Magnetism of free and deposited magnetic molecules

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UNIVERSITÄT BIELEFELD
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Irz

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.

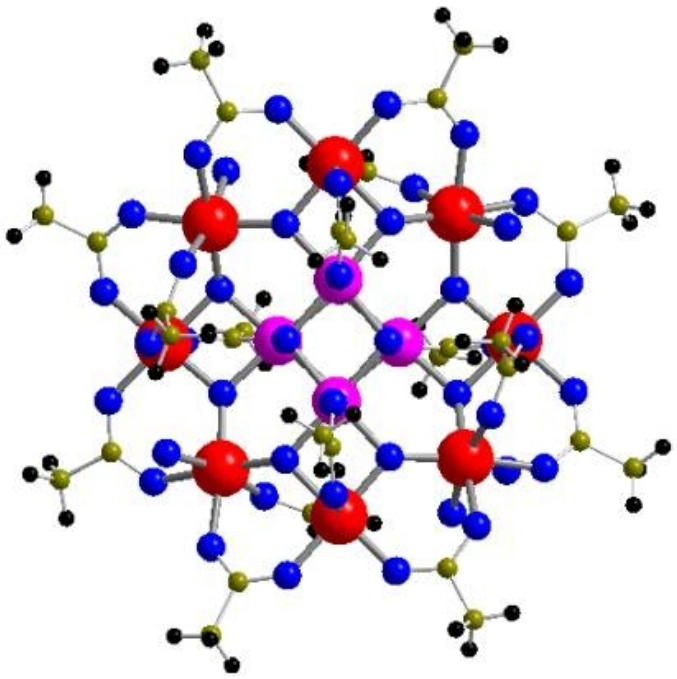
The origins of and reasons for this conspiracy are not a part of the original theory. Speculated originators jokingly include the CIA, Mossad, or aliens who use Bielefeld University as a disguise for their spaceship.

Do you know anybody from Bielefeld?

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

Beauty of Magnetic Molecules

The beauty of magnetic molecules I

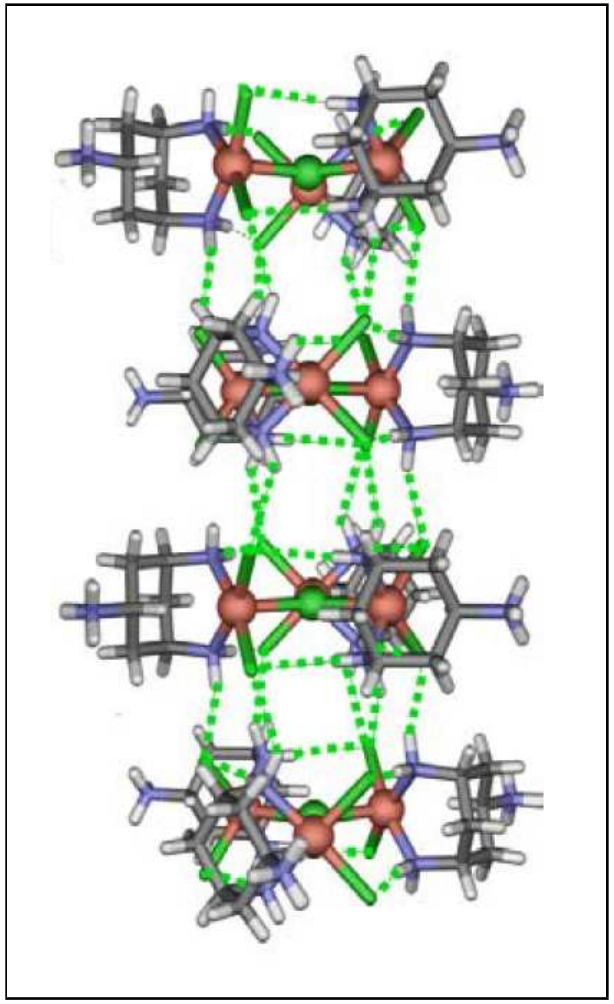


Mn_{12}

- Inorganic or organic macro molecules, e.g. polyoxometalates, where paramagnetic ions such as Iron (Fe), Chromium (Cr), Copper (Cu), Nickel (Ni), Vanadium (V), Manganese (Mn), or rare earth ions are embedded in a host matrix;
- Pure organic magnetic molecules: magnetic coupling between high spin units (e.g. free radicals);
- Single spin quantum number $1/2 \leq s \leq 7/2$;
- Intermolecular interaction relatively small, therefore measurements reflect the thermal behaviour of a single molecule.

Magnetism goes Nano, Ed. Stefan Blügel, Thomas Brückel, and Claus M. Schneider, FZ Jülich, Institute of Solid State Research, Lecture Notes **36** Jülich 2005

The beauty of magnetic molecules II



- Dimers (Fe_2), tetrahedra (Cr_4), cubes (Cr_8);
- Rings, especially iron rings (Fe_6, Fe_8, Fe_{10}, . . .);
- Complex structures (Mn_{12}) – drosophila of molecular magnetism;
- “Soccer balls”, more precisely icosidodecahedra (Fe_{30}) and other macro molecules;
- Chain like and planar structures of interlinked magnetic molecules, e.g. triangular Cu chain:

  J. Schnack, H. Nojiri, P. Kögerler, G. J. T. Cooper, L. Cronin, Phys. Rev. B 70, 174420 (2004)

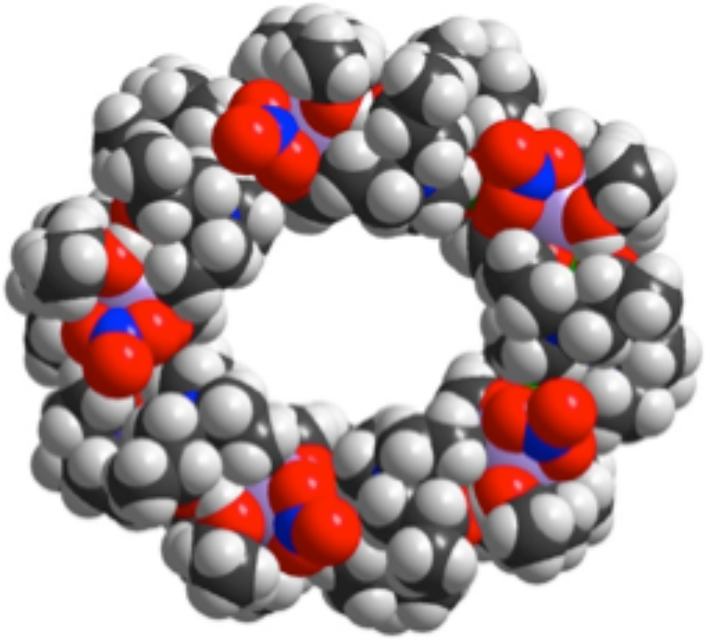
Contents for you today

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

1. Typicality-based estimates
2. The magnetocaloric effect
3. A quantum phase transition
4. Deposited molecules
5. Finite-Temperature Lanczos for anisotropic systems

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

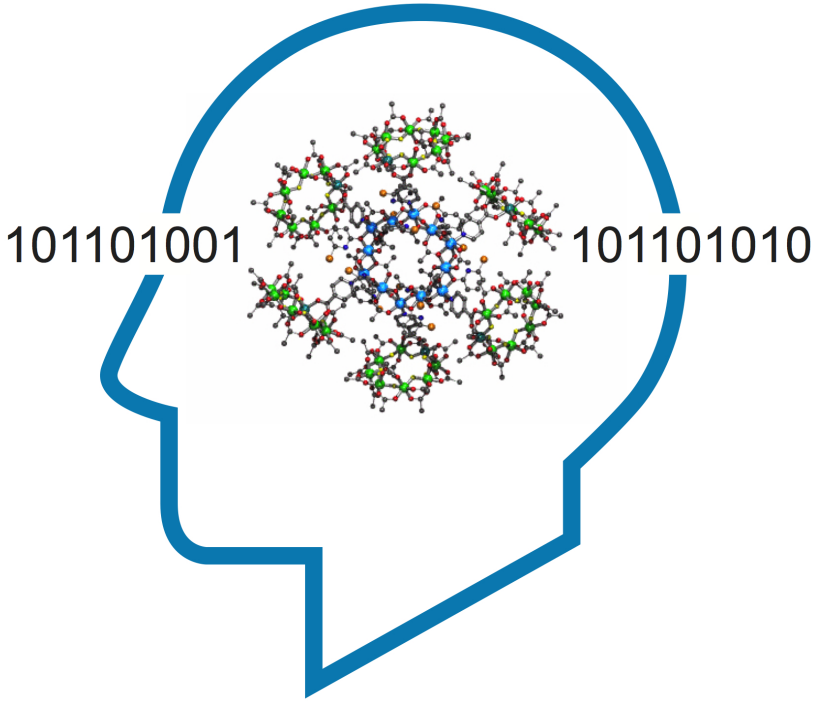
You have got a molecule!



$S = 60$!

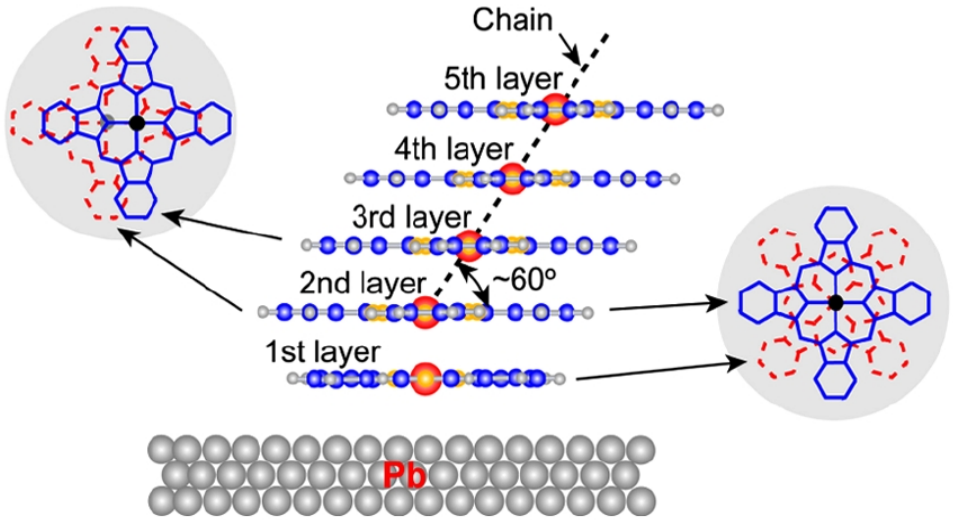
Congratulations!

You want to build a quantum computer!



Very smart!

You want to deposit your molecule!

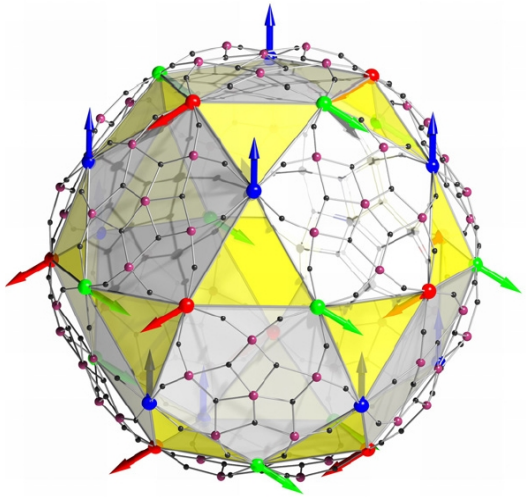


Next generation magnetic storage!

You have got an idea about the modeling!

$$\underset{\sim}{H} = -2\sum_{i<j} J_{ij}\,\underset{\sim}{\vec{s}}(i)\cdot\underset{\sim}{\vec{s}}(j) + g\,\mu_B\,B\sum_{i}^{N}\underset{\sim}{s}_z(i)$$

Heisenberg Zeeman



Frustration effects!

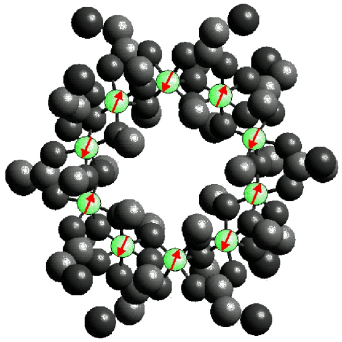
You have to solve the Schrödinger equation!

$$\underset{\sim}{H} \left| \phi_n \right\rangle = E_n \left| \phi_n \right\rangle$$

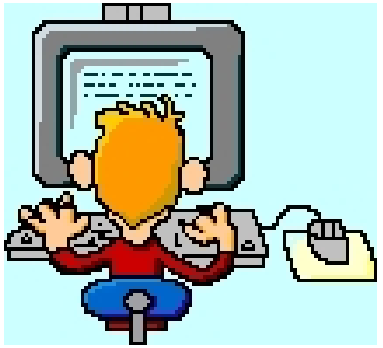
Eigenvalues E_n and eigenvectors $\left| \phi_n \right\rangle$

- 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!



$$\Rightarrow \begin{pmatrix} -27.8 & 3.46 & 0.18 & \cdots \\ 3.46 & -2.35 & -1.7 & \cdots \\ 0.18 & -1.7 & 5.64 & \cdots \\ \vdots & \vdots & \vdots & \cdots \end{pmatrix} \Rightarrow$$



Fe^{III}_{10}: $N = 10, s = 5/2$

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

Can we evaluate the partition function

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

without diagonalizing the Hamiltonian?

Solution I: trace estimators

$$\mathrm{tr}\left(\underset{\sim}{Q}\right) \approx \langle r | \underset{\sim}{Q} | r \rangle$$

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

- $|\nu\rangle$ some orthonormal basis of your choice;
  not the eigenbasis of $\underset{\sim}{Q}$, 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

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

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

$$\underset{\sim}{1}\,|\,r\,\rangle, \quad \underset{\sim}{H}\,|\,r\,\rangle, \quad \underset{\sim}{H}^2\,|\,r\,\rangle, \quad \ldots \underset{\sim}{H}^{N_L-1}\,|\,r\,\rangle\,.$$

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

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

Partition function I: simple approximation

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

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

- 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

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

- 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: $R = 1\ldots 100, N_L \approx 100$.

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

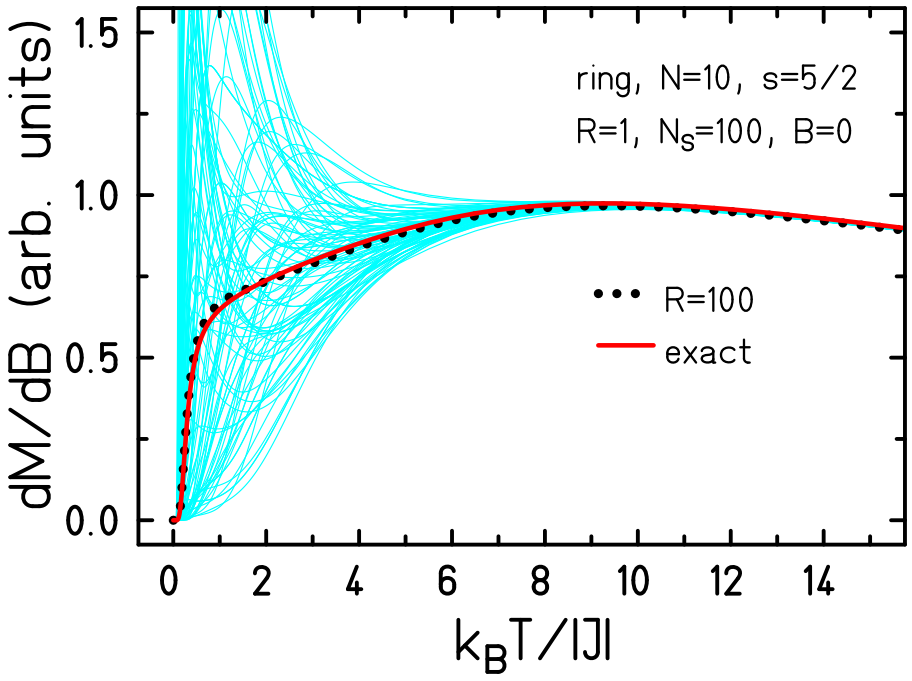
Partition function III: use symmetries if you can

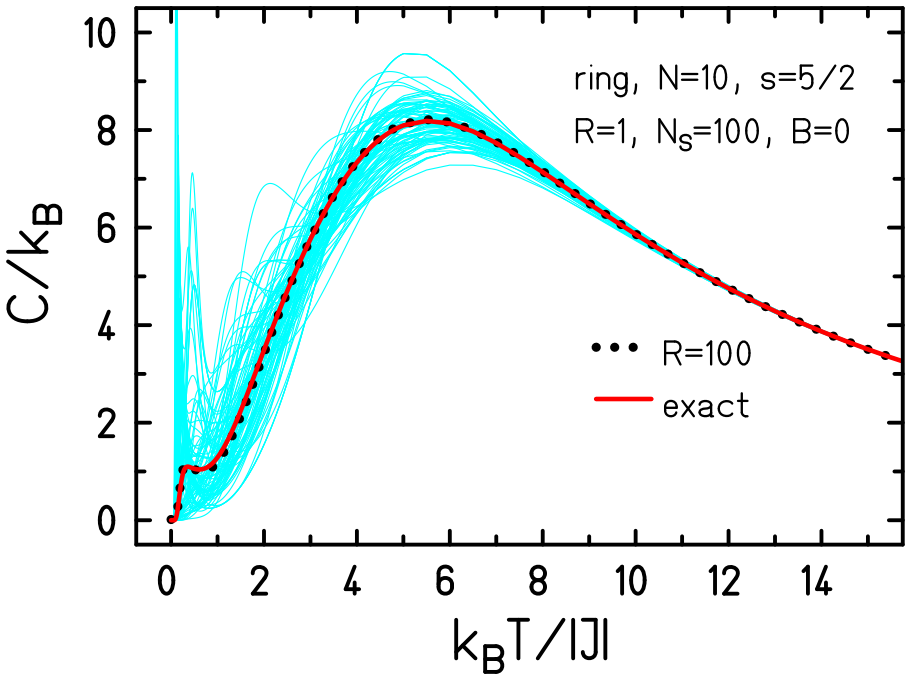
$$Z^{\mathsf{FTLM}}(T,B) \approx \sum_{\gamma=1}^{\Gamma} \frac{1}{R} \sum_{r=1}^{R} \sum_{n=1}^{N_L} e^{-\beta\epsilon_n^{(r)}} |\langle\, n(r) \,|\, r \,\rangle|^2$$

- 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

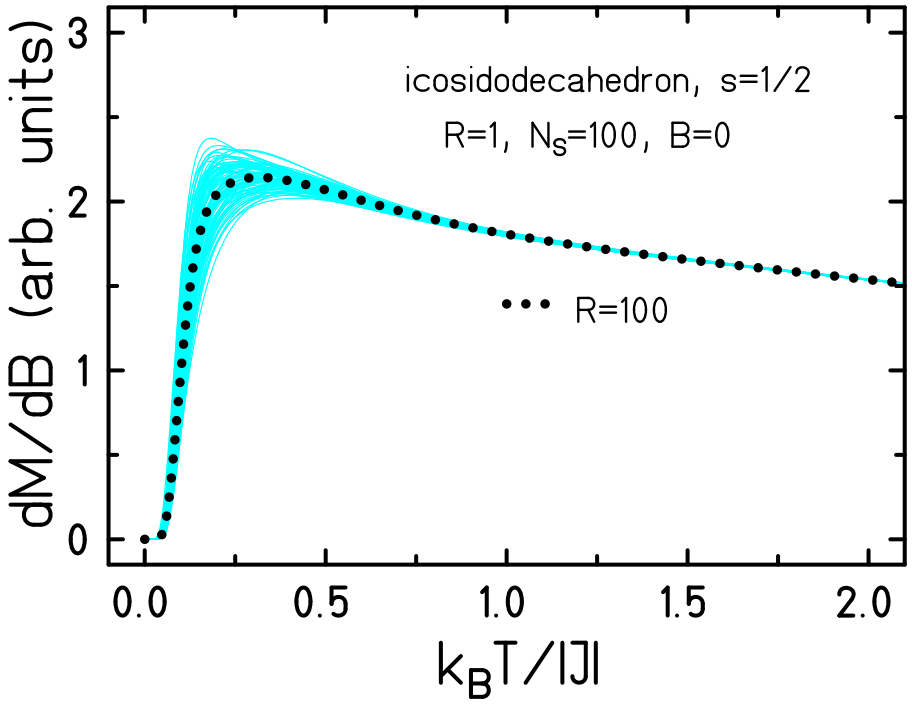
FTLM 1: ferric wheel

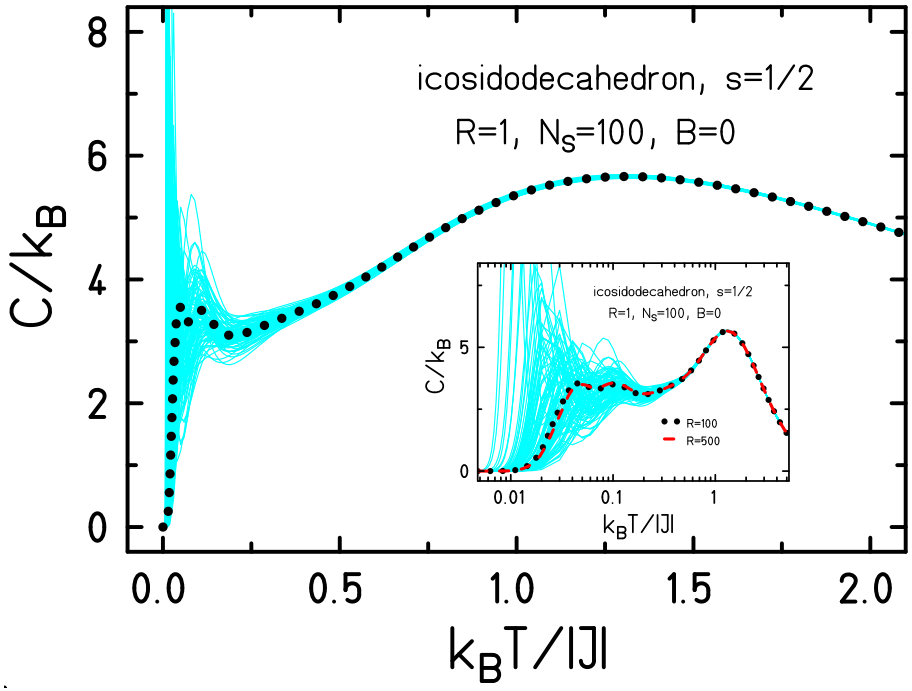




J. Schnack, J. Richter, R. Steinigeweg, arXiv:1911.08838

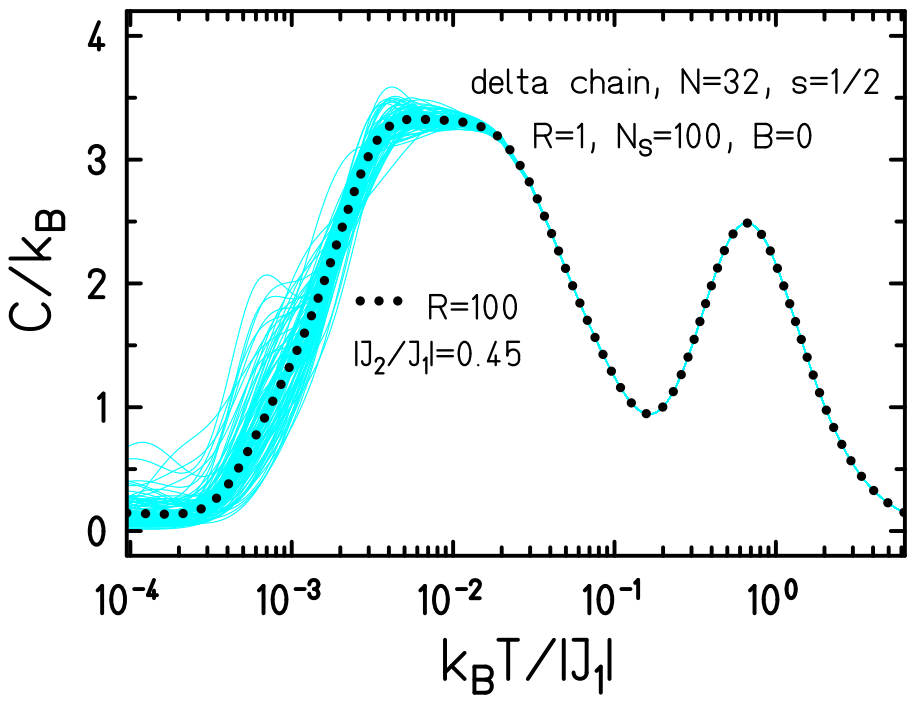
FTLM 2: icosidodecahedron

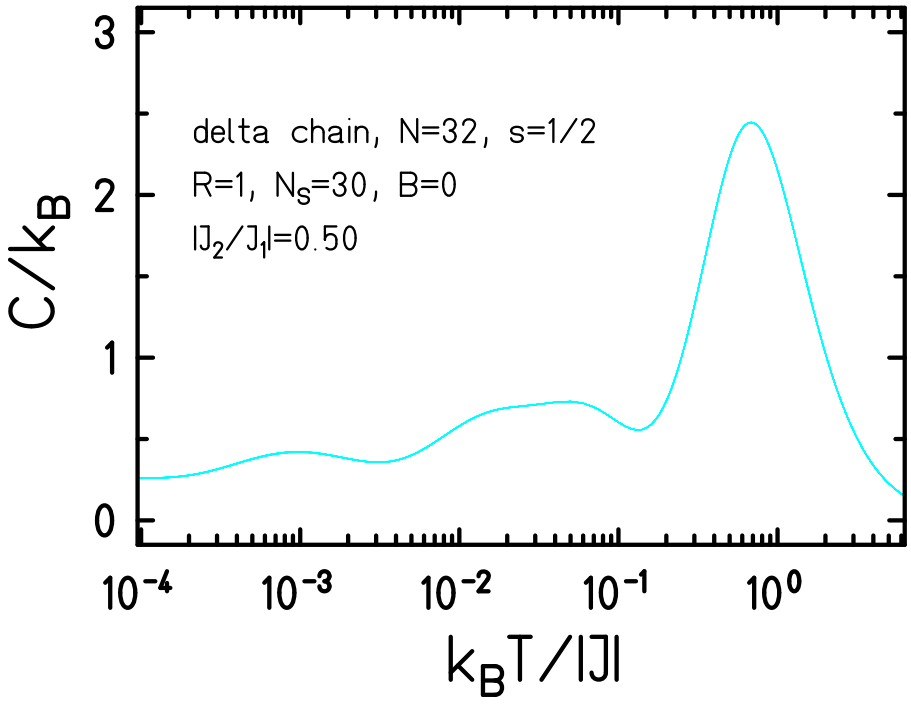




J. Schnack, J. Richter, R. Steinigeweg, arXiv:1911.08838

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.

J. Schnack, J. Richter, R. Steinigeweg, arXiv:1911.08838,
J. Schnack, J. Richter, T. Heitmann, J. Richter, R. Steinigeweg, arXiv:2002.00411

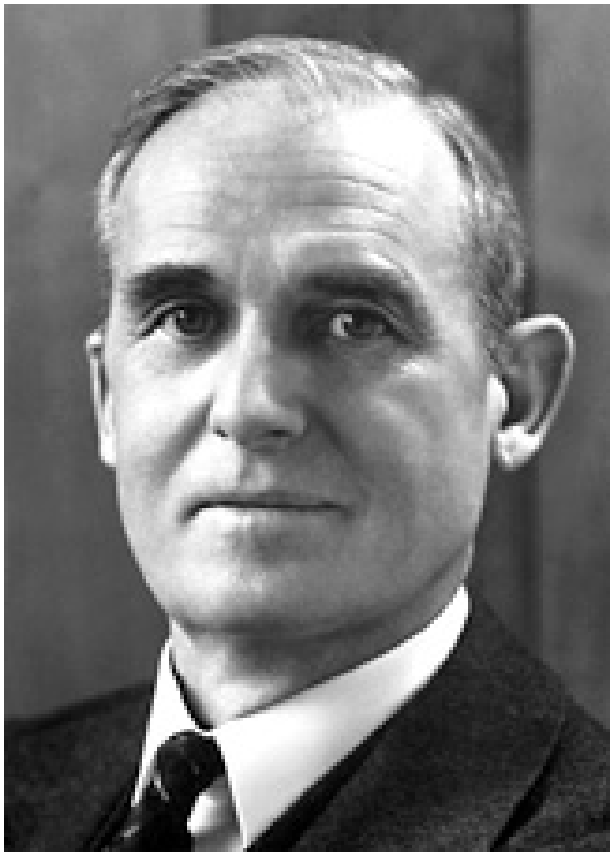
The magnetocaloric effect

Magnetocaloric effect – Basics

- Heating or cooling in a varying magnetic field. Predicted, discussed, discovered by Thomson, Warburg, Weiss, and Piccard (1).
- Typical rates: $0.5 \ldots 2$ K/T.
- Giant magnetocaloric effect: $3 \ldots 4$ K/T e.g. in $Gd_5(Si_xGe_{1-x})_4$ 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. Giauque *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

Attainment of Temperatures Below 1° Absolute by Demagnetization of $Gd_2(SO_4)_3 \cdot 8H_2O$

We have recently carried out some preliminary experiments on the adiabatic demagnetization of $Gd_2(SO_4)_3 \cdot 8H_2O$ 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 $Gd_2(SO_4)_3 \cdot 8H_2O$ 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.

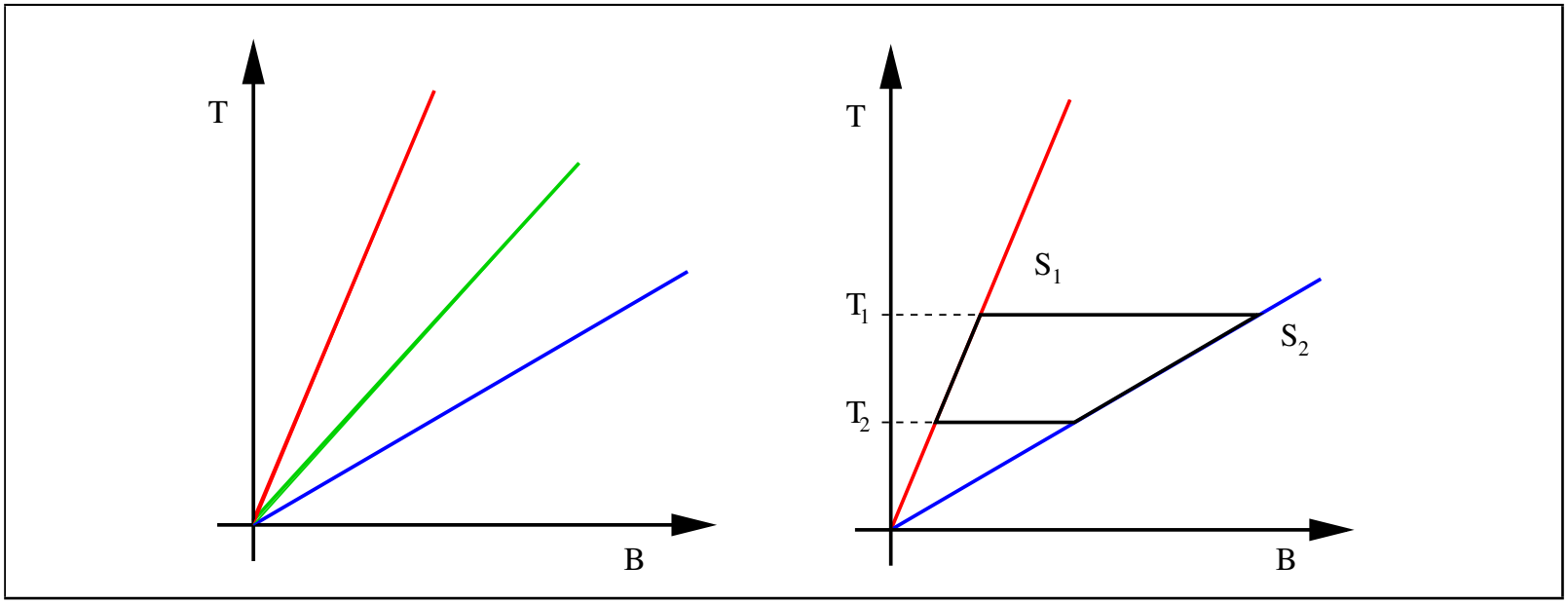
It is apparent that it will be possible to obtain much lower temperatures, especially when successive demagnetizations are utilized.

W. F. GIAUQUE
D. P. MACDOUGALL

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

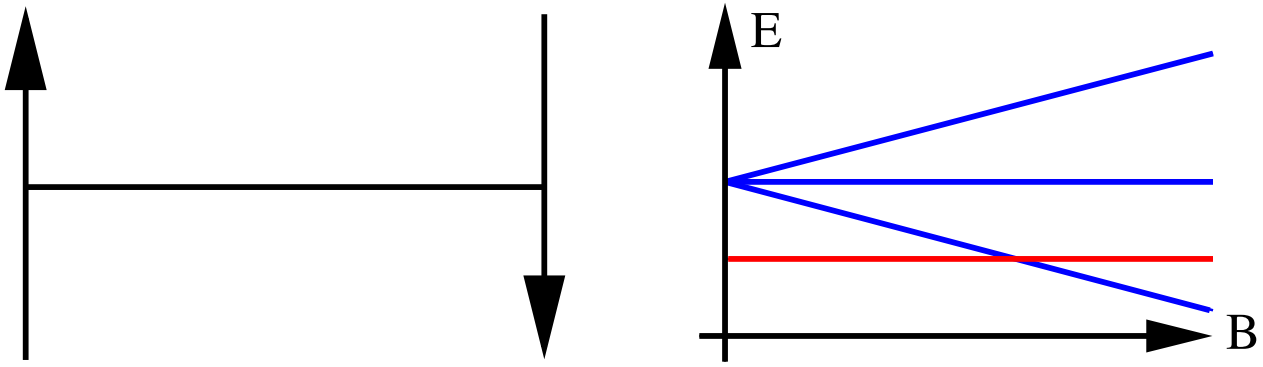
W. F. Giauque and D. MacDougall, Phys. Rev. **43**, 768 (1933).

Magnetocaloric effect – Paramagnets



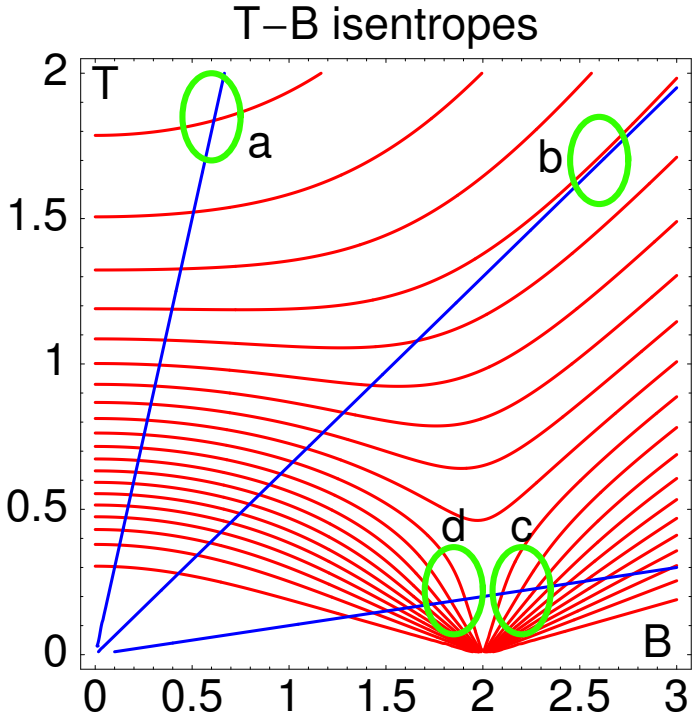
- Ideal paramagnet: $S(T,B) = f(B/T)$, i.e. $S = const \Rightarrow T \propto B$.
- At low T pronounced effects of dipolar interaction prevent further effective cooling.

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; $\quad S(T = 0, B_c) = k_B \ln 2$, otherwise zero.

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



blue lines: ideal paramagnet, red curves: af dimer

Magnetocaloric effect:

(a) reduced,

(b) the same,

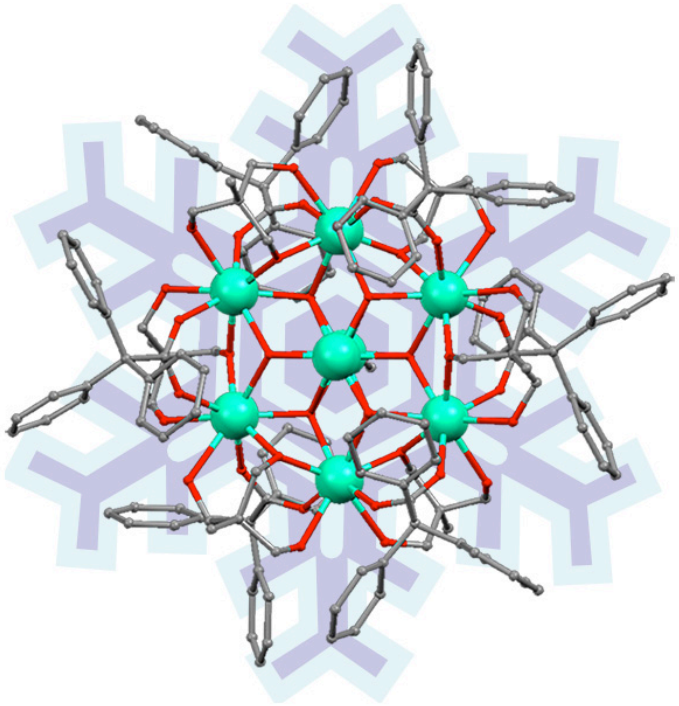
(c) enhanced,

(d) opposite

when compared to an ideal paramagnet.

Case (d) does not occur for a paramagnet.

Gd$_7$ – Basics

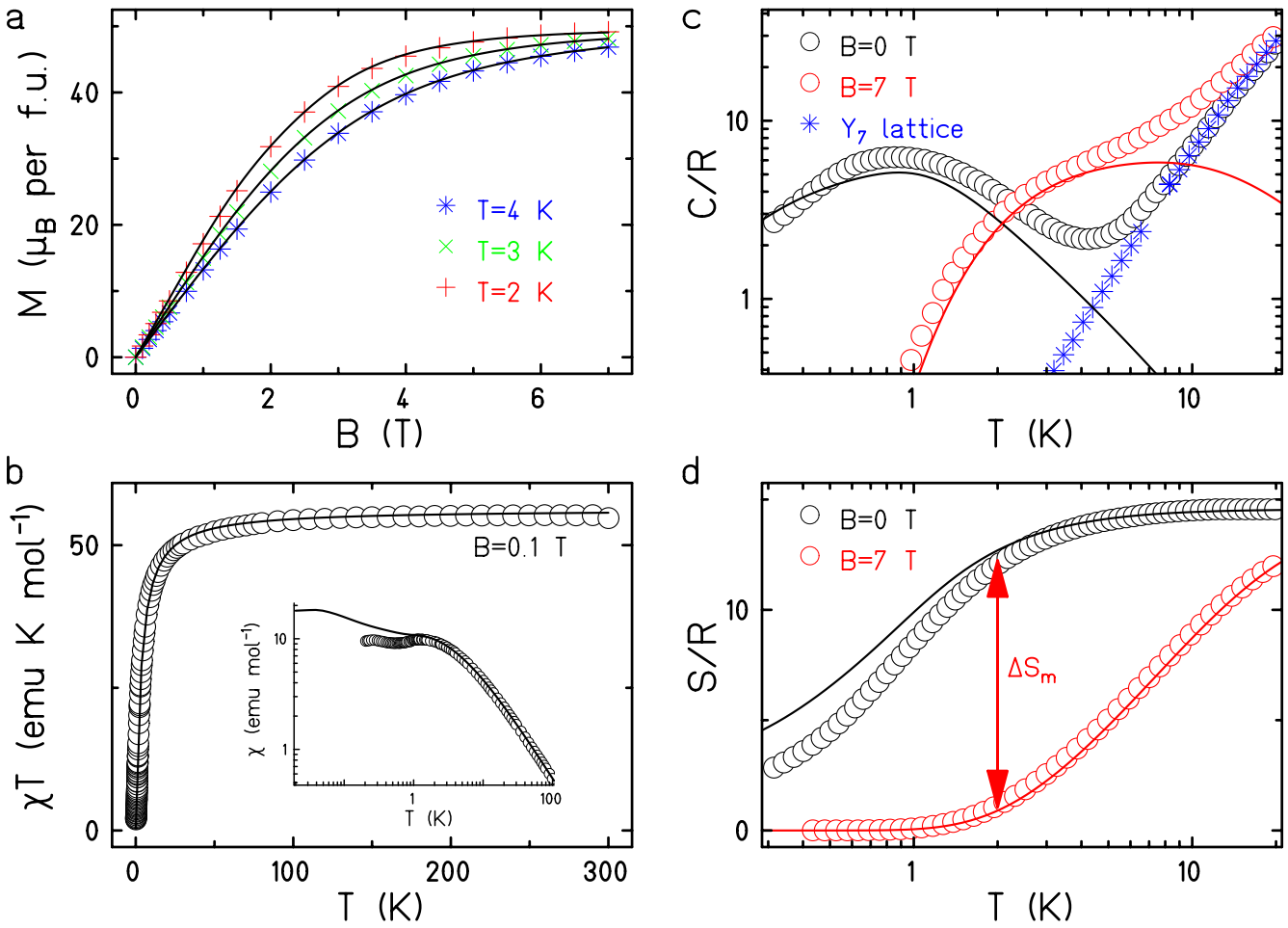


- Often magnetocaloric observables not directly measured, but inferred from Maxwell's relations.
- First real cooling experiment with a molecule.
- $\underset{\sim}{H} = -2 \sum_{i<j} J_{ij}\, \underset{\sim}{\vec{s}}_i \cdot \underset{\sim}{\vec{s}}_j + g\,\mu_B\, B \sum_i^N \underset{\sim}{s}_i^z$

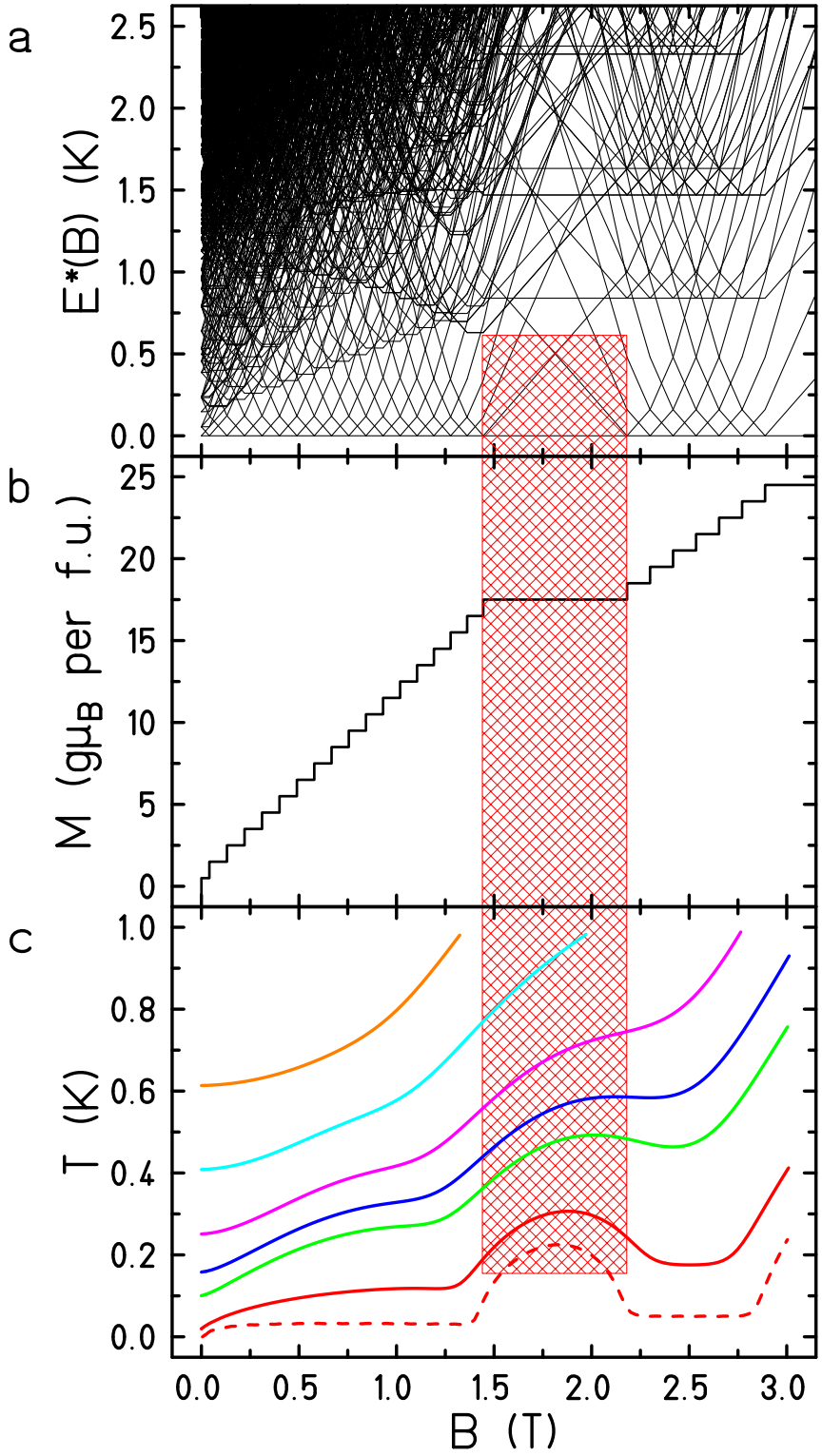
  $J_1 = -0.090(5)$ K, $J_2 = -0.080(5)$ K and $g = 2.02$.
- Very good agreement down to the lowest temperatures.

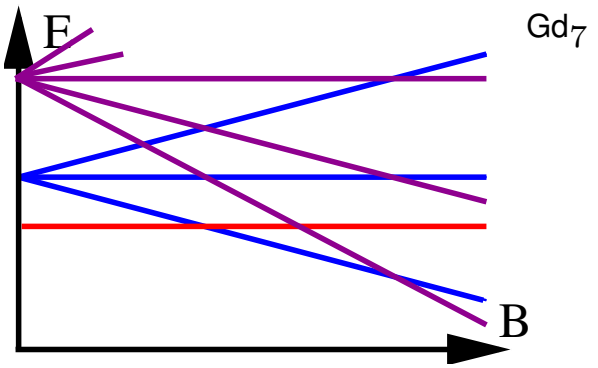
J. W. Sharples, D. Collison, E. J. L. McInnes, J. Schnack, E. Palacios, M. Evangelisti, Nat. Commun. **5**, 5321 (2014).

Gd$_7$ – experiment & theory

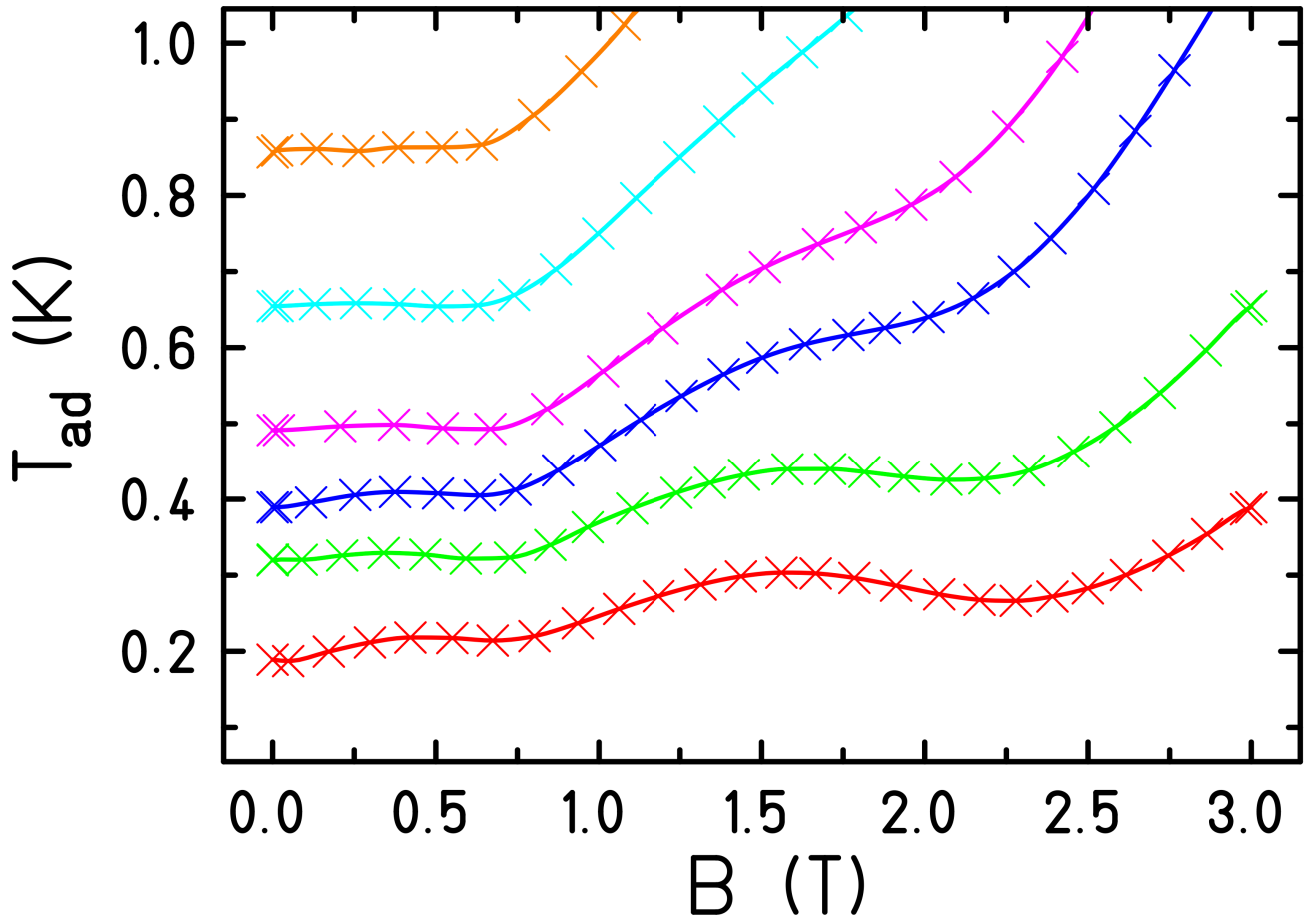


J. W. Sharples, D. Collison, E. J. L. McInnes, J. Schnack, E. Palacios, M. Evangelisti, Nat. Commun. **5**, 5321 (2014).


a
b
c
E*(B) (K)
M (gμB per f.u.)
T (K)
B (T)
0.0
0.5
1.0
1.5
2.0
2.5
3.0
0.2
0.4
0.6
0.8
5
10
15
20
25


E
B
Gd7

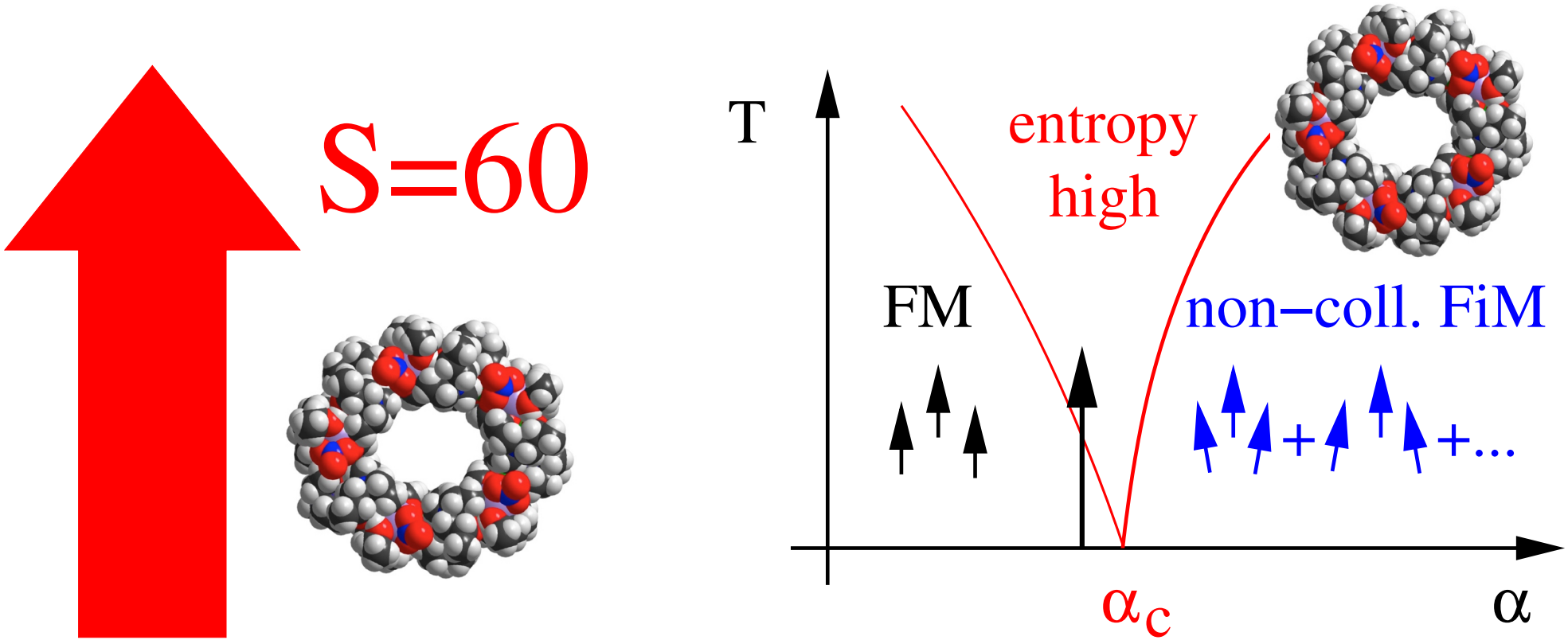
Gd$_7$ – Experimental cooling



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

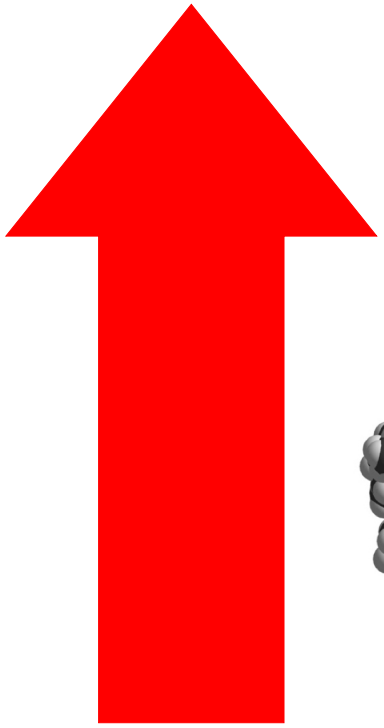
A quantum phase transition

$Gd_{10}Fe_{10}$ – summary

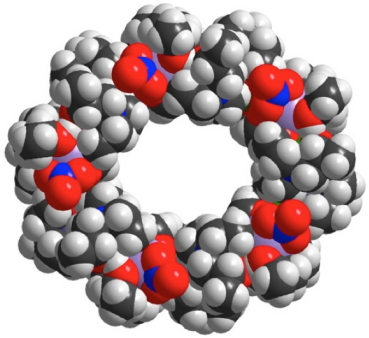


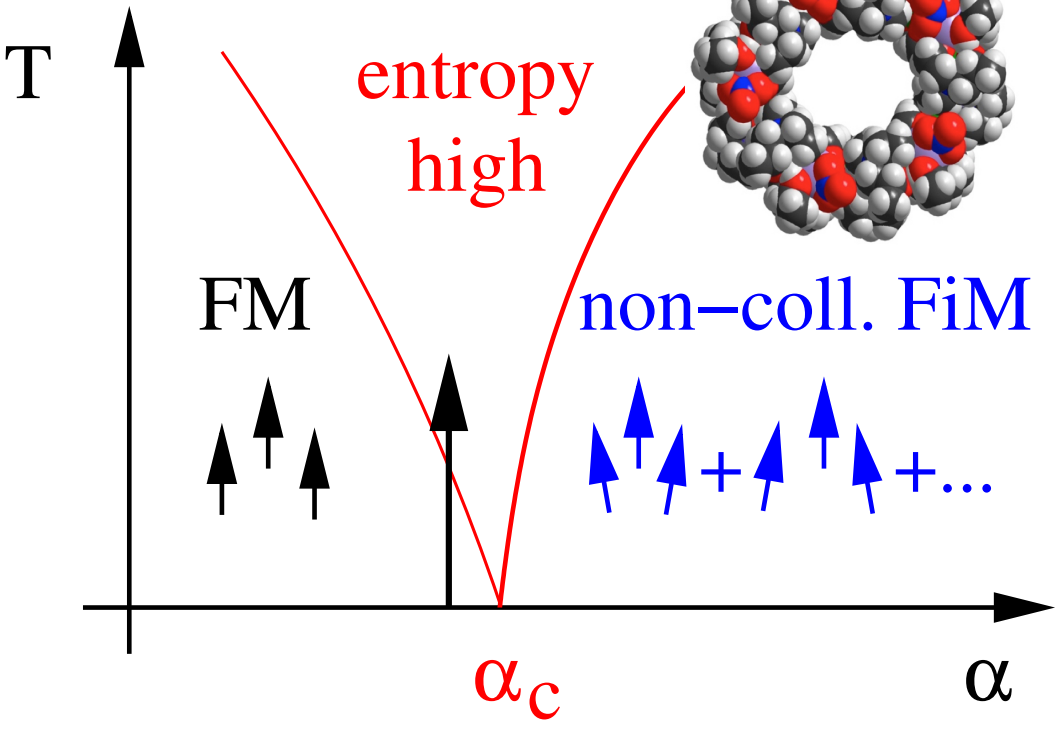
A. Baniodeh, N. Magnani, Y. Lan, G. Buth, C.E. Anson, J. Richter, M. Affronte, J. Schnack, A.K. Powell,
High Spin Cycles: Topping the Spin Record for a Single Molecule verging on Quantum Criticality,
npj Quantum Materials **3**, 10 (2018)

$Gd_{10}Fe_{10}$ – summary



S=60

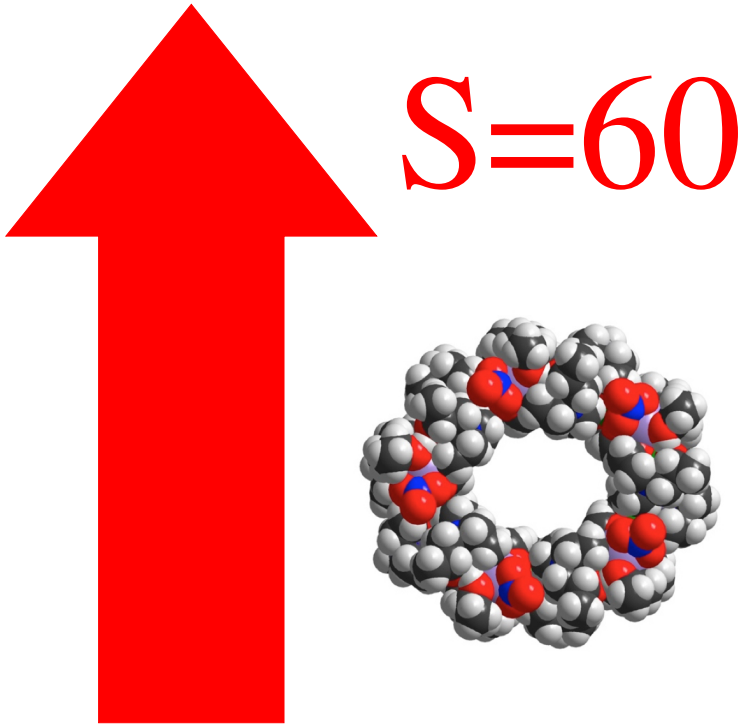


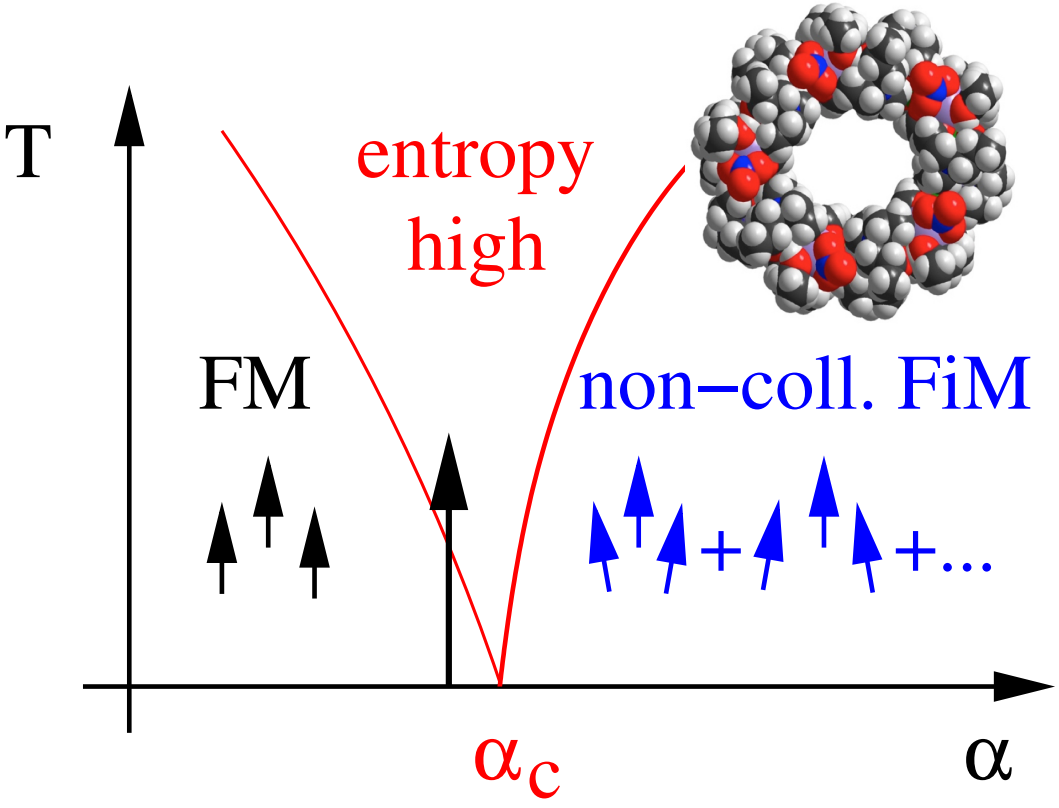


How do we know?

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

$Gd_{10}Fe_{10}$ – summary



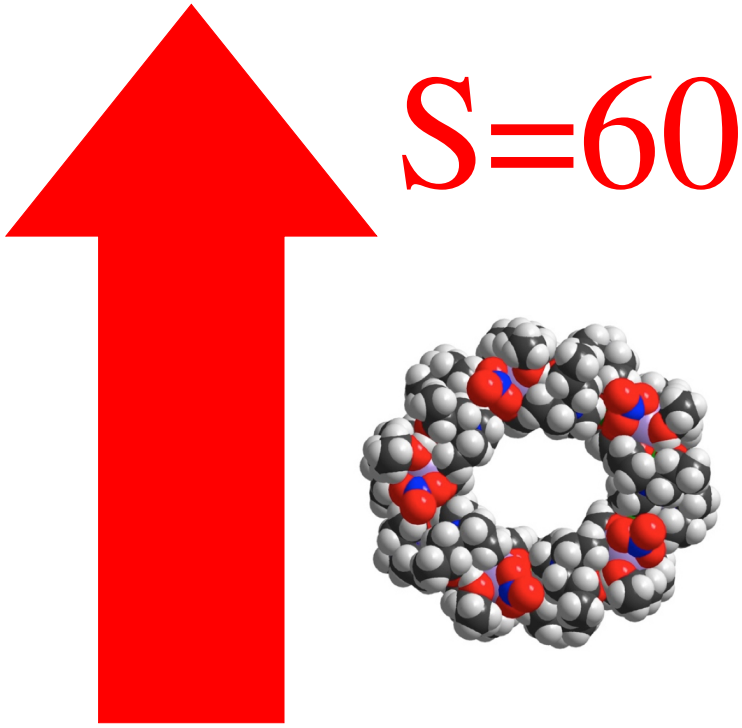


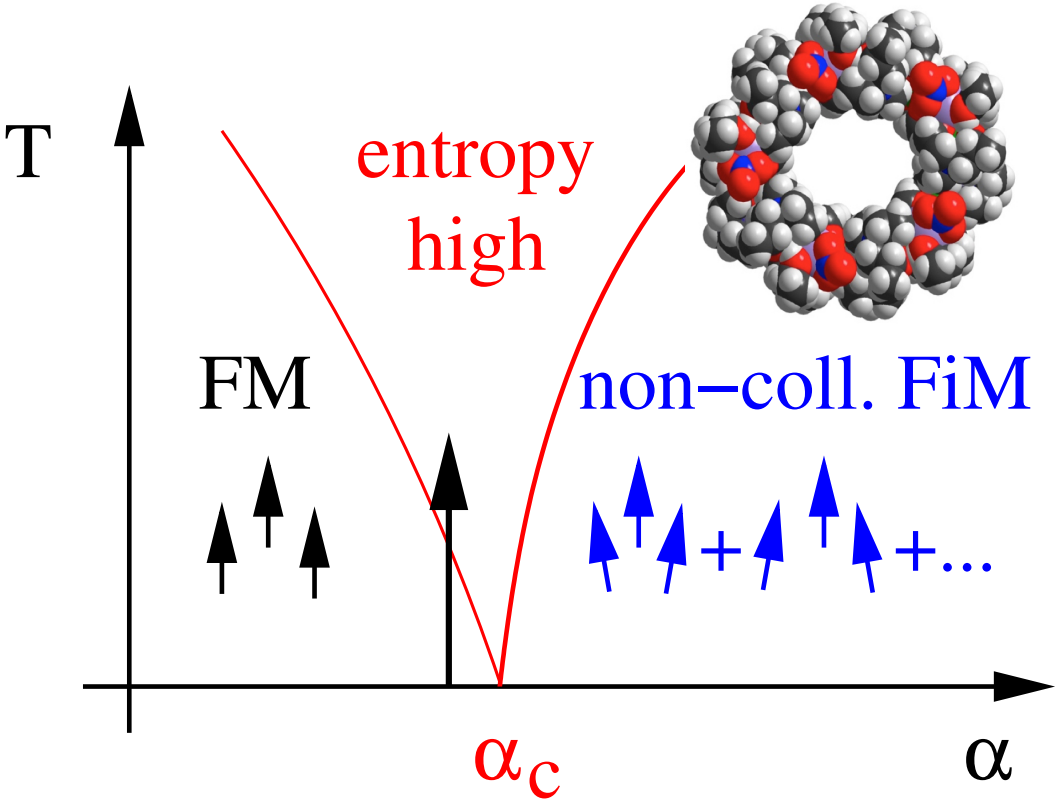
How do we know?

What is a QPT?

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

$Gd_{10}Fe_{10}$ – summary





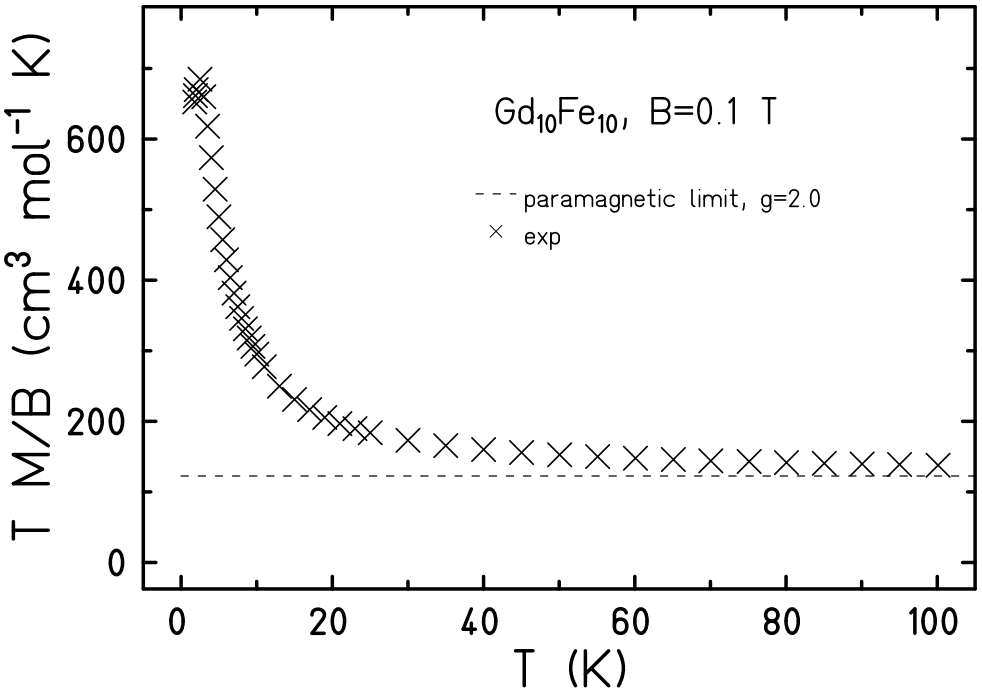
How do we know?

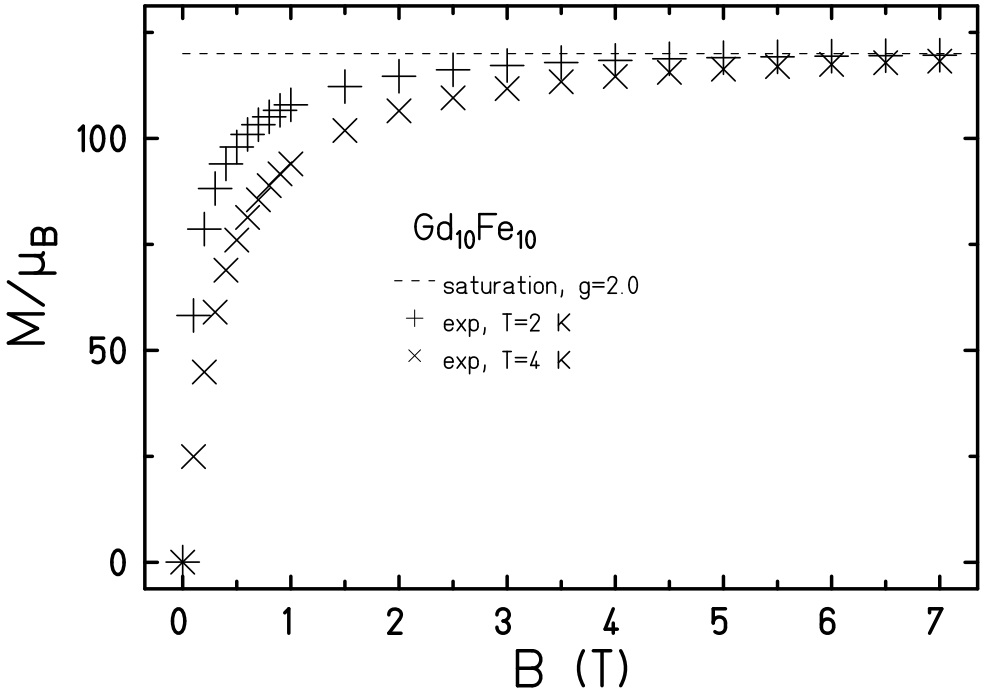
What is a QPT?
In $Gd_{10}Fe_{10}$?

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

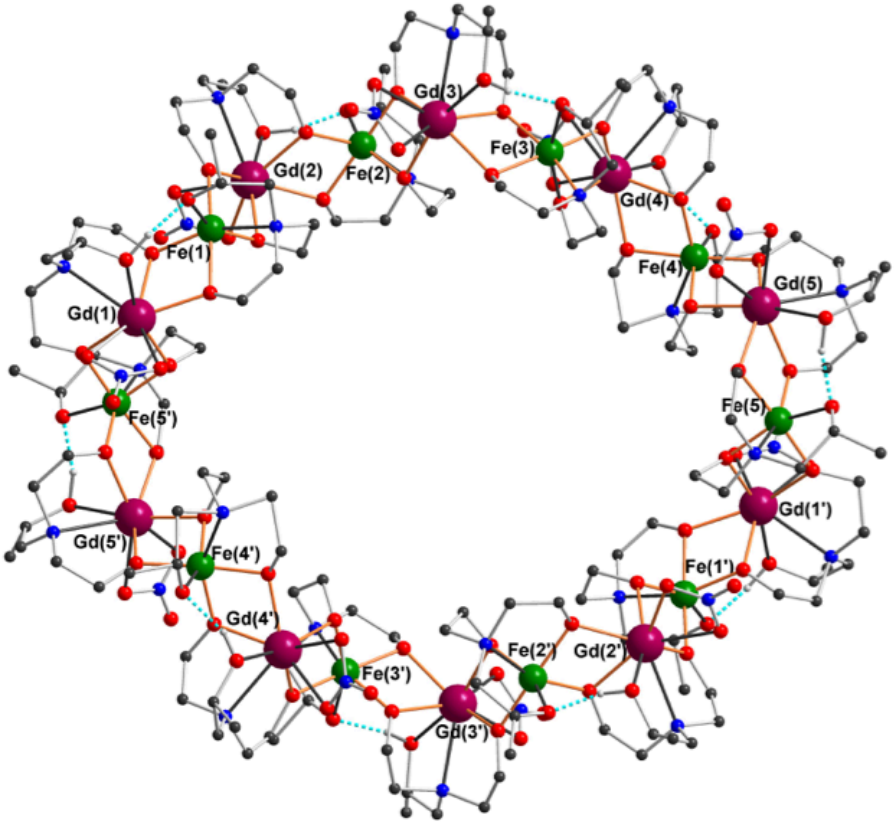
Start: experimental data

