Large-scale numerical investigations of the antiferromagnetic Heisenberg icosidodecahedron

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MA 40.5

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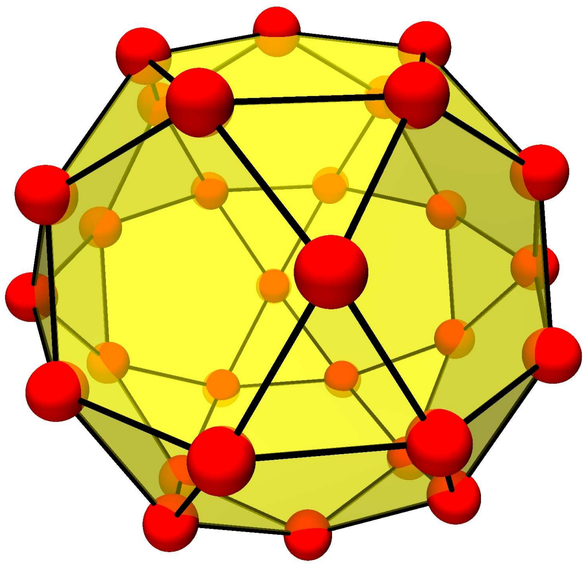
The icosidodecahedron

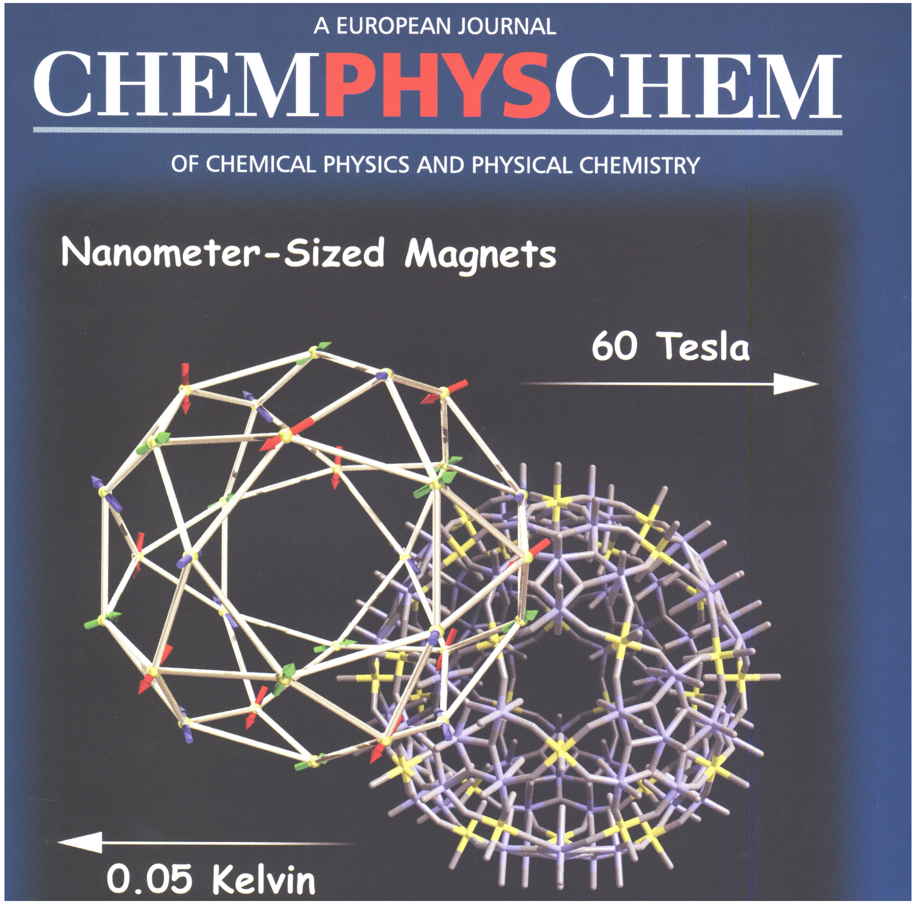


– History –

Celebrating 10+ years of

Searching in the dark!

In 2001 (we thought) we solved the problem!



A. Müller *et al.*, Chem. Phys. Chem. **2**, 517 (2001).

Again in 2001 (we thought) we solved the problem!

