

Enhanced magnetocaloric effect in frustrated magnetic molecules with icosahedral symmetry

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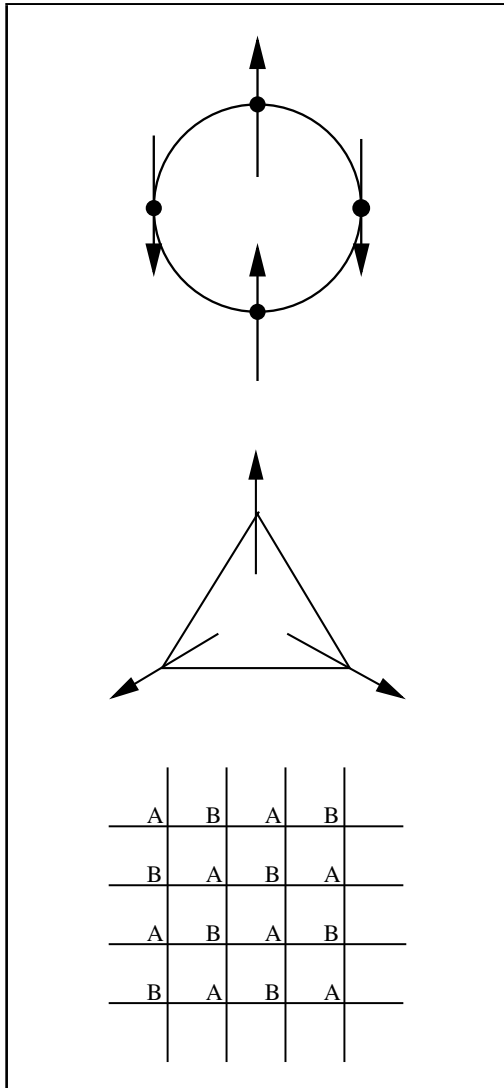


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Hamiltonian and frustration



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

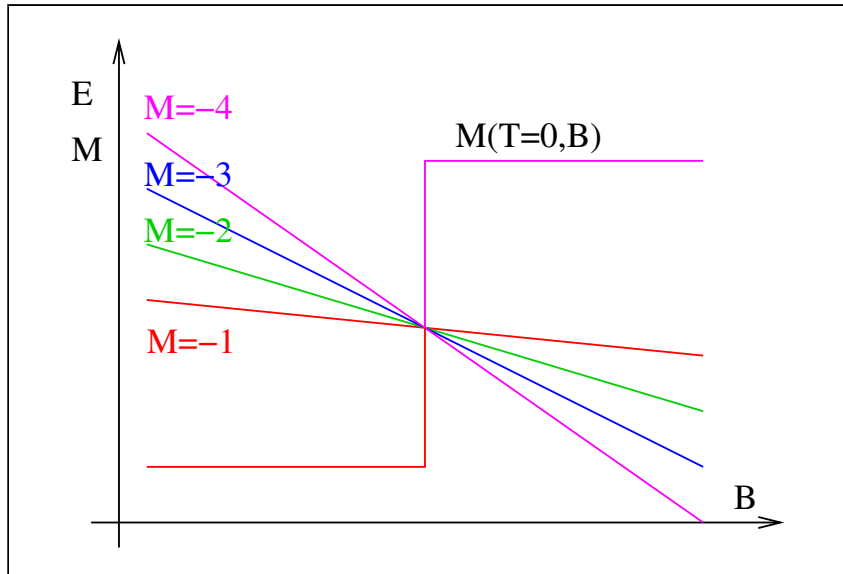
- Frustration (simple): An antiferromagnet is frustrated if in the ground state of the corresponding classical spin system not all interactions can be minimized simultaneously.

- Frustration (advanced): A non-bipartite antiferromagnet is frustrated. A bipartite spin system can be decomposed into two sublattices A and B such that for all exchange couplings:

$$J(x_A, y_B) \leq g^2, J(x_A, y_A) \geq g^2, J(x_B, y_B) \geq g^2, \text{ cmp. (1,2).}$$

(1) E.H. Lieb, T.D. Schultz, and D.C. Mattis, Ann. Phys. (N.Y.) **16**, 407 (1961)
 (2) E.H. Lieb and D.C. Mattis, J. Math. Phys. **3**, 749 (1962)

Magnetocaloric effect I



- $$\left(\frac{\partial T}{\partial B}\right)_S = -\frac{T}{C} \left(\frac{\partial S}{\partial B}\right)_T$$
- High degeneracy of ground state levels
 \Rightarrow large residual entropy at $T = 0$.
- Advantageous: many Zeeman levels crossing at one and the same magnetic field.

