

The power of typicality applied to magnetic molecules and low-dimensional quantum spin systems

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Seminar,
Centre for Science at Extreme Conditions, Edinburgh, 24 February 2020

The Bielefeld conspiracy



The story goes that the city of **BIELEFELD** in the German state of North Rhine-Westphalia **DOES NOT** actually **EXIST**. Rather, its existence is merely propagated by an entity known only as **THEM**, which has conspired with the authorities to create the illusion of the city's existence.

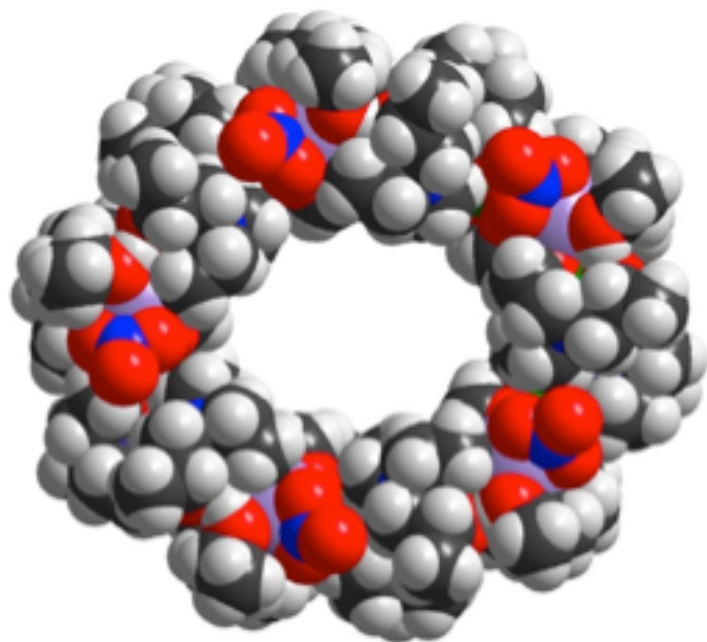
The origins of and reasons for this conspiracy are not a part of the original theory. Speculated originators jokingly include the CIA, Mossad, or aliens who use Bielefeld University as a disguise for their spaceship.

Do you know anybody from Bielefeld?

https://en.wikipedia.org/wiki/Bielefeld_Conspiracy

We investigate magnetic molecules

You have got a molecule!

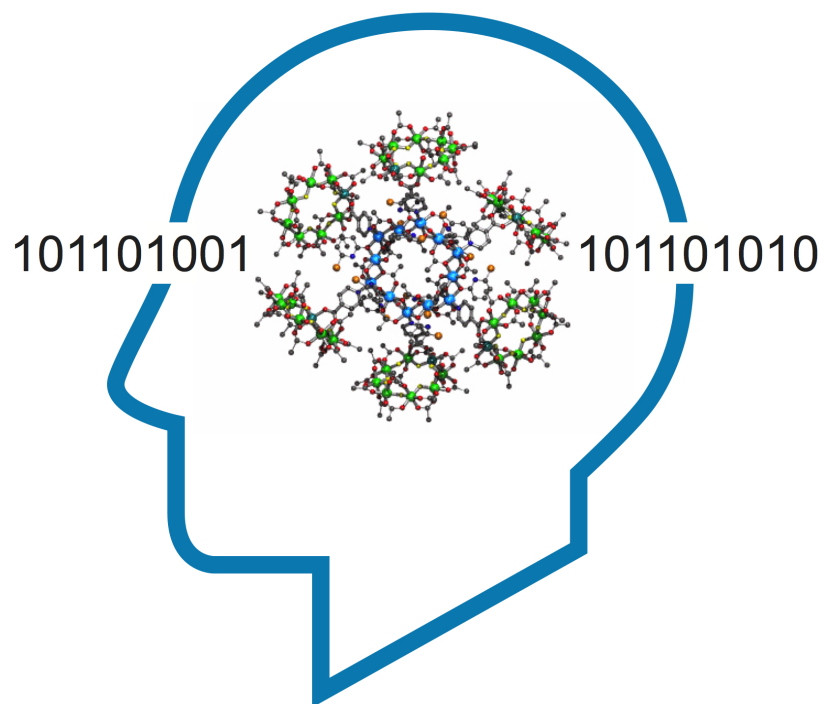


$$S = 60!$$

Congratulations!

Powell group: npj Quantum Materials **3**, 10 (2018)

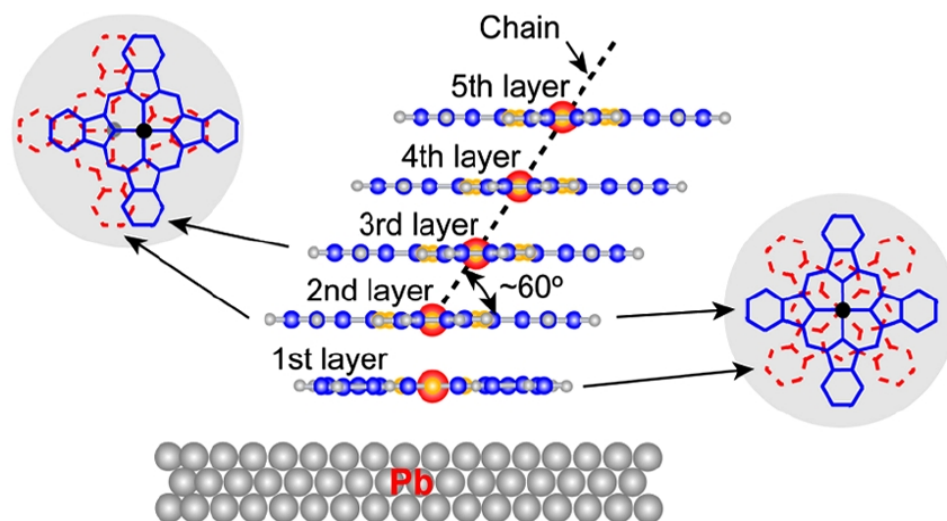
You want to build a quantum computer!



Very smart!

Wernsdorfer group: Phys. Rev. Lett. **119**, 187702 (2027)

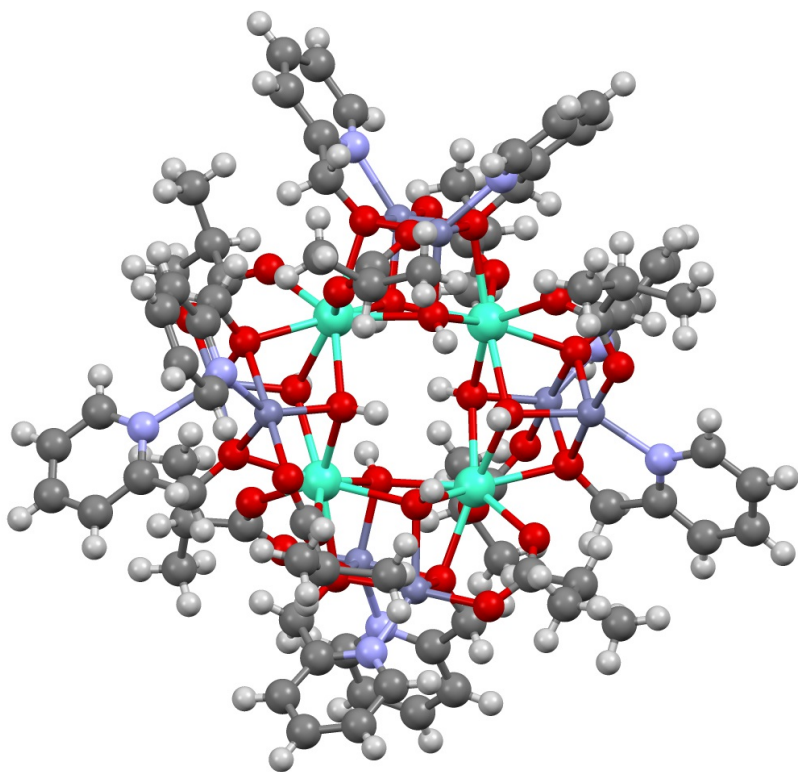
You want to deposit your molecule!



Next generation magnetic storage!

Xue group: Phys. Rev. Lett. **101**, 197208 (2008)

You want molecular magnetocalorics!



Brilliant!

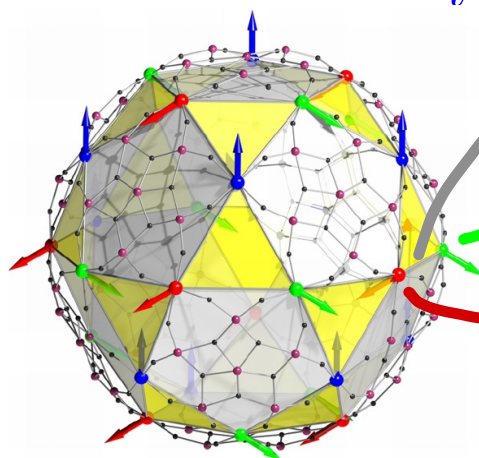
Brechin group: *Angew. Chem. Int. Ed.* **51**, 4633 (2012)

You have got an idea about the modeling!

Heisenberg

Zeeman

$$\underline{H} = -2 \sum_{i < j} J_{ij} \vec{s}(i) \cdot \vec{s}(j) + g \mu_B B \sum_i^N s_z(i)$$



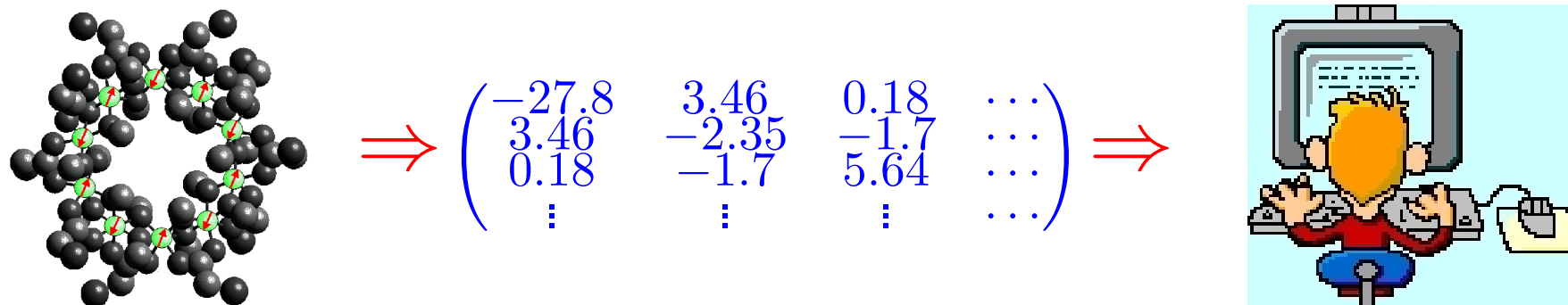
You have to solve the Schrödinger equation!

$$\hat{H} | \phi_n \rangle = E_n | \phi_n \rangle$$

Eigenvalues E_n and eigenvectors $| \phi_n \rangle$

- needed for spectroscopy (EPR, INS, NMR);
- needed for thermodynamic functions (magnetization, susceptibility, heat capacity);
- needed for time evolution (pulsed EPR, simulate quantum computing, thermalization).

In the end it's always a big matrix!



$$\text{Fe}_{10}^{\text{III}}: N = 10, s = 5/2, \dim(\mathcal{H}) = (2s + 1)^N$$

Dimension=60,466,176. Maybe too big?

Can we evaluate the partition function

$$Z(T, B) = \text{tr} \left(\exp \left[-\beta \underline{H} \right] \right)$$

without diagonalizing the Hamiltonian?

Yes, we can!



$$\begin{pmatrix} 3 & 42 & 4711 \\ 42 & 0 & 3.14 \\ 4711 & 3.14 & 8 \\ -17 & 007 & 13 \\ 1.8 & 15 & 081 \end{pmatrix}$$

1. Typicality-based estimates
2. The magnetocaloric effect
3. A quantum phase transition
4. Kagome lattice antiferromagnet

We are the sledgehammer team of matrix diagonalization.
Please send inquiries to jschnack@uni-bielefeld.de!

Solution I: trace estimators

$$\text{tr}(\mathcal{Q}) \approx \langle r | \mathcal{Q} | r \rangle$$

$$|r\rangle = \sum_{\nu} r_{\nu} |\nu\rangle, \quad r_{\nu} = \pm 1$$

- $|\nu\rangle$ some orthonormal basis of your choice;
not the eigenbasis of $\mathcal{Q}$, since we don't know it.
- $r_{\nu} = \pm 1$ random, equally distributed. Rademacher vectors.
- Amazingly accurate, bigger (Hilbert space dimension) is better.

M. Hutchinson, Communications in Statistics - Simulation and Computation **18**, 1059 (1989).

Solution II: Krylov space representation

$$\exp \left[-\beta \tilde{H} \right] \approx \tilde{1} - \beta \tilde{H} + \frac{\beta^2}{2!} \tilde{H}^2 - \dots \frac{\beta^{N_L-1}}{(N_L-1)!} \tilde{H}^{N_L-1}$$

applied to a state $|r\rangle$ yields a superposition of

$$\tilde{1}|r\rangle, \quad \tilde{H}|r\rangle, \quad \tilde{H}^2|r\rangle, \quad \dots \tilde{H}^{N_L-1}|r\rangle.$$

These (linearly independent) vectors span a small space of dimension N_L ; it is called Krylov space.

Let's diagonalize $\tilde{H}$ in this space!

Partition function I: simple approximation

$$Z(T, B) \approx \langle r | e^{-\beta \tilde{H}} | r \rangle \approx \sum_{n=1}^{N_L} e^{-\beta \epsilon_n^{(r)}} |\langle n(r) | r \rangle|^2$$

$$O^r(T, B) \approx \frac{\langle r | Q e^{-\beta \tilde{H}} | r \rangle}{\langle r | e^{-\beta \tilde{H}} | r \rangle}$$

- Wow!!!
- One can replace a trace involving an intractable operator by an expectation value with respect to just ONE random vector evaluated by means of a Krylov space representation???

J. Jaklic and P. Prelovsek, Phys. Rev. B **49**, 5065 (1994).

Partition function II: Finite-temperature Lanczos Method

$$Z^{\text{FTLM}}(T, B) \approx \frac{1}{R} \sum_{r=1}^R \sum_{n=1}^{N_L} e^{-\beta \epsilon_n^{(r)}} |\langle n(r) | r \rangle|^2$$

- Averaging over R random vectors is better.
- $|n(r)\rangle$ n -th Lanczos eigenvector starting from $|r\rangle$ (Rademacher vectors).
- Partition function replaced by a small sum: $R = 1 \dots 100, N_L \approx 100$.

