Simulations of magnetic molecules

Jürgen Schnack,

Dept. of Physics – University of Osnabrück, Germany

http://obelix.physik.uni-osnabrueck.de/∼schnack/

Bull HPC User Convention

Paris, September 28 & 29th 2006

Deutsche Forschungsgemeinschaft DFG

UNIVERSITÄT OSNABRÜCK

文部科学省

unilogo-m-rot.jpg

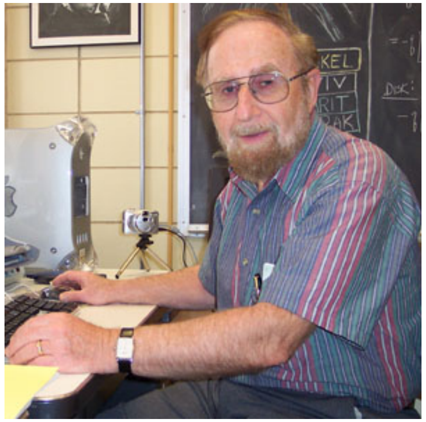
In late 20th century people coming from

transport theory

general relativity

nuclear physics

Schottky diodes



were triggered by a “magnetic” enthusiast.

Meanwhile a big collaboration has been established

- K. Bärwinkel, H.-J. Schmidt, J. S., 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 (UOS);

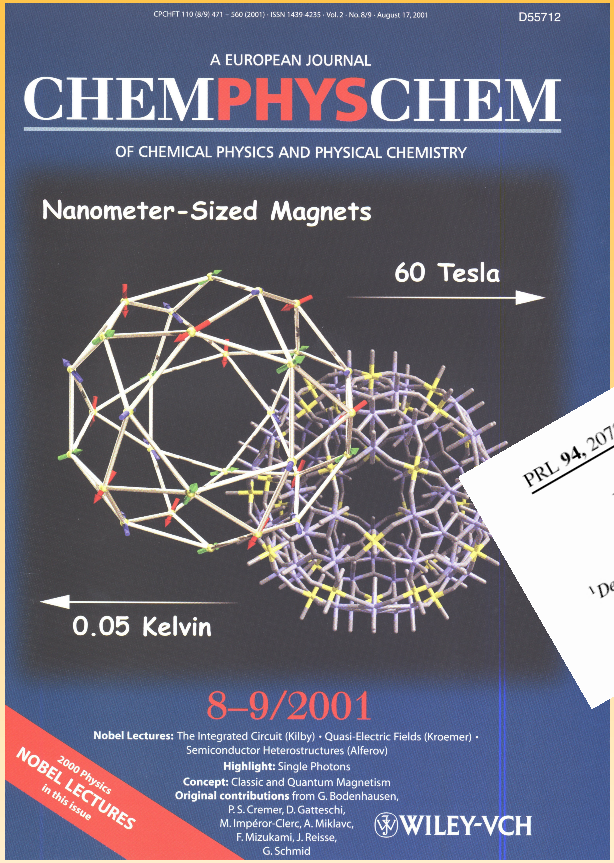
- M. Luban, P. Kögerler, D. Vaknin (Ames Lab, USA);
  J. Musfeld (U. of Tennessee, USA); N. Dalal (Florida State, USA);

- R.E.P. Winpenny (Man U, UK); L. Cronin (U. of Glasgow, UK);
  H. Nojiri (Tohoku University, Japan);

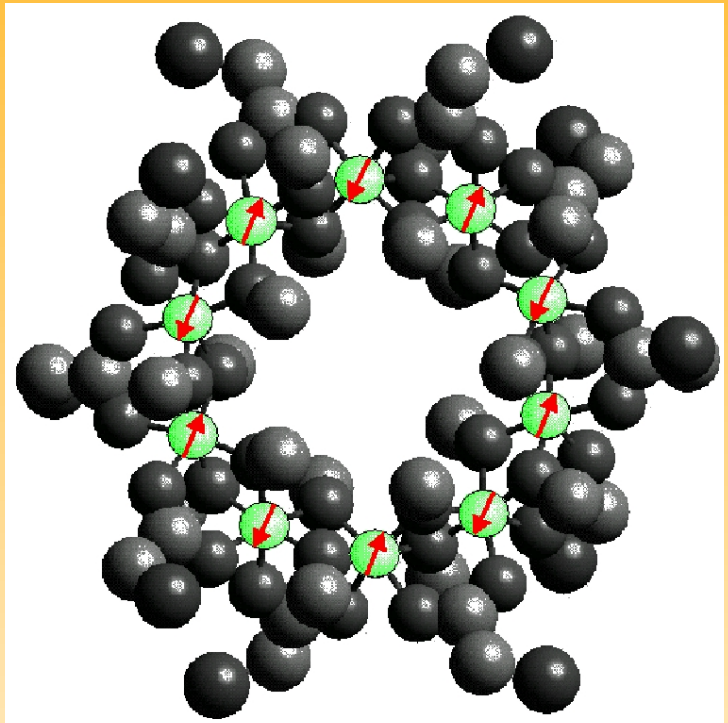
- A. Müller (U. Bielefeld) & Chr. Schröder (FH Bielefeld);
  J. Richter, J. Schulenburg, R. Schmidt (U. Magdeburg);
  S. Blügel, A. Postnikov (FZ Jülich); A. Honecker (U. Göttingen);
  E. Rentschler (U. Mainz); U. Kortz (IUB); A. Tennant, B. Lake (HMI Berlin);