EUROPHYSICS LETTERS 15 December 2001

Europhys. Lett., **56** (6), pp. 863–869 (2001)

Quantum rotational band model for the Heisenberg molecular magnet $\{Mo_{72}Fe_{30}\}$

J. Schnack[1], M. Luban[2] and R. Modler[2]

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(received 27 April 2001; accepted in final form 4 October 2001)

PACS. 75.10.Jm – Quantized spin models.
PACS. 75.50.Xx – Molecular magnets.

J. Schnack, M. Luban, and R. Modler, Europhys. Lett. **56**, 863 (2001).

The following solutions were so good,

they all appeared in Phys. Rev. Lett.!

In 2002 (we thought) we solved the problem!

VOLUME 88, NUMBER 16 PHYSICAL REVIEW LETTERS 22 APRIL 2002

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

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[2]*Institut für Theoretische Physik, TU Braunschweig, Mendelssohnstrasse 3, D-38106 Braunschweig, Germany*

[3]*Universität Osnabrück, Fachbereich Physik, Barbarastrasse 7, D-49069 Osnabrück, Germany*

(Received 29 August 2001; published 8 April 2002)

For a class of frustrated spin lattices including the Kagomé lattice we construct exact eigenstates consisting of several independent, localized one-magnon states and argue that they are ground states for high magnetic fields. If the maximal number of local magnons scales with the number of spins in the system, which is the case for the Kagomé lattice, the effect persists in the thermodynamic limit and gives rise to a macroscopic jump in the zero-temperature magnetization curve just below the saturation field. The effect decreases with increasing spin quantum number and vanishes in the classical limit. Thus it is a true macroscopic quantum effect.

DOI: 10.1103/PhysRevLett.88.167207 PACS numbers: 75.10.Jm, 75.45.+j, 75.50.Ee, 75.60.Ej

J. Schulenburg *et al.*, Phys. Rev. Lett. **88**, 167207 (2002).

In 2005 (we thought) we solved the problem!

PRL 94, 017205 (2005) PHYSICAL REVIEW LETTERS week ending 14 JANUARY 2005

Competing Spin Phases in Geometrically Frustrated Magnetic Molecules

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Marshall Luban and Paul Kögerler
Ames Laboratory & Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA
(Received 18 May 2004; revised manuscript received 27 November 2004; published 11 January 2005)

We had to *discuss* the experimental data somewhat. ⇒ !!!

C. Schröder *et al.*, Phys. Rev. Lett. **94**, 017205 (2005).

In 2008 even the editor thought that the problem was solved!

PHYSICAL REVIEW B **77**, 224409 (2008)

Multiple nearest-neighbor exchange model for the frustrated magnetic molecules $\{Mo_{72}Fe_{30}\}$ and $\{Mo_{72}Cr_{30}\}$

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Akira Matsuo and Koichi Kindo
Institute for Solid State Physics, University of Tokyo, Kashiwanoha 5-1-5, Kashiwa, Chiba 277-8581, Japan

Achim Müller and Ana Maria Todea
Fakultät für Chemie, Universität Bielefeld, D-33501 Bielefeld, Germany

(Received 27 December 2007; revised manuscript received 9 May 2008; published 4 June 2008)

C. Schröder *et al.*, Phys. Rev. B **77**, 224409 (2008).

Finally in 2010: Hare Krishna!

PERSPECTIVE www.rsc.org/dalton | Dalton Transactions

Structure-related frustrated magnetism of nanosized polyoxometalates: aesthetics and properties in harmony†

Paul Kögerler,*[a] Boris Tsukerblat[b] and Achim Müller[c]

Received 1st June 2009, Accepted 1st September 2009
First published as an Advance Article on the web 12th October 2009
DOI: 10.1039/b910716a

P. Kögerler, B. Tsukerblat, and A. Müller, Dalton Trans. **39**, 1 (2010).

This world could be

so nice and harmonic . . .

. . . except:

IT IS NOT!

So, what is the problem?