J. Jaklic and P. Prelovsek, Phys. Rev. B **49**, 5065 (1994).

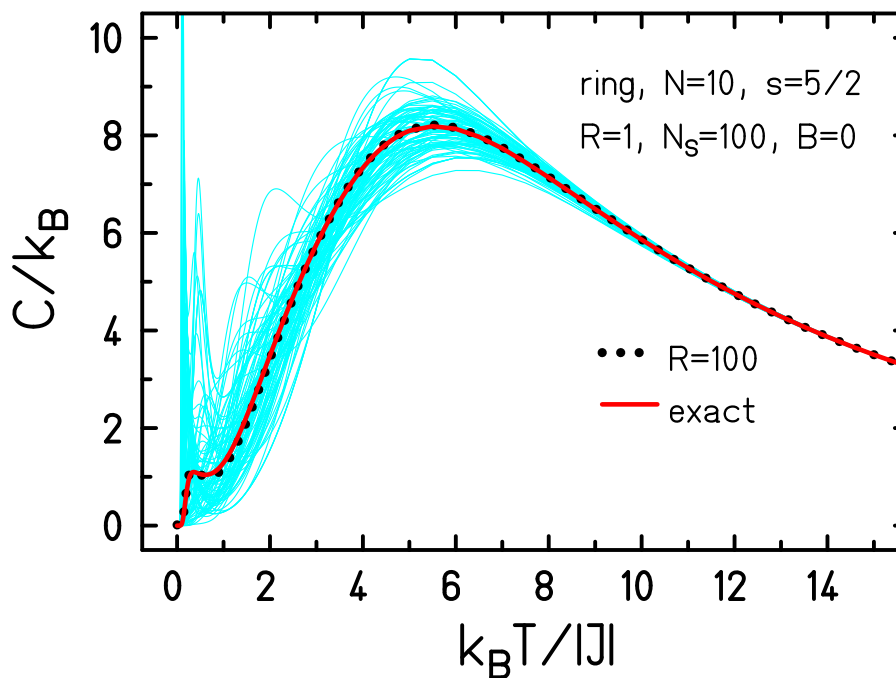
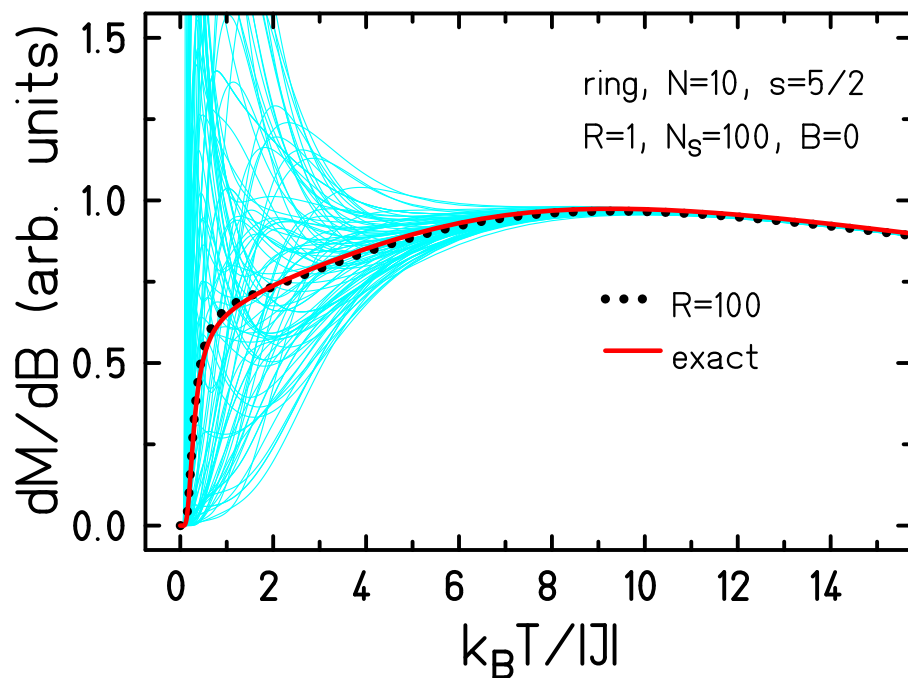
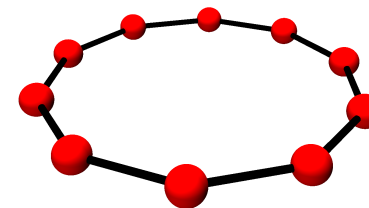
Partition function III: use symmetries if you can

$$Z^{\text{FTLM}}(T, B) \approx \sum_{\gamma=1}^{\Gamma} \frac{1}{R} \sum_{r=1}^R \sum_{n=1}^{N_L} e^{-\beta \epsilon_n^{(r)}} |\langle n(r) | r \rangle|^2$$

- γ labels all the symmetries you use in your calculation (all irreducible representations).
- $|r\rangle$ is then drawn from the respective subspace with this symmetry.

J. Schnack and O. Wendland, Eur. Phys. J. B **78** (2010) 535-541

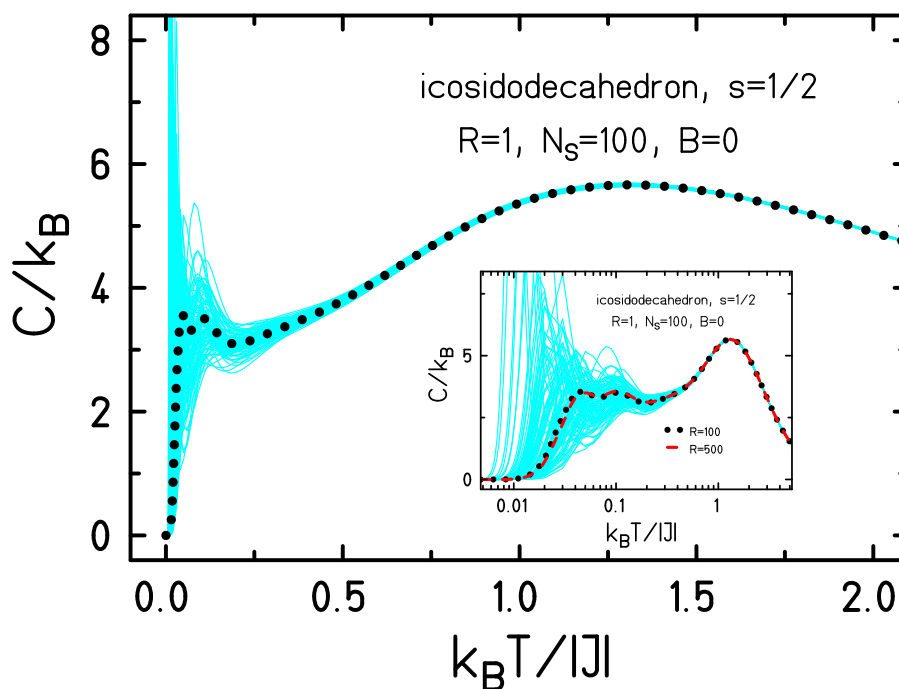
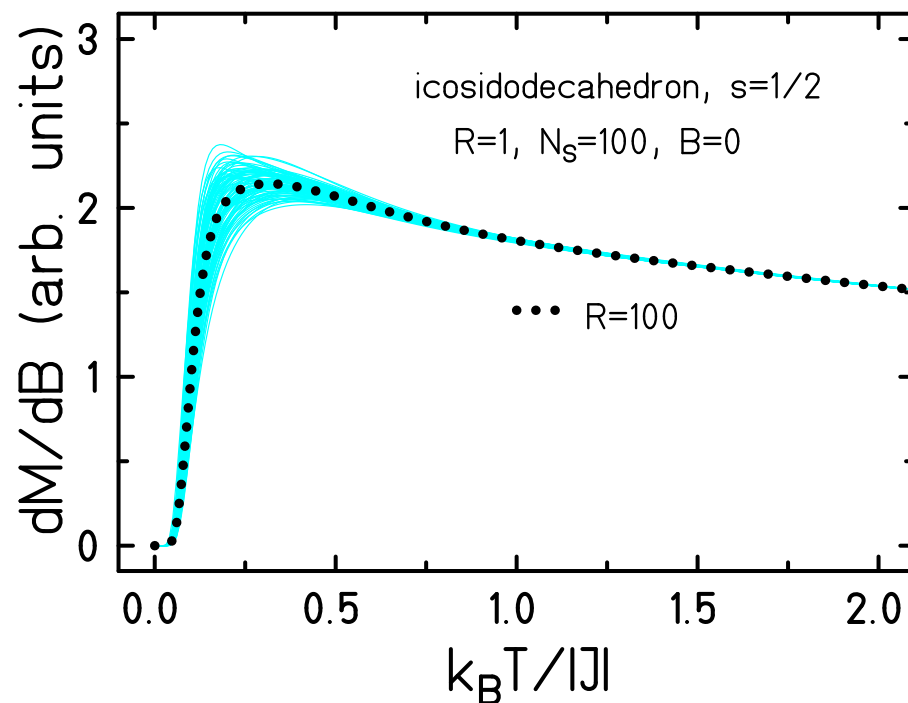
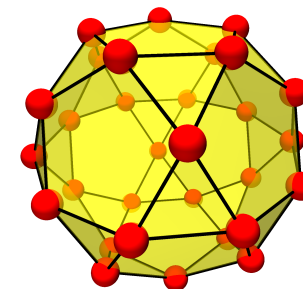
FTLM 1: ferric wheel



(1) J. Schnack, J. Richter, R. Steinigeweg, Phys. Rev. Research **2**, 013186 (2020).

(2) R. Schnalle and J. Schnack, Int. Rev. Phys. Chem. **29**, 403 (2010).

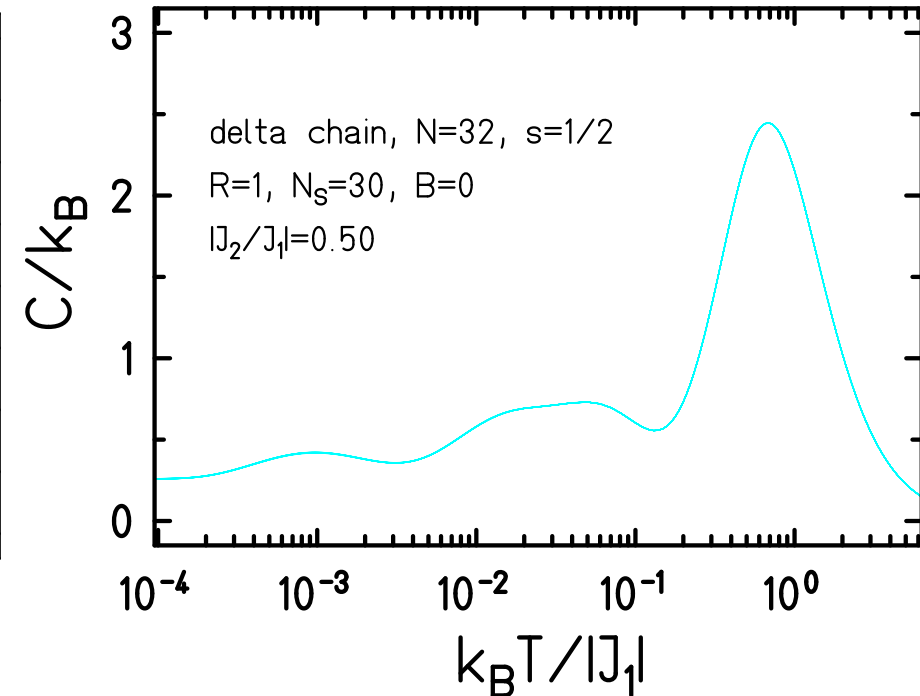
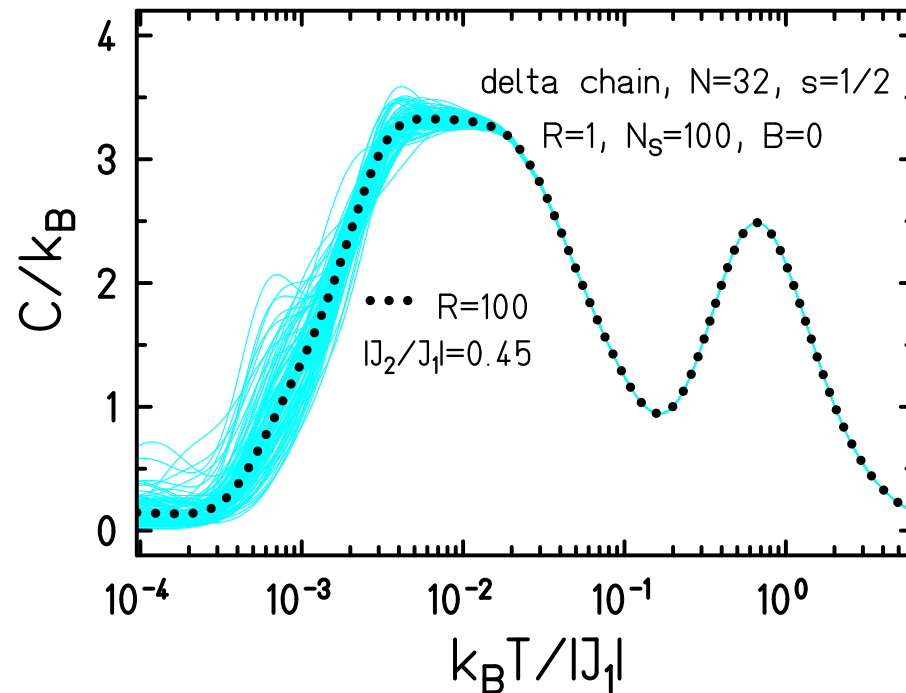
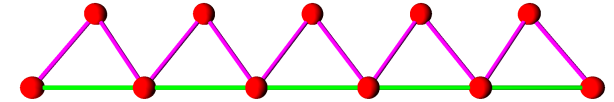
FTLM 2: icosidodecahedron



(1) J. Schnack, J. Richter, R. Steinigeweg, Phys. Rev. Research **2**, 013186 (2020).

(2) J. Schnack and O. Wendland, Eur. Phys. J. B **78**, 535 (2010).

FTLM 3: sawtooth chain



$|J_2/J_1| = 0.45$ – near critical, $|J_2/J_1| = 0.50$ – critical.

Frustration, technically speaking, works in your favour.

(1) J. Schnack, J. Richter, R. Steinigeweg, Phys. Rev. Research **2**, 013186 (2020)

(2) J. Schnack, J. Richter, T. Heitmann, J. Richter, R. Steinigeweg, Z. Naturforsch. A (2020) accepted, arXiv:2002.00411

The magnetocaloric effect

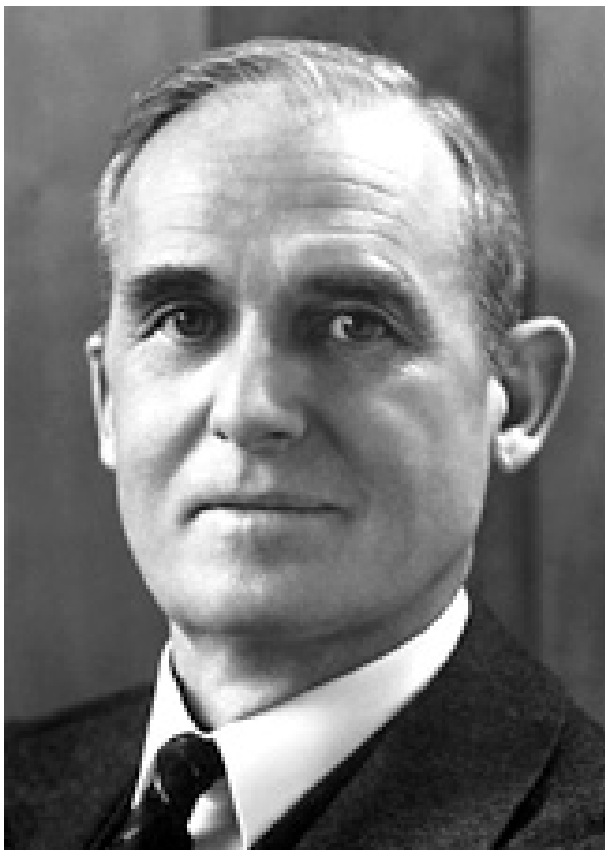
Magnetocaloric effect – Basics



- Heating or cooling in a varying magnetic field. Predicted, discussed, discovered by Thomson, Warburg, Weiss, and Piccard (1).
- Typical rates: 0.5 ... 2 K/T.
- Giant magnetocaloric effect: 3 ... 4 K/T e.g. in $\text{Gd}_5(\text{Si}_x\text{Ge}_{1-x})_4$ alloys ($x \leq 0.5$).
- **Scientific goal I: room temperature applications.**
- **Scientific goal II: sub-Kelvin cooling.**

(1) A. Smith, Eur. Phys. J. H **38**, 507 (2013).

Sub-Kelvin cooling: Nobel prize 1949



The Nobel Prize in Chemistry 1949 was awarded to William F. Giaque *for his contributions in the field of chemical thermodynamics, particularly concerning the behaviour of substances at extremely low temperatures.*

Sub-Kelvin cooling: Nobel prize 1949

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LETTERS TO THE EDITOR

Attainment of Temperatures Below 1° Absolute by Demagnetization of $\text{Gd}_2(\text{SO}_4)_3 \cdot 8\text{H}_2\text{O}$

We have recently carried out some preliminary experiments on the adiabatic demagnetization of $\text{Gd}_2(\text{SO}_4)_3 \cdot 8\text{H}_2\text{O}$ at the temperatures of liquid helium. As previously predicted by one of us, a large fractional lowering of the absolute temperature was obtained.