- B. Büchner, V. Kataev, R. Klingeler (IFW Dresden)

. . . and various general results could be achieved



Contents for you today

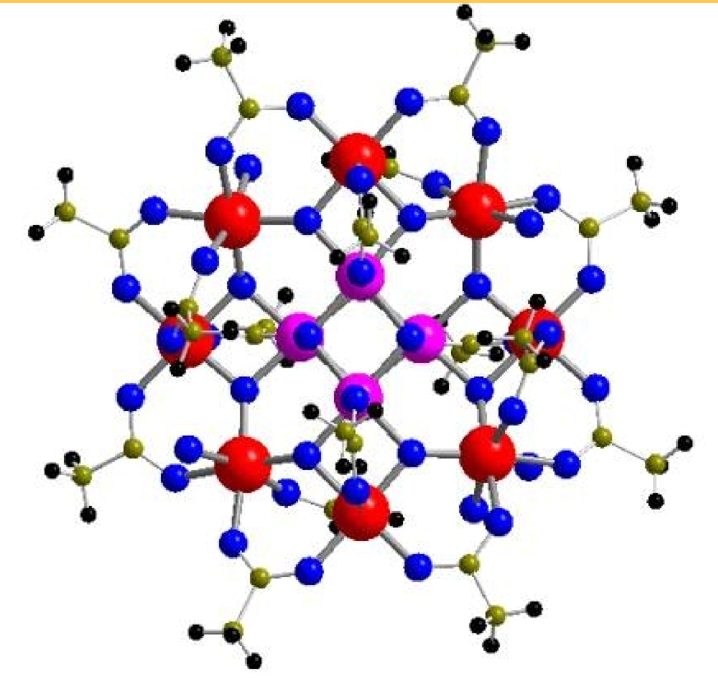


Fe_{10}

1. The suspects: magnetic molecules
2. The thumbscrew: Heisenberg model
3. Giant magnetization jumps in frustrated antiferromagnets
4. Hysteresis without anisotropy
5. NovaScale 4040: Power for a small university

