

Giant magnetization jumps in high fields: a new macroscopic quantum effect

Jürgen Schnack, Heinz-Jürgen Schmidt (University of Osnabrück)

Johannes Richter, Jörg Schulenburg (University of Magdeburg)

Andreas Honecker (University of Braunschweig)

<http://obelix.physik.uni-osnabrueck.de/~schnack/>

JEMS, Dresden, September 2004

Contents

- Model Hamiltonian: Heisenberg Hamiltonian & Zeeman term
- Molecular Magnetism point of view: Rotational bands
- Strange magnetic molecule $\{\text{Mo}_{72}\text{Fe}_{30}\}$
- Magnetization jumps
- Independent magnons
- Example spin systems
- Solid state point of view: Flat band
- Outlook

Model Hamiltonian – Heisenberg-Model

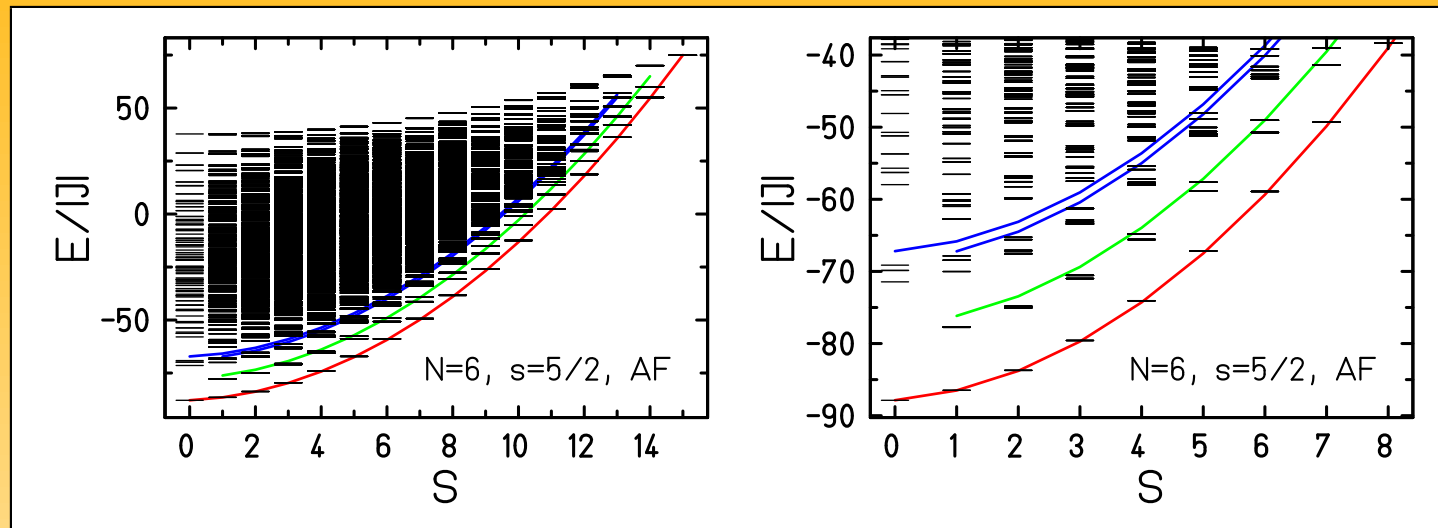
$$\underline{H} = - \sum_{i,j} J_{ij} \vec{\underline{S}}(i) \cdot \vec{\underline{S}}(j) + g \mu_B B \sum_i^N \underline{S}_z(i)$$

Heisenberg
Zeeman

The Heisenberg Hamilton operator together with a Zeeman term are used for the following considerations.

$J < 0$: antiferromagnetic coupling.