An iron-free solenoid producing a field of about 8000 gauss was used for all the measurements. The amount of $\text{Gd}_2(\text{SO}_4)_3 \cdot 8\text{H}_2\text{O}$ was 61 g. The observations were checked by many repetitions of the cooling. The temperatures were measured by means of the inductance of a coil surrounding the gadolinium sulfate. The coil was immersed in liquid helium and isolated from the gadolinium by means of an evacuated space. The thermometer was in excellent agreement with the temperature of liquid helium as indicated by its vapor pressure down to 1.5°K.

On March 19, starting at a temperature of about 3.4°K, the material cooled to 0.53°K. On April 8, starting at about 2°, a temperature of 0.34°K was reached. On April 9, starting at about 1.5°, a temperature of 0.25°K was attained.

It is apparent that it will be possible to obtain much lower temperatures, especially when successive demagnetizations are utilized.

W. F. GIAUQUE
D. P. MACDOUGALL

Department of Chemistry,
University of California,
Berkeley, California,
April 12, 1933.

W. F. Giauque and D. MacDougall, *Phys. Rev.* **43**, 768 (1933).

Sub-Kelvin cooling with molecules

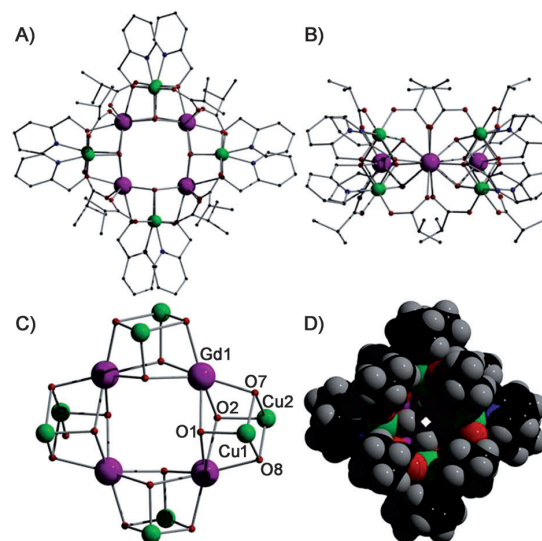
The Importance of Being Exchanged: $[\text{Gd}^{\text{III}}_4\text{M}^{\text{II}}_8(\text{OH})_8(\text{L})_8(\text{O}_2\text{CR})_8]^{4+}$ Clusters for Magnetic Refrigeration**

Thomas N. Hooper, Jürgen Schnack, Stergios Piligkos,* Marco Evangelisti,* and Euan K. Brechin*

One of the most promising applications for molecules built from paramagnetic metal ions is low-temperature magnetic refrigeration.^[1] Indeed, recent studies have suggested that molecular coolers can outperform any conventionally employed solid-state refrigerant material by orders of magnitude.^[2] In order to do so, molecules must possess a combination of a large spin ground state (S), with negligible anisotropy ($D_{\text{cluster}} = 0$), weak magnetic exchange between the constituent metal ions, and a relatively large metal:non-metal mass ratio (that is, a large magnetic density).^[1b] These molecular prerequisites suggest the use of lanthanide ions and, in particular, the f^7 ion Gd^{3+} in the construction of homo- and heterometallic (Gd-3d) clusters, and a sensible starting point is the synthesis of $\text{Gd}^{\text{III}}\text{--Cu}^{\text{II}}$ clusters, as previous studies have shown this combination favors ferromagnetic exchange.^[3]

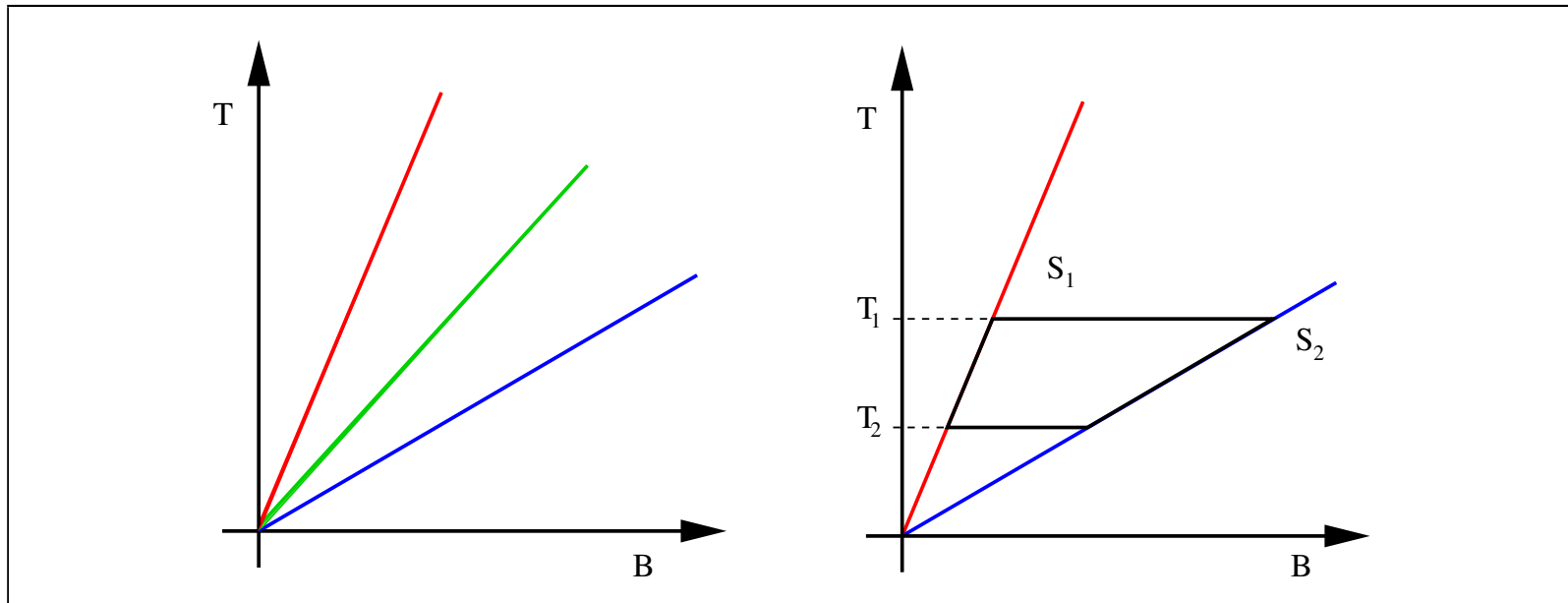
Herein we introduce a rather remarkable new family of compounds of general formula $[\text{Ln}^{\text{III}}_4\text{M}^{\text{II}}_8(\text{OH})_8(\text{L})_8(\text{O}_2\text{CR})_8](\text{X})_4$ in which almost all the constituent parts, namely the lanthanide ions Ln^{3+} , the transition-metal ions M^{2+} , the bridging ligand L , the carboxylates, and the counterions X can be exchanged. In each case, the structure remains essentially the same and this allows for a thorough understanding of the individual contributions to the magnetocaloric effect (MCE). Herein we describe the three family members $[\text{Gd}^{\text{III}}_4\text{M}^{\text{II}}_8(\text{OH})_8(\text{L})_8(\text{O}_2\text{CR})_8](\text{ClO}_4)_4$ ($\text{M} = \text{Zn}$, $\text{R} = \text{CHMe}_2$,

1; $\text{M} = \text{Cu}$, $\text{R} = \text{CHMe}_2$, **2**; $\text{M} = \text{Ni}$, $\text{R} = \text{CH}_2\text{Me}$, **3**; $\text{LH} = 2$ - (hydroxymethyl)pyridine) and show how the identity of the transition metal and the sign of the magnetic exchange are vital components to consider when designing molecular coolers.



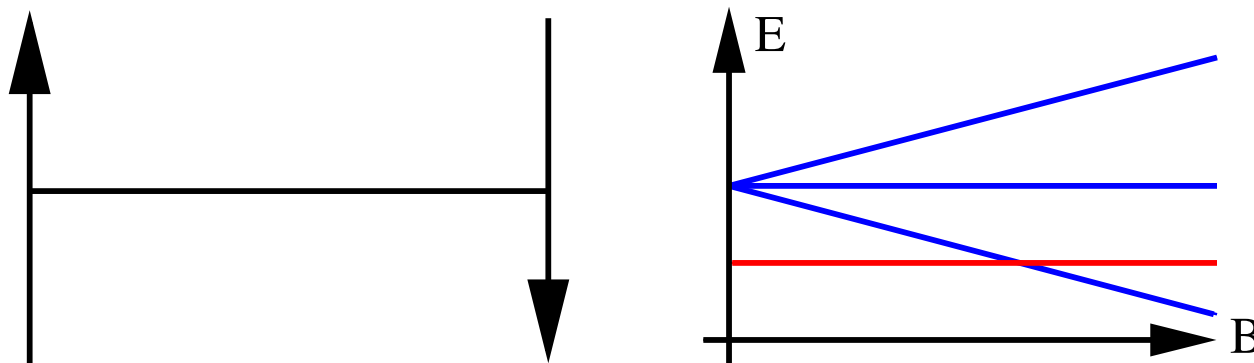
T. N. Hooper, J. Schnack, S. Piligkos, M. Evangelisti, and E. K. Brechin, *Angew. Chem. Int. Ed.* **51**, 4633 (2012).

Magnetocaloric effect – Paramagnets



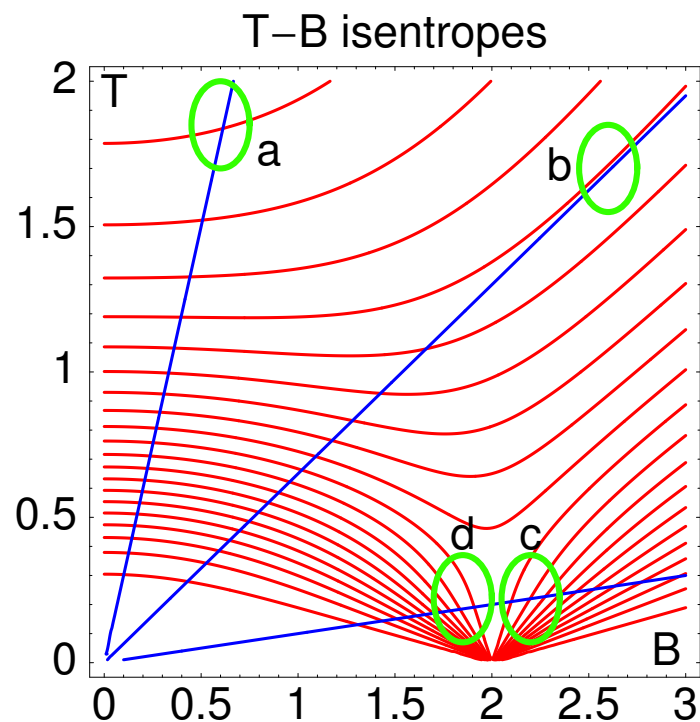
- Ideal paramagnet: $S(T, B) = f(B/T)$, i.e. $S = \text{const} \Rightarrow T \propto B$.
- At low T pronounced effects of dipolar interaction prevent further effective cooling.

Magnetocaloric effect – af $s = 1/2$ dimer



- Singlet-triplet level crossing causes a peak of S at $T \approx 0$ as function of B .
- $M(T = 0, B)$ and $S(T = 0, B)$ not analytic as function of B .
- $M(T = 0, B)$ jumps at B_c ; $S(T = 0, B_c) = k_B \ln 2$, otherwise zero.

Magnetocaloric effect – af $s = 1/2$ dimer



blue lines: ideal paramagnet, red curves: af dimer

Magnetocaloric effect:

(a) reduced,

(b) the same,

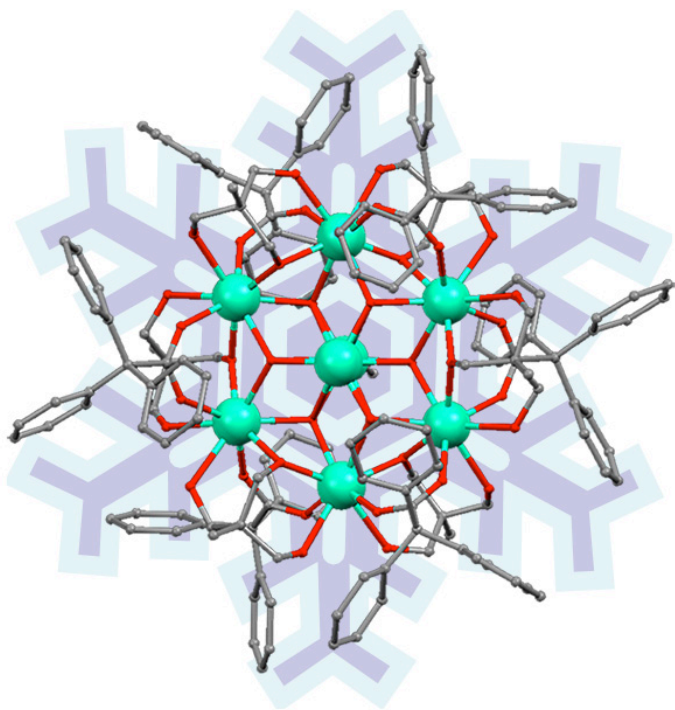
(c) enhanced,

(d) opposite

when compared to an ideal paramagnet.

Case (d) does not occur for a paramagnet.