Magnetic Molecules

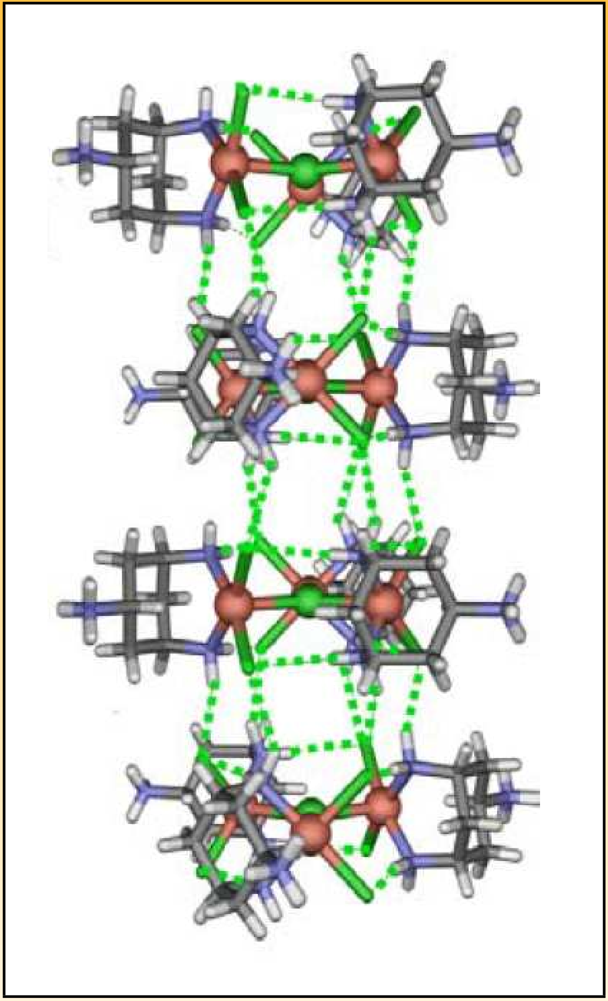
The beauty of magnetic molecules I



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);
- Spin = magnetic moment ("compass needle"): Molecule has magnetic properties.
- Speculative applications: magnetic storage devices, magnets in biological systems, light-induced nano switches, displays, catalysts, transparent magnets, qubits for quantum computers.

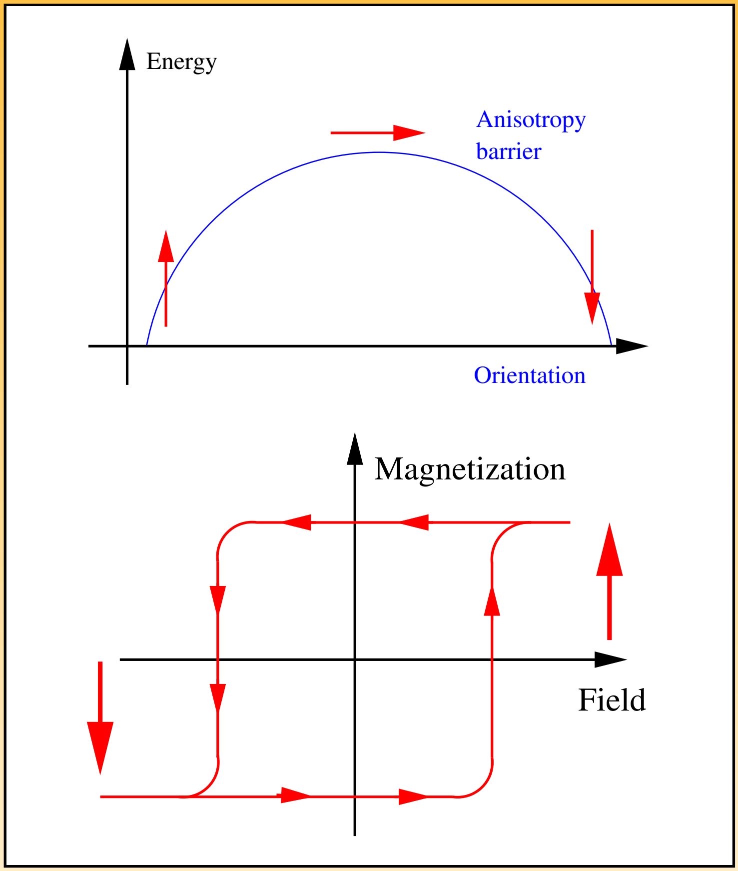
The beauty of magnetic molecules II



- Dimers (Fe_2), tetrahedra (Cr_4), cubes (Cr_8);
- Rings, especially iron rings (Fe_6, Fe_8, Fe_{10}, ...);
- 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)

The beauty of magnetic molecules III



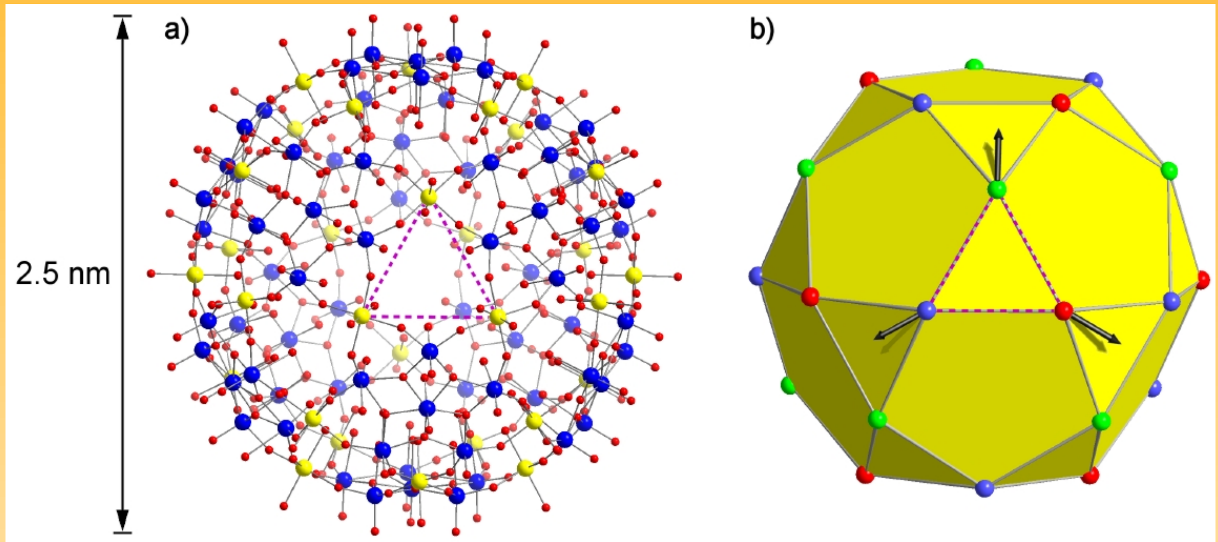
- Single Molecule Magnets (SMM): magnetic molecules with large ground state moment; e.g. $S = 10$ for Mn_{12} or Fe_8