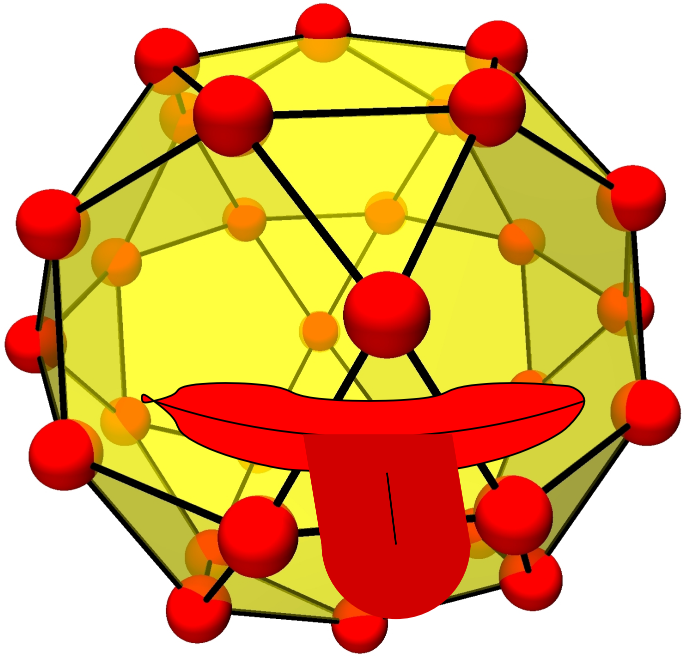
Well, we all thought that $\{(\mathrm{Mo/W})_{72}(\mathrm{Fe/Cr/V})_{30}\}$ is

"The Kagome on a sphere".

But it is not.