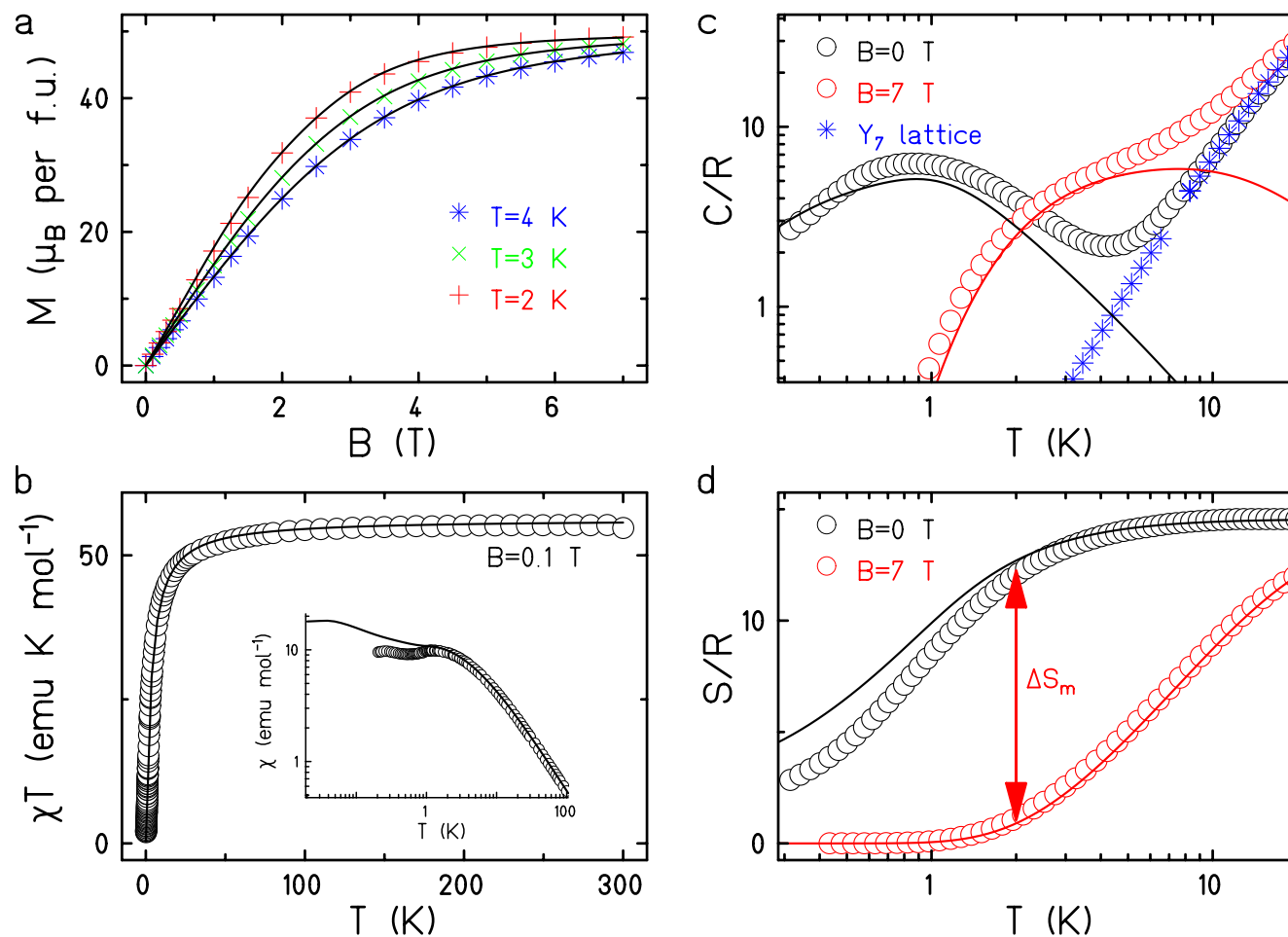
Gd₇ – Basics



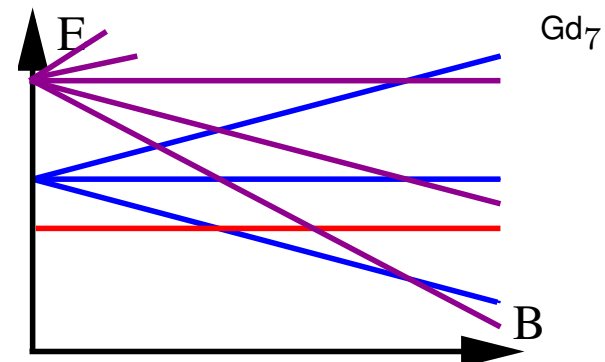
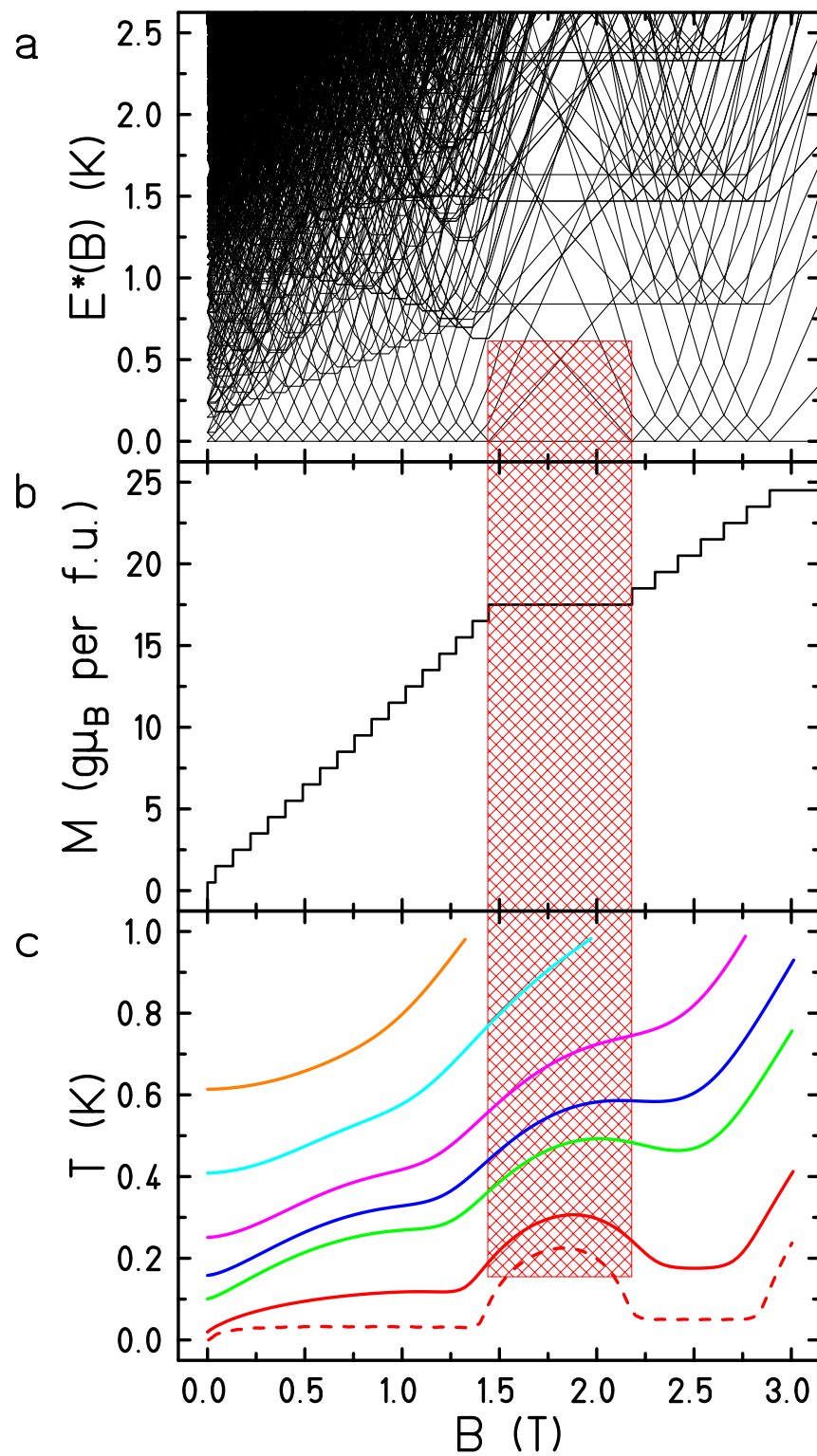
- Often magnetocaloric observables not directly measured, but inferred from Maxwell's relations.
- First real cooling experiment with a molecule.
- $$\underline{H} = -2 \sum_{i < j} J_{ij} \vec{s}_i \cdot \vec{s}_j + g \mu_B B \sum_i^N s_i^z$$
$$J_1 = -0.090(5) \text{ K}, J_2 = -0.080(5) \text{ K}$$
and $g = 2.02$.
- **Very good agreement down to the lowest temperatures.**

J. W. Sharples, D. Collison, E. J. L. McInnes, J. Schnack, E. Palacios, M. Evangelisti, Nat. Commun. **5**, 5321 (2014).

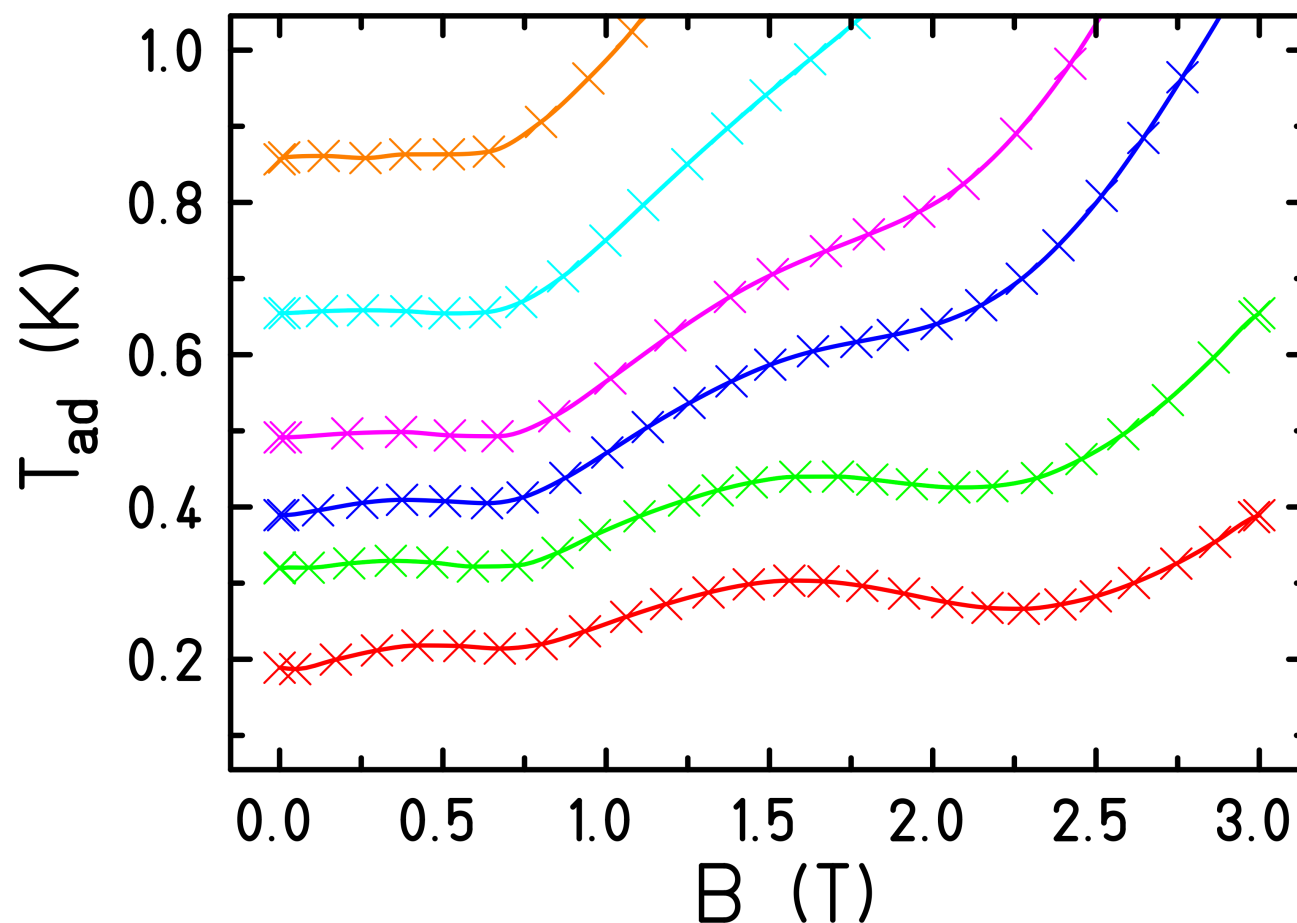
Gd₇ – experiment & theory



J. W. Sharples, D. Collison, E. J. L. McInnes, J. Schnack, E. Palacios, M. Evangelisti, Nat. Commun. **5**, 5321 (2014).



Gd₇ – Experimental cooling



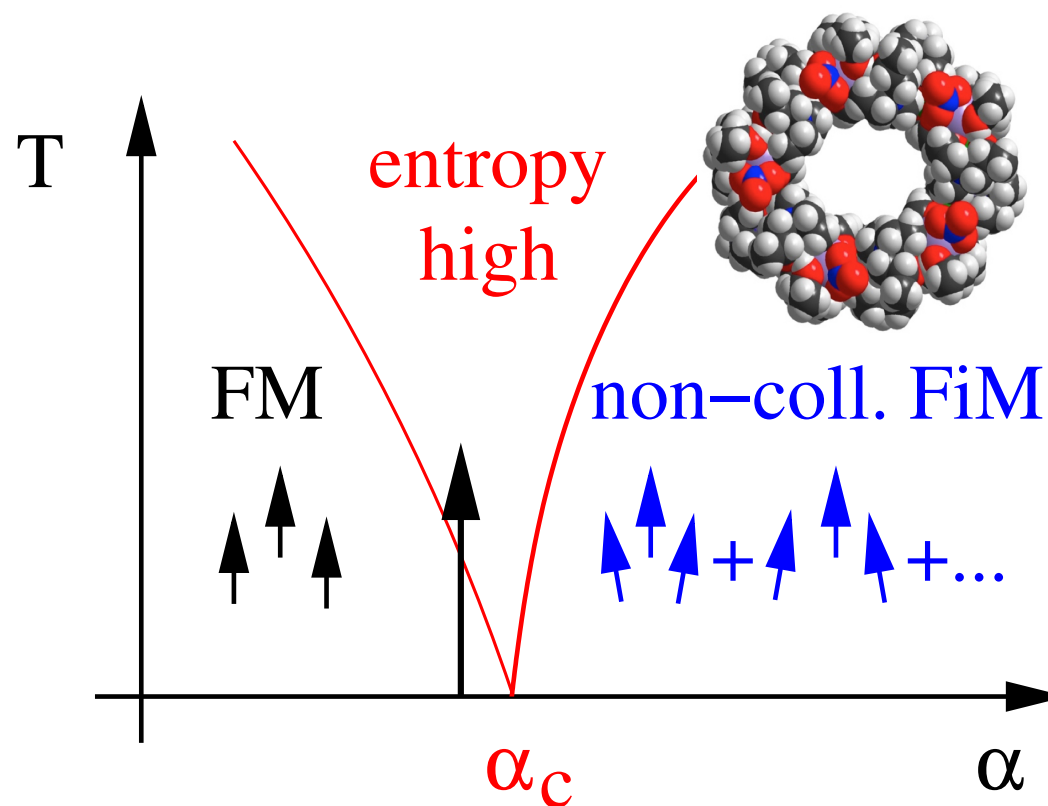
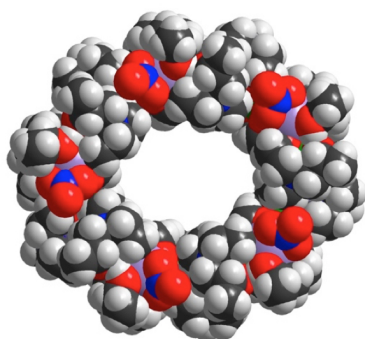
J. W. Sharples, D. Collison, E. J. L. McInnes, J. Schnack, E. Palacios, M. Evangelisti, Nat. Commun. **5**, 5321 (2014).