- 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.

$\{Mo_{72}Fe_{30}\}$ – a giant magnetic Keplerate molecule



- Structure: Fe - yellow, Mo - blue,
  O - red;
- Exciting magnetic properties (1).
- Quantum treatment very complicated, dimension of Hilbert space $(2s+1)^N \approx 10^{23}$ (2).

(1) A. Müller *et al.*, Chem. Phys. Chem. **2**, 517 (2001) , (2) M. Exler and J. Schnack, Phys. Rev. B **67**, 094440 (2003)

Numerics

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 . . .

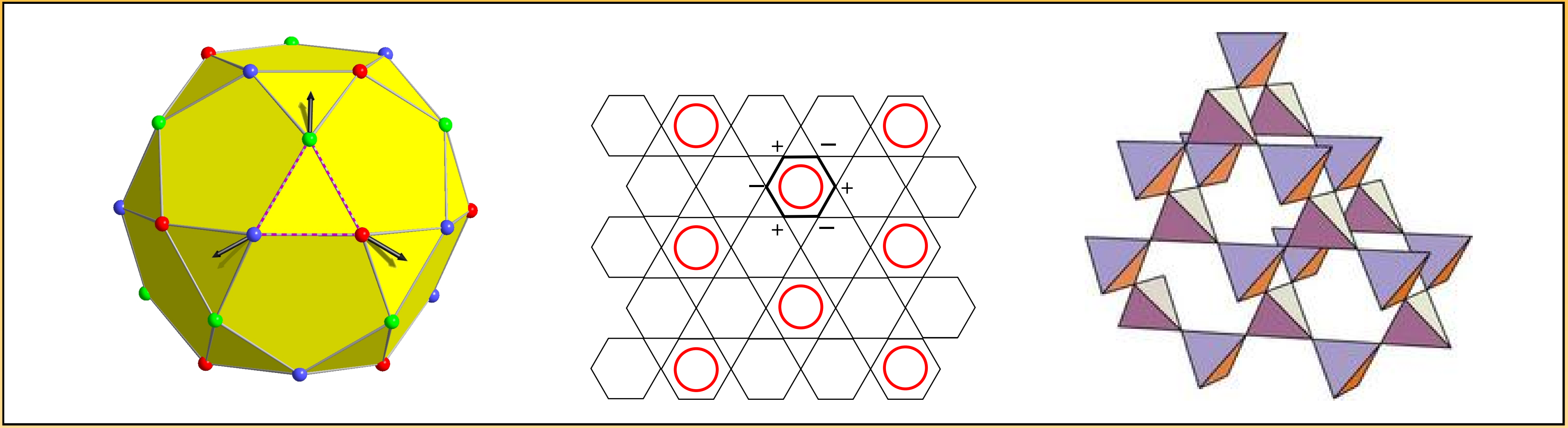
$$\underset{\sim}{H} = -\sum_{i,j} J_{ij} \underset{\sim}{\vec{s}}(i) \cdot \underset{\sim}{\vec{s}}(j) + g \mu_B B \sum_{i}^{N} \underset{\sim}{s}_z(i)$$

Heisenberg Zeeman

The Hamilton operator is represented as a matrix whose eigenvalues and eigenvectors have to be computed.