I. Rousochatzakis, A. M. Läuchli, and F. Mila, Phys. Rev. B **77**, 094420 (2008).

Contents for you today



1. History $\surd$
2. Expectations
3. The Reality
4. Speculation: random J (CS)
5. $\{$W$_{72}$V$_{30}\}$

Expectations

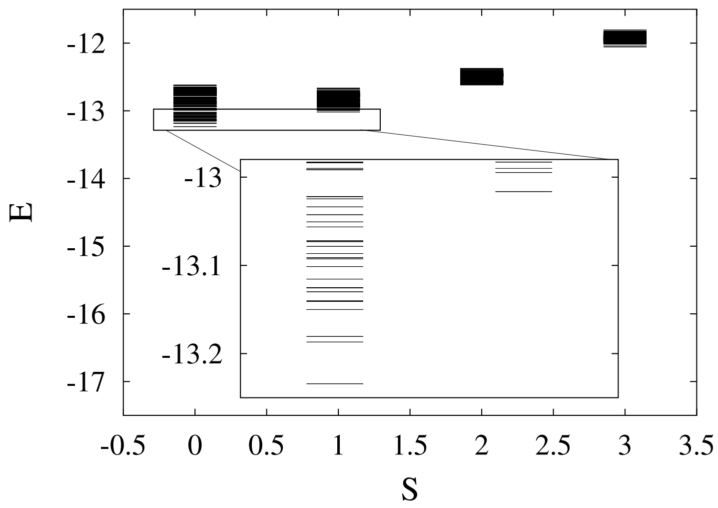
Icosidodecahedron

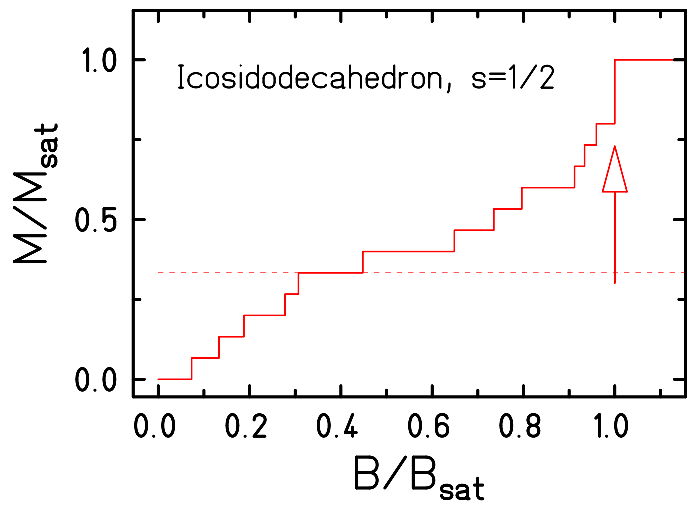
$$+$$

Heisenberg model

$$=$$

Expectations: Singlets, Plateau, and Jump

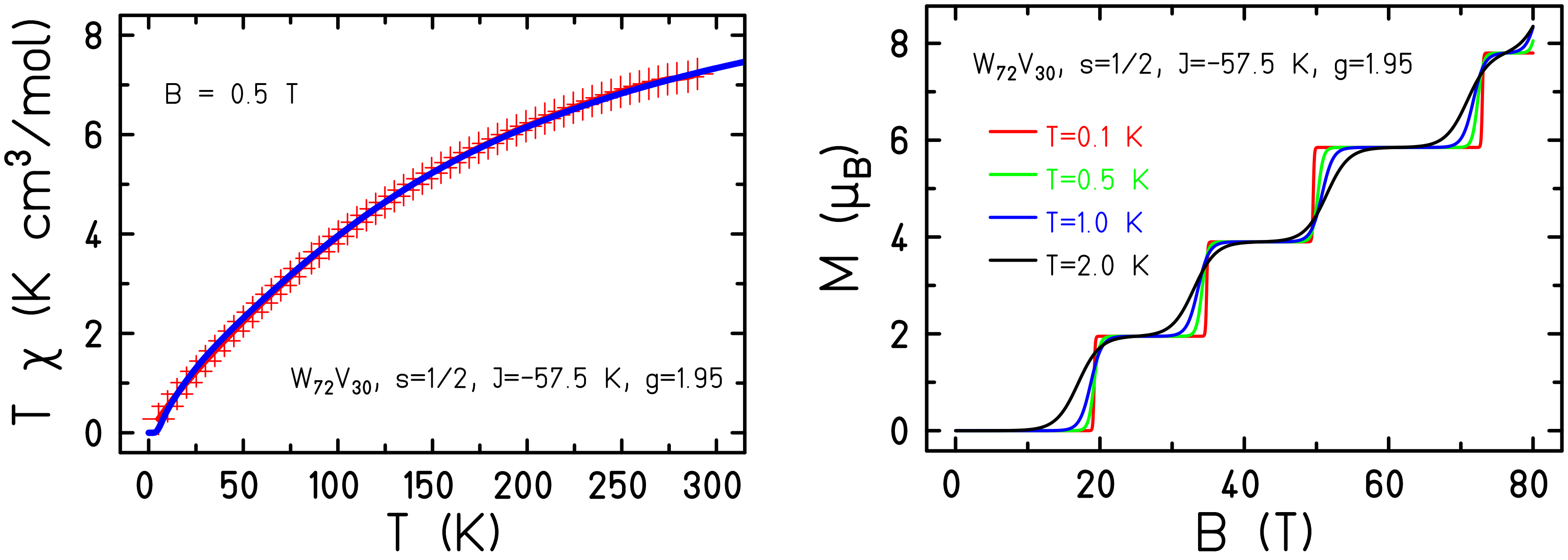




- Many singlet levels below the first triplet;
- Plateau at $\mathcal{M} = \mathcal{M}_{\text{sat}}/3$;
- Unusually large jump to saturation.

R. Schmidt, J. Schnack, and J. Richter, J. Magn. Magn. Mater. **295**, 164 (2005).
J. Schnack, Dalton Trans. **39**, 4677 (2010).

