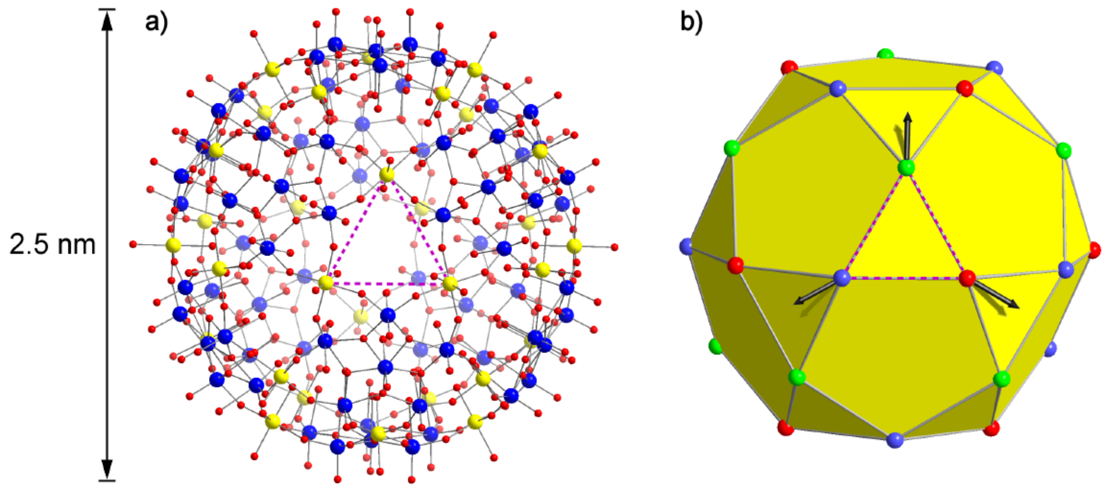
What does the icosidodecahedron teach us about magnetism?

Jürgen Schnack

Universität Osnabrück, D-49069 Osnabrück, Germany



thanks to Paul Kögerler

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

Contents

Heisenberg model

Hamilton operator (AF: $J > 0$[a])

$$\underset{\sim}{H} \;=\; J \sum_{(u,v)} \underset{\sim}{\vec{s}}(u) \cdot \underset{\sim}{\vec{s}}(v) + g\,\mu_B\,B \sum_{u}^{N} \underset{\sim}{s}_z(u)$$

Symmetries and good quantum numbers

$$\left[\underset{\sim}{H}, \underset{\sim}{\vec{S}}^2\right] = 0 \quad \& \quad \left[\underset{\sim}{H}, \underset{\sim}{S}_z\right] = 0 \quad \& \quad \left[\underset{\sim}{\vec{S}}^2, \underset{\sim}{S}_z\right] = 0 \quad , \quad \underset{\sim}{S}_z = \sum_{u}^{N} \underset{\sim}{s}_z(u)$$

For this talk I will assume that all spins have the same length s.

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[a] Don't worry. This definition looks different in every publication, even in our own.