MM point of view: Rotational bands



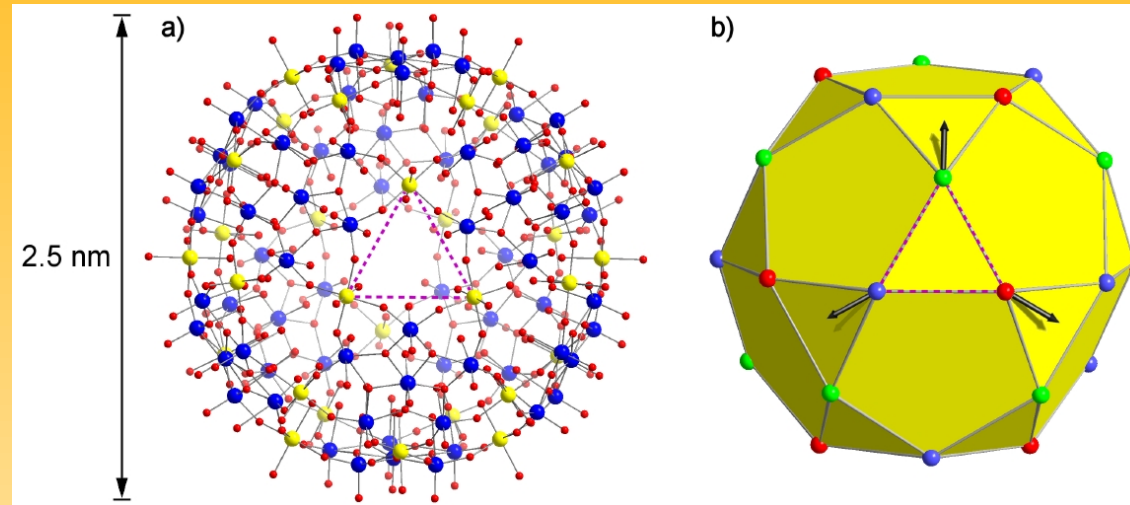
- For magnetic molecules the minimal energies $E_{min}(S)$ often form a rotational band, i. e. depend quadratically on S : Landé interval rule (1);
- Most pronounced for bipartite systems (2), good approximation for more general systems;
- Sometimes low-lying spectrum is a sequence of rotational bands (3).

(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)

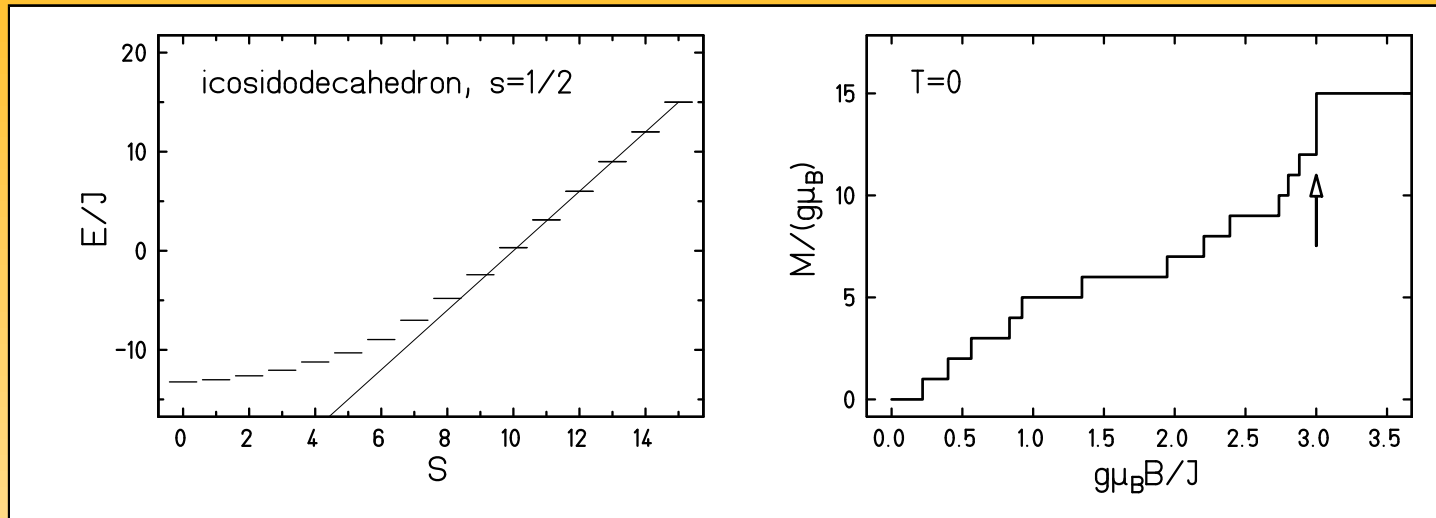
Strange magnetic molecule {Mo₇₂Fe₃₀}



- Structure of {Mo₇₂Fe₃₀}: Fe - yellow, Mo - blue, O - red,
- Antiferromagnetic interaction mediated by O-Mo-O bridges (1).
- Classical ground state of {Mo₇₂Fe₃₀}: three sublattice structure, coplanar spins (2);
- Quantum mechanical ground state $S = 0$ can only be approximated (3,4), dimension of Hilbert space $(2s + 1)^N \approx 10^{23}$.