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

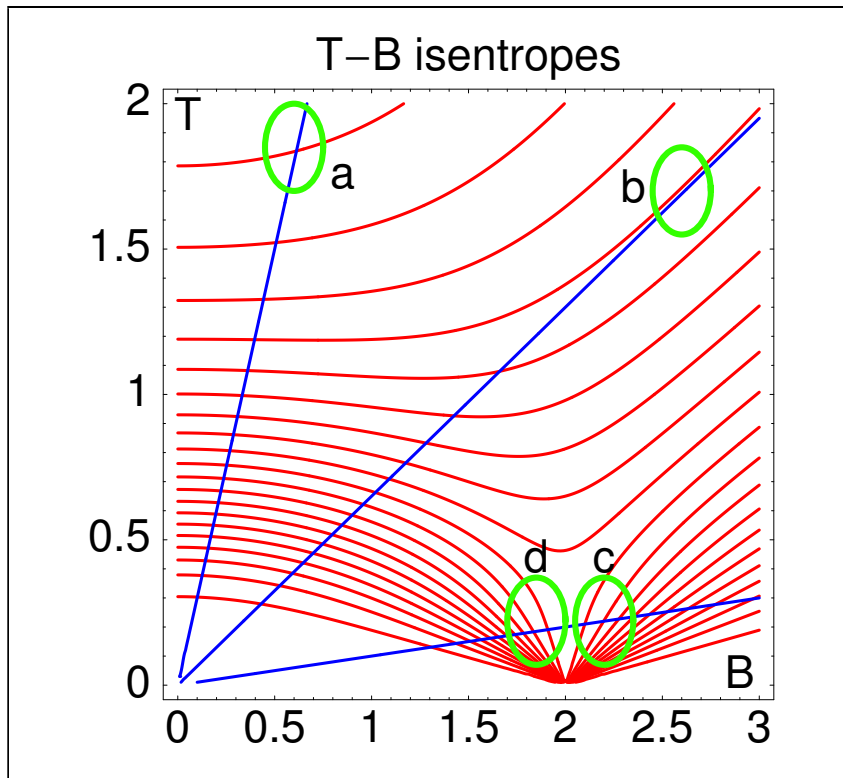
A. Honecker, J. Richter, Condensed Matter Physics **8**, 813 (2005)

H.-J. Schmidt, J. Richter, R. Moessner, J. Phys. A: Math. Gen. **39**, 10673 (2006)

O. Derzhko, J. Richter, A. Honecker, H.-J. Schmidt, Low Temp. Phys. **33**, 745 (2007)

Magnetocaloric effect II

Isentropes of an $s = 1/2$ dimer



blue lines: ideal paramagnet, red curves: af dimer

Magnetocaloric effect:

(a) reduced,

(b) the same,

(c) enhanced,

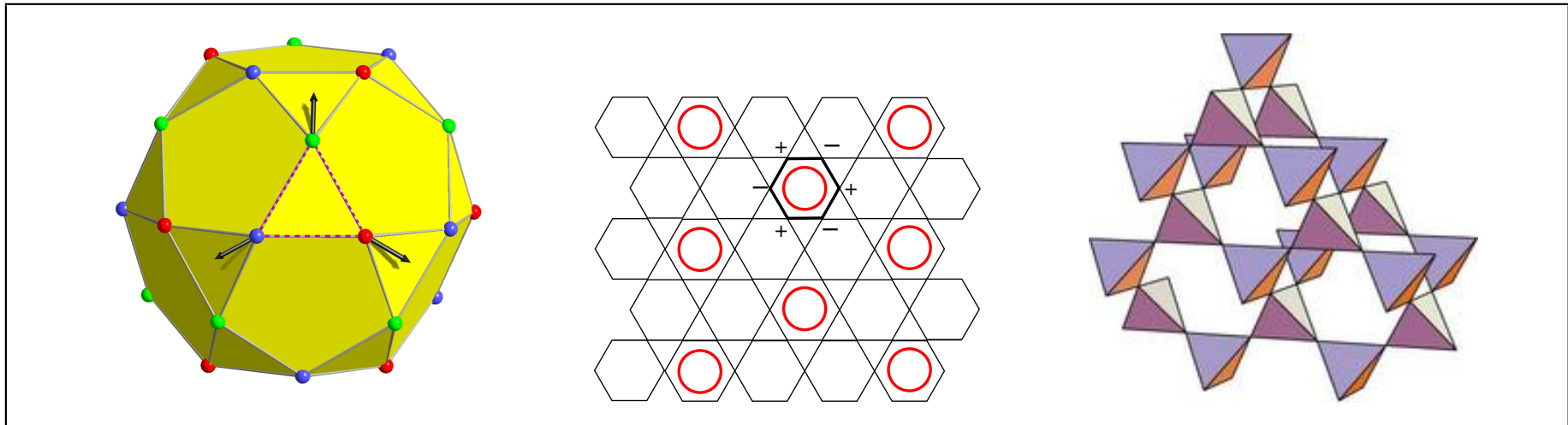
(d) opposite

when compared to an ideal paramagnet.

Case (d) does not occur for a paramagnet.

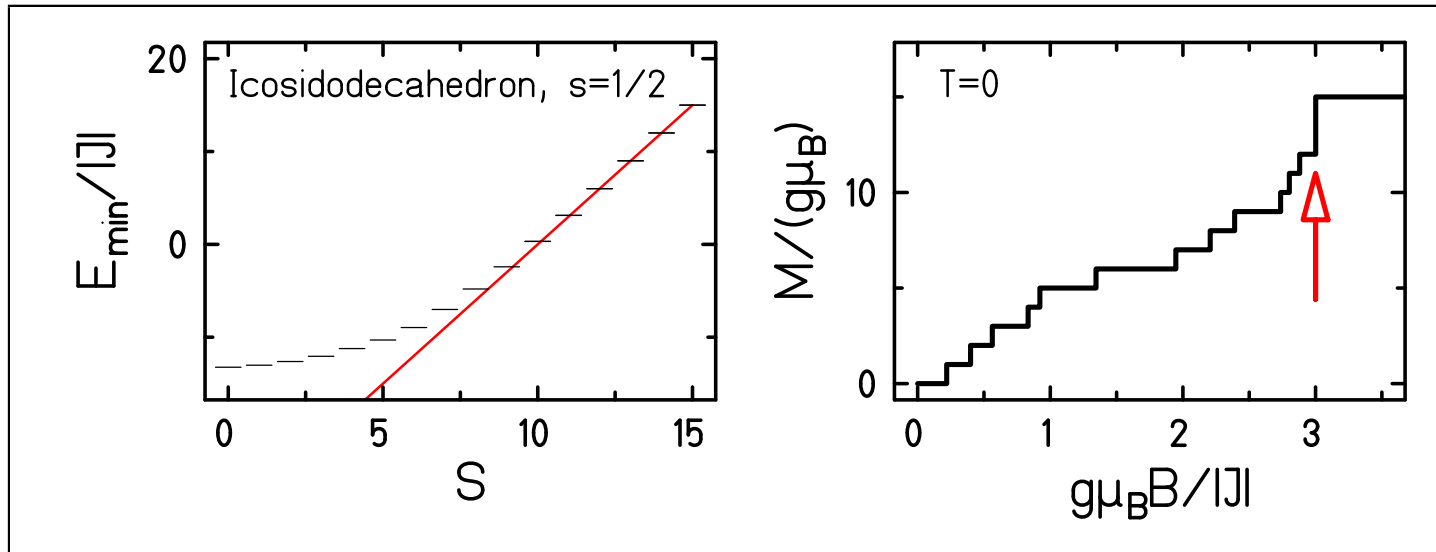
Magnetocaloric effect III

Corner sharing triangles and tetrahedra



- Several frustrated antiferromagnets – e.g. icosidodecahedron, kagome lattice, pyrochlore – possess large degeneracies of levels close to saturation.
- This leads to an unusual magnetization behavior and to unusual magnetocaloric properties.

