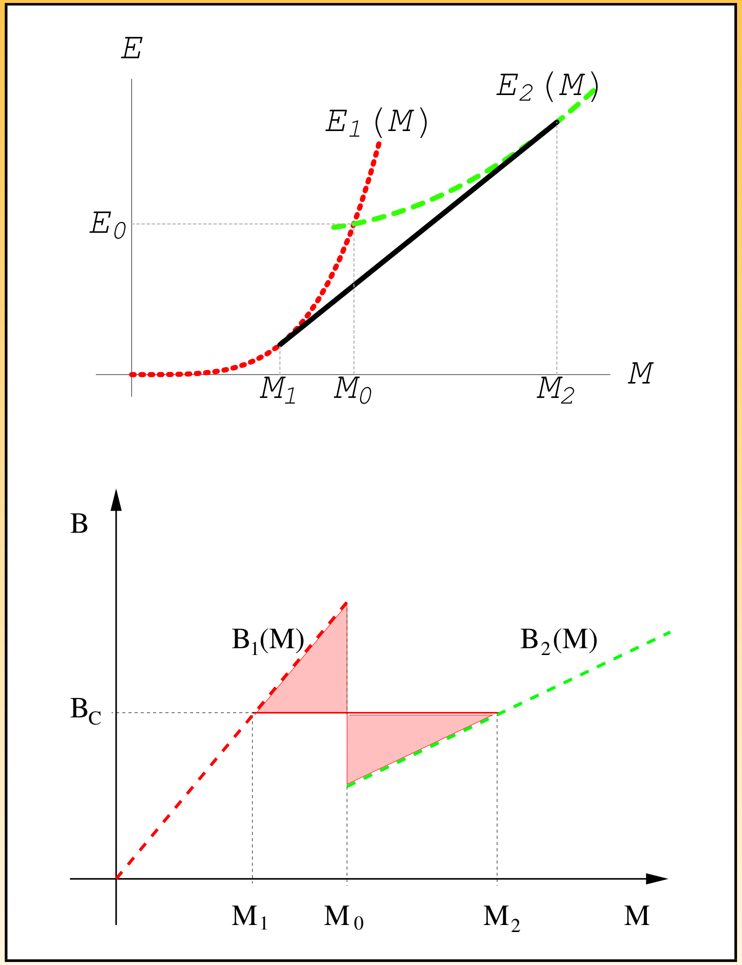
Metamagnetic phase transition I
Hysteresis without anisotropy



- Heisenberg model with isotropic nearest neighbor exchange
- Hysteresis behavior of the classical icosahedron 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)

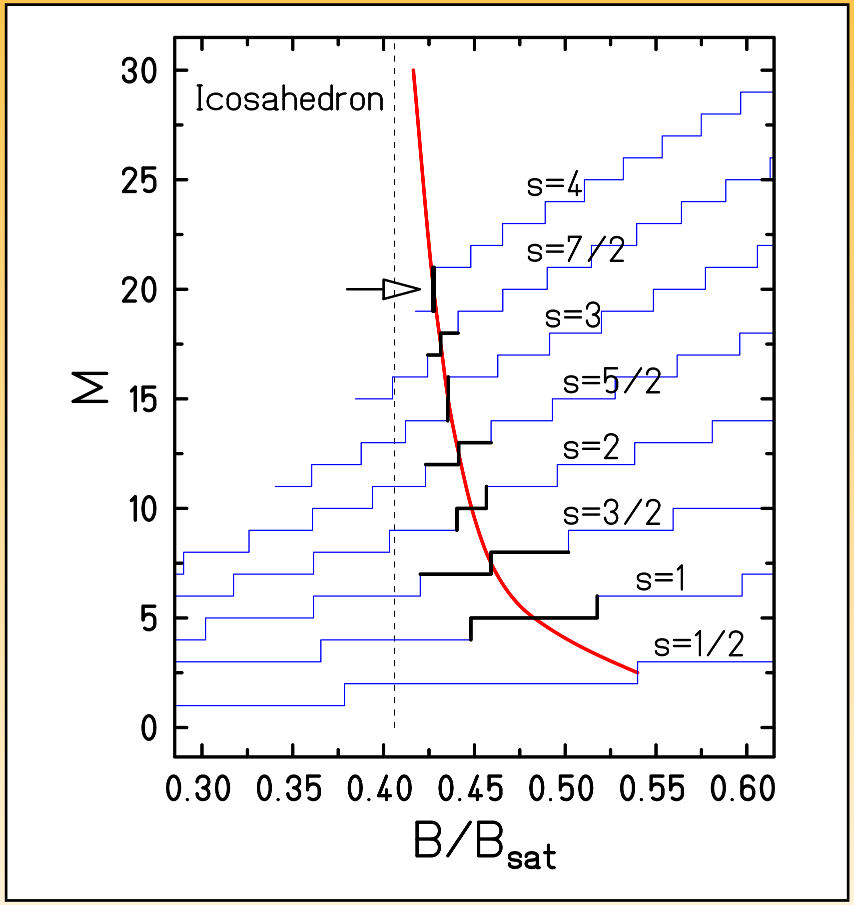
Metamagnetic phase transition II
Non-convex minimal energy