Giant Magnetization Jumps

Giant magnetization jumps in frustrated antiferromagnets I
Systems

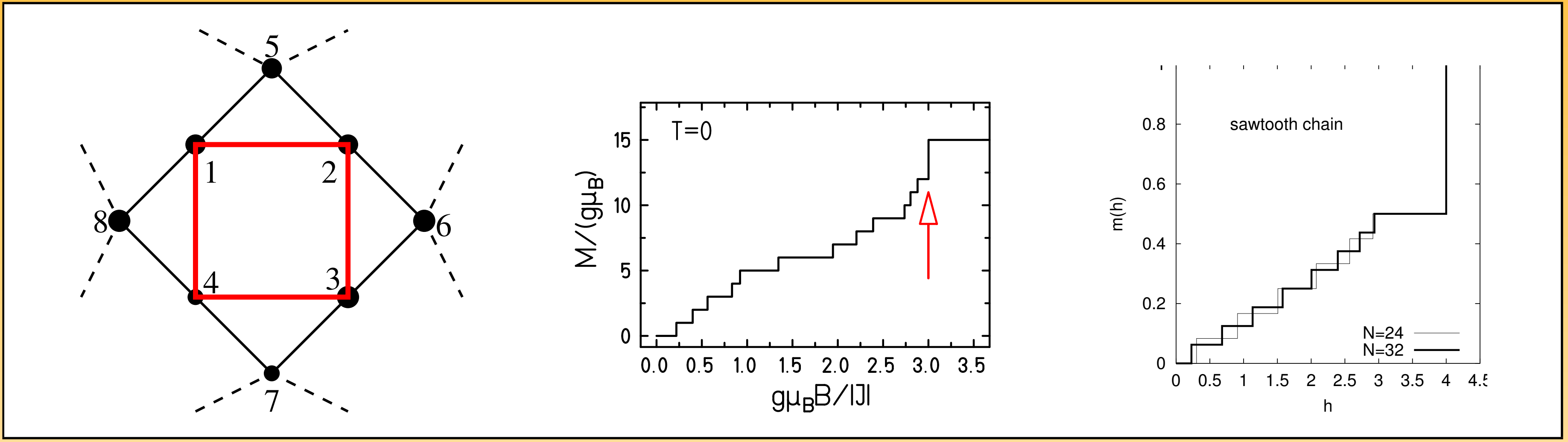


- Several frustrated antiferromagnets show an unusual behavior at the saturation field (1,2).

- E.g., icosidodecahedron, kagome lattice, pyrochlore lattice.

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

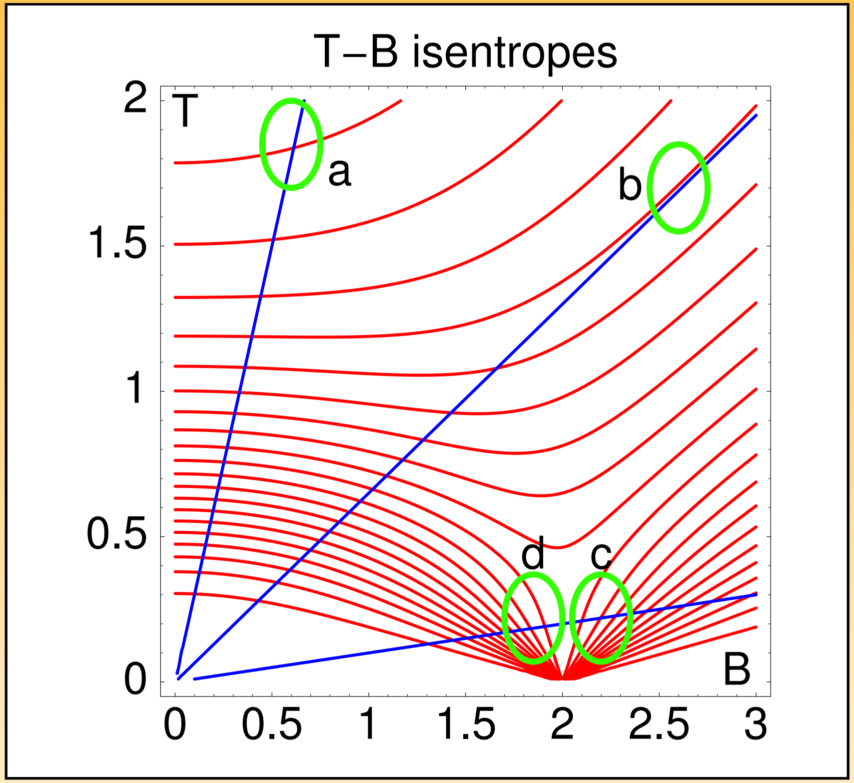
Giant magnetization jumps in frustrated antiferromagnets II
Magnetization jumps due to independent magnons



- Usually a magnetization curve is rather smooth.
- Unusually high magnetization jump at the saturation field.