Giant magnetization jumps in frustrated antiferromagnets I Icosidodecahedron



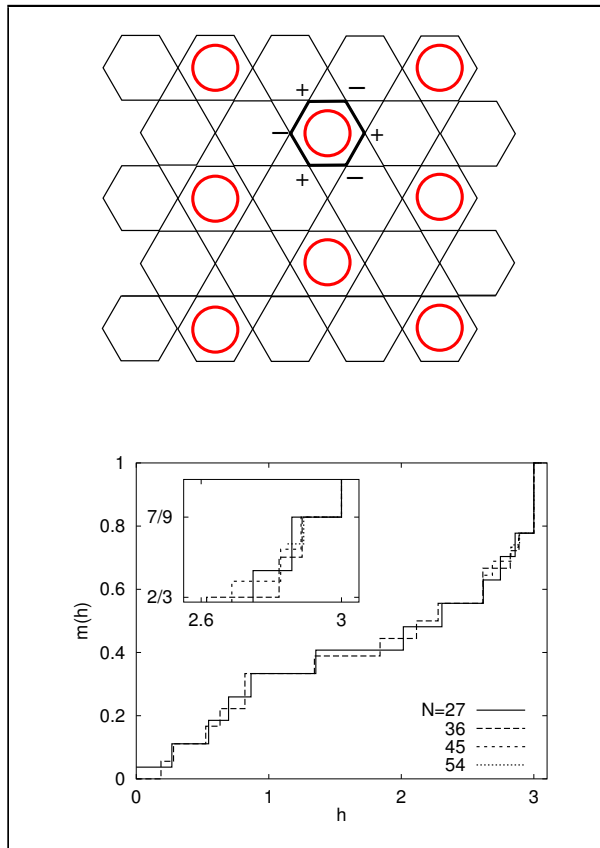
- Close look: $E_{\min}(S)$ linear in S for high S instead of being quadratic (1);
- Heisenberg model: property depends only on the structure but not on s (2);
- Alternative formulation: independent localized magnons (3);

(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**, 167207 (2002)