Typical observables in the canonical ensemble

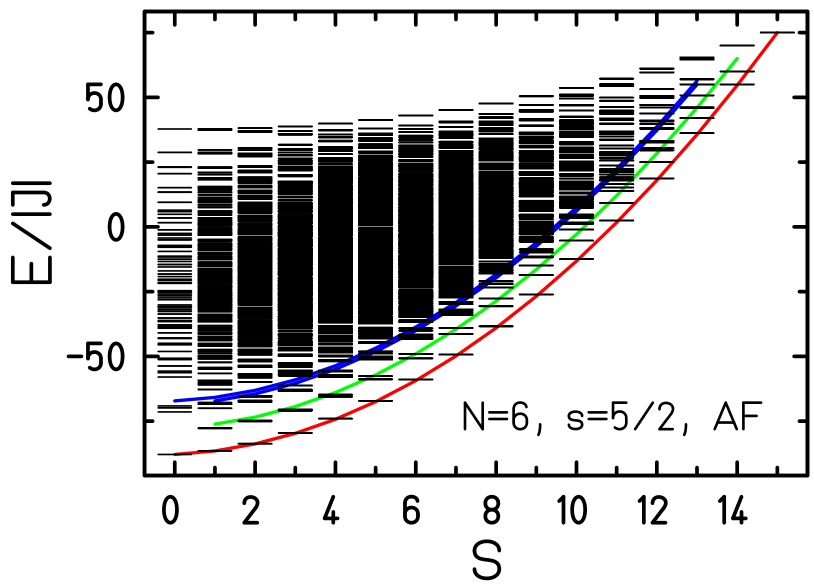
Mean energy and specific heat

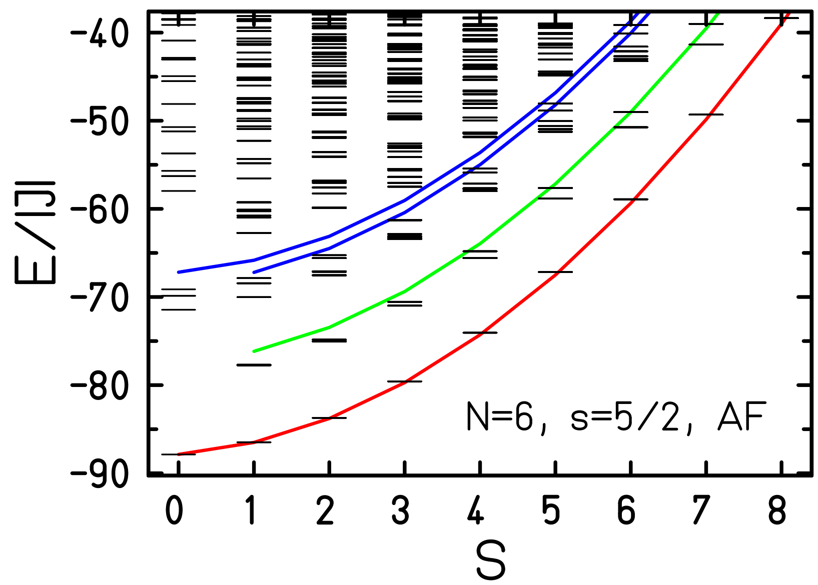
$$\begin{aligned}\langle\langle\, \underset{\sim}{H} \,\rangle\rangle &= \frac{1}{Z}\,\mathrm{tr}\left\{\underset{\sim}{H}\, e^{-\beta \underset{\sim}{H}}\right\} \quad , \quad Z = \mathrm{tr}\left\{e^{-\beta \underset{\sim}{H}}\right\} \quad , \quad \beta = \frac{1}{kT} \\ C &= \frac{d}{dT}\,\langle\langle\, \underset{\sim}{H} \,\rangle\rangle = \frac{1}{kT^2}\left(\langle\langle\, \underset{\sim}{H}^2 \,\rangle\rangle - \langle\langle\, \underset{\sim}{H} \,\rangle\rangle^2\right)\end{aligned}$$

Magnetisation and magnetic susceptibility

$$\begin{aligned}\mathcal{M} &= g\mu_B\left(\frac{1}{Z}\,\mathrm{tr}\left\{\underset{\sim}{S}_z \mathrm{e}^{-\beta \underset{\sim}{H}}\right\}\right) \\ \chi &= \left(\frac{\partial\,\mathcal{M}}{\partial\, B}\right) = g^2\mu_B^2\beta\left(\langle\langle\, \left(\underset{\sim}{S}_z\right)^2 \,\rangle\rangle - \langle\langle\, \underset{\sim}{S}_z \,\rangle\rangle^2\right)\end{aligned}$$

Rotational bands in AF Heisenberg rings





Very often the minimal energies $E_{min}(S)$ form a rotational band, i. e. depend approximately quadratically on the total spin quantum number S (Landé interval rule).[a]
Sometimes the low-lying spectrum is dominated by a sequence of rotational bands.

[a] Chem. Eur. J. **2**, 1379 (1996); G. L. Abbati *et al.*, Inorg. Chim. Acta **297**, 291 (2000); J. Schnack and M. Luban, Phys. Rev. B **63**, 014418 (2001).

Rotational band Hamiltonian for Fe_{30}

$$
\begin{aligned}
\underset{\sim}{H} = -2\,J \sum_{(u<v)} \underset{\sim}{\vec{s}}(u) \cdot \underset{\sim}{\vec{s}}(v) \quad &\approx \quad -\frac{D\,J}{N}\left[\underset{\sim}{\vec{S}}^2 - \sum_{j=1}^{N_{SL}} \underset{\sim}{\vec{S}}_j^2\right] = \underset{\sim}{H}_1^{\mathrm{eff}} \\
&\approx \quad -J\,\frac{D(N,s)}{N}\left[\underset{\sim}{\vec{S}}^2 - \gamma(N,s)\left(\sum_{j=1}^{N_{SL}} \underset{\sim}{\vec{S}}_j^2\right)\right] = \underset{\sim}{H}_2^{\mathrm{eff}}
\end{aligned}
$$