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)

Giant magnetization jumps in frustrated antiferromagnets III
Giant magnetocaloric effect



blue lines: ideal paramagnet, red curves: af dimer

Magnetocaloric effect, i.e. temperature change when changing the applied magnetic field:

(a) reduced,

(b) the same,

(c) enhanced,

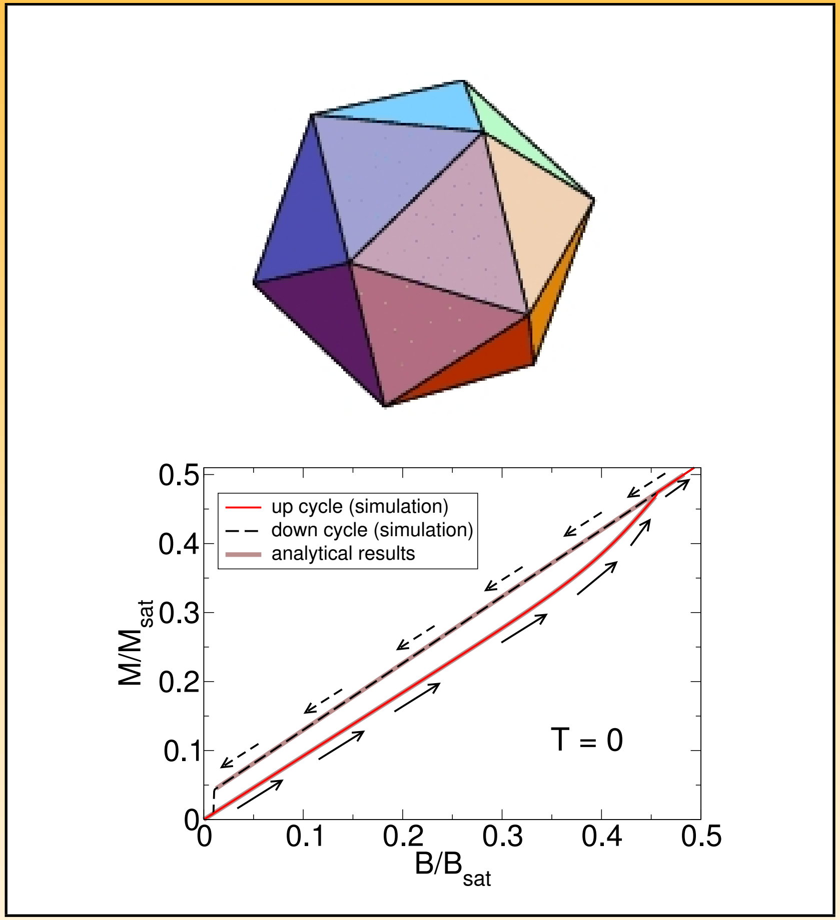
(d) opposite

when compared to an ideal paramagnet.

Case (d) does not occur for a paramagnet.