(1) A. Müller *et al.*, Chem. Phys. Chem. **2**, 517 (2001) , (2) M. Axenovich and M. Luban, Phys. Rev. B **63**, 100407 (2001) , (3) J. Schnack, M. Luban, R. Modler, Europhys. Lett. **56** 863 (2001) 863 , (4) M. Exler, J. Schnack, Phys. Rev. B **67** (2003) 094440

{Mo₇₂Fe₃₀} - magnetization jump



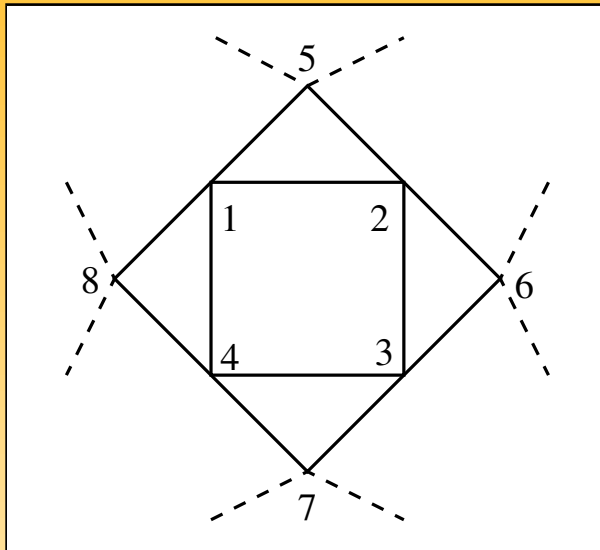
- $E_{\min}(S)$ linear in S for high S instead of being quadratic (1);
- Heisenberg model: property depends only on the structure but not on s (2);
- Alternative formulation: independent localized magnons (3);

(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** (2002) 167207

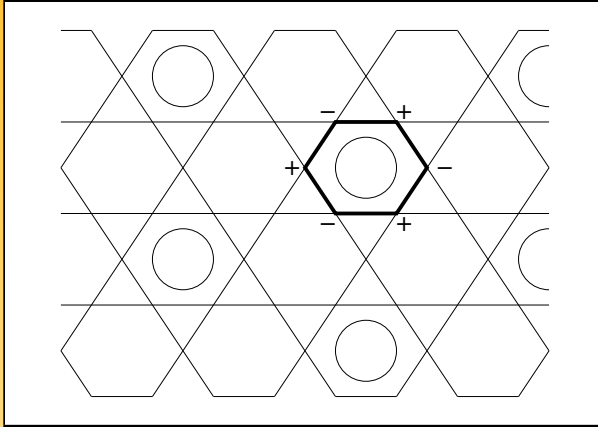
Localized Magnons



- $|\text{localized magnon}\rangle = \frac{1}{2}(|1\rangle - |2\rangle + |3\rangle - |4\rangle)$
- $|u\rangle = \tilde{s}^-(u)|\Omega\rangle$; $|\Omega\rangle$ – magnon vacuum;
 $u = 1, 2, 3, 4$
- $\tilde{H}|1\rangle = J\{|1\rangle + 1/2(|2\rangle + |4\rangle + |5\rangle + |8\rangle)\}$
- $\tilde{H}|\text{localized magnon}\rangle \propto |\text{localized magnon}\rangle$