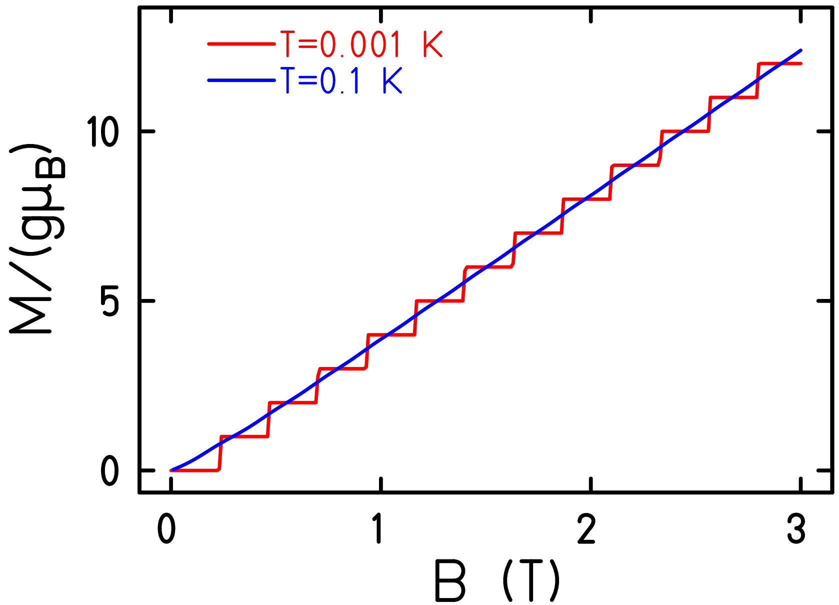
N_{SL} – number of sublattices, $\underset{\sim}{\vec{S}}_j$ – sublattice spin;

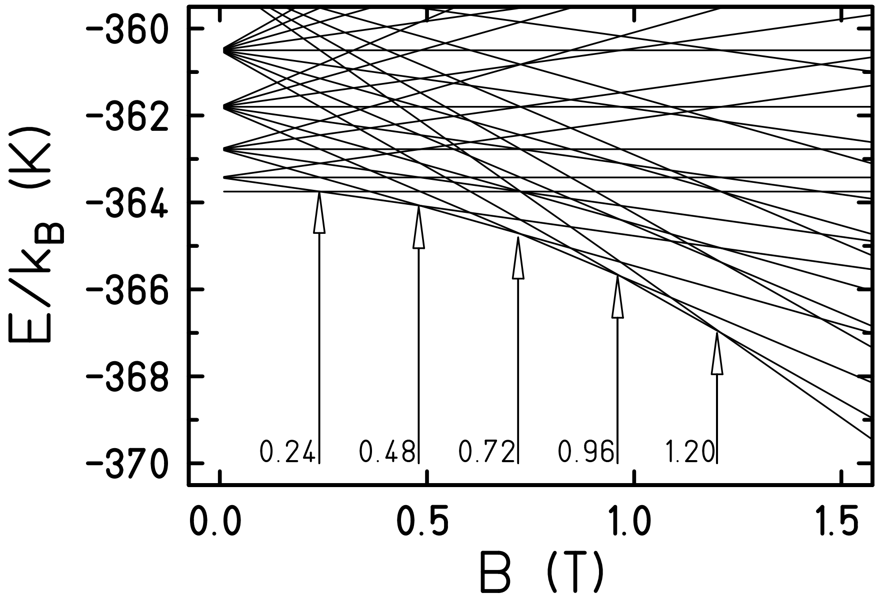
$\{Mo_{72}Fe_{30}\}$[a]**:**

- $N_{SL} = 3$, $S_A, S_B, S_C = 0, 1, \dots, 25$, $S = 0, 1, \dots, 75$;
- $D = 6$ determined from corresponding classical system or equivalently from sublattice structure;
- finite size effect: $D(N,s) = 6.23$, $\gamma(N,s) = 1.07$.

[a] J. Schnack, M. Luban, R. Modler, *Quantum rotational band model for the Heisenberg molecular magnet $\{Mo_{72}Fe_{30}\}$*, Europhys. Lett. (2001) submitted.

Can one detect rotational bands?