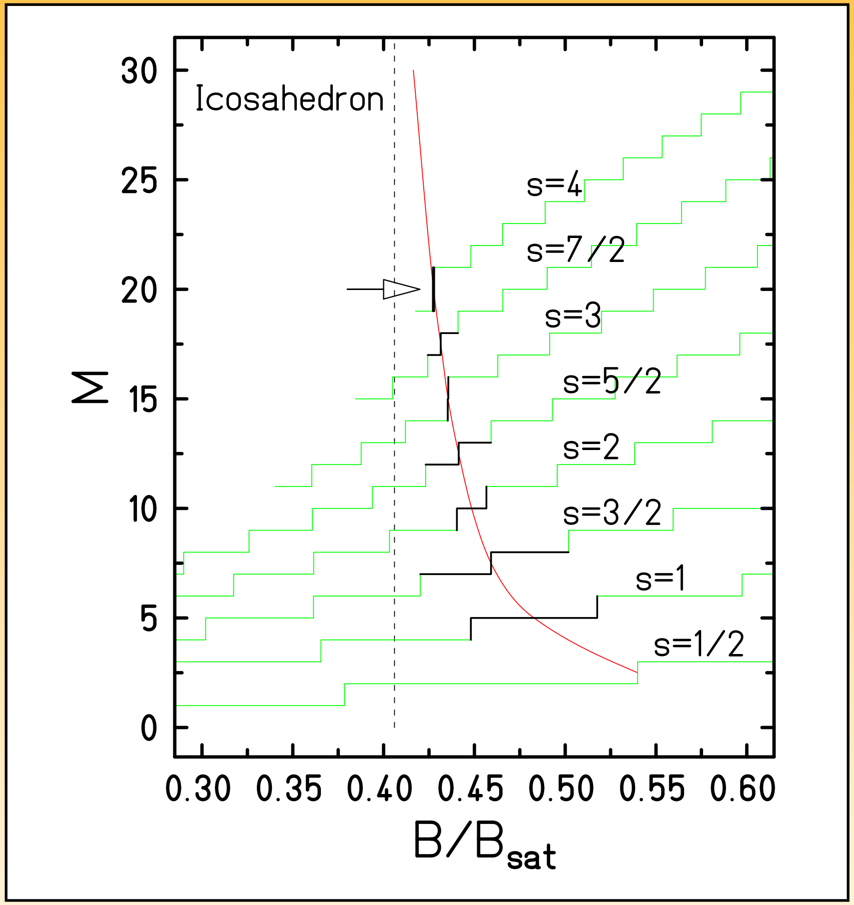
Hysteresis without Anisotropy

Metamagnetic phase transition I
Hysteresis without anisotropy



- Hysteresis is usually caused by anisotropy
- Hysteresis behavior of the classical isotropic Heisenberg 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
Quantum icosahedron



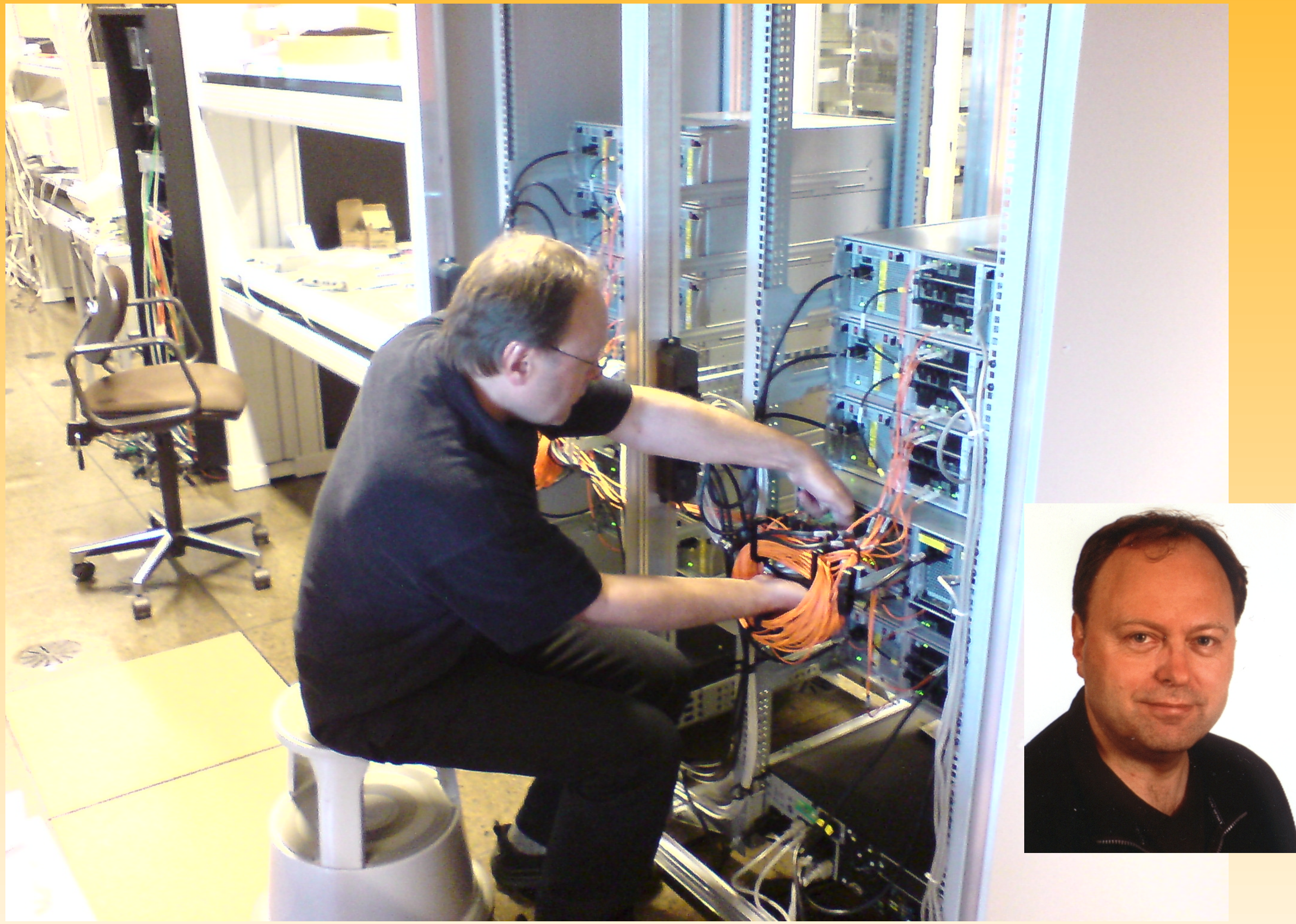
- Quantum analog:
  Non-convex minimal energy levels
  $\Rightarrow$ magnetization jump of $\Delta M > 1$.
- Lanczos diagonalization for various s.
- True jump of $\Delta M = 2$ for $s = 4$.
- Polynomial fit in $1/s$ yields the classically observed transition field.
- Numerics: Lanczos with vectors of max. length 1,342,275,012!