Giant magnetization jumps in frustrated antiferromagnets II Kagome Lattice

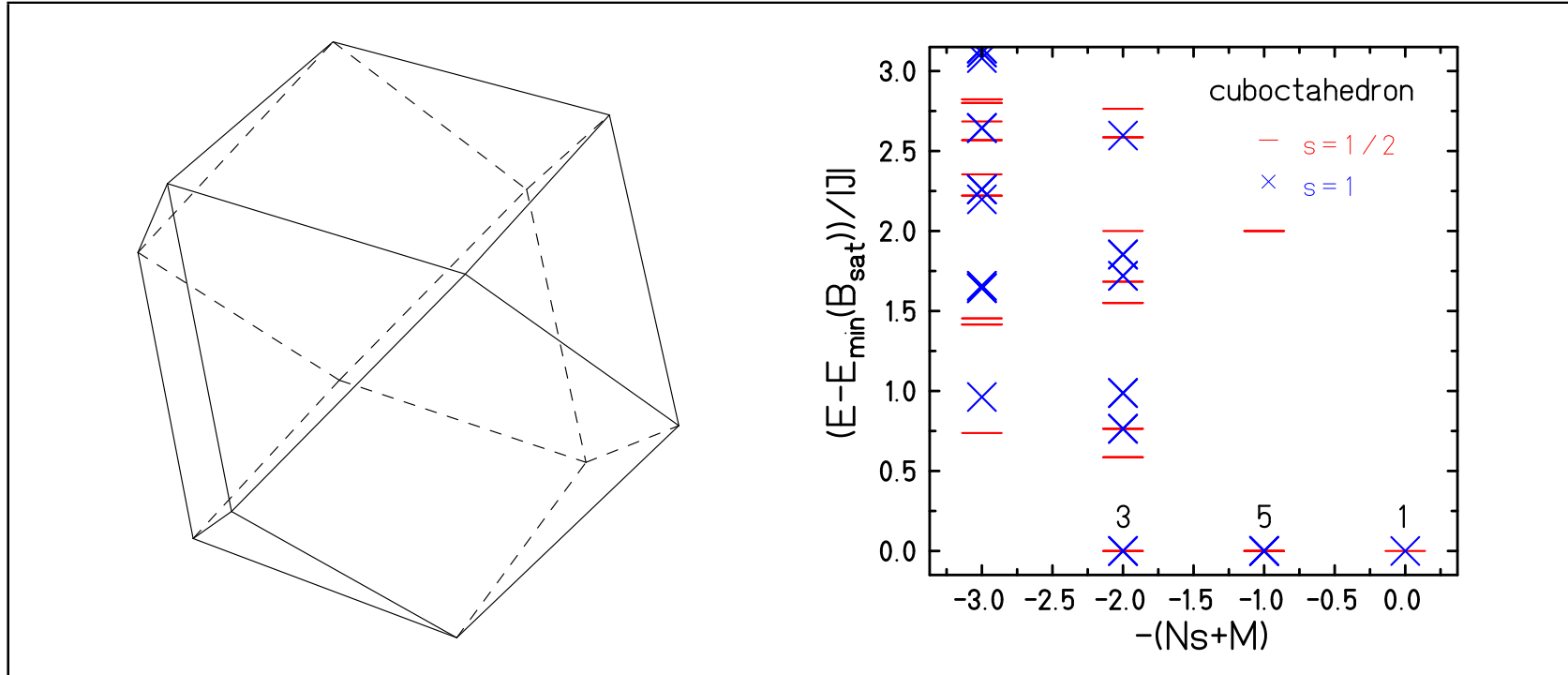


- Non-interacting one-magnon states can be placed on various lattices, e. g. kagome or pyrochlore;
- Each state of n independent magnons is the ground state in the Hilbert subspace with $M = Ns - n$;
Kagome: max. number of indep. magnons is $N/9$;
- Linear dependence of E_{\min} on M
 \Rightarrow ($T = 0$) magnetization jump;
- Jump is a macroscopic quantum effect!
- A rare example of analytically known many-body states!

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)

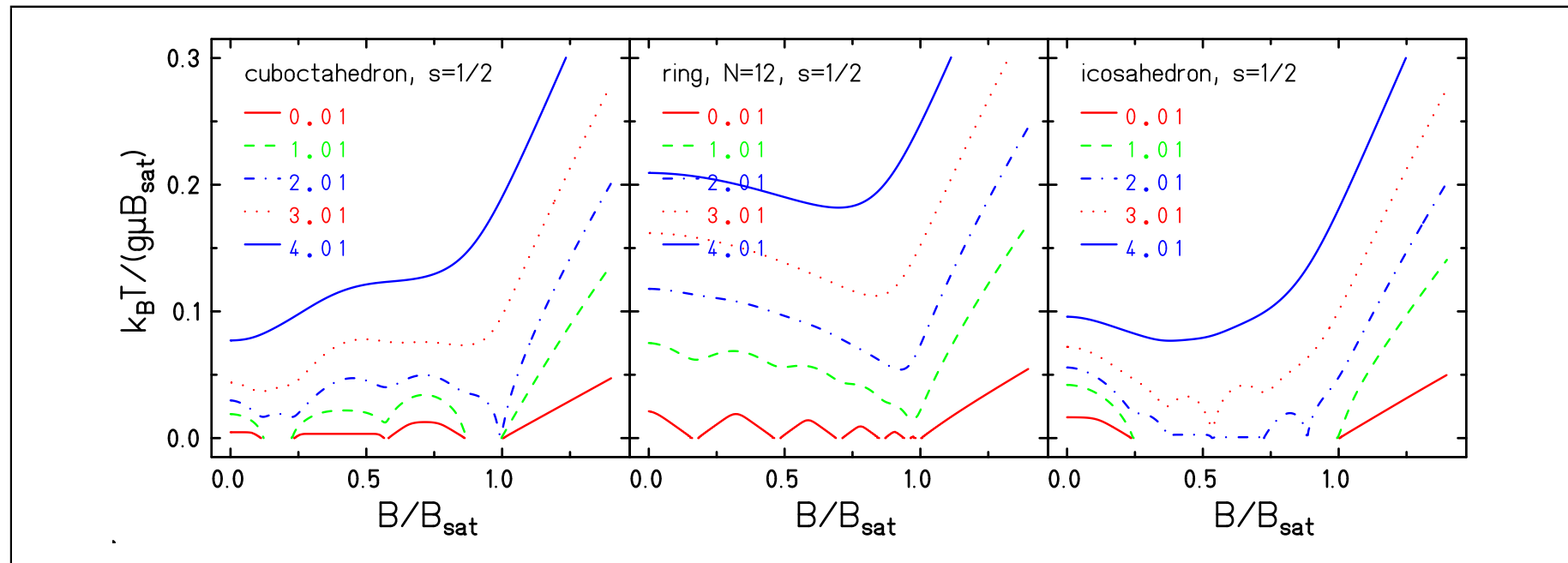
Magnetocaloric effect IV – Cuboctahedron



- Independent magnons; Additional degeneracy of levels.