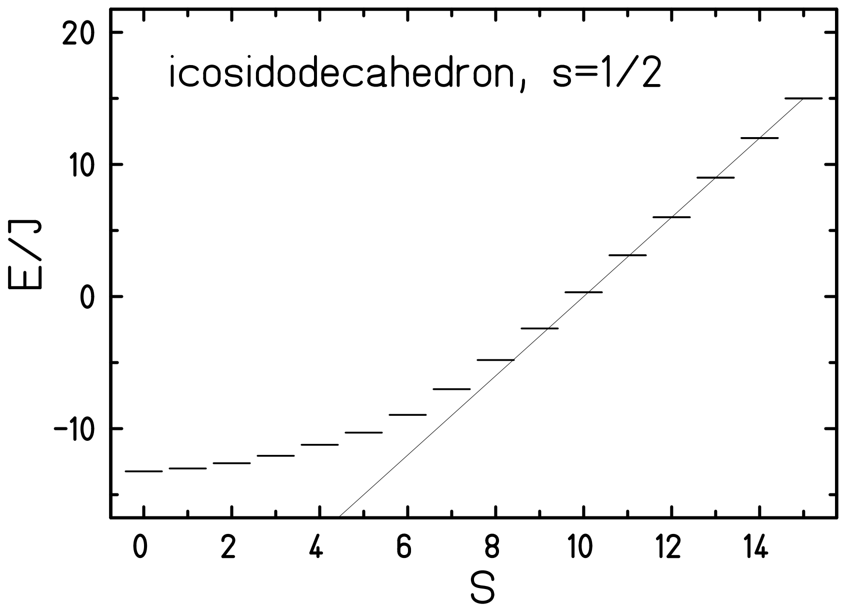


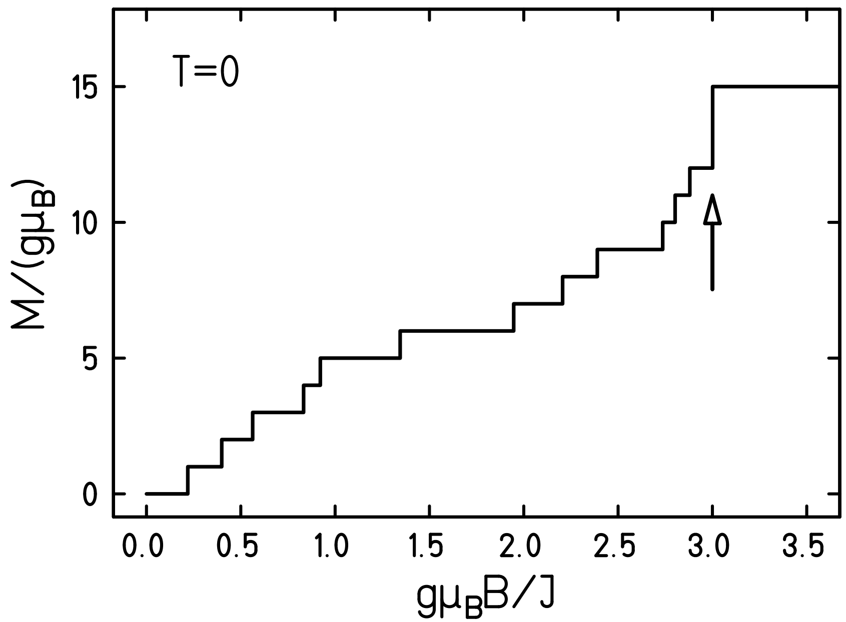


Low-temperature magnetisation measurements as well as low-temperature NMR can detect the ground state band. Higher bands might be accessible by neutron scattering or ESR.[a]

[a] J. Schnack, M. Luban, R. Modler, *Quantum rotational band model for the Heisenberg molecular magnet* $\{Mo_{72}Fe_{30}\}$, Europhys. Lett. (2001) submitted.