Expectation: $\{\mathbf{W}_{72}\mathbf{V}_{30}\}$

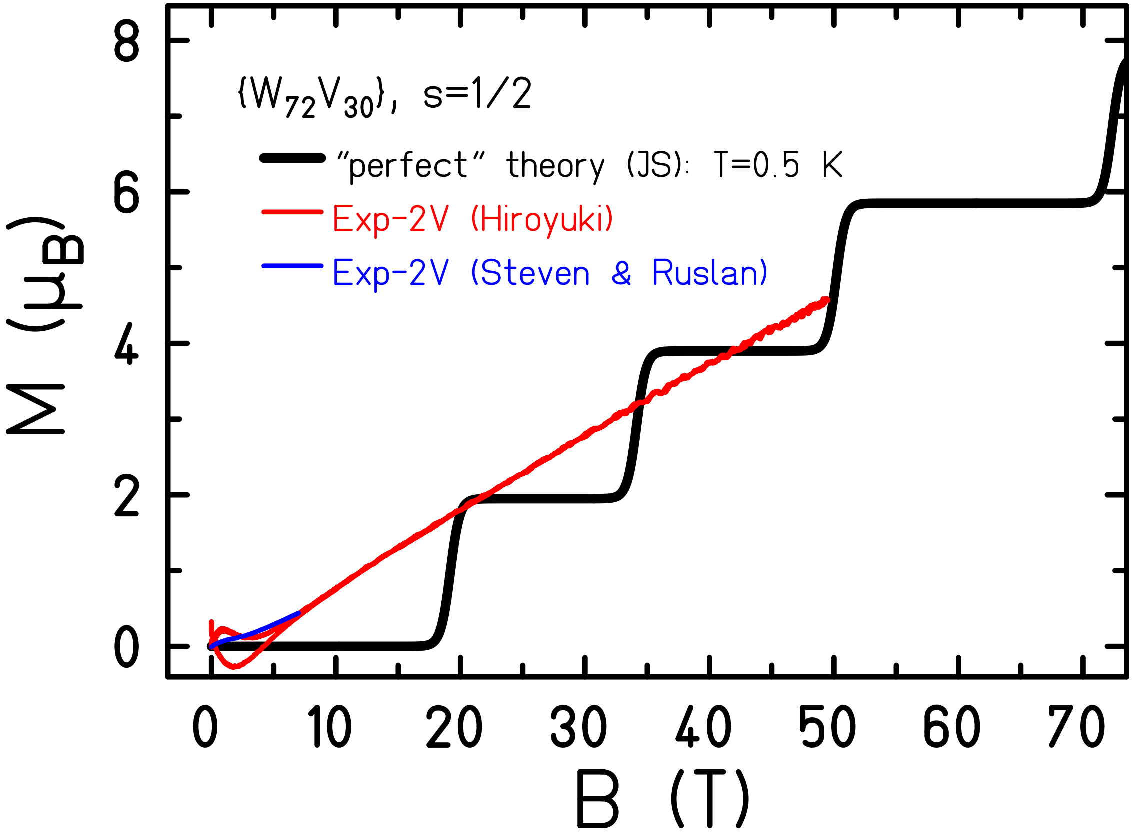


- Perfect fit of susceptibility (FTLM);
- Expect magnetization steps in high-field measurements.

exp. data: A. M. Todea, A. Merca, H. Bögge, T. Glaser, L. Engelhardt, R. Prozorov, M. Luban, A. Müller, Chem. Commun., 3351 (2009).
J. Schnack, arXiv:1012.4980

Reality

Reality: magnetization curve without steps



Speculations

Speculation I: random J

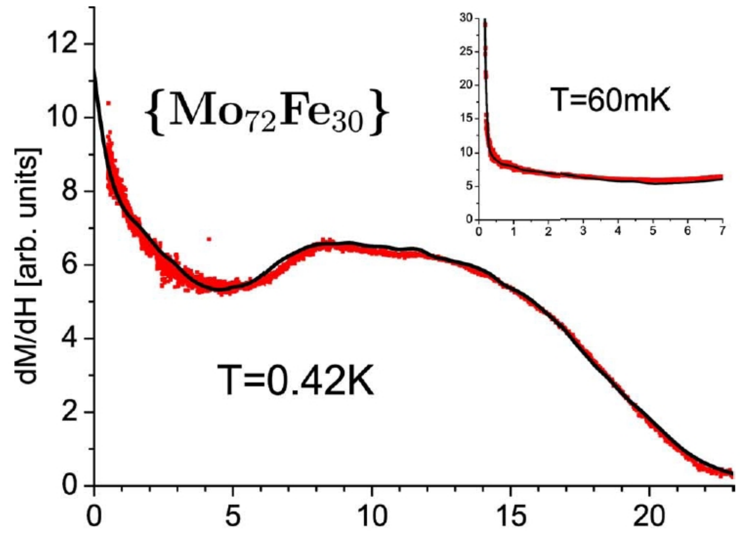
$$\underset{\sim}{H} = -2 \sum_{i<j} J_{ij}\, \underset{\sim}{\vec{s}}(i) \cdot \underset{\sim}{\vec{s}}(j) \quad + \quad g\, \mu_B\, B \sum_{i}^{N} \underset{\sim}{s}_z(i)$$

Heisenberg Zeeman

Idea of Christian Schröder: J_{ij} fluctuate (J-strain), therefore, are chosen according to a random distribution.

