

Simulations of magnetic molecules

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Bull HPC User Convention

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文部科学省

In late 20th century people coming from



transport theory



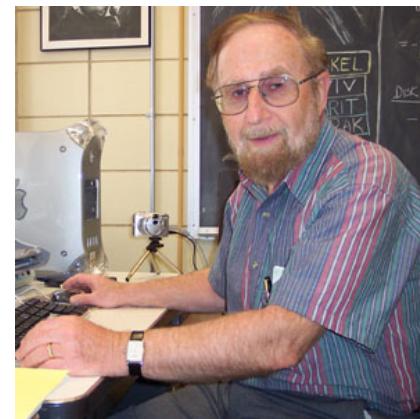
general relativity



nuclear physics



Schottky diodes

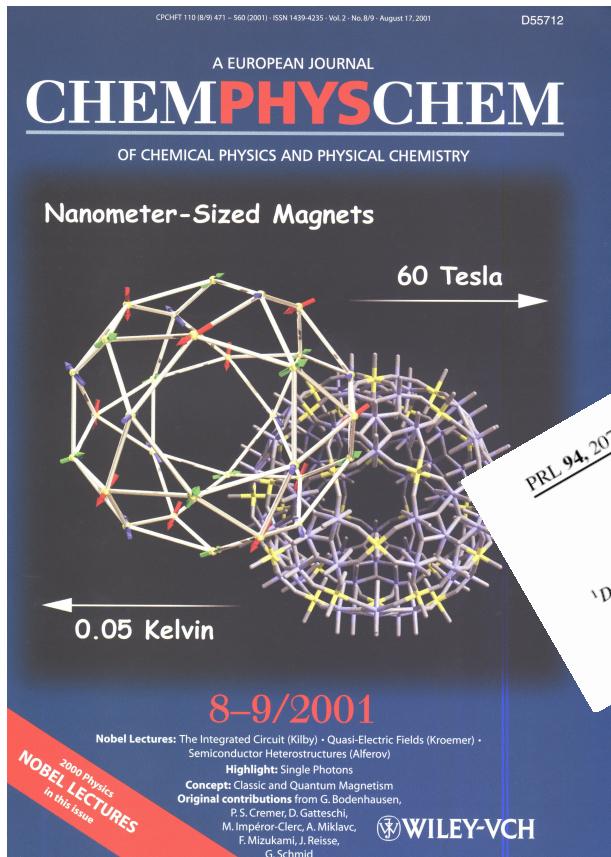


were triggered by a “magnetic” enthusiast.

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. Tenant, B. Lake (HMI Berlin);
- B. Büchner, V. Kataev, R. Klingeler (IFW Dresden)

... and various general results could be achieved



4, 207203 (2005)

Metamagnetic Phase Transition of the Antifer

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PHYSICAL REVIEW LETTERS

Macroscopic Magnetization Jumps due to Independent Mass in Frustrated Quantum Spin Lattices

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(Received 29 August 2001; published 8 April 2002)

PHYSICAL REVIEW B, VOLUME 63, 014418

Rotational modes in molecular magnets with antiferromagnetic Heisenberg exchange

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(Received 13 July 2000; published 12 December 2000)

PHYSICAL REVIEW B, VOLUME 63, 054401

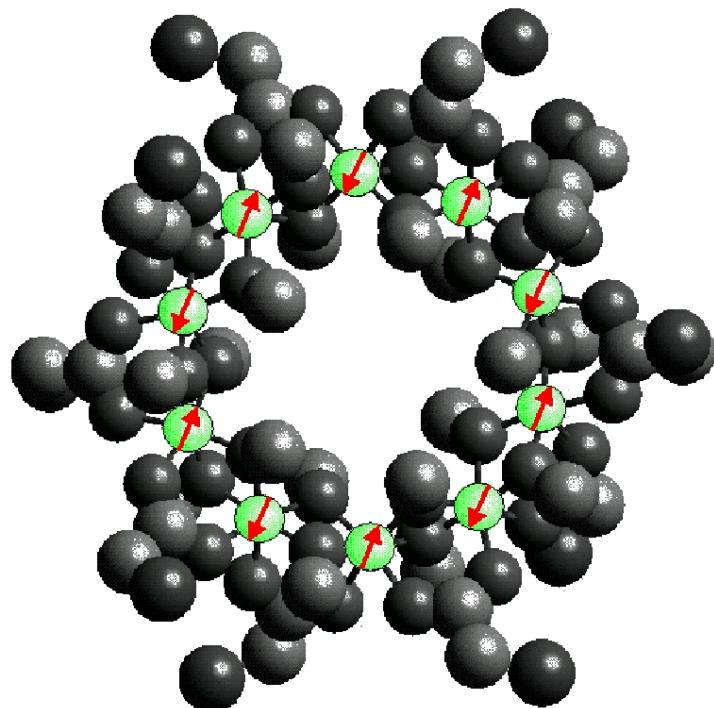
Quantum numbers for relative ground states