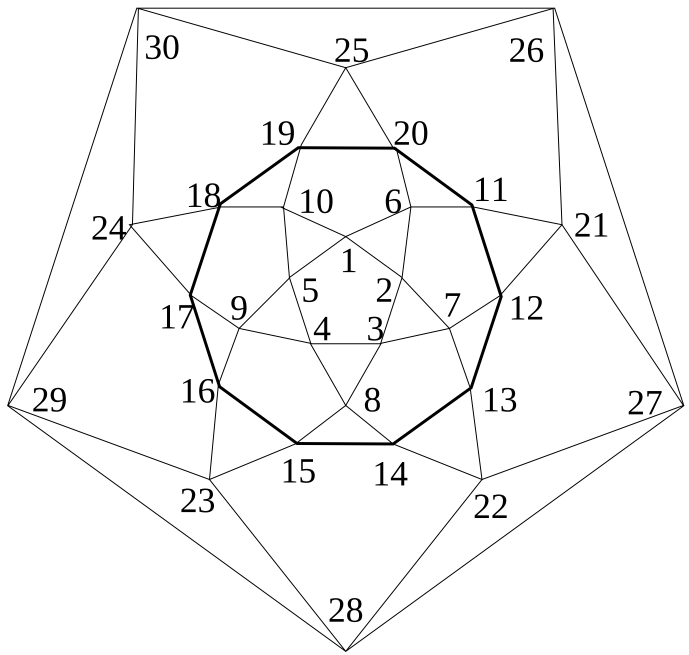
Icosidodecahedron with $s = 1/2$

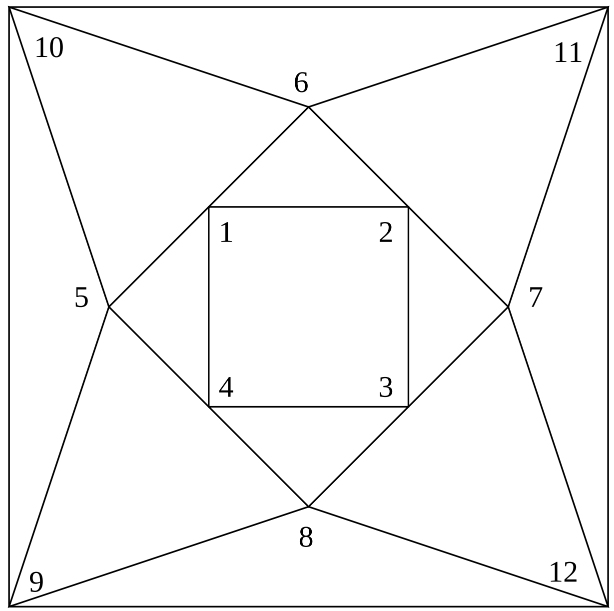




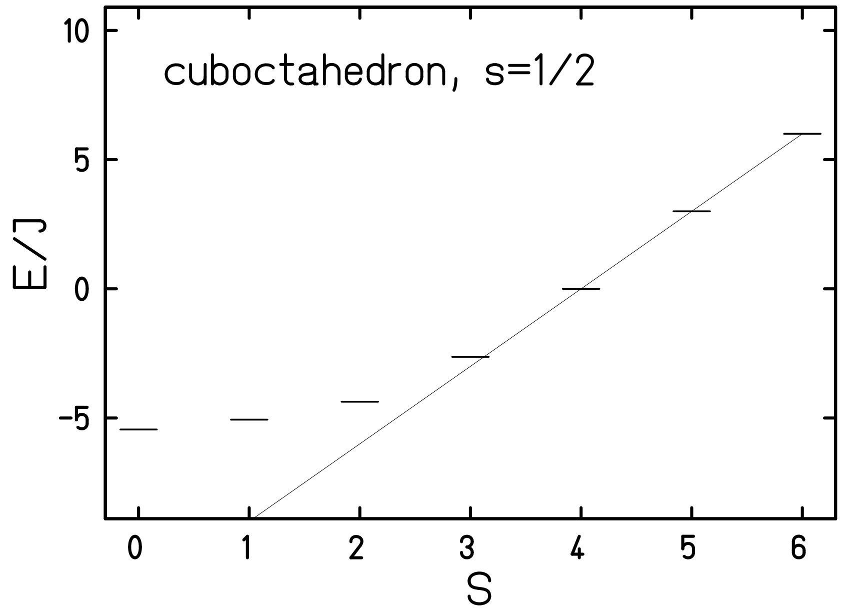
J. Schnack, H.-J. Schmidt, J. Richter, J. Schulenburg, *Independent magnon states on magnetic polytopes*, Eur. Phys. J. B (2001) submitted; cond-mat/0108432

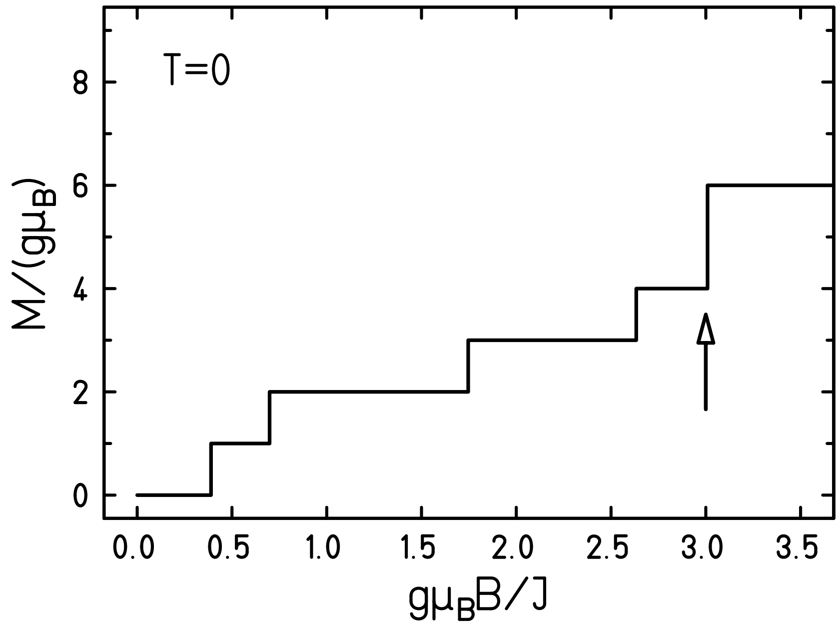
Structure of Icosidodecahedron and Cuboctahedron