C. Schröder *et al.*, Phys. Rev. B **77**, 224409 (2008).

Speculation I: random J

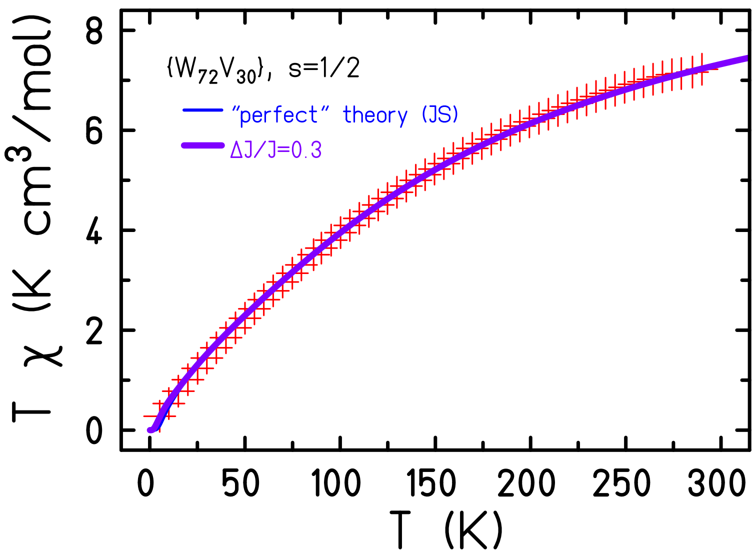


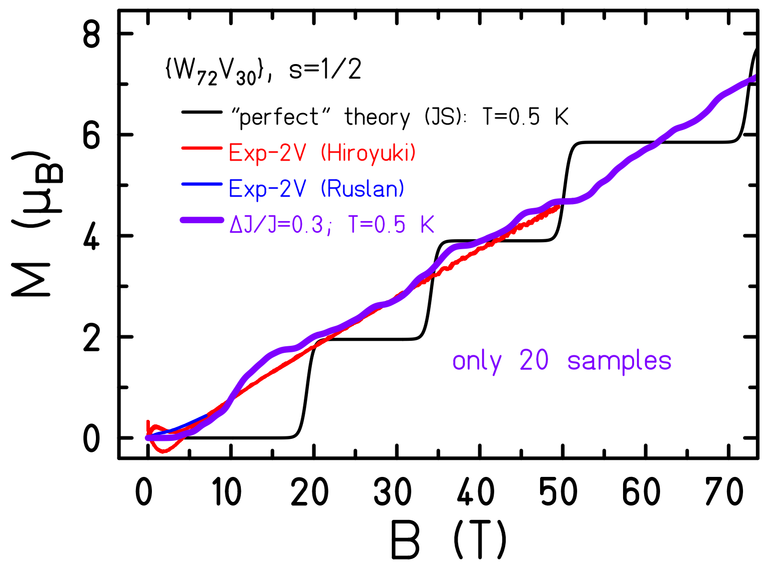
- Classical spin dynamics with random J for $\{\text{Mo}_{72}\text{Fe}_{30}\}$ and $\{\text{Mo}_{72}\text{Cr}_{30}\}$;
- Absolutely astonishing accuracy.