Klaus Bärwinkel,* Peter Hage,^{1,†}
Universität Osnabrück,¹ (Received 24 April 2001; published 24 June 2001)

PHYSICAL REVIEW B, VOLUME 63, 054401

**week ending
27 MAY 2005**

Contents for you today

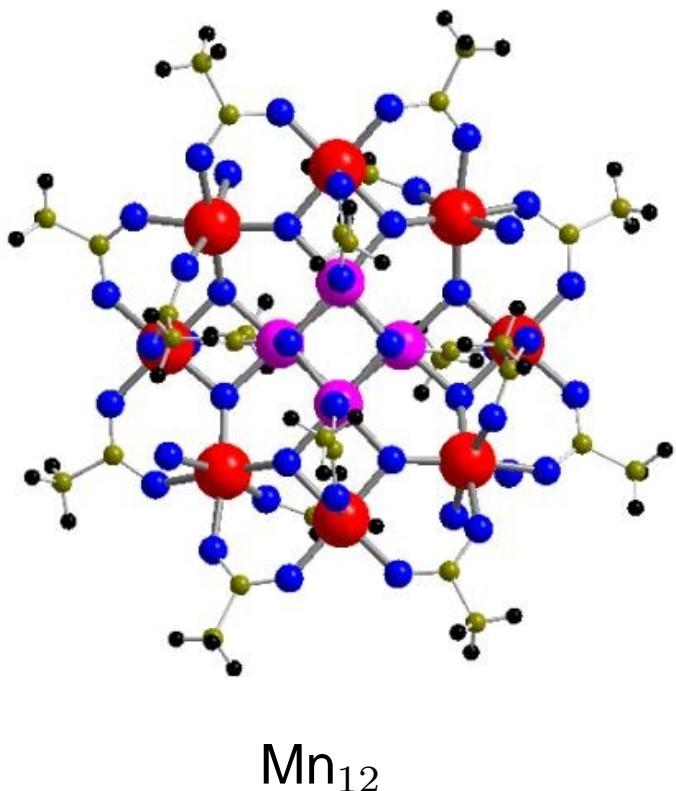


Fe₁₀

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

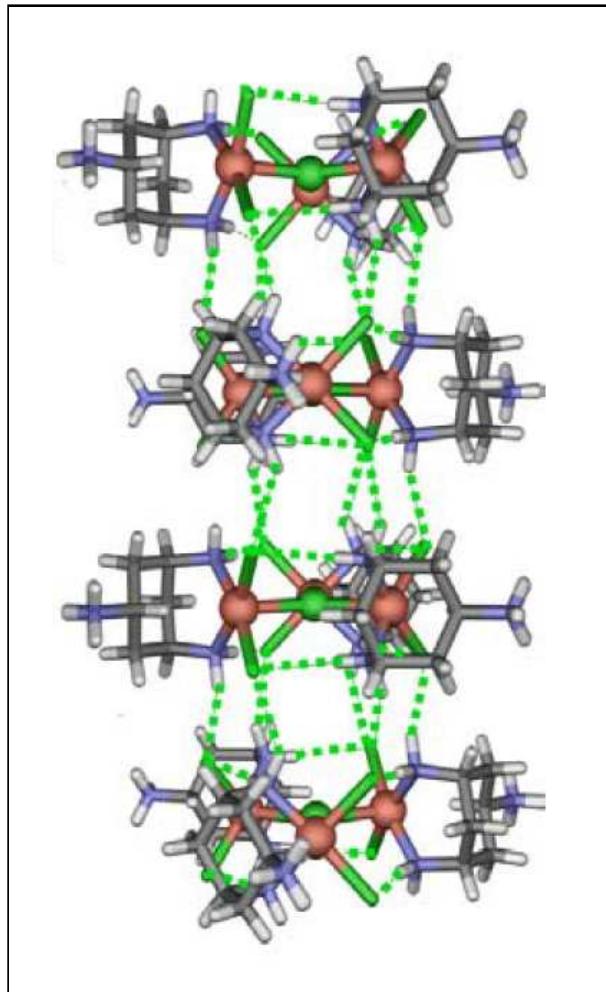
Magnetic Molecules

The beauty of magnetic molecules I