J. Schnack, R. Schmidt, J. Richter, Phys. Rev. B **76**, 054413 (2007)

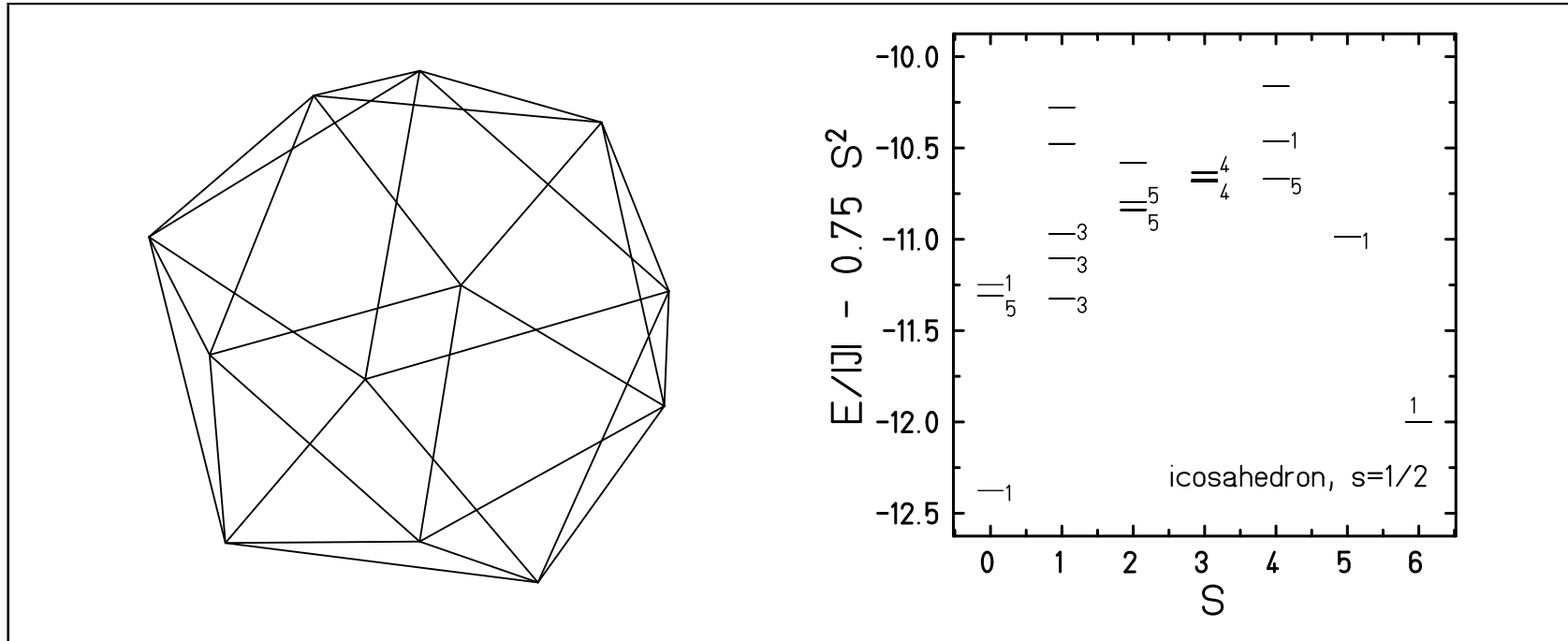
Magnetocaloric effect V – Molecular systems



- Cuboctahedron: high cooling rate due to independent magnons;
- Ring: normal level crossing, normal jump;
- Icosahedron: unusual behavior due to edge-sharing triangles, high degeneracies all over the spectrum; high cooling rate.