C. Schröder *et al.*, Phys. Rev. B **77**, 224409 (2008).

$$\left\{W_{72}V_{30}\right\}$$

$\{\mathbf{W}_{72}\mathbf{V}_{30}\}$

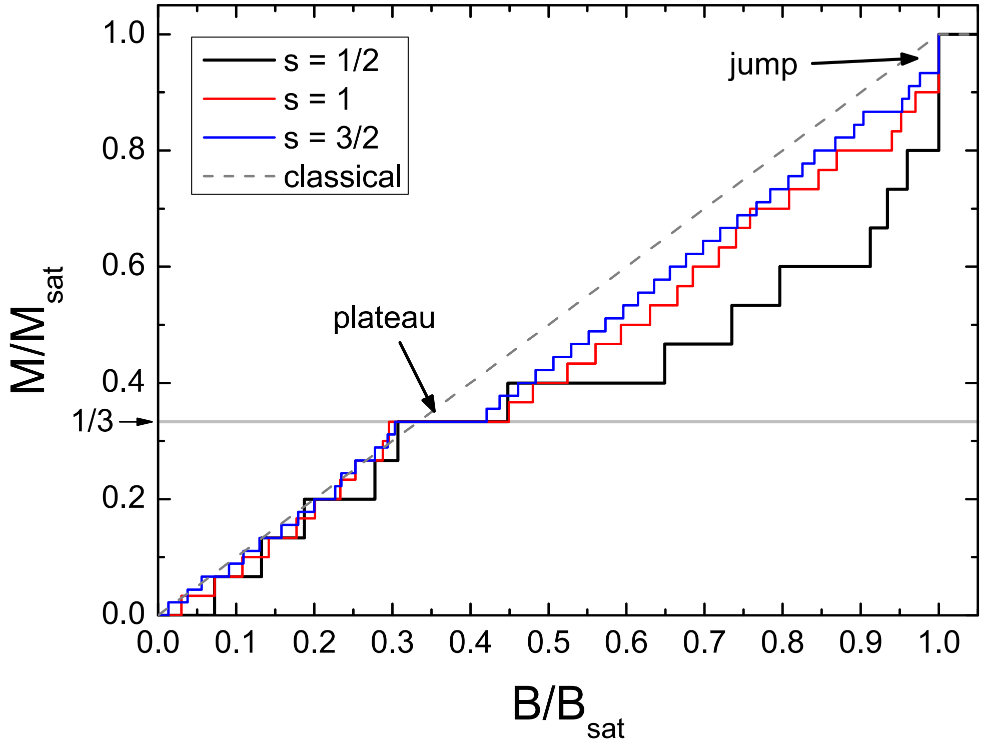




- $\{\mathrm{W}_{72}\mathrm{V}_{30}\}$ is the MOST symmetric Keplerate (AM).
- Nevertheless, it needs a J variation of about 30%.
- Full FTLM quantum calculations, 15 hours on 510 cores for a single parameter set.

Outlook

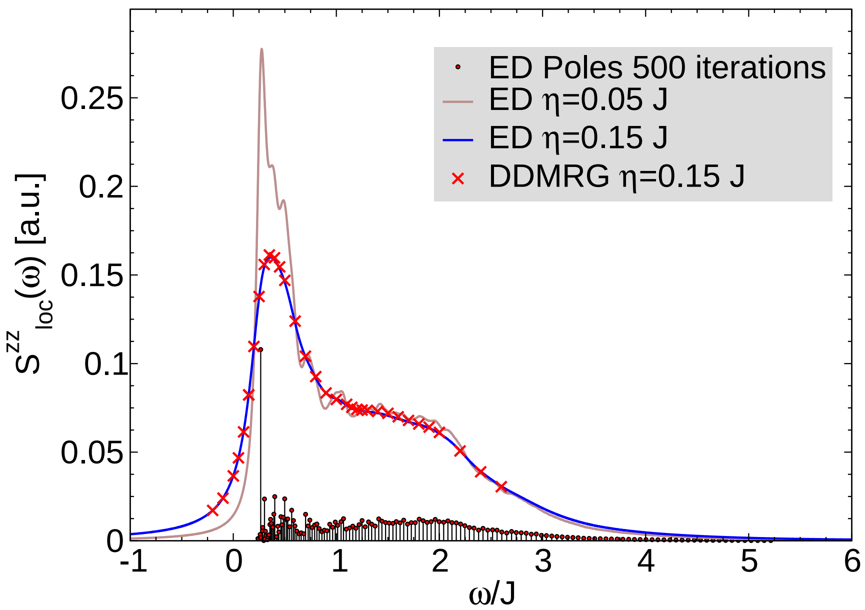
DMRG & FTLM provide full details I



- DMRG yields ground states + very few low-lying states in orthogonal subspaces.
- Magnetization curve for $T = 0$, resonance energies for spectroscopy.