- 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.**

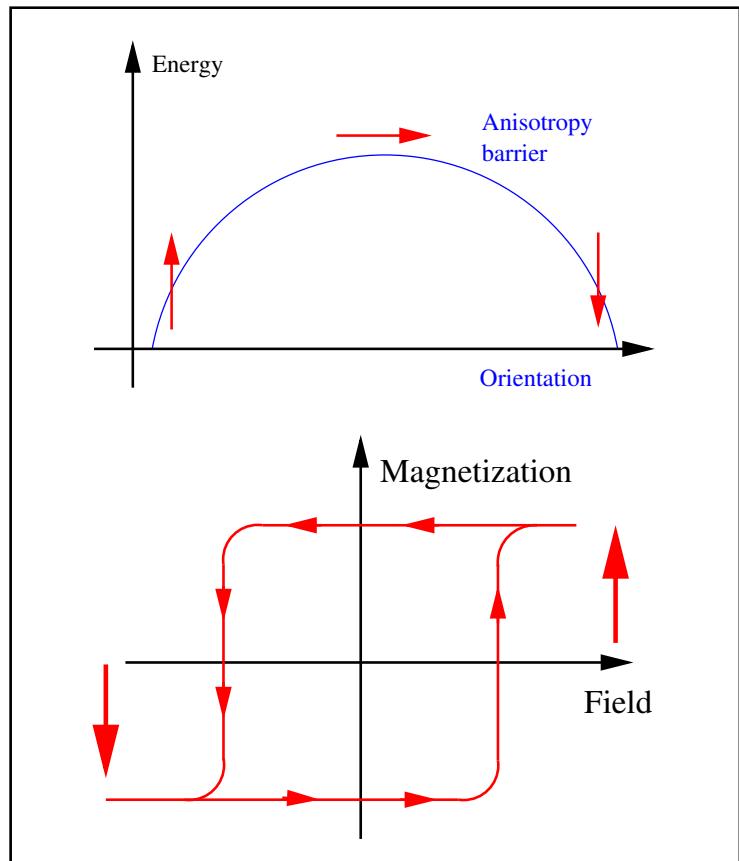
The beauty of magnetic molecules II



- 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:

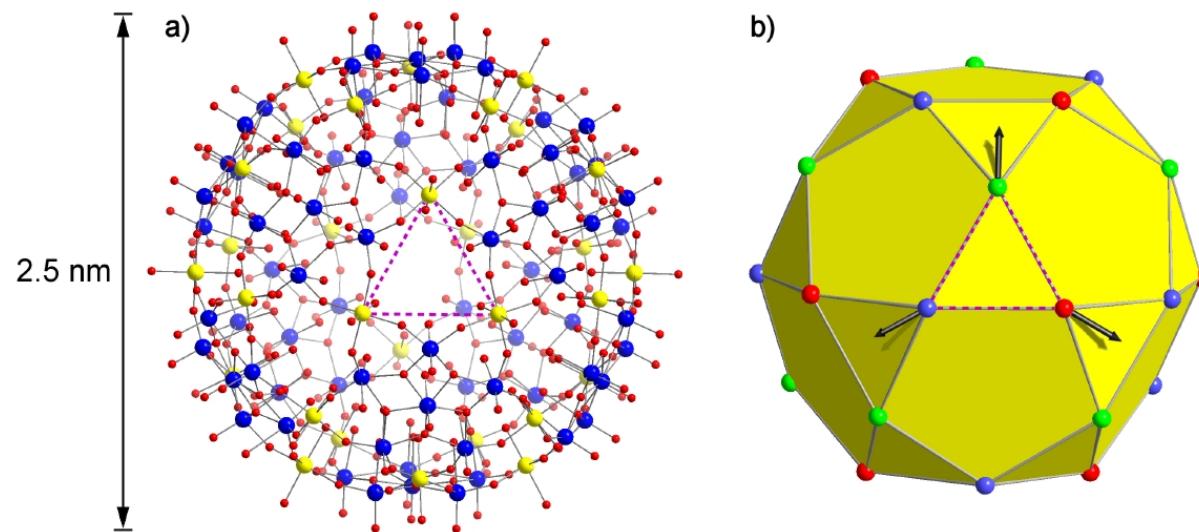
J. Schnack, H. Nojiri, P. Kögerler, G. J. T. Cooper, L. Cronin, Phys. Rev. B 70, 174420 (2004)

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.