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

Kagome Lattice

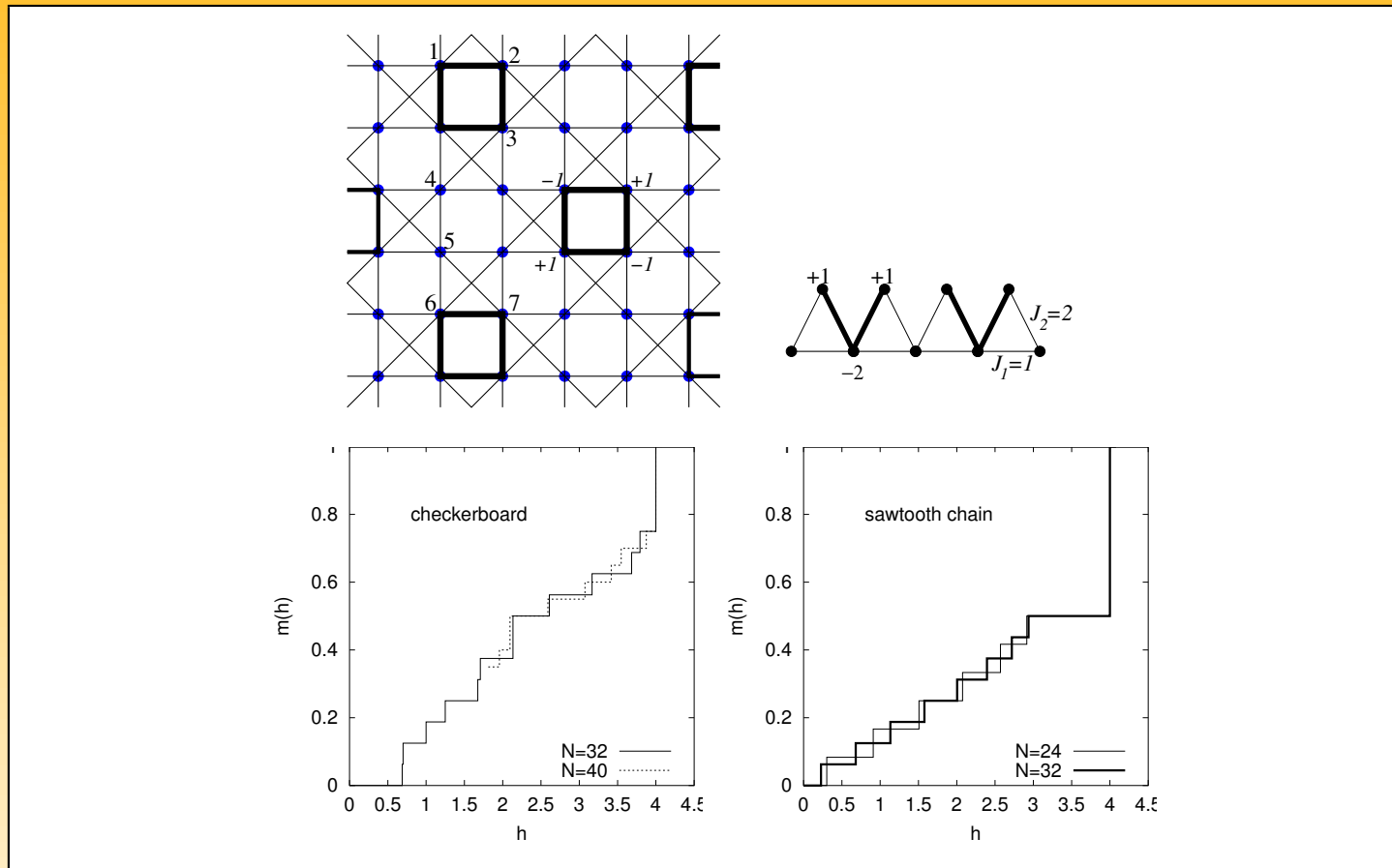


- Localized one-magnon state indicated by bold lines;
- Non-interacting one-magnon states can be placed on the grid; each state of n independent magnons is the ground state in the Hilbert subspace with $M = Ns - n$;

- \Rightarrow Linear dependence of E_{\min} on M ; magnetization jump;
- Maximal number of independent magnons: $N/9$;
- Magnetization jump is a macroscopic quantum effect!

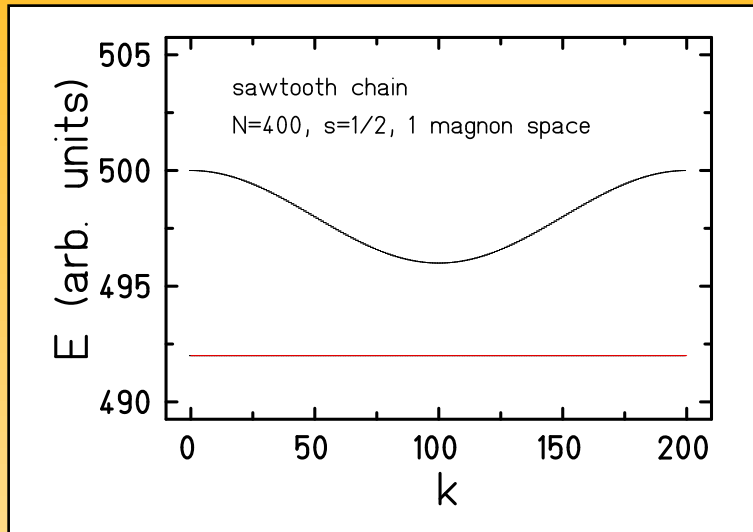
J. Schulenburg, A. Honecker, J. Schnack, J. Richter, H.-J. Schmidt, Phys. Rev. Lett. **88** (2002) 167207