J. Schnack, R. Schmidt, J. Richter, Phys. Rev. B **76**, 054413 (2007)

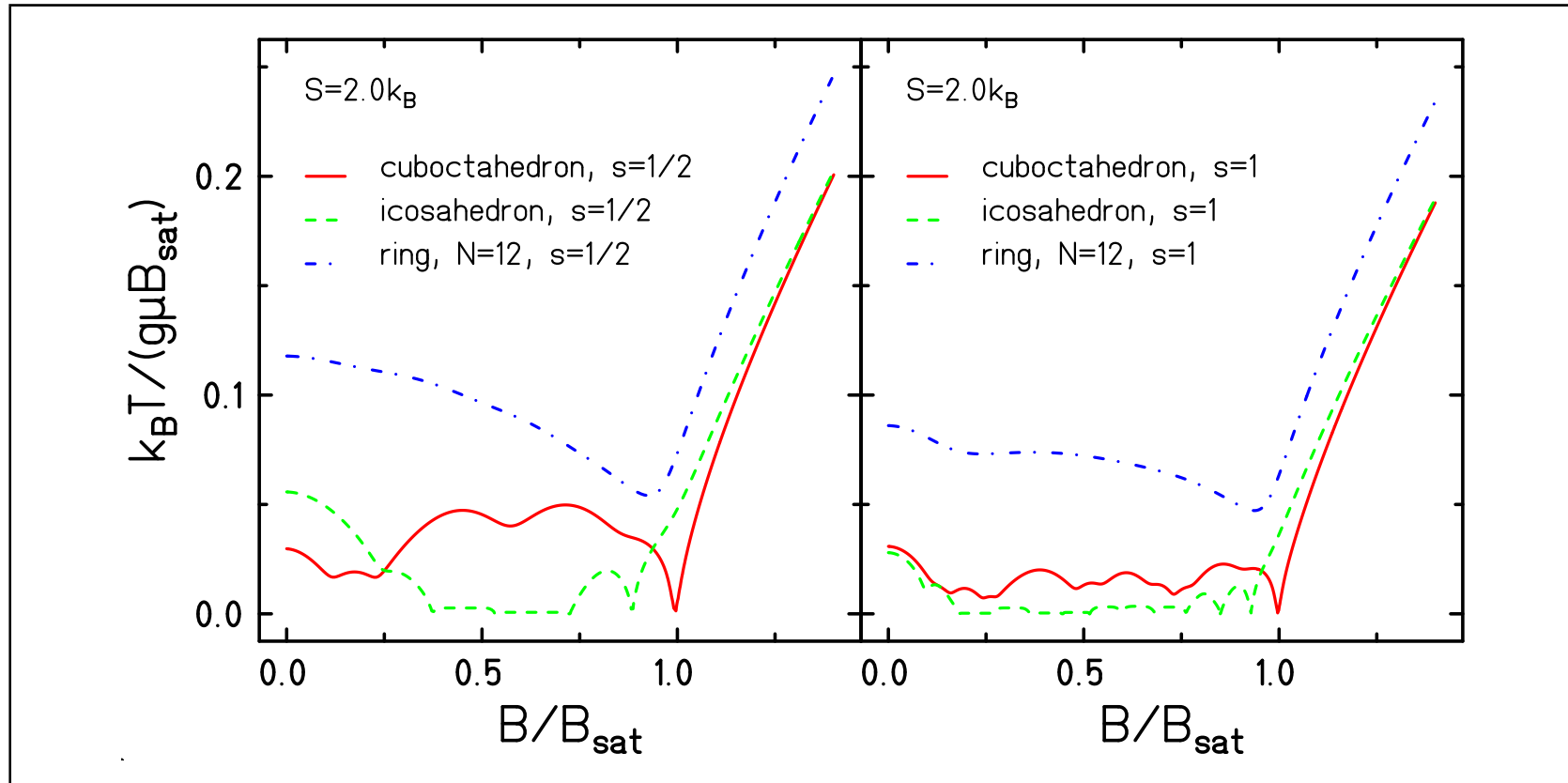
Magnetocaloric effect VI – Icosahedron



- Icosahedron: unusual behavior due to edge-sharing triangles, high degeneracies all over the spectrum;

J. Schnack, R. Schmidt, J. Richter, Phys. Rev. B **76**, 054413 (2007)

Magnetocaloric effect VII – Comparison



- Frustration leads to increased low-temperature entropy.

J. Schnack, R. Schmidt, J. Richter, Phys. Rev. B **76**, 054413 (2007)

Thank you very much for your attention.

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www.molmag.de

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