A quantum phase transition

Gd₁₀Fe₁₀ – summary



$S=60$

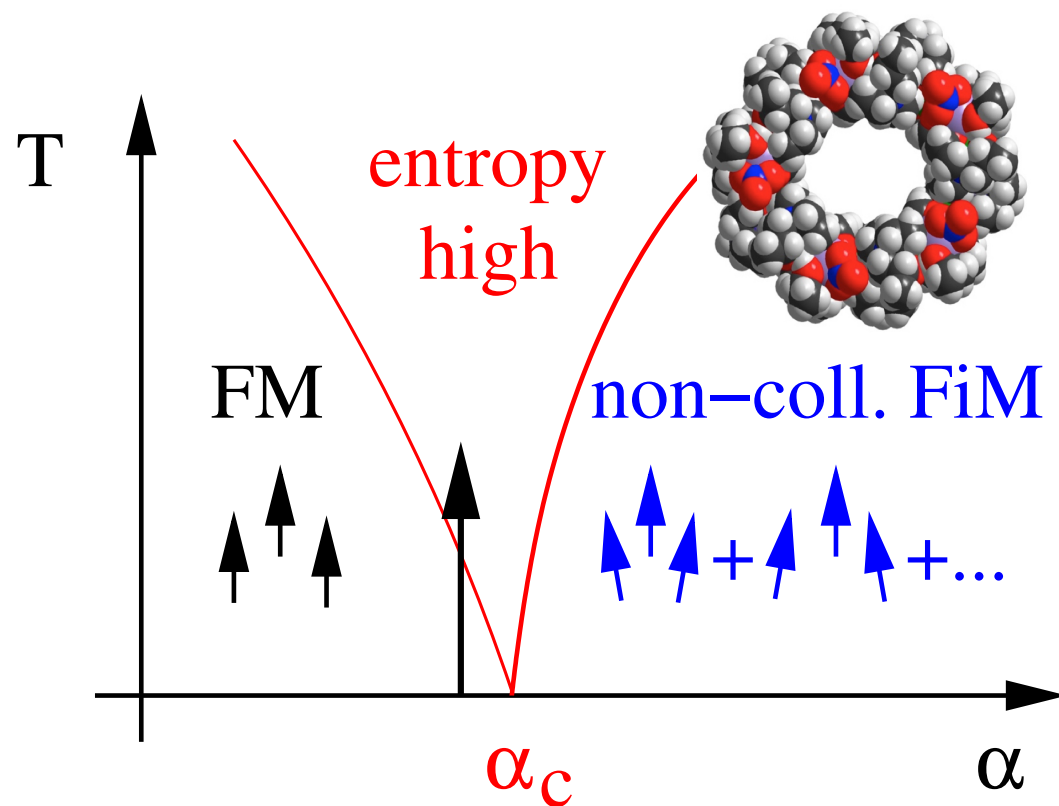
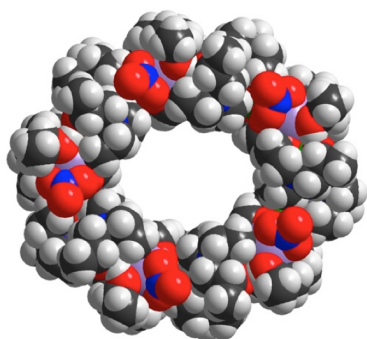


A. Baniodeh, N. Magnani, Y. Lan, G. Buth, C.E. Anson, J. Richter, M. Affronte, J. Schnack, A.K. Powell,
High Spin Cycles: Topping the Spin Record for a Single Molecule verging on Quantum Criticality,
 npj Quantum Materials **3**, 10 (2018)

Gd₁₀Fe₁₀ – summary



$S=60$

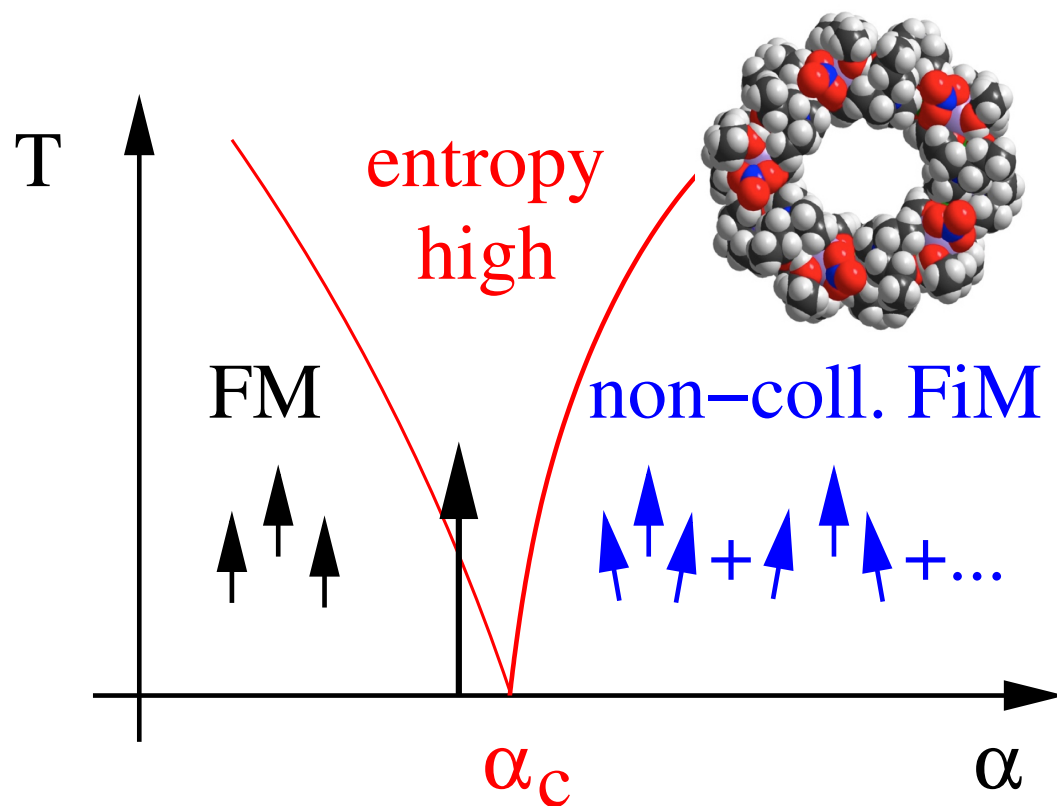
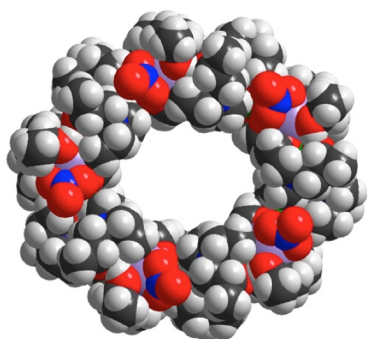


How do we know?

Gd₁₀Fe₁₀ – summary



$S=60$



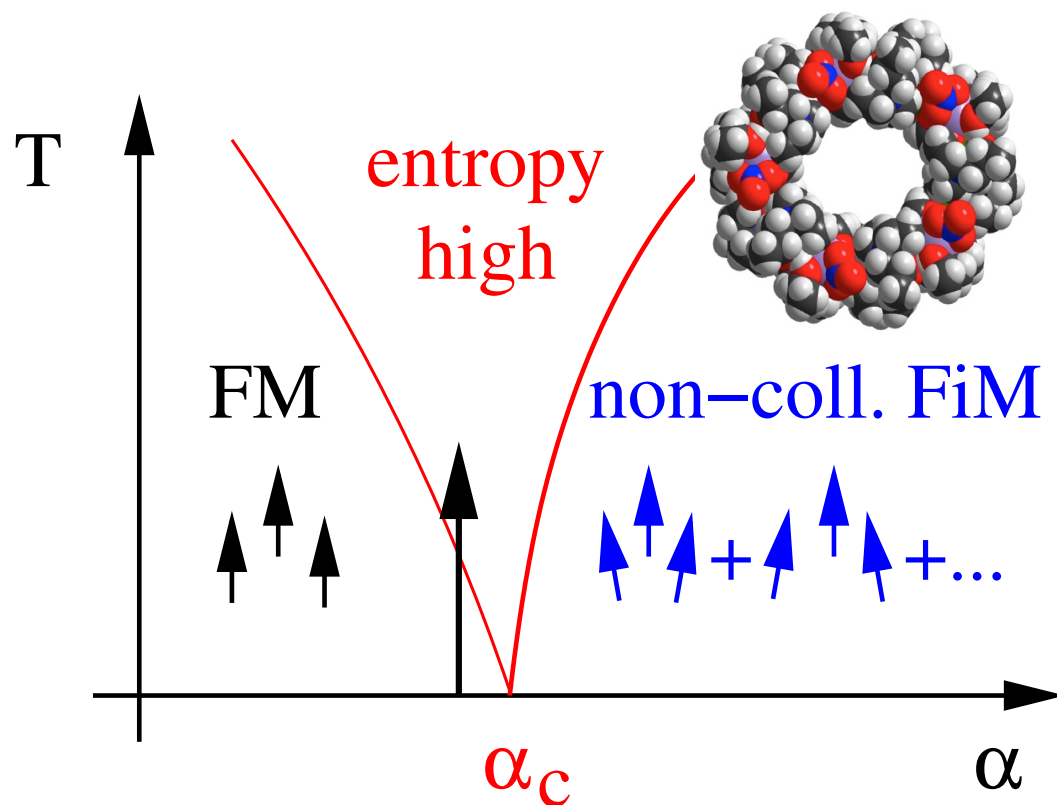
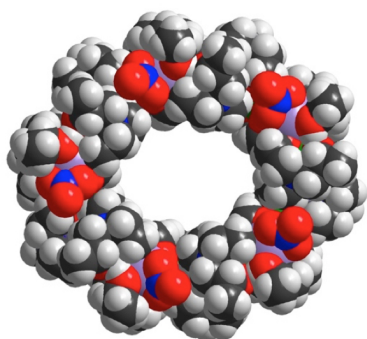
How do we know?

What is a QPT?

Gd₁₀Fe₁₀ – summary



$S=60$

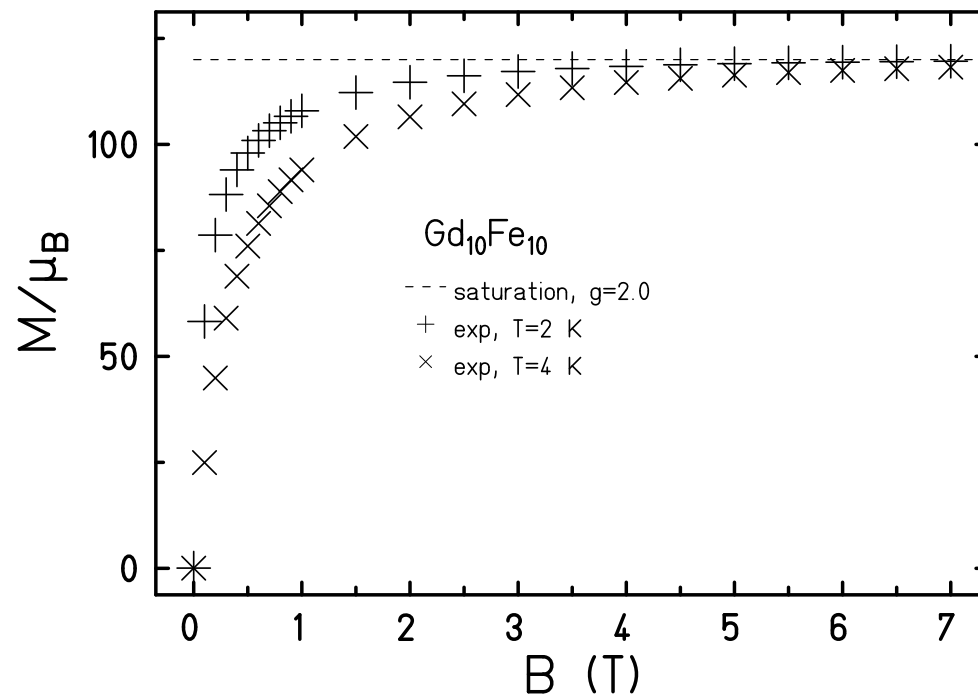
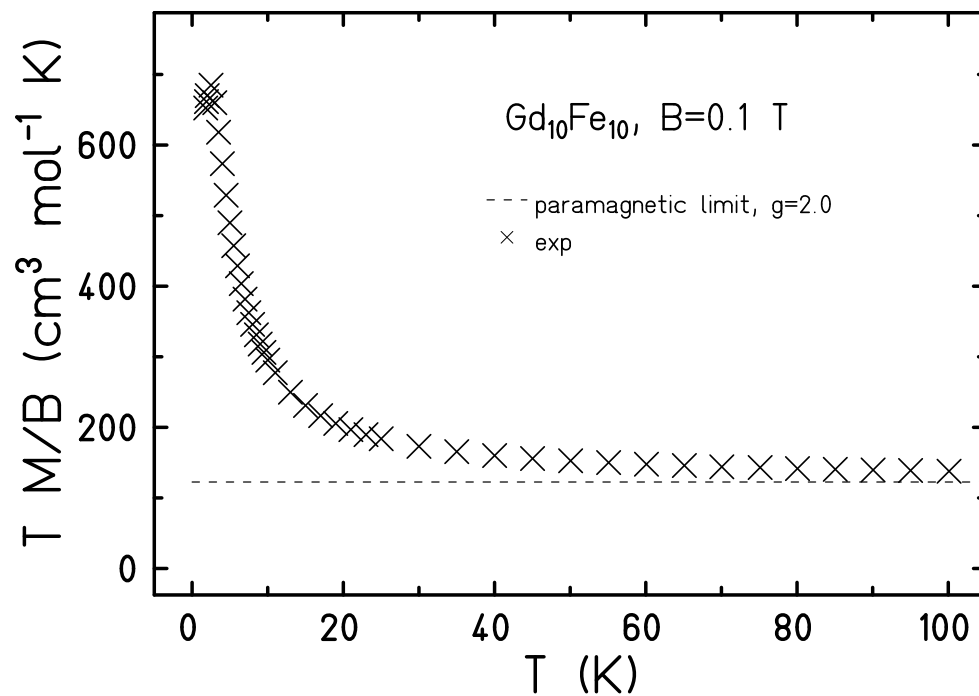


How do we know?

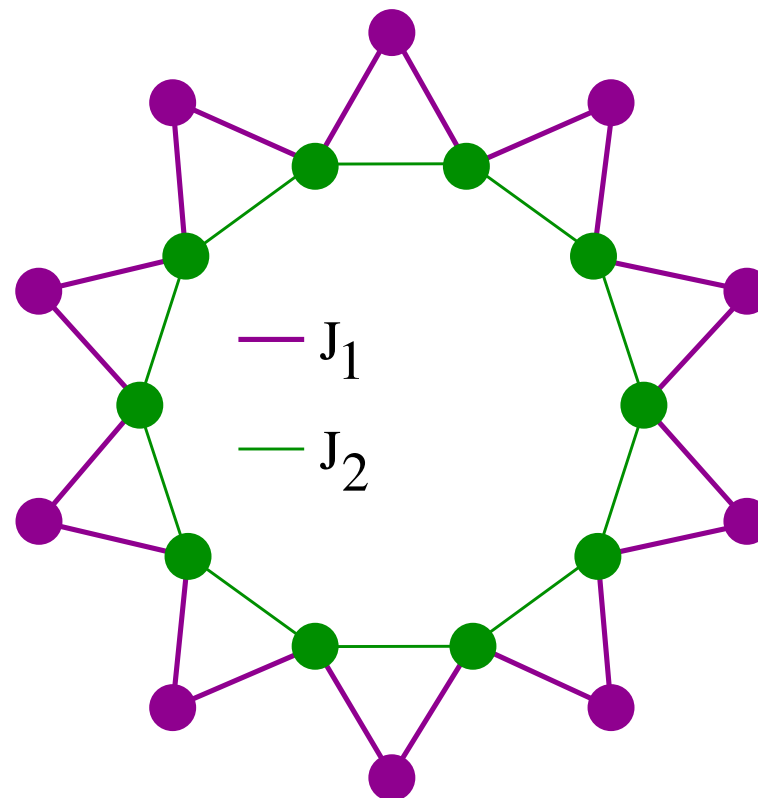
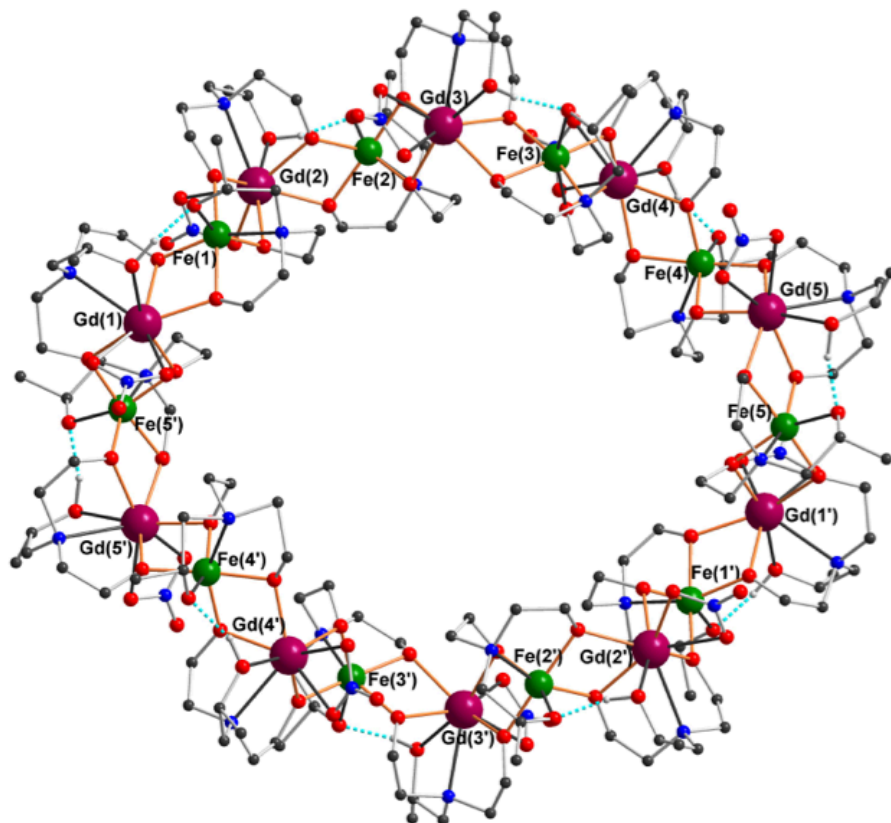
What is a QPT?
In Gd₁₀Fe₁₀?

Start: experimental data

Gd₁₀Fe₁₀ – How to rationalize the experimental data?



Gd₁₀Fe₁₀ – structure = delta chain



green: Fe ($s = 5/2$), purple: Gd ($s = 7/2$)

A. Baniodeh *et al.*, *npj Quantum Materials* **3**, 10 (2018)

Model Hamiltonian

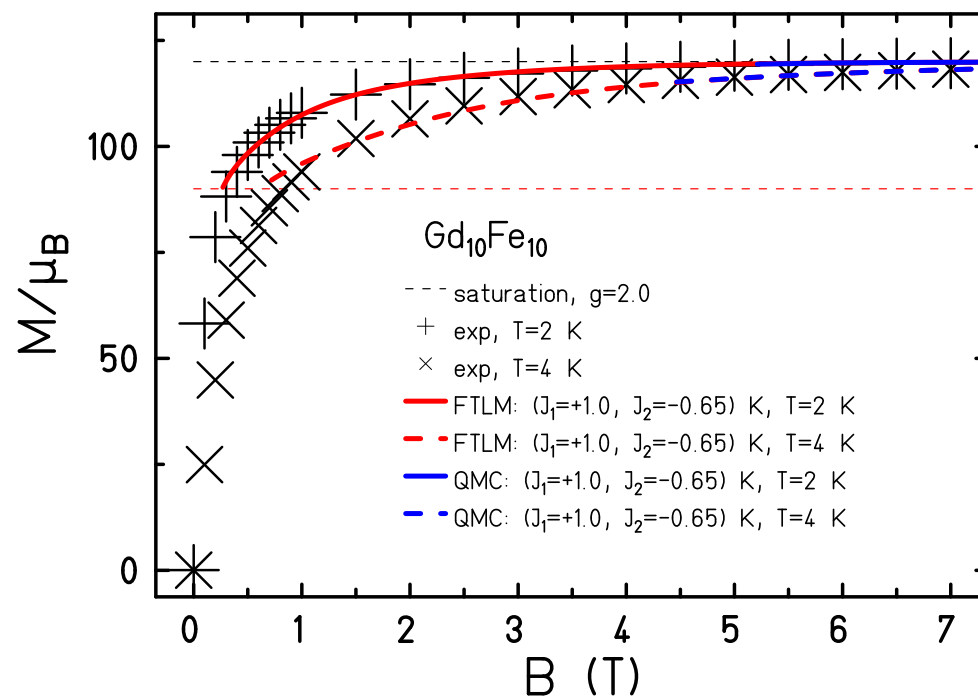
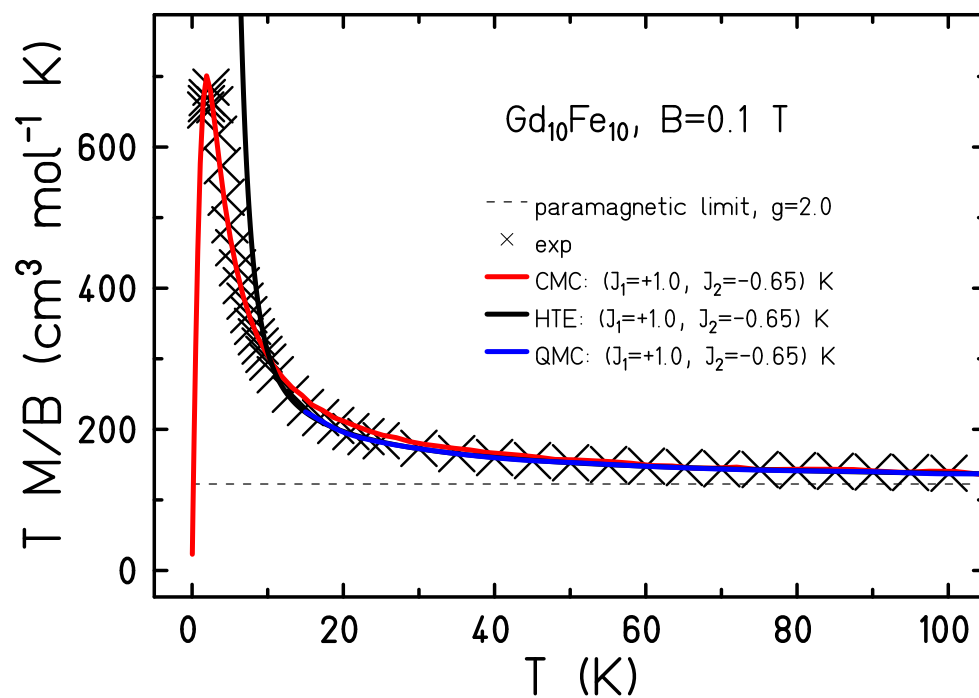
$$\begin{aligned} \underline{H} = & -2J_1 \sum_i \underline{\vec{S}}_{\text{Gd},i} \cdot \left(\underline{\vec{S}}_{\text{Fe},i} + \underline{\vec{S}}_{\text{Fe},i+1} \right) \\ & -2J_2 \sum_i \underline{\vec{S}}_{\text{Fe},i} \cdot \underline{\vec{S}}_{\text{Fe},i+1} + g \mu_B B \sum_i \left(\underline{S}_{\text{Gd},i}^z + \underline{S}_{\text{Fe},i}^z \right) \end{aligned}$$

Dimension of Hilbert space

$$(2s_{\text{Gd}} + 1)^{10} (2s_{\text{Fe}} + 1)^{10} \approx 6.5 \cdot 10^{16}$$

What would you do?

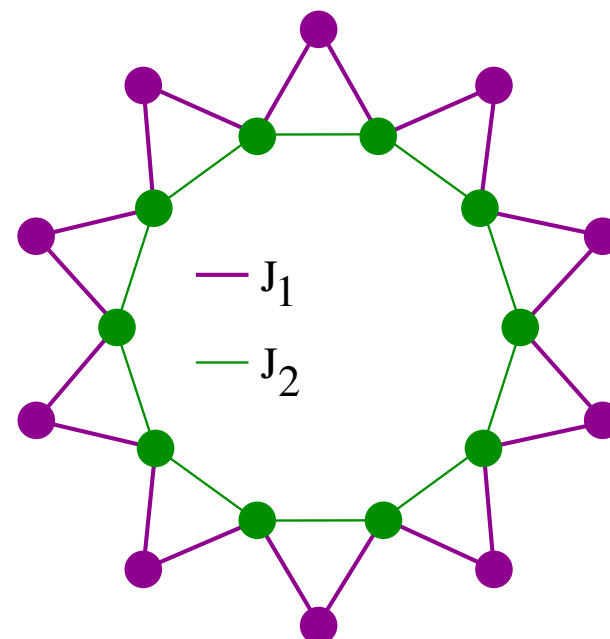
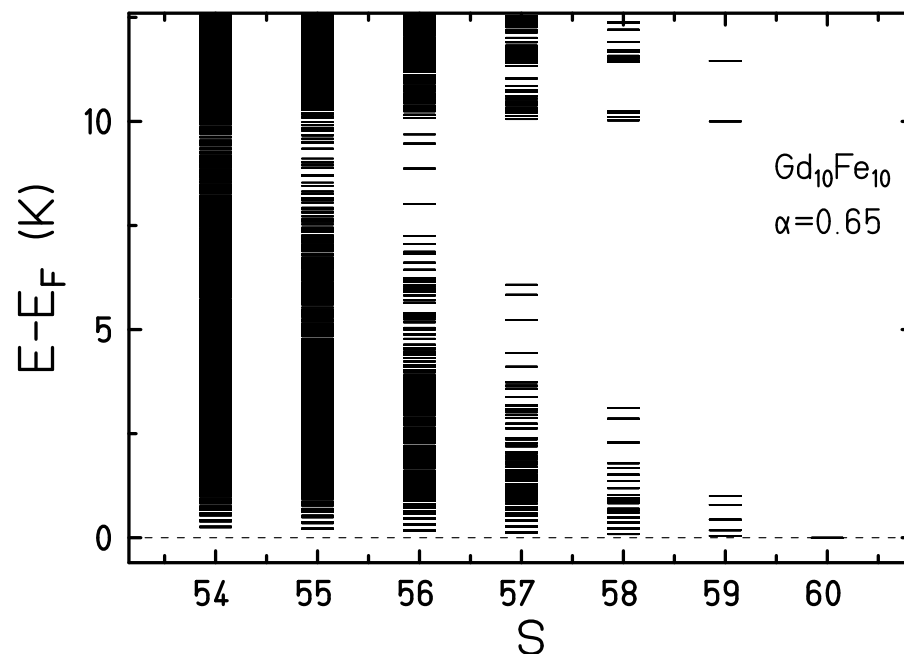
Gd₁₀Fe₁₀ – Methods



Methods: HTE, QMC, CMC, FTLM $\Rightarrow J_1 = 1.0$ K, $J_2 = -0.65$ K

A. Baniodeh *et al.*, *npj Quantum Materials* **3**, 10 (2018)

Gd₁₀Fe₁₀ – $S = 60$

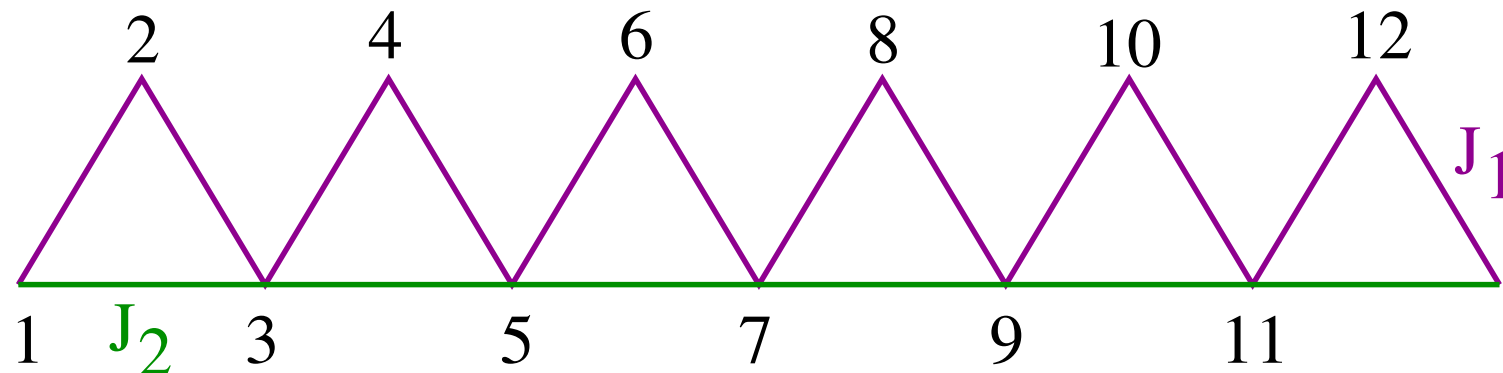


⇒ $S = 60$, largest ground state spin of a molecule to date

⇒ $\alpha_{\text{Gd}_{10}\text{Fe}_{10}} = |J_2|/J_1 = 0.65$ What if J_2 stronger?

A. Baniodeh *et al.*, *npj Quantum Materials* **3**, 10 (2018)

Excursus: sawtooth (delta) chain



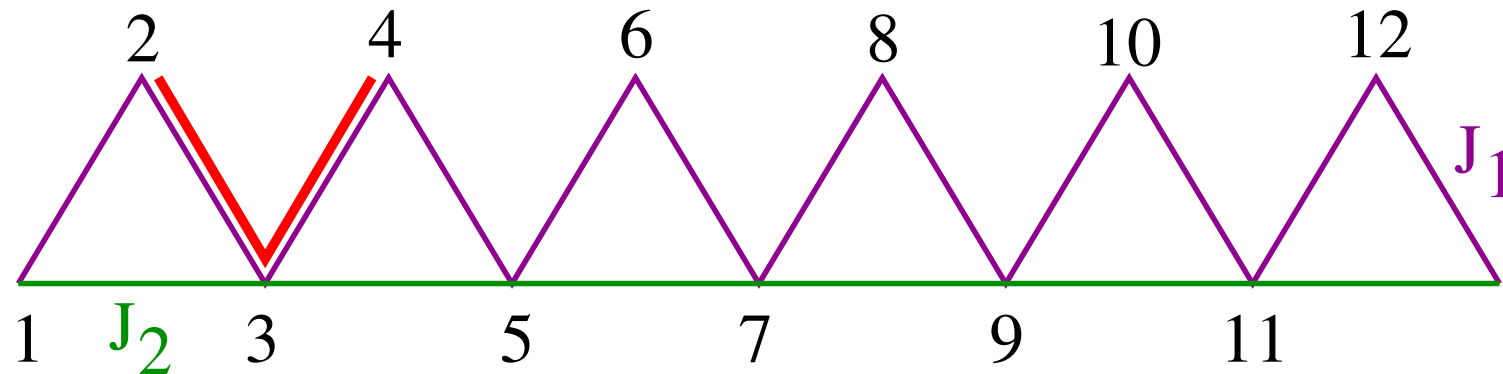
⇒ special properties for $J_1 > 0$ (ferro) and $J_2 < 0$ (af) at certain α_c

e.g. $\alpha_c = |J_2|/J_1 = 0.5$ if $s_i = 1/2 \forall i$

⇒ flat band of (multi-) magnon states; huge ground state degeneracy (1,2)

- (1) V. Y. Krivnov, D. V. Dmitriev, S. Nishimoto, S.-L. Drechsler, and J. Richter, Phys. Rev. B **90**, 014441 (2014).
- (2) D. V. Dmitriev and V. Y. Krivnov, Phys. Rev. B **92**, 184422 (2015).
- (3) D. V. Dmitriev and V. Y. Krivnov, J. Richter, J. Schnack, Phys. Rev. B **99**, 094410 (2019)

Excursus: sawtooth (delta) chain



$\Rightarrow |F\rangle = |S = S_{\max}, M = S_{\max}\rangle$ fully polarized ferromagnetic state

$\Rightarrow |1 \text{ localized magnon at } (2,3,4)\rangle = (\tilde{s}_2^- + \tilde{s}_4^- + 2\tilde{s}_3^-)|F\rangle;$

$$E = E_F, M = S_{\max} - 1$$

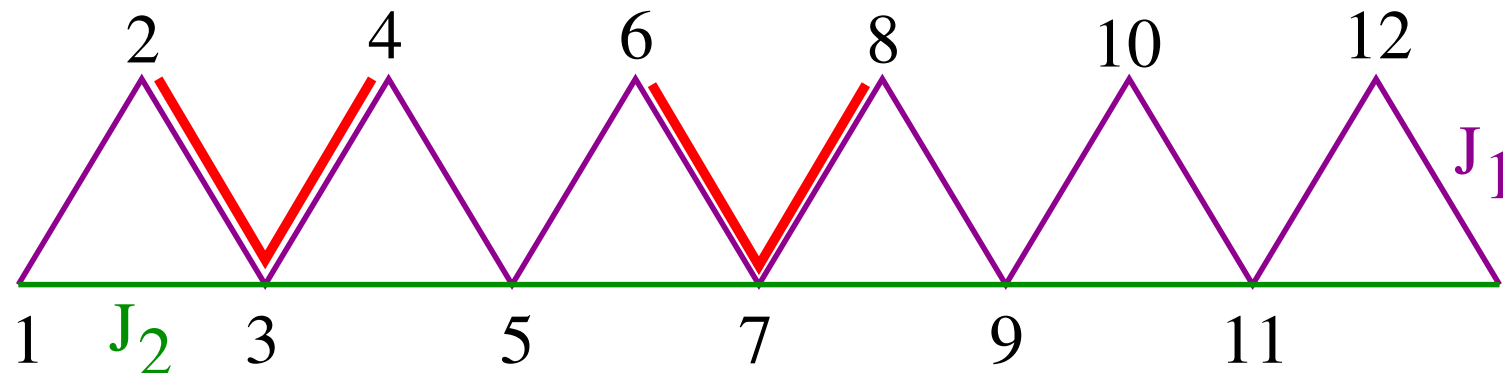
$\Rightarrow$ Can be everywhere. Flat band in one-magnon space. Degenerate with $|F\rangle$.

(1) V. Y. Krivnov, D. V. Dmitriev, S. Nishimoto, S.-L. Drechsler, and J. Richter, Phys. Rev. B **90**, 014441 (2014).

(2) D. V. Dmitriev and V. Y. Krivnov, Phys. Rev. B **92**, 184422 (2015).

(3) D. V. Dmitriev and V. Y. Krivnov, J. Richter, J. Schnack, Phys. Rev. B **99**, 094410 (2019)

Excursus: sawtooth (delta) chain

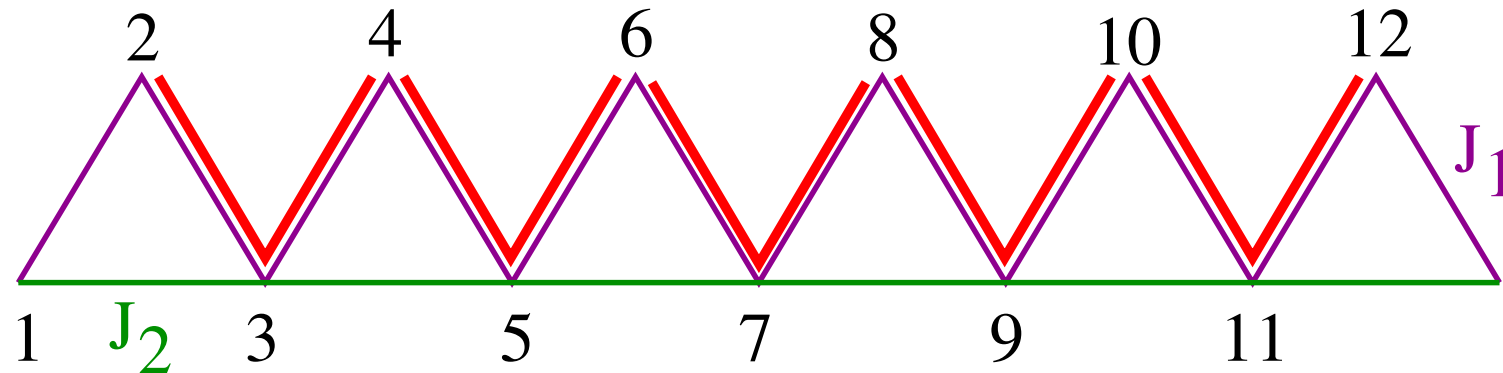


$\Rightarrow | 2 \text{ localized magnons} \rangle; E = E_F, M = S_{\max} - 2$

$\Rightarrow$ Can be everywhere. Flat band in two-magnon space. Degenerate with $| F \rangle$.

- (1) V. Y. Krivnov, D. V. Dmitriev, S. Nishimoto, S.-L. Drechsler, and J. Richter, Phys. Rev. B **90**, 014441 (2014).
- (2) D. V. Dmitriev and V. Y. Krivnov, Phys. Rev. B **92**, 184422 (2015).
- (3) D. V. Dmitriev and V. Y. Krivnov, J. Richter, J. Schnack, Phys. Rev. B **99**, 094410 (2019)

Excursus: sawtooth (delta) chain



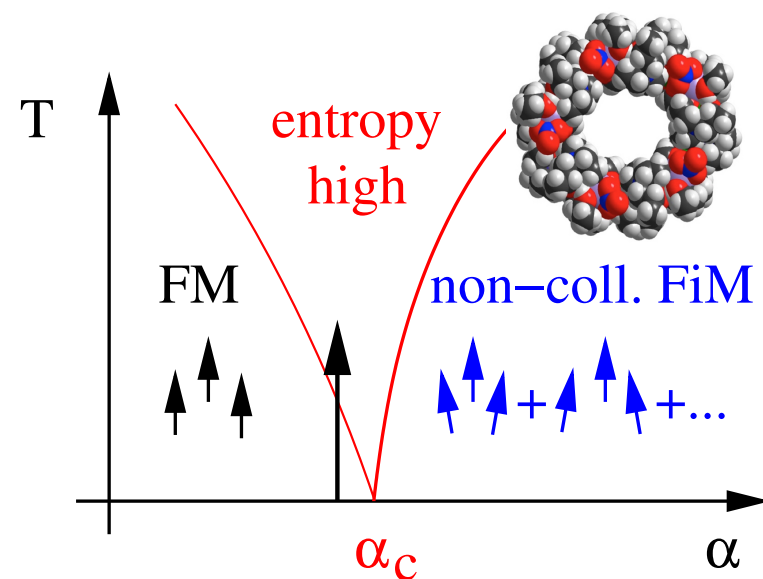
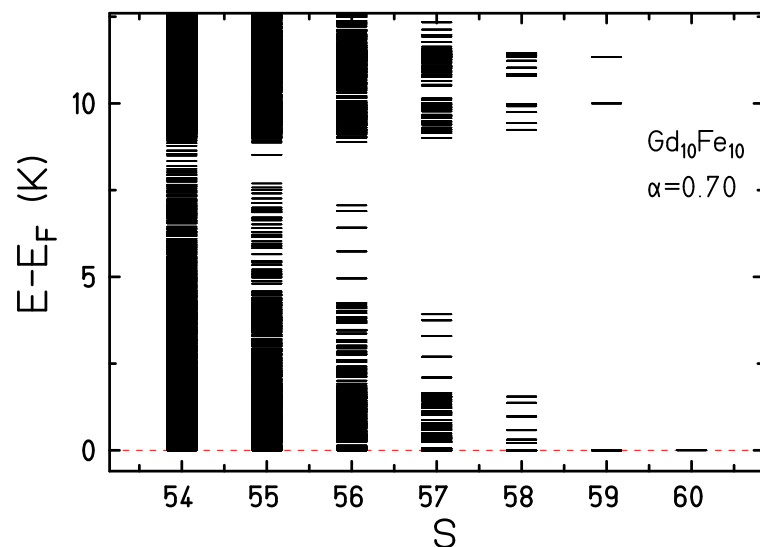
⇒ | max. number of localized magnons $\rangle$; $E = E_F$, $M = S_{\max} - N/2$

⇒ Macroscopic number of localized magnons. Degenerate with $|F\rangle$.

⇒ Extensive entropy.

- (1) V. Y. Krivnov, D. V. Dmitriev, S. Nishimoto, S.-L. Drechsler, and J. Richter, Phys. Rev. B **90**, 014441 (2014).
- (2) D. V. Dmitriev and V. Y. Krivnov, Phys. Rev. B **92**, 184422 (2015).
- (3) D. V. Dmitriev and V. Y. Krivnov, J. Richter, J. Schnack, Phys. Rev. B **99**, 094410 (2019)

Gd₁₀Fe₁₀ – QCP



⇒ for $s_1 = 5/2$ and $s_2 = 7/2$: $\alpha_c = 0.70$

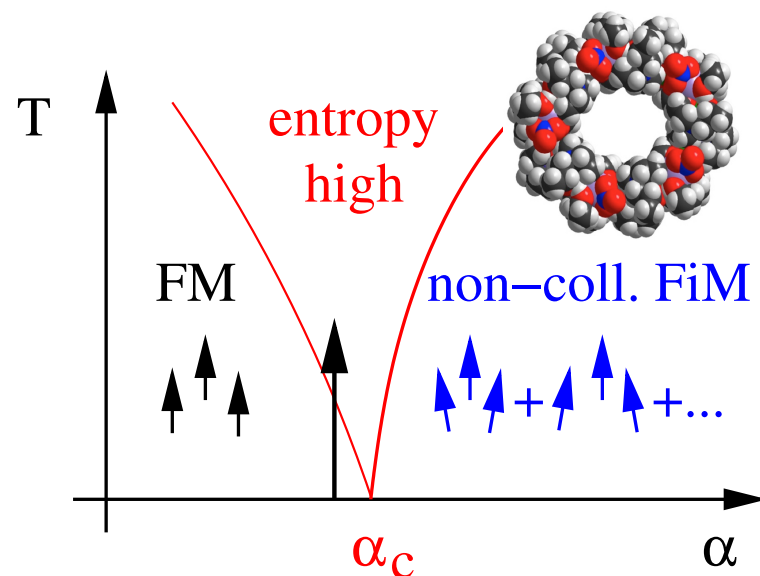
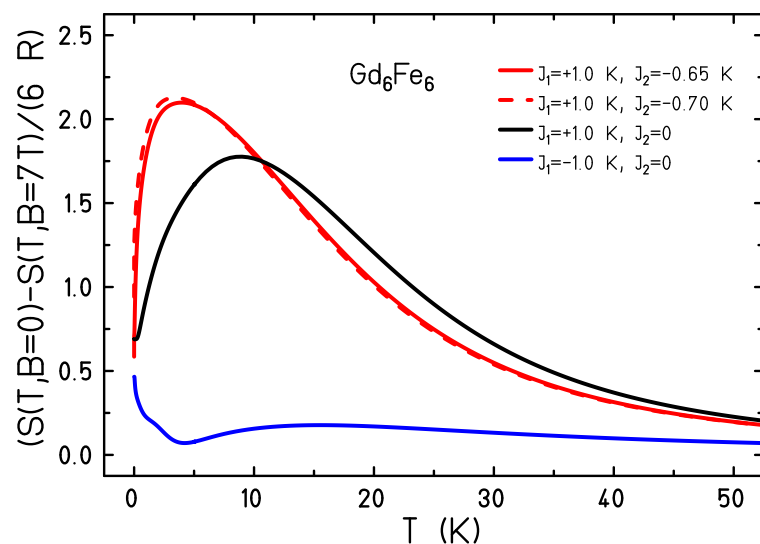
⇒ as function of α Quantum Phase Transition at α_c
 from $S = 60$ ground state to ground state with $S = 54$.
 ($\Delta S = N/4 + 1$ in general)

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Quantum Phase Transition

Non-analytic behavior of thermodynamic functions at $T = 0$ for variation of another external parameter, e.g. field, pressure; here α – maybe varied by pressure.

Gd₁₀Fe₁₀ – $T > 0$

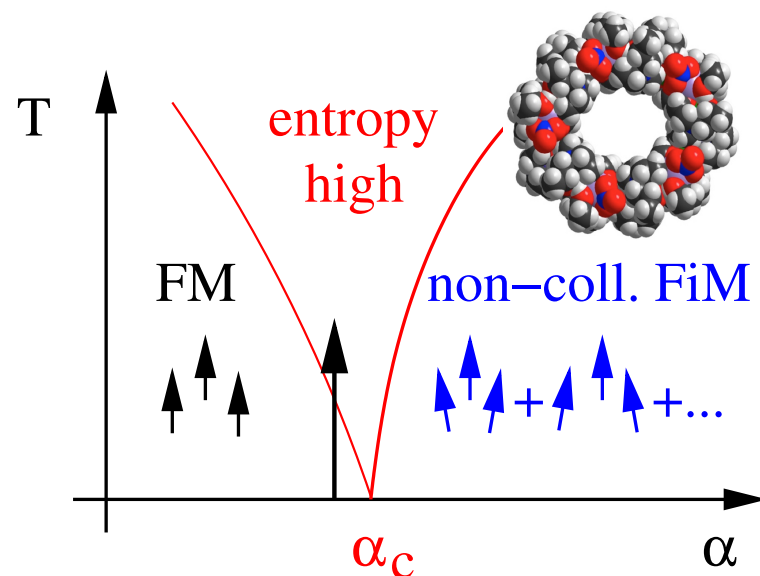
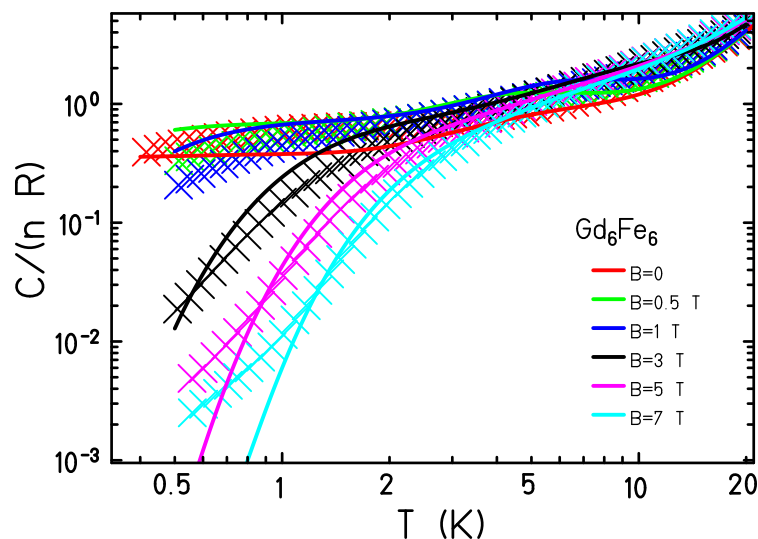


⇒ although QPT and QCP at $T = 0$,
noticeable at elevated temperatures (arrow);

⇒ **example isothermal entropy change:**
little difference between $\alpha = 0.70$ and $\alpha = 0.65$.

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Gd₁₀Fe₁₀ – heat capacity



⇒ heat capacity assumes very large values even down to lowest temperatures;

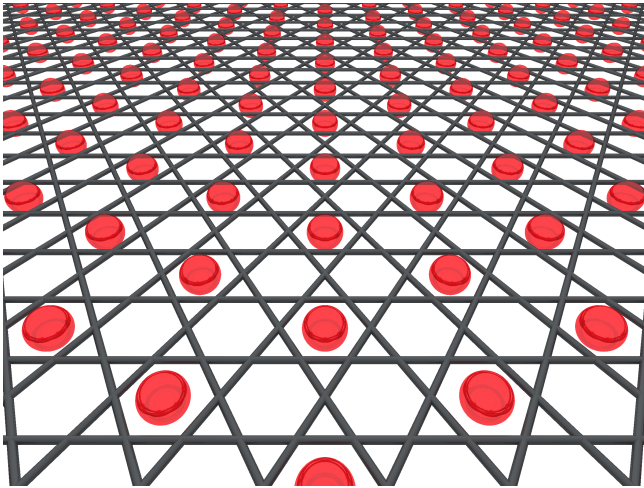
⇒ evaluated by means of FTLM for a smaller (hypothetical) system Gd₆Fe₆;

⇒ magnetic field separates $S = 60$ ground state, C drops.

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Kagome lattice antiferromagnet

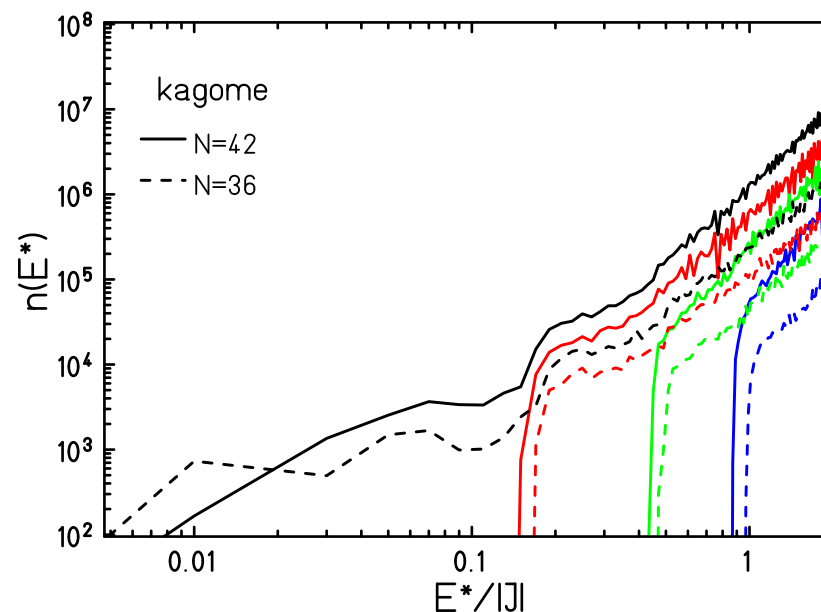
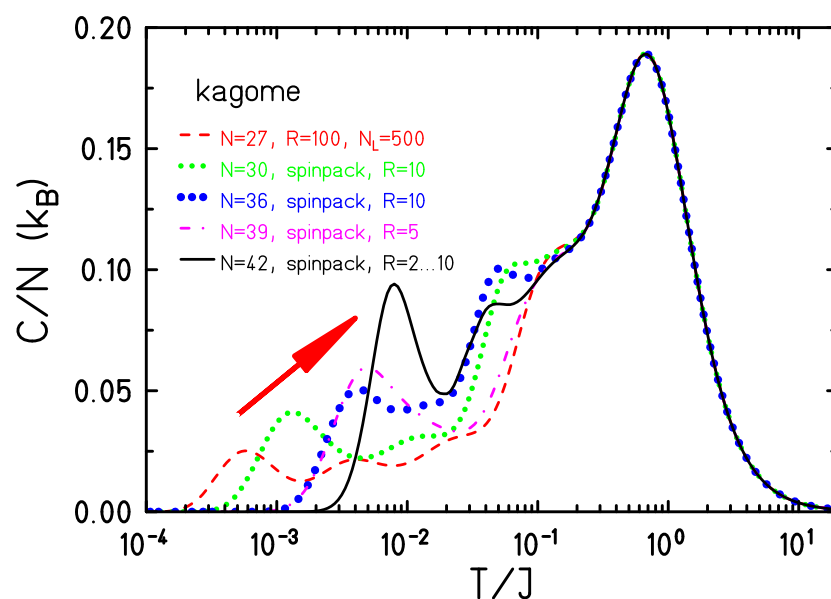
Kagome lattice antiferromagnet – scientific problems



- Thermodynamic functions, in particular heat capacity and susceptibility
- “Condensation” of low-lying singlets below the first triplet?
- Magnetization jump to saturation
- Thermal stability of magnetization plateaus, e.g. at $\mathcal{M}_{\text{sat}}/3$.
- Crystallization of localized magnons?

J. Schnack, J. Schulenburg, J. Richter, Phys. Rev. B **98**, 094423 (2018)

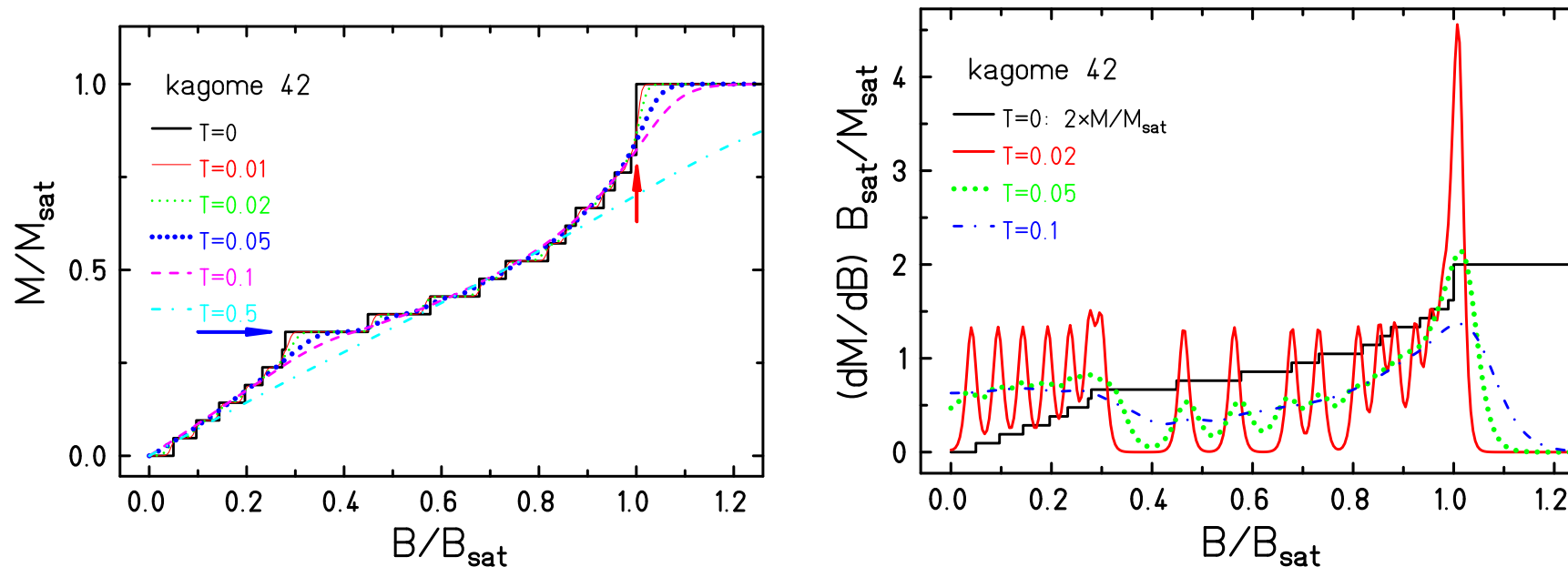
Kagome 42 – heat capacity



- Low- T peak moves to higher T with increasing N .
- Density of low-lying singlets seems to move to higher excitation energies.

J. Schnack, J. Schulenburg, J. Richter, Phys. Rev. B **98**, 094423 (2018)

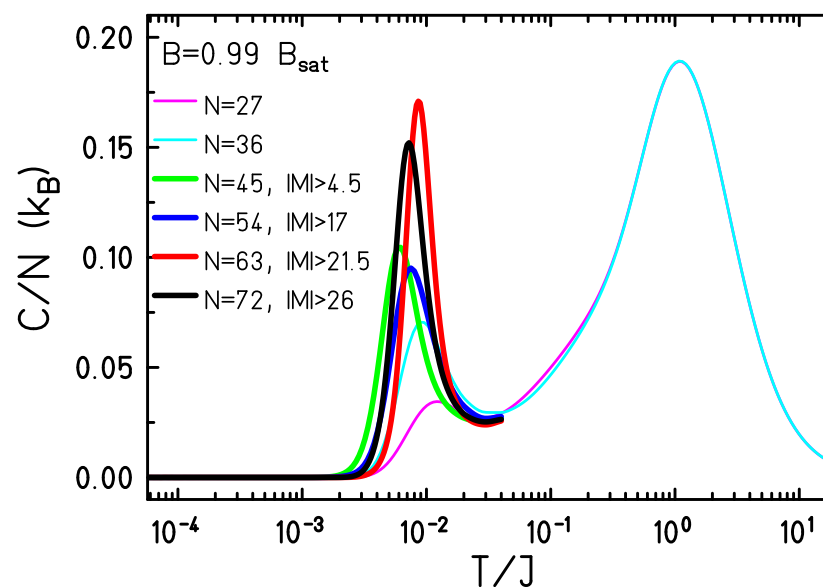
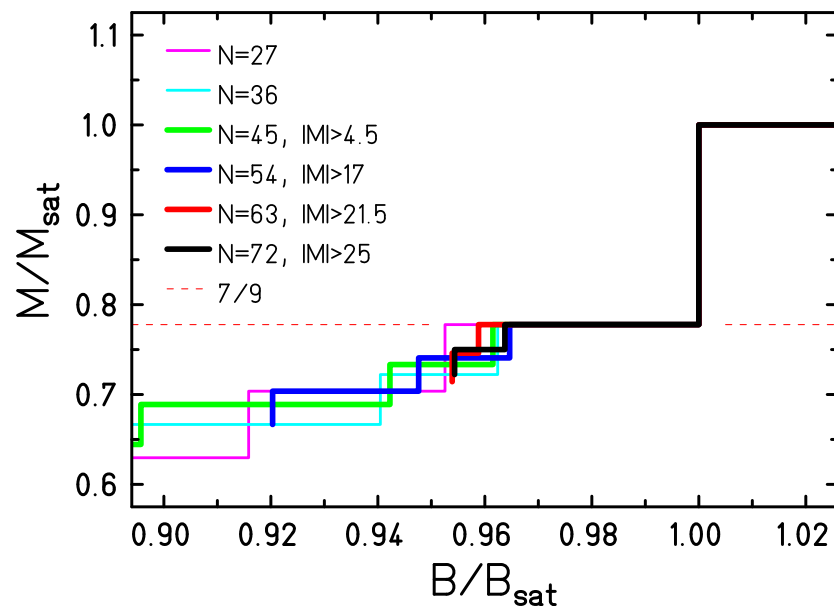
Kagome 42 – magnetization



- Plateaus and jump; asymmetric melting of the plateau at $M_{\text{sat}}/3$.

- (1) S. Capponi, O. Derzhko, A. Honecker, A. M. Laeuchli, J. Richter, Phys. Rev. B **88**, 2 144416 (2013).
- (2) J. Schulenburg, A. Honecker, J. Schnack, J. Richter, H.-J. Schmidt, Phys. Rev. Lett. **88**, 167207 (2002).
- (3) H. Nakano and T. Sakai, J. Phys. Soc. Jpn. **83**, 104710 (2014).

Kagome 42 – magnonon crystallization

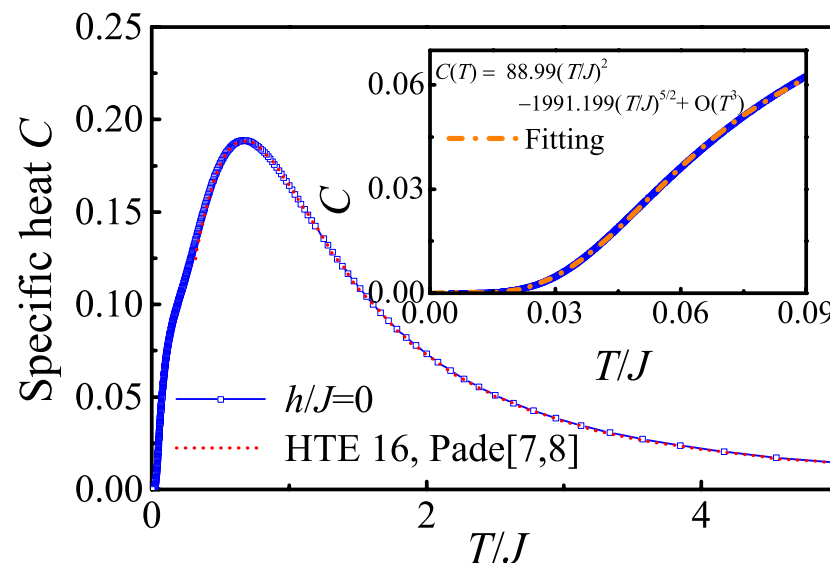
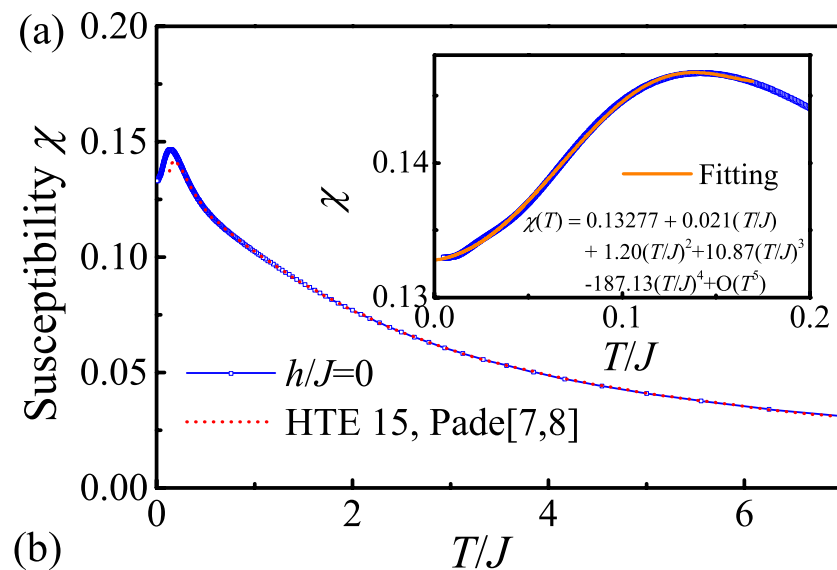


- Phase transition similar to two-dimensional three-state Potts model.

J. Schnack, J. Schulenburg, A. Honecker, J. Richter, arXiv:1910.10448

Is 42 the final answer?

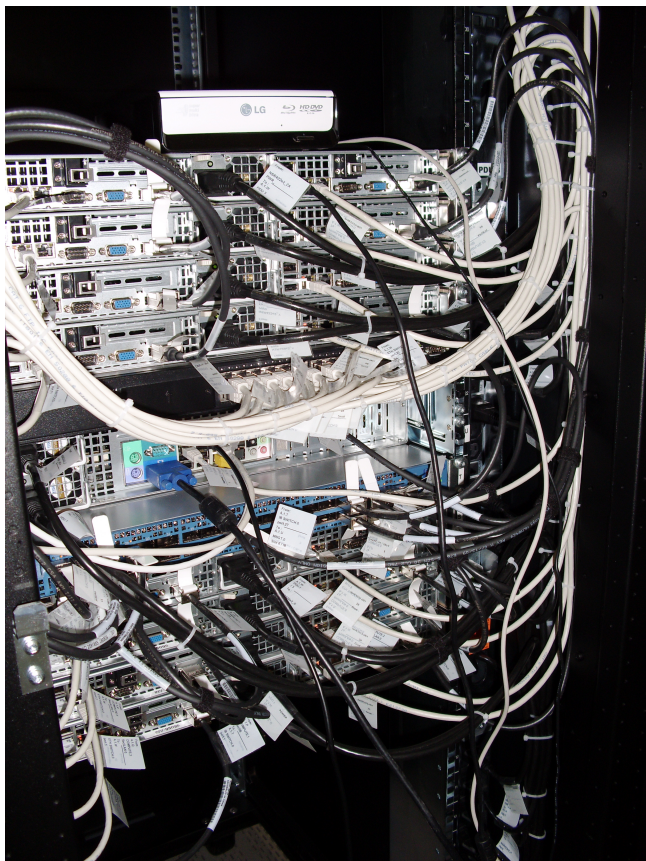
Kagome – tensor network calculations



- Tensor network calculations for the infinite system (1).

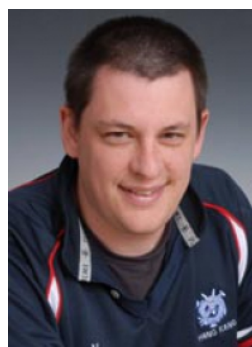
(1) Xi Chen, Shi-Ju Ran, Tao Liu, Cheng Peng, Yi-Zhen Huang, Gang Su, Science Bulletin **63**, 1545 (2018).

Summary



- Magnetic molecules for storage, q-bits, MCE, and since they are nice.
- Molecules taught us about frustrated systems.
- Isentropes for interacting systems are much richer than for paramagnets. Good for applications away from $(T = 0, B = 0)$.
- Quantum phase transitions may allow barocaloric applications.
- ED, HTE, CMC, QMC, FTLM, DMRG, DDMRG, thDMRG for magnetic molecules.

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Thank you very much for your
attention.

The end.

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