Cuboctahedron with $s = 1/2$





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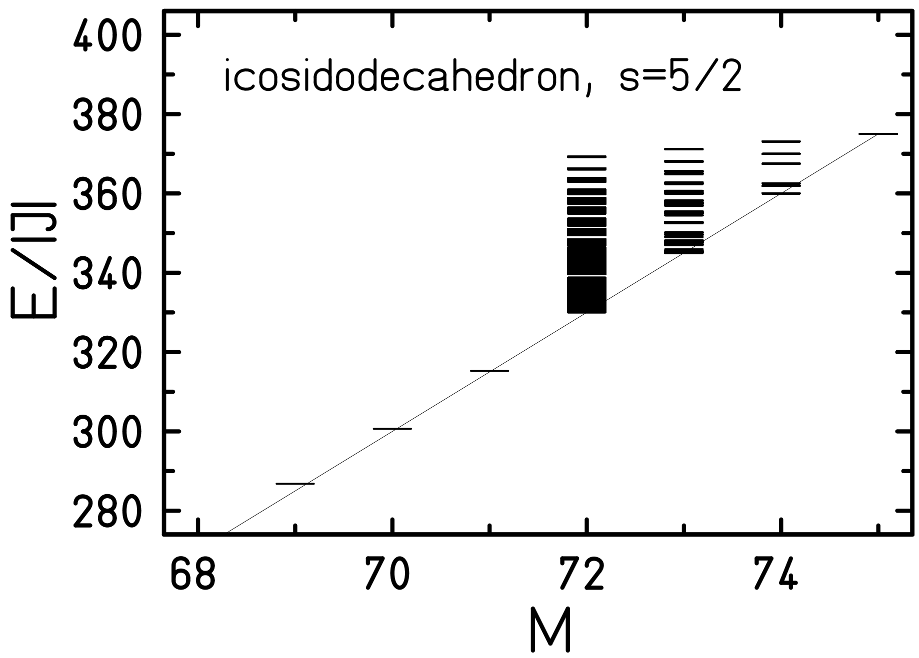
Questions

- Magnetisation curve shows plateaus and jumps!
- Where are the rotational bands?
- Accident ?
- How can one understand the jumps, i.e. the linear behaviour in $E_{\mathrm{min}}(S)$?
- Are there other structures with such properties?
- Who saves our brilliant ideas[a] about Fe_{30}?

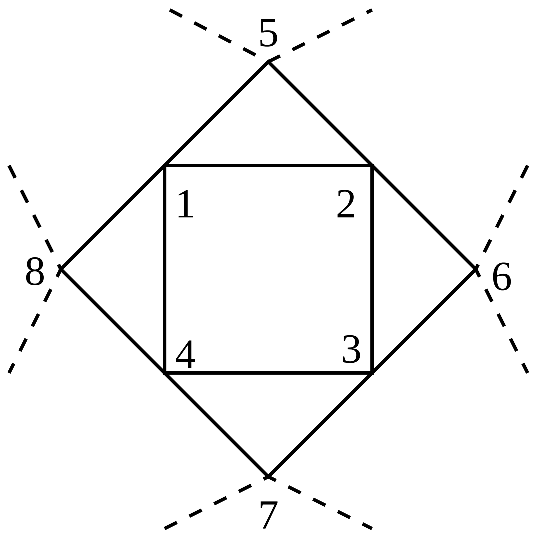
[a] J. Schnack, M. Luban, R. Modler, *Quantum rotational band model for the Heisenberg molecular magnet* $\{Mo_{72}Fe_{30}\}$, Europhys. Lett. (2001) submitted.

Independent Magnons



- magnon vacuum: $M = 75$, one-magnon space: $M = 74$
- one-magnon ground state highly degenerate
- localized one-magnon states can be constructed
- if spin array large enough several localized one-magnon states can be placed on the grid without interaction
- minimal energy, i.e. ground state energy in the n-magnon spaces, is linear in M