$\{\text{Mo}_{72}\text{Fe}_{30}\}$ – 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

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

Exchange/Anisotropy Dzyaloshinskii-Moriya Zeeman

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

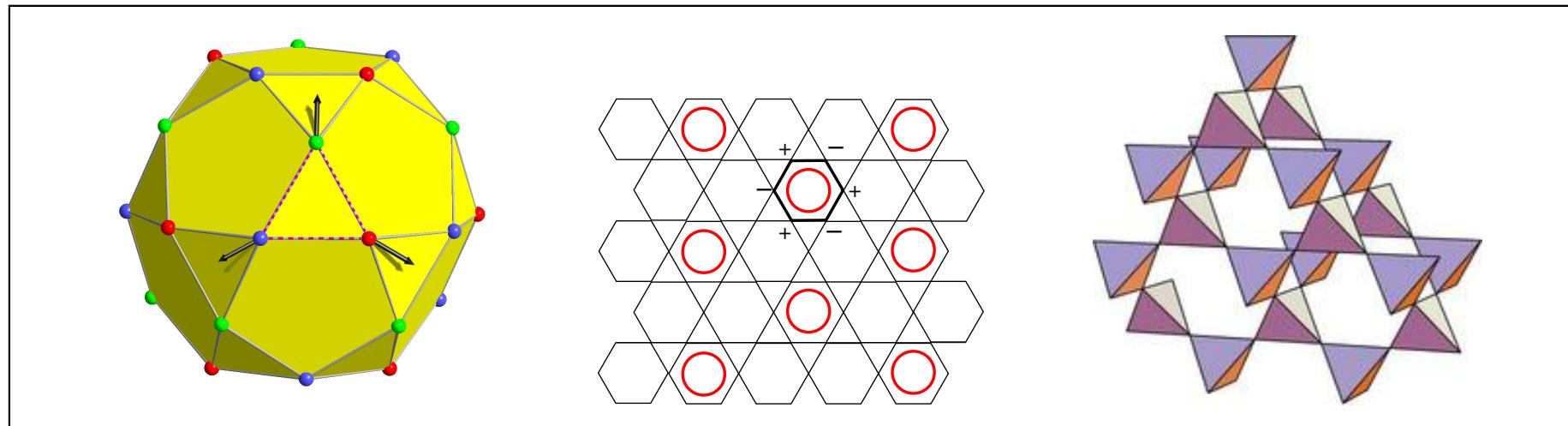
$$\tilde{H} = - \sum_{i,j} J_{ij} \vec{s}(i) \cdot \vec{s}(j) + g \mu_B B \sum_i^N \tilde{s}_z(i)$$