- 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
  Theory achievement: work with vectors with 10^9 entries.
- True jump of $\Delta M = 2$ for $s = 4$.
- Polynomial fit in $1/s$ yields the classically observed transition field.

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

If it comes to numerics:

we don’t know any fear!

Numerics I – IBM 3090 at GSI

- One day in the early 90s Prof. Nörenberg came and showed a kind of bill where computer time on the IBM 3090 was listed. A guy (TP38 – Guess who it was?) had used 1/3 of GSI's annual computer time!

Numerics II – today I am using 100 %

- BULL NovaScale Server 3045:

- Future: wide open
  8 ITANIUM TUKWILA (a 4 cores),
  512 GB RAM
  (an amazing computer power)

- Now:
  4 ITANIUM MONTECITO (a 2 cores),
  64 GB RAM
  (already an amazing computer power,
  but one can get used to it ;-))

Many thanks to my collaborators worldwide

- T. Englisch, T. Glaser, S. Leiding, A. Müller, Chr. Schröder (Bielefeld)
- K. Bärwinkel, H.-J. Schmidt, M. Allalen, M. Brüger, D. Mentrup, D. Müter, M. Exler, P. Hage, F. Hesmer, K. Jahns, F. Ouchni, R. Schnalle, P. Shchelokovskyy, S. Torbrügge & M. Neumann, K. Küpper, M. Prinz (Osnabrück);
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  J. Musfeld (U. of Tennessee, USA); N. Dalal (Florida State, USA);
  R.E.P. Winpenny (Man U, UK); L. Cronin (U. of Glasgow, UK);
  H. Nojiri (Tohoku University, Japan); A. Postnikov (U. Metz)
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  S. Blügel (FZ Jülich); A. Honecker (U. Göttingen);
  E. Rentschler (U. Mainz); U. Kortz (IUB); A. Tennant, B. Lake (HMI Berlin);
  B. Büchner, V. Kataev, R. Klingeler, H.-H. Klauß (Dresden)

It all started at GSI with . . .

- Hans Feldmeier
- Konrad Bieler, Jörg Lindner, Thomas Neff, Robert Roth, J.S.
- L. Mornas, L. Razumov, G. Papp, . . .
- J. Knoll, B. Friman, P. Henning, W. Nörenberg, Chr. Sauermann, W. Weinhold, J. Randrup, . . .

It was a good time I

- I learned physics during my Ph.D.!

Many-body physics in action

spectator

two-body correlation

Information

German Molecular Magnetism Web

www.molmag.de

Highlights. Tutorials. Who is who. DFG SPP 1137