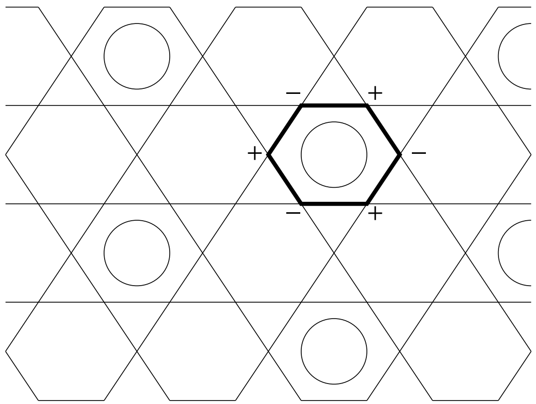
Localized Magnon – Example



- $|\,\text{localized magnon}\,\rangle = \frac{1}{2}\left(|\,1\,\rangle - |\,2\,\rangle + |\,3\,\rangle - |\,4\,\rangle\right)$
- $|\,u\,\rangle = \underset{\sim}{s}^{-}(u)\,|\,\Omega\,\rangle$; $|\,\Omega\,\rangle$ – magnon vacuum
- $\underset{\sim}{H}\,|\,1\,\rangle = J\{\,|\,1\,\rangle + 1/2(\,|\,2\,\rangle + |\,4\,\rangle + |\,5\,\rangle + |\,8\,\rangle)\}$
- $\underset{\sim}{H}\,|\,\text{localized magnon}\,\rangle \propto |\,\text{localized magnon}\,\rangle$
- triangles trap the localized magnon, amplitudes cancel at outer vertices
- proven for $s = 1/2$, one exchange constant J, and same number of interactions for each site[a]
- result also holds for $s > 1/2$ and XXZ model $(\Delta \geq 0)$.

[a] J. Schnack, H.-J. Schmidt, J. Richter, J. Schulenburg, *Independent magnon states on magnetic polytopes*, Eur. Phys. J. B (2001) submitted; cond-mat/0108432

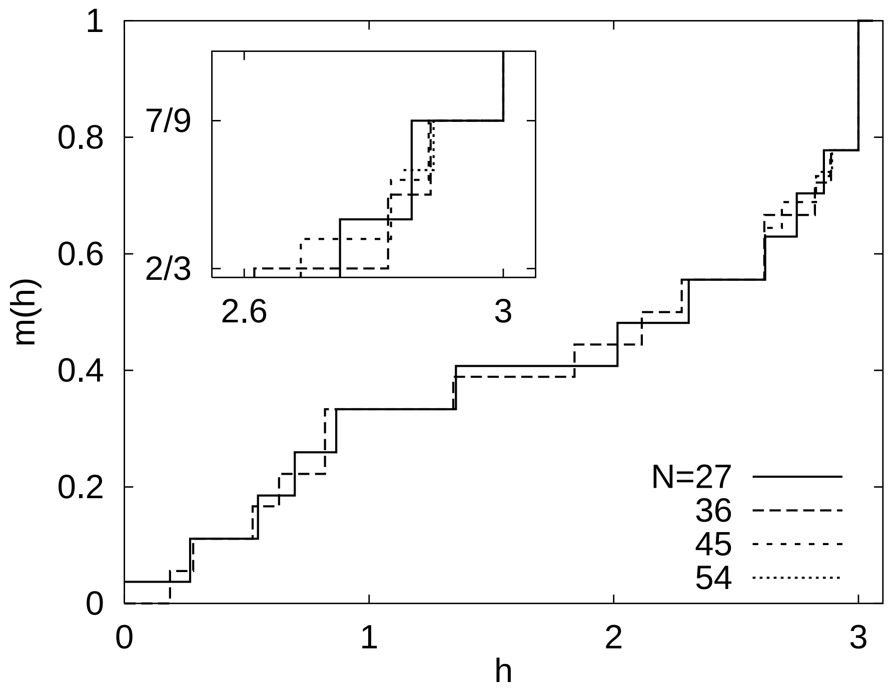
Kagomé Lattice – Independent Magnons



- localized one-magnon state indicated by bold lines;
- independent (non-interacting) one-magnon states can be placed on the grid (circles);
- due to the absence of attractive interaction, 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;
- $\Rightarrow$ magnetisation jump;
- maximal number of independent magnons: N/9;
- magnetisation jump is a macroscopic quantum effect!