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



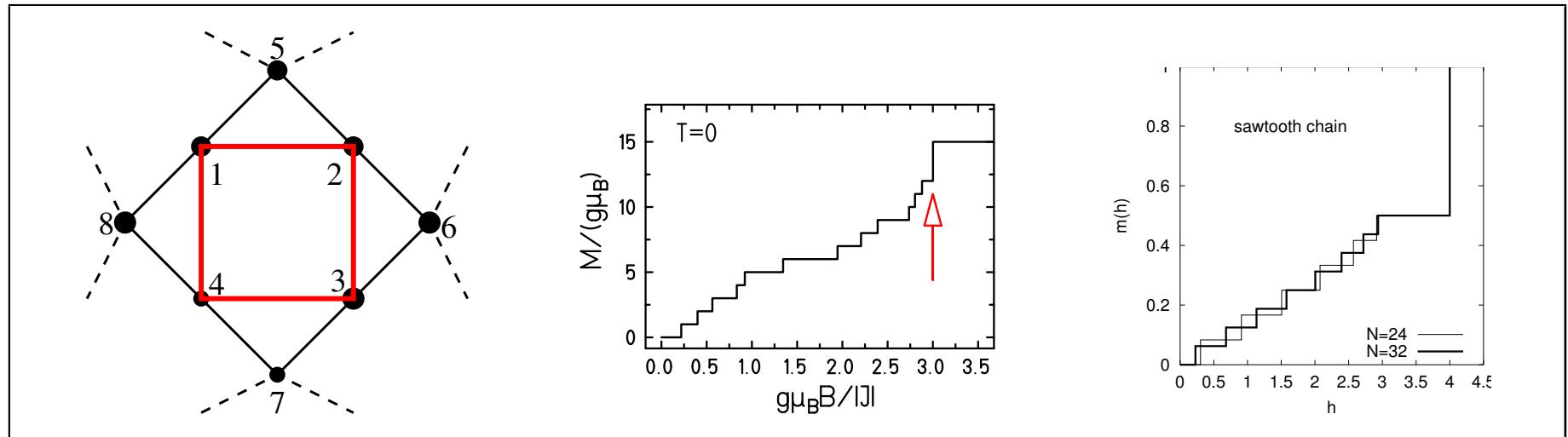
- Several frustrated antiferromagnets show an unusual behavior at the saturation field (1,2).
- E.g., icosidodecahedron, kagome lattice, pyrochlore lattice.

(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

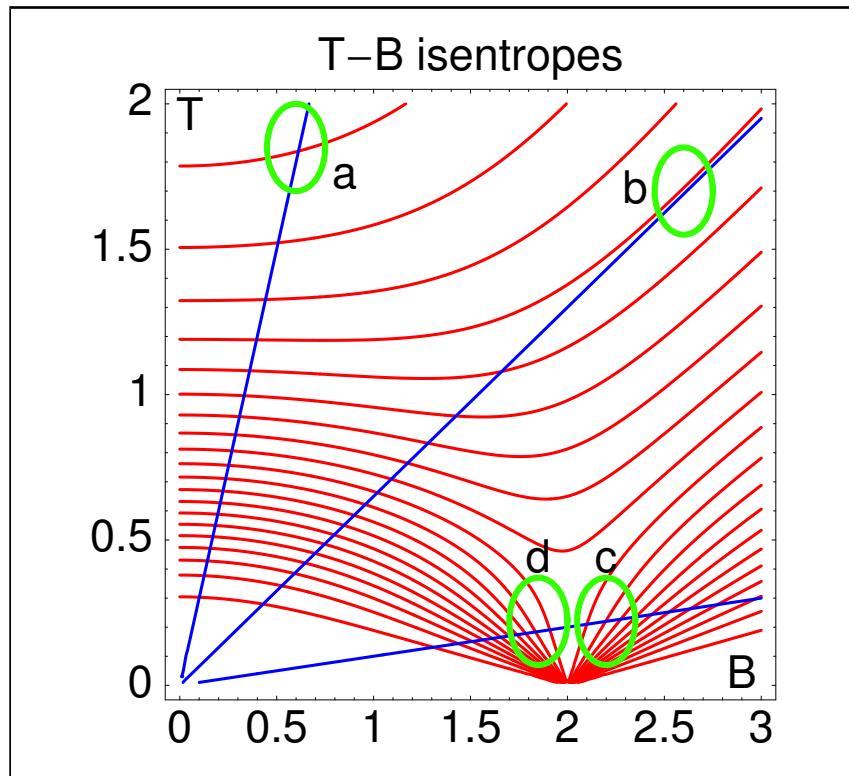


- Usually a magnetization curve is rather smooth.
- Unusually high magnetization jump at the saturation field.