NovaScale 4040: Power for a Small University

NovaScale 4040: small is beautiful

4 Itanium II (1595.658 MHz, 5 MB cache), 32 GB RAM

Werner Nienhüser – the master of our computer power



NovaScale 4040: typical usage

```
xterm
top - 13:32:29 up 31 days, 20:13,  4 users,  load average: 4.07, 4.10, 4.03
Tasks: 103 total,   5 running,  98 sleeping,   0 stopped,   0 zombie
Cpu(s): 99.9% us,  0.1% sy,  0.0% ni,  0.0% id,  0.0% wa,  0.0% hi,  0.0% si
Mem:   33286736k total, 28525104k used,  4761632k free,   325440k buffers
Swap:  49937344k total,      176k used, 49937168k free, 10743616k cached

  PID USER      PR  NI  VIRT  RES  SHR S %CPU %MEM    TIME+  COMMAND
 8392 apostnik  25   0 3320m 2.7g 8352 R 99.9  8.6 886:03.15 siesta
25487 apostnik  25   0  748m 720m 8304 R 99.9  2.2 326:21.32 siesta
29647 jschnack  25   0 4809m 4.5g 2688 R 99.9 14.0 189:47.94 hbodyr-17-22-20
29633 jschnack  25   0 17.8g 8.1g 2656 R 99.1 25.4 191:24.24 hbodyr-18-23-20
29389 jschnack  15   0 23280  11m 8080 S  0.4  0.0   0:02.47 sshd
30401 jschnack  16   0 11120 5936 4352 R  0.2  0.0   0:25.90 top
29421 jschnack  15   0 82688  22m  11m S  0.1  0.1   0:03.14 emacs
 2975 root      16   0 16864  13m 4096 S  0.1  0.0   8:10.57 hald
29709 jschnack  15   0 64384 8032 5248 S  0.1  0.0   0:04.18 xterm
    1 root      16   0  3440 1520 1232 S  0.0  0.0   0:02.34 init
    2 root      RT   0     0    0    0 S  0.0  0.0   0:01.62 migration/0
    3 root      34  19     0    0    0 S  0.0  0.0   0:00.05 ksoftirqd/0
    4 root      RT   0     0    0    0 S  0.0  0.0   0:01.56 migration/1
    5 root      34  19     0    0    0 S  0.0  0.0   0:00.07 ksoftirqd/1
    6 root      RT   0     0    0    0 S  0.0  0.0   0:01.40 migration/2
    7 root      34  19     0    0    0 S  0.0  0.0   0:00.11 ksoftirqd/2
    8 root      RT   0     0    0    0 S  0.0  0.0   0:00.98 migration/3
```

NovaScale 4040: benchmarks for diagonalization

architecture	software	time (s)
Xeon 5160 @ 3 GHz, 4 MB	ifort & MKL 9.0	976
Opteron 246 @ 2 GHz, 1 MB	g77 & ACML	2760
Itanium 2 @ 1.5GHz, 6 MB	ifort & MKL 8.0	916
CRAY SV1ex, Jülich (4 proc., 8 GFlops, 2002)	vectorized LAPACK	2903

Determination of all eigenvalues of a 9225×9225 hermitean matrix using the LAPACK routine ZHEEV (my benchmark problem).

Summary

There is a big demand
for fast and accurate numerics
in the theory of magnetism.

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

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

Thank you very much for your attention.

German Molecular Magnetism Web

www.molmag.de

Highlights. Tutorials. Who is who. DFG SPP 1137