(1) J. Ummethum, J. Schnack, and A. Laeuchli, J. Magn. Magn. Mater. **327** (2013) 103

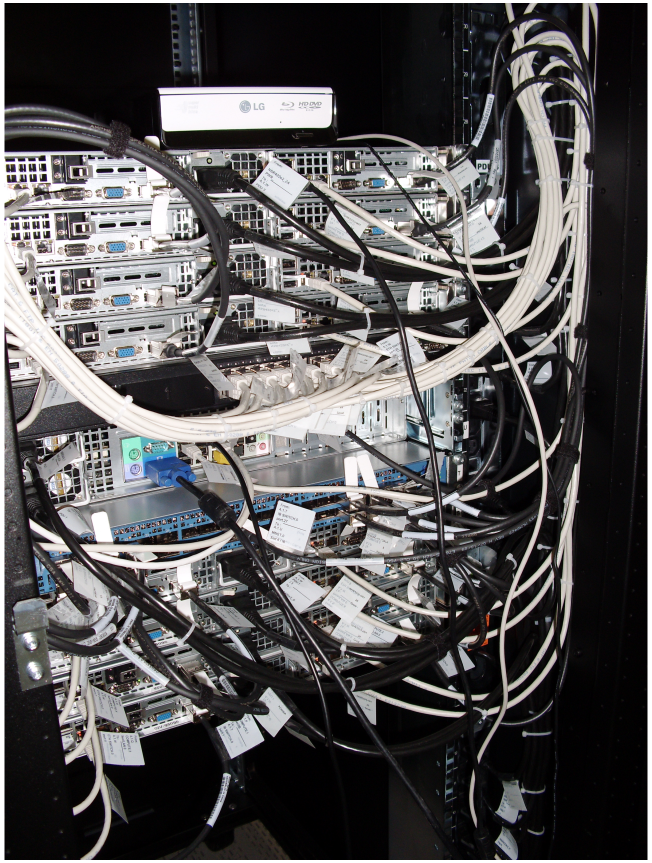
DMRG & FTLM provide full details II



- V_{30}: $S^{zz}_{\text{loc}}(\omega) = -\frac{1}{\pi}\text{Im}\langle\text{GS}|S^z_0 \frac{1}{\omega-(H-E_{\text{GS}})+i\eta} S^z_0|\text{GS}\rangle$
- Aim: better understanding of low-lying levels, **INS**.

(1) J. Ummethum, J. Schnack, and A. Laeuchli, J. Magn. Magn. Mater. **327** (2013) 103

Summary



- The Keplerate molecules remain my hobby.
- Finite-temperature Lanczos is perfect to deal with larger systems and to go beyond Heisenberg models.
- J-strain should be visible elsewhere!
- If you have no explanation, try Dzyaloshinskii-Moriya! This is our next step.

Many thanks to my collaborators worldwide

- T. Glaser, Chr. Heesing, M. Höck, N.B. Ivanov, J. Korenke, H.T. Langwald, S. Leiding, A. Müller, Chr. Schröder, J. Ummethum, O. Wendland (Bielefeld)

- K. Bärwinkel, H.-J. Schmidt, M. Neumann (Osnabrück)

- M. Luban (Ames Lab, USA); P. Kögerler (Aachen, Jülich, Ames); R.E.P. Winpenny, E.J.L. McInnes (Man U, UK); L. Cronin, M. Murrie (Glasgow, UK); E. Brechin (Edinburgh, UK); H. Nojiri (Sendai, Japan); A. Postnikov (Metz, France); M. Evangelisti (Zaragosa, Spain)

- J. Richter, J. Schulenburg (Magdeburg); A. Honecker (Göttingen); U. Kortz (Bremen); A. Tennant, B. Lake (HMI Berlin); B. Büchner, V. Kataev, H.-H. Klauß (Dresden); P. Chaudhuri (Mühlheim); J. Wosnitza (Dresden-Rossendorf); J. van Slageren (Stuttgart); R. Klingeler (Heidelberg); O. Waldmann (Freiburg)

Thank you very much for your attention.

The end.

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