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

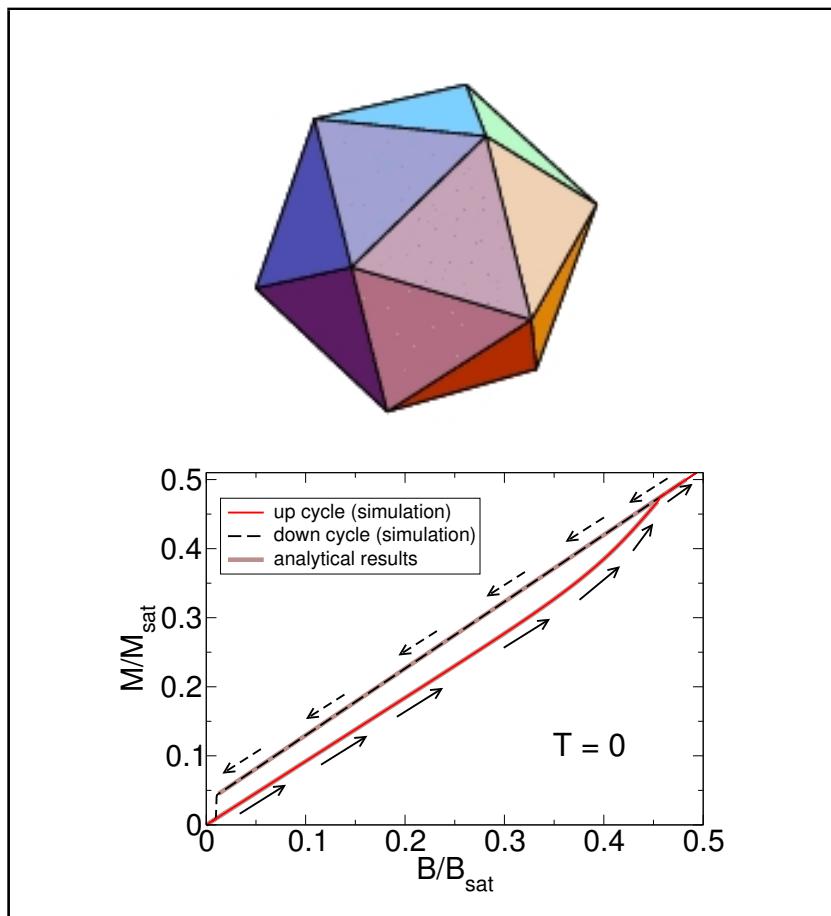
when compared to an ideal paramagnet.

Case (d) does not occur for a paramagnet.

Hysteresis without Anisotropy

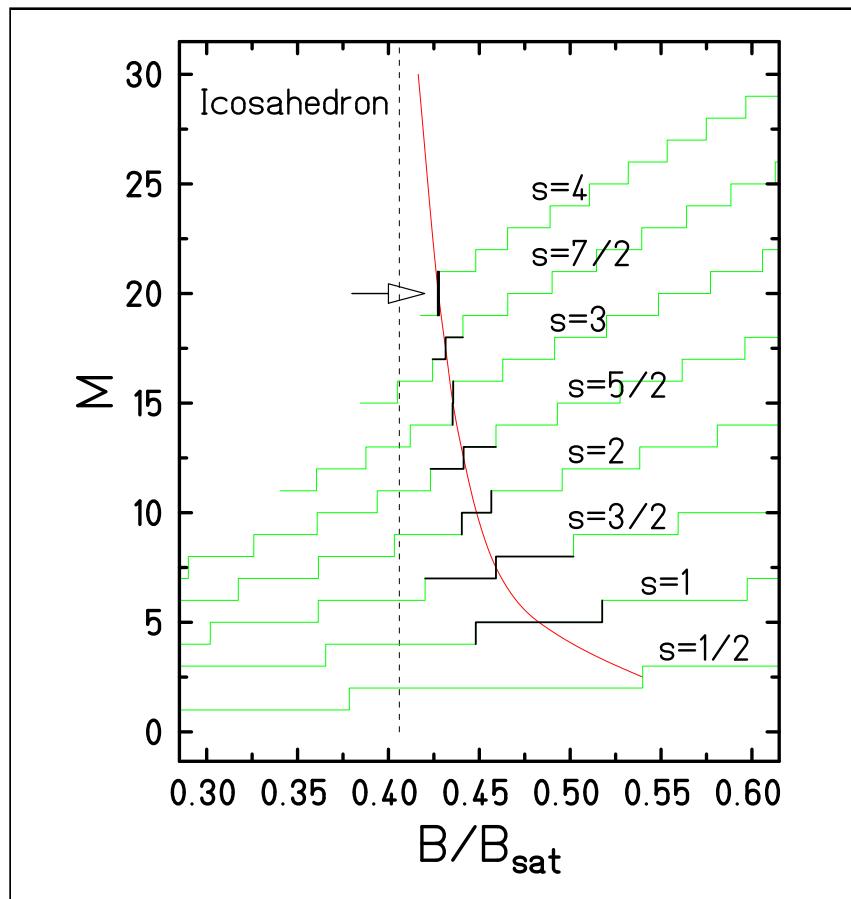
Metamagnetic phase transition I

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!