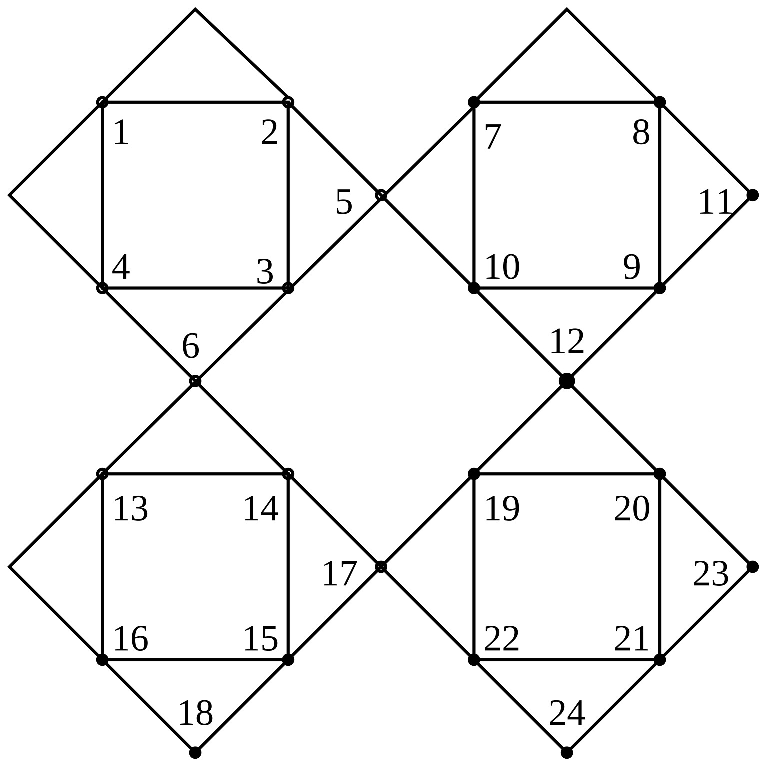
J. Schulenburg, A. Honecker, J. Schnack, J. Richter, H.-J. Schmidt, *Macroscopic magnetization jumps due to independent magnons in frustrated quantum spin lattices*, Phys. Rev. Lett. (2001) submitted; cond-mat/0108498

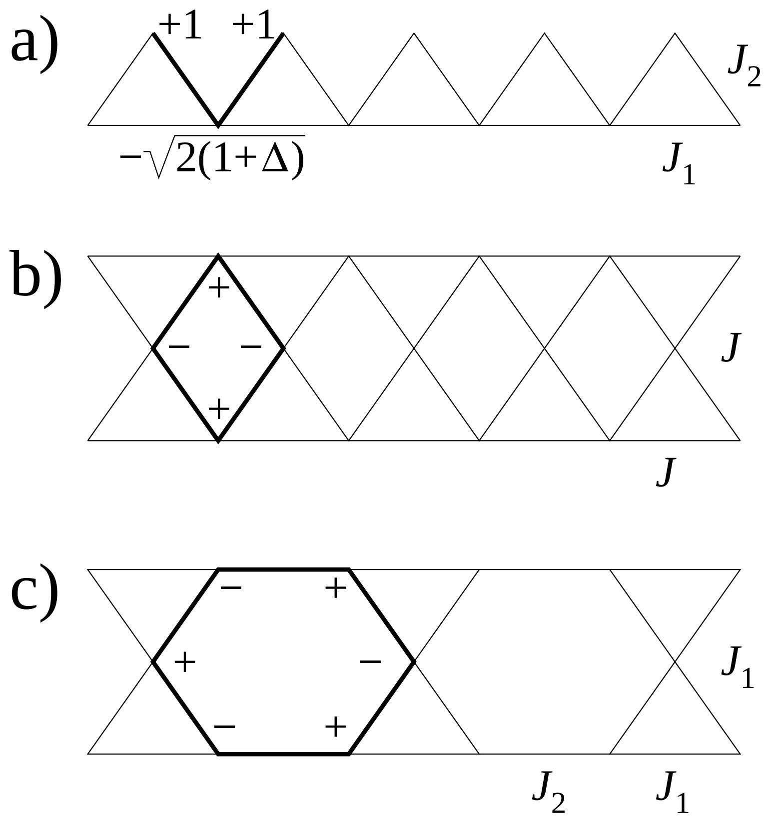
Kagomé Lattice
Giant Magnetisation Jump



J. Schulenburg, A. Honecker, J. Schnack, J. Richter, H.-J. Schmidt, *Macroscopic magnetization jumps due to independent magnons in frustrated quantum spin lattices*, Phys. Rev. Lett. (2001) submitted; cond-mat/0108498

Structures With Magnetisation Jump





Who saves our brilliant ideas about Fe_{30}?

Marshall Luban and Heinz-Jürgen Schmidt

&

Matthias Exler

There's still a lot to be done.

List of whishes for Christmas:

- Paul Kögerler – please synthesise an icosidodecahedron with $s = 1/2$. What about Cu_{30} or V_{30}?
- Marshall Luban and Heinz-Jürgen Schmidt – please publish your proof.
- Robert Modler – Can't we go to 50 mK with Fe_{30}?
- understand specific heat of Fe_{30} $\Rightarrow$ need better low-energy spectrum;
- Neutron scattering with Fe_{30}?
- find material with giant magnetisation jump

Meanwhile, what I have to do

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