Example spin systems



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

Solid state point of view: Flat band

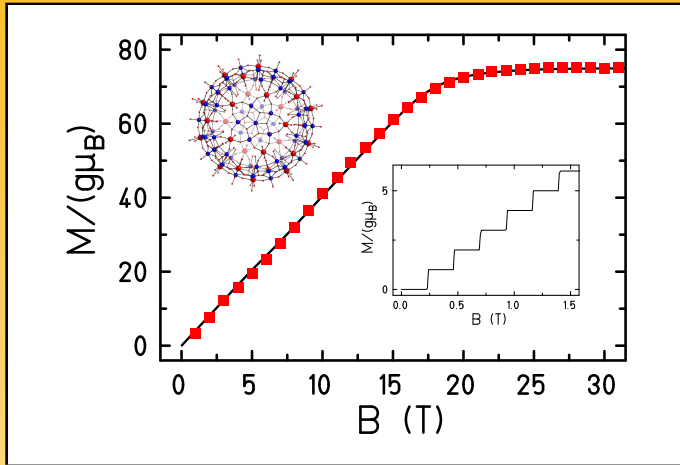


- Flat band of minimal energy in one-magnon space, i. e. high degeneracy of ground state energy in $\mathcal{H}(M = Ns - 1)$;
- Localized magnons can be built from eigenstates of the shift (translation) operator;
- Sawtooth chain exceptional since degeneracy is $N/2$ (very high).

Yet another point of view

- Localized magnons are special solitons;
- They are well localized and have dispersionless time-evolution;
- But they are also stationary, i. e. do not move.

Outlook



- Magnetization jump in $\{\text{Mo}_{72}\text{Fe}_{30}\}$ not detectable: too small, temperature too high;
- A material like Kagome, checkerboard or saw-tooth chain would be preferable since there the effect is of macroscopic nature;

- Our hope is that dipolar interactions smear out the magnetization jump only weakly.
- Magnetocaloric effect presumably especially strong close to the jump (compare symposium on MC and (1-3)).

(1) O. Derzhko, J. Richter, cond-mat/0404204;
 (2) M. Zhitomirsky, A. Honecker, J. Stat. Mech.: Theor. Exp. (2004) P07012;
 (3) M. Zhitomirsky, H. Tsunetsugu, cond-mat/0405578

Thank you very much for your attention.

Collaboration

- Prof. K. Bärwinkel, Prof. H.-J. Schmidt, M. Allalen, M. Brüger, D. Mentrup, M. Exler, P. Hage, F. Hesmer, F. Ouchni, P. Shechelokovskyy (Uni Osnabrück);
- Prof. M. Luban, Dr. P. Kögerler, Dr. Chr. Schröder (Ames Lab, Iowa, USA);
- Prof. H. Nojiri (Tohoku University, Japan);
- Prof. R. Winpenny (Manchester), Dr. L. Cronin (Glasgow);
- Prof. B. Büchner, Dr. R. Klingeler (IFW Dresden);
- Prof. J. Richter, Dr. J. Schulenburg (Uni Magdeburg);
- Dr. A. Honecker (Uni Braunschweig); Prof. S. Blügel (FZ Jülich);

Buy now!

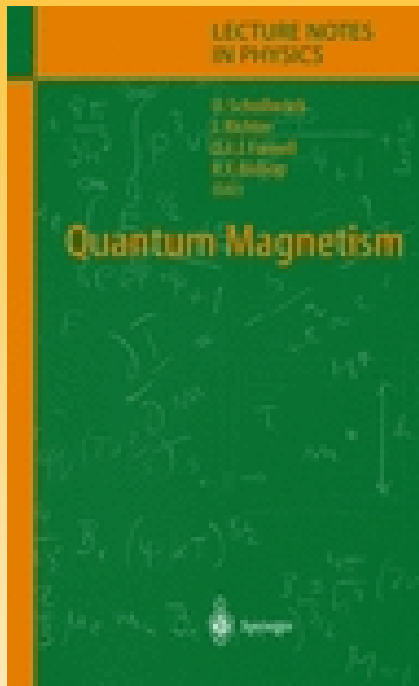
Quantum Magnetism

Lecture Notes in Physics , Vol. 645

Schollwöck, U.; Richter, J.; Farnell, D.J.J.; Bishop, R.F.
(Eds.)

2004, XII, 478 p., Hardcover, 69,95 €

ISBN: 3-540-21422-4



Mikeska, Kolezhuk, *One-dimensional magnetism*

Richter, Schulenburg, Honecker, *Q. Mag. in 2-D*

Schnack, *Molecular Magnetism*

Ivanov, Sen, *Spin Wave Analysis*

Laflorie, Poilblanc, *Low-Dim. Gapped Systems*

Cabra, Pujol, *Field-Theoretical Methods*

Farnell, Bishop, *Coupled Cluster Method*

Klümper, *Integrability of Quantum Chains*

Sachdev, *Mott Insulators*

Lemmens, Millet, *Spin Orbit Topology, a Triptych*