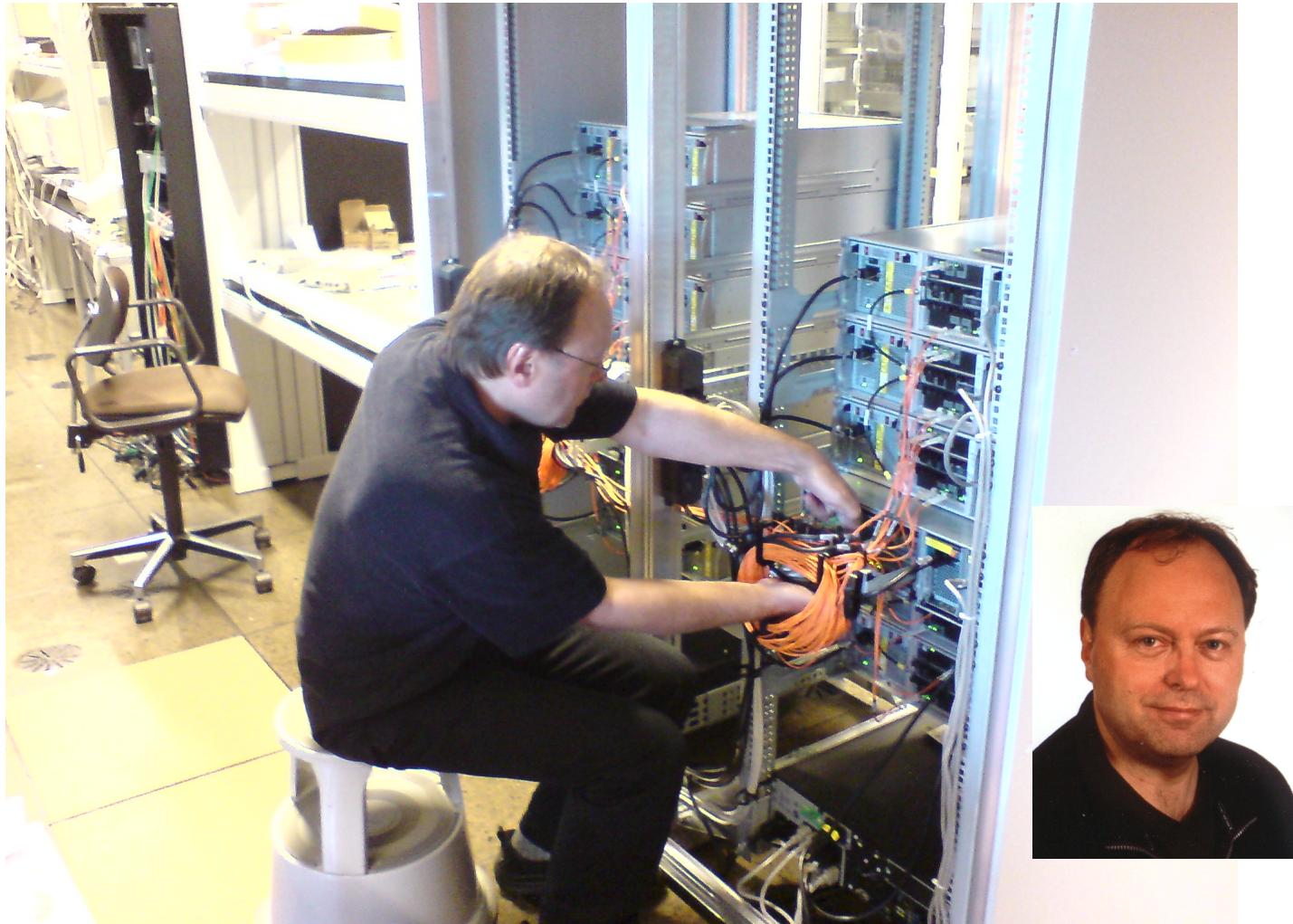
NovaScale 4040: Power for a Small University

NovaScale 4040: small is beautiful



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

Werner Nienhäuser – 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 halld
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