Basics of (frustrated) quantum spin systems

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Philosophy

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few → many ← infinite

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energy eigenvalues
degeneracies
analytic for $T > 0$

phases
quasi particles
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I work here.

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Does not exist.

Philosophy

few → many ← infinite

energy eigenvalues
degeneracies
analytic for $T > 0$

phases
quasiparticles
maybe,
non-analytic
for $T > 0$

However, damn useful.

Some spin gymnastics

Ising gym of two spins (f/af)

Ising gym of three spins (f/af; obc/pbc)

Heisenberg gym of two classical spins (f/af; SU(2))

Heisenberg gym of three classical spins

(f/af; obc/pbc; SU(2))

Heisenberg gym of two quantum spins (f/af; SU(2))

Heisenberg gym of three quantum spins (f/af; obc/pbc; SU(2))

Model Hamiltonian (spin only)

$$\underset{\sim}{H} = \sum_{i \leq j} \underset{\sim}{\vec{s}}_i \cdot \mathbf{J}_{ij} \cdot \underset{\sim}{\vec{s}}_j + \sum_{i<j} \vec{D}_{ij} \cdot \left[\underset{\sim}{\vec{s}}_i \times \underset{\sim}{\vec{s}}_j \right] + \mu_B \vec{B} \sum_i^N \mathbf{g}_i \underset{\sim}{\vec{s}}_i$$

Exchange/Anisotropy Dzyaloshinskii-Moriya Zeeman

Isotropic Hamiltonian

$$\underset{\sim}{H} = \sum_{i<j} J_{ij} \underset{\sim}{\vec{s}}_i \cdot \underset{\sim}{\vec{s}}_j + g \mu_B B \sum_i^N \underset{\sim}{s}_i^z$$

Heisenberg Zeeman

openAI on frustration

Frustration in quantum spin models occurs when the spin interactions cannot be simultaneously satisfed, preventing the system from reaching a single, lowest-energy configuration.

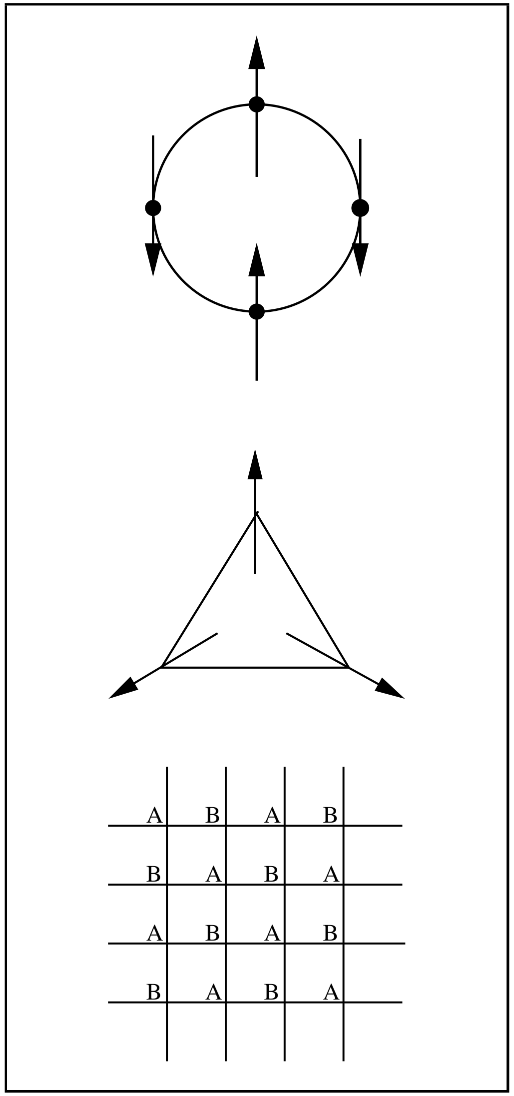
This can be due to the geometry of the lattice (e.g., odd-length loops like triangles, which leads to geometrical frustration) or the nature of the interactions themselves (e.g., a mix of ferromagnetic and antiferromagnetic bonds). The result is a highly degenerate ground state, often leading to exotic phenomena like quantum spin liquids.

The Triangle: Consider three spins on a triangle with antiferromagnetic interactions. If one spin points up and another points down, the third spin cannot be both aligned and anti-aligned with its two neighbors, leading to frustration.

Frustrated Lattices: The kagome lattice (like a basket weave) and the pyrochlore lattice (corner-sharing tetrahedra) are well-known examples of geometrically frustrated structures that favor exotic magnetic states.

Novel Phenomena: Frustration can lead to a wide range of exotic phases and phenomena, including quantum spin liquids, spin glasses, quantum criticality, and topological states, making it a rich area of research.

Definition of frustration



- Competing interactions lead to frustration.
- Simple: An antiferromagnet is frustrated if in the ground state of the corresponding classical spin system not all interactions can be minimized simultaneously.
- 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 (1):
  $J(x_A, y_B) \geq g^2$, $J(x_A, y_A) \leq g^2$, $J(x_B, y_B) \leq g^2$.

  This is not a strict definition since there are exceptions for small systems. And, what about competing interactions of other types?

(1) E.H. Lieb and D.C. Mattis, J. Math. Phys. **3**, 749 (1962)

Heisenberg dimer

$$\underset{\sim}{H} \quad = \quad -2J \quad \underset{\sim}{\vec{s}}_1 \cdot \underset{\sim}{\vec{s}}_2$$

Please calculate analytically and plot spectrum versus total spin.

Heisenberg trimer

$$\underset{\sim}{H} = -2J \left[\underset{\sim}{\vec{s}}_1 \cdot \underset{\sim}{\vec{s}}_2 + \underset{\sim}{\vec{s}}_2 \cdot \underset{\sim}{\vec{s}}_3 + \underset{\sim}{\vec{s}}_3 \cdot \underset{\sim}{\vec{s}}_1 \right]$$

Please calculate analytically and plot spectrum versus total spin.

Heisenberg square

$$\underset{\sim}{H} = -2J \left[\underset{\sim}{\vec{s}}_1 \cdot \underset{\sim}{\vec{s}}_2 + \underset{\sim}{\vec{s}}_2 \cdot \underset{\sim}{\vec{s}}_3 + \underset{\sim}{\vec{s}}_3 \cdot \underset{\sim}{\vec{s}}_4 + \underset{\sim}{\vec{s}}_4 \cdot \underset{\sim}{\vec{s}}_1 \right]$$

Please calculate analytically and plot spectrum versus total spin.

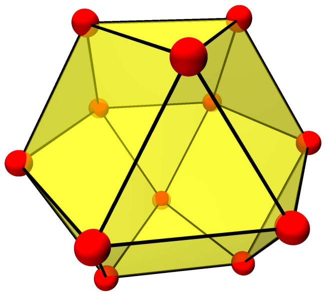
Complete diagonalization:

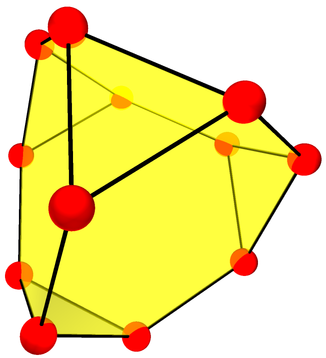
SU(2) & point group symmetry

Quantum chemists need to be much smarter since they have smaller computers!

(1) D. Gatteschi and L. Pardi, Gazz. Chim. Ital. **123**, 231 (1993).
(2) J. J. Borras-Almenar, J. M. Clemente-Juan, E. Coronado, and B. S. Tsukerblat, Inorg. Chem. **38**, 6081 (1999).
(3) B. S. Tsukerblat, *Group theory in chemistry and spectroscopy: a simple guide to advanced usage*, 2nd ed. (Dover Publications, Mineola, New York, 2006).

Irreducible Tensor Operator approach





Spin rotational symmetry SU(2):

- $\underset{\sim}{H} = -2\sum_{i<j} J_{ij}\ \underset{\sim}{\vec{s}}_i \cdot \underset{\sim}{\vec{s}}_j + g\mu_B \underset{\sim}{\vec{S}} \cdot \vec{B}$;
- Physicists employ: $\left[\underset{\sim}{H}, \underset{\sim}{S}_z\right] = 0;$
- Chemists employ: $\left[\underset{\sim}{H}, \underset{\sim}{\vec{S}}^2\right] = 0,\ \left[\underset{\sim}{H}, \underset{\sim}{S}_z\right] = 0;$

  Irreducible Tensor Operator (ITO) approach;
  Free program MAGPACK (2) available.

(1) D. Gatteschi and L. Pardi, Gazz. Chim. Ital. **123**, 231 (1993).
(2) J. J. Borras-Almenar, J. M. Clemente-Juan, E. Coronado, and B. S. Tsukerblat, Inorg. Chem. **38**, 6081 (1999).
(3) B. S. Tsukerblat, *Group theory in chemistry and spectroscopy: a simple guide to advanced usage*, 2nd ed. (Dover Publications, Mineola, New York, 2006).

Point Group Symmetry

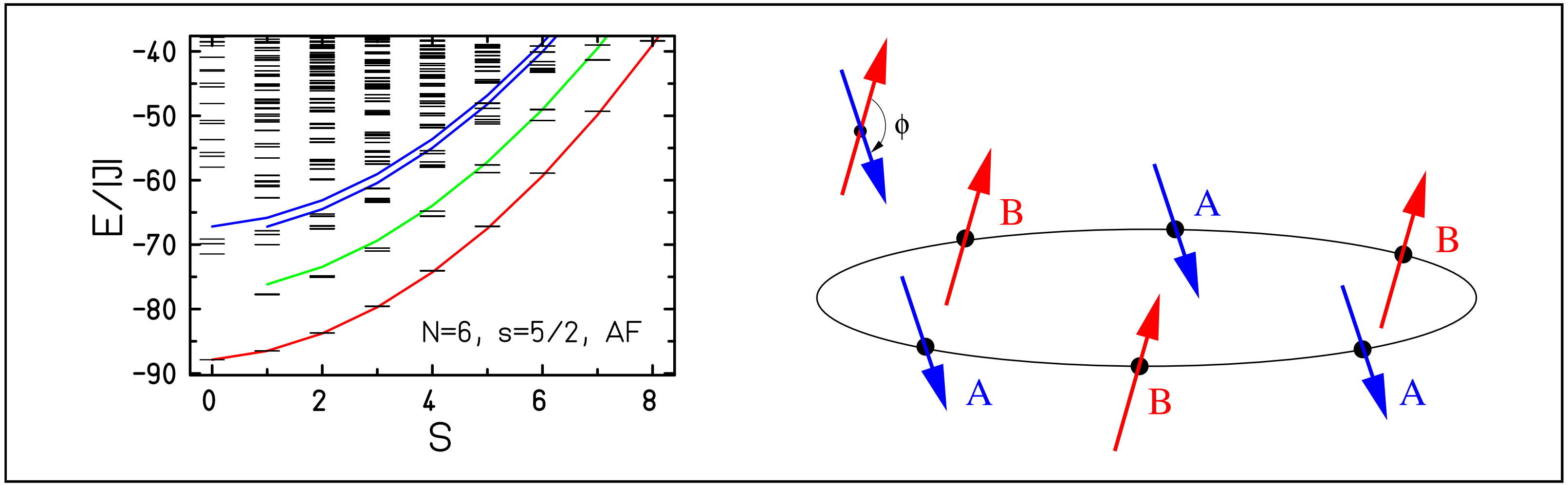
$$| \, \alpha' \, S \, M \, \Gamma \, \rangle = \mathcal{P}^{(\Gamma)} \, | \, \alpha \, S \, M \, \rangle = \left(\frac{l_\Gamma}{h} \sum_R \left(\chi^{(\Gamma)}(R) \right)^* \underset{\sim}{G}(R) \right) | \, \alpha \, S \, M \, \rangle$$

Method:

- Projection onto irreducible representations Γ of the point group (1,2);
- No free program, things are a bit complicated (3,4).

(1) M. Tinkham, *Group Theory and Quantum Mechanics*, Dover.
(2) D. Gatteschi and L. Pardi, Gazz. Chim. Ital. **123**, 231 (1993).
(3) O. Waldmann, Phys. Rev. B **61**, 6138 (2000).
(4) R. Schnalle and J. Schnack, Int. Rev. Phys. Chem. **29**, 403-452 (2010) $\Leftarrow$ contains EVERYTHING.

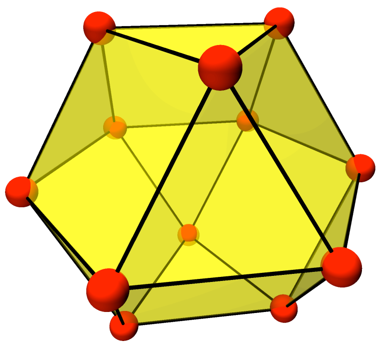
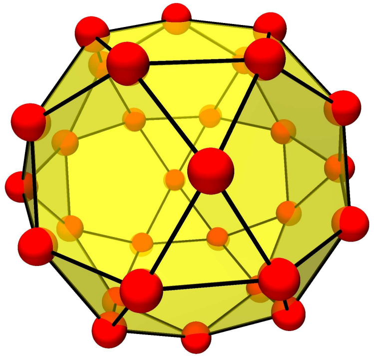
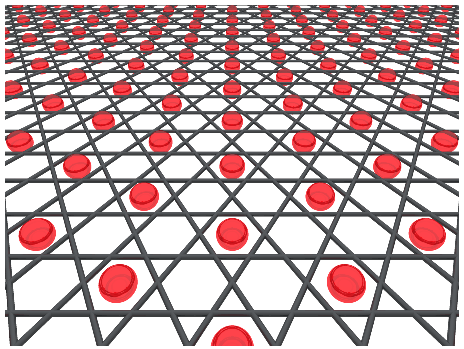
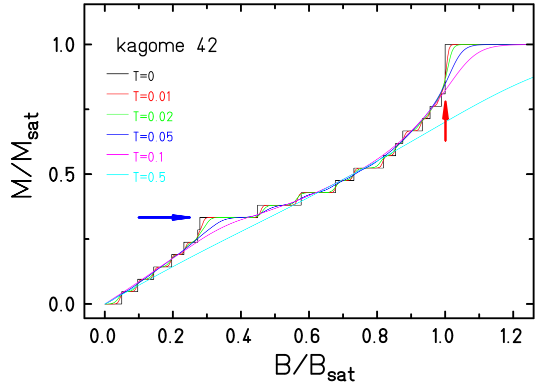
Rotational bands in non-frustrated antiferromagnets



- Often minimal energies $E_{min}(S)$ form a rotational band: Landé interval rule (1);
- For bipartite systems (2,3): $\underset{\sim}{H}^{\text{eff}} = -2\, J_{\text{eff}}\, \underset{\sim}{\vec{S}}_A \cdot \underset{\sim}{\vec{S}}_B$;
- Lowest band – rotation of Néel vector, second band – spin wave excitations (4).

(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)
(4) P.W. Anderson, Phys. Rev. B **86**, 694 (1952), O. Waldmann *et al.*, Phys. Rev. Lett. **91**, 237202 (2003).

Three spins – triangles and frustration

- Antiferromagnetic frustrated molecules and lattices may exhibit fascinating properties: unusual magnetization curves, plateaus and jumps, magnon crystallization, strange ground states , e.g. spin liquids, spin ice, . . .

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C. Castelnovo, R. Moessner, S.L. Sondhi, Nature **451**, 42 (2008).
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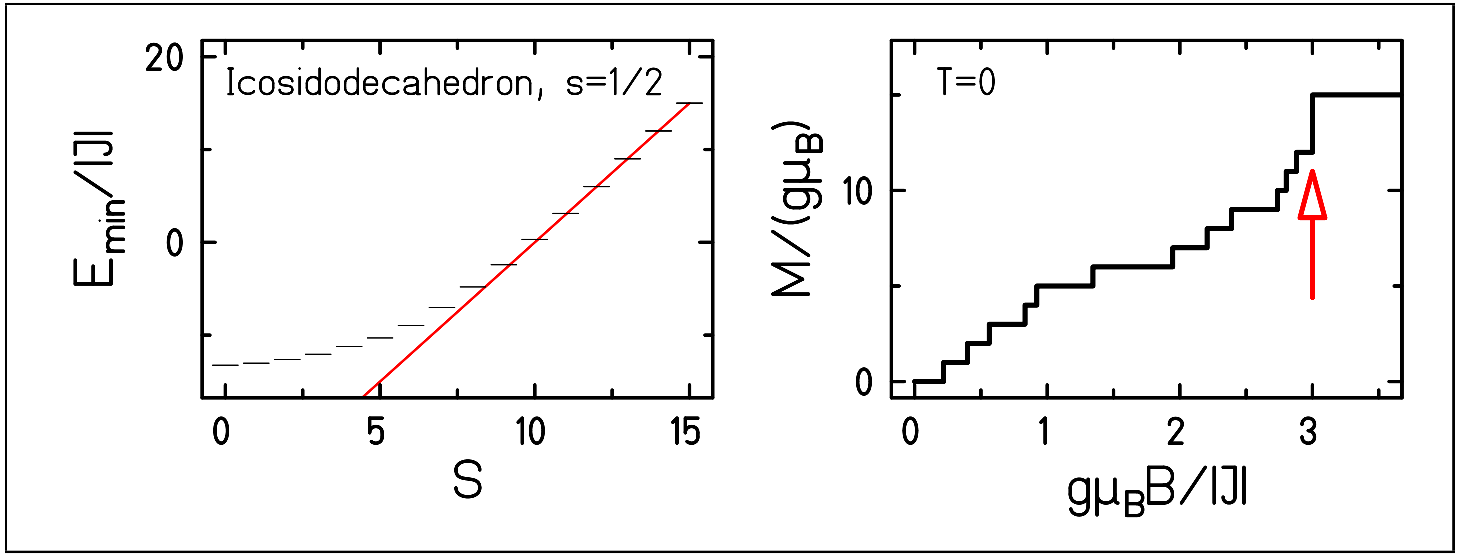
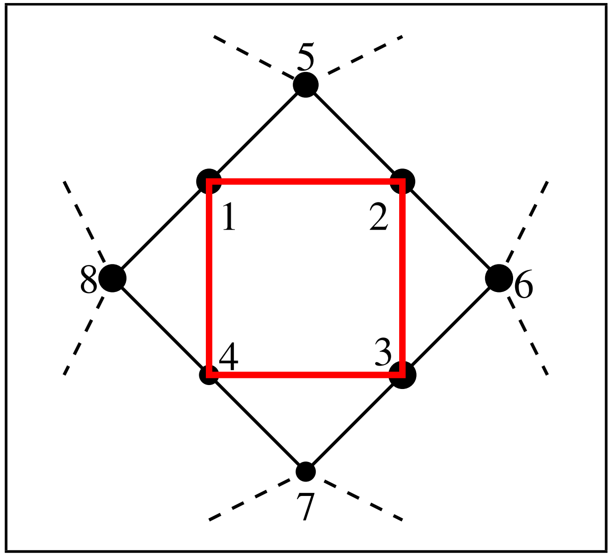
Giant magnetization jumps in frustrated antiferromagnets I
$\{$Mo$_{72}$Fe$_{30}\}$



- Close look: $E_{\text{min}}(S)$ 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 Localized Magnons

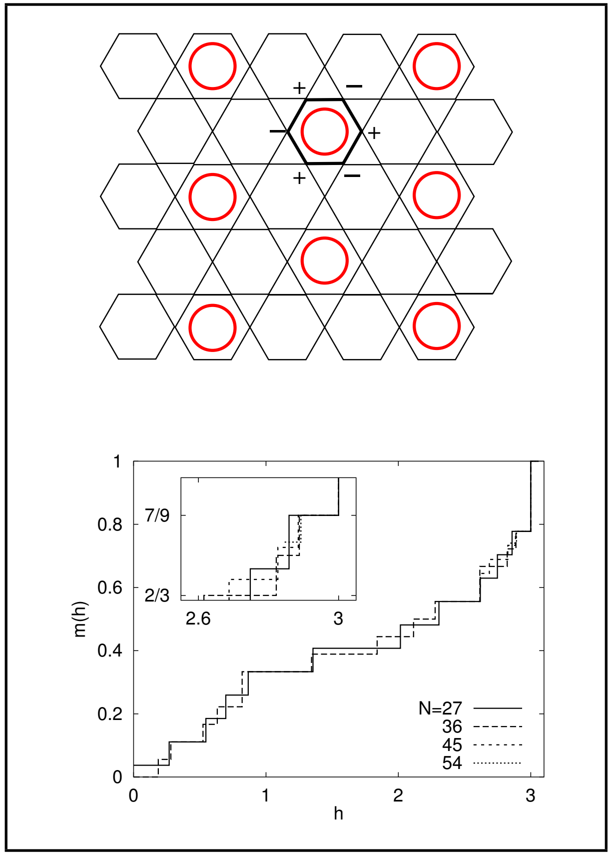


- $|\,\text{localized magnon}\,\rangle = \frac{1}{2}(\,|\,1\,\rangle - |\,2\,\rangle + |\,3\,\rangle - |\,4\,\rangle)$
- $|\,1\,\rangle = \underset{\sim}{s}^{-}(1)\,|\uparrow\uparrow\uparrow\ \ldots\rangle$ etc.
- $\underset{\sim}{H}\,|\,\text{localized magnon}\,\rangle \propto |\,\text{localized magnon}\,\rangle$
- Localized magnon is state of lowest energy (1,2).

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

(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)

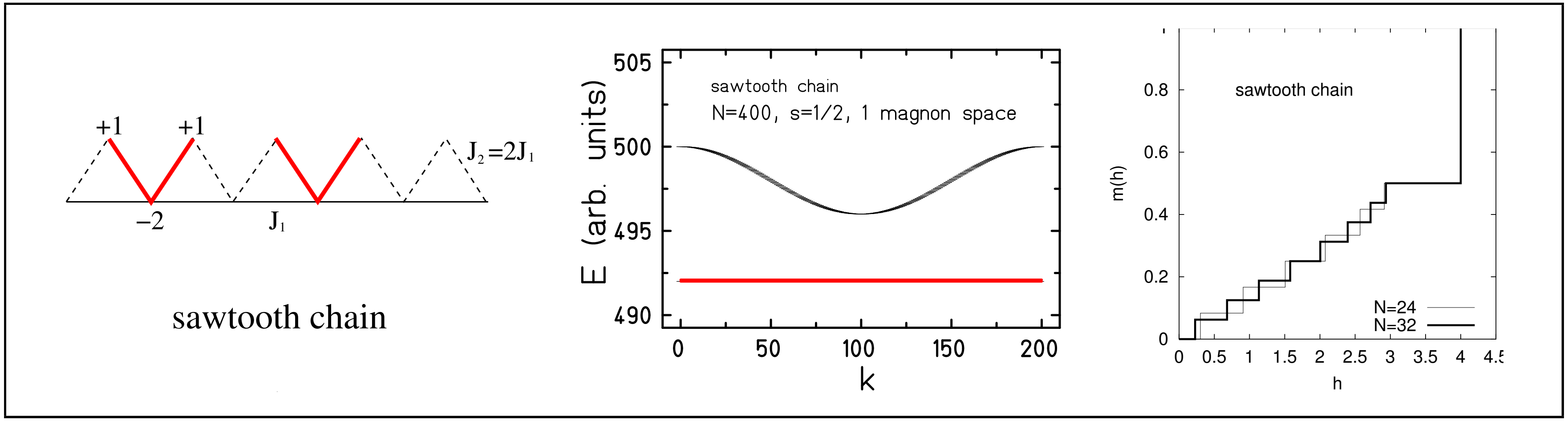
Giant magnetization jumps in frustrated antiferromagnets III Kagome Lattice



- 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)

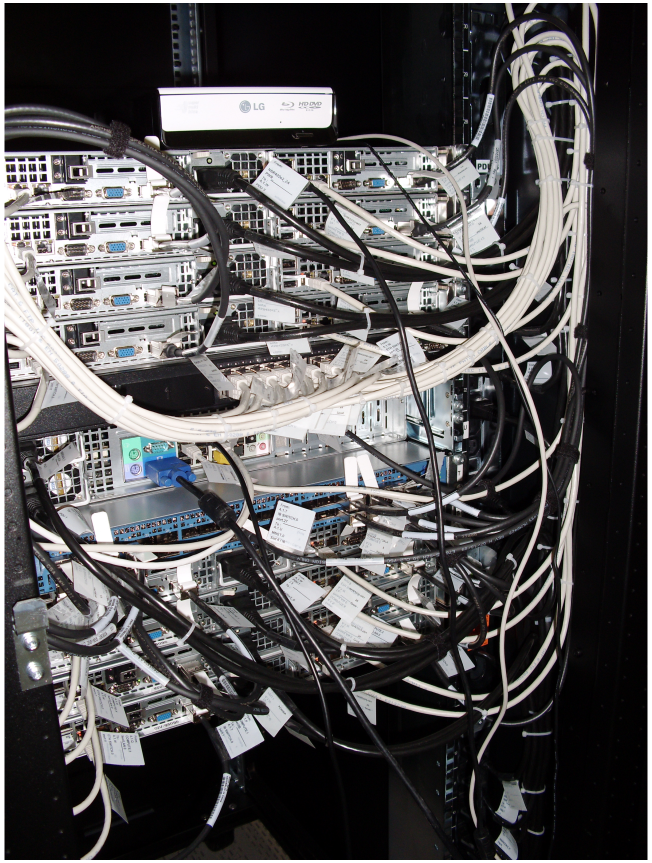
Condensed matter physics point of view: Flat band



- Flat band of minimal energy in one-magnon space; localized magnons can be built from delocalized states in the flat band.
- Entropy can be evaluated using hard-object models (1); universal low-temperature behavior.
- Same behavior for Hubbard model; flat band ferromagnetism (Tasaki & Mielke), jump of N with μ (2).

(1) H.-J. Schmidt, J. Richter, R. Moessner, J. Phys. A: Math. Gen. **39**, 10673 (2006)
(2) A. Honecker, J. Richter, Condens. Matter Phys. **8**, 813 (2005)

Summary



- Spin systems, spin models – great!
  But why can we use them?

- Great physics and nice playground for models, methods, and fundamental science, e.g., thermalization.

- Frustration is the normal state of matter.
  The opposite is rare.

Many thanks to my collaborators














- C. Beckmann, M. Czopnik, T. Glaser, O. Hanebaum, Chr. Heesing, M. Höck, K. Irländer, N.B. Ivanov, H.-T. Langwald, A. Müller, H. Schlüter, R. Schnalle, Chr. Schröder, J. Ummethum, P. Vorndamme, J. Waltenberg, D. Westerbeck (Bielefeld)
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Thank you very much for your attention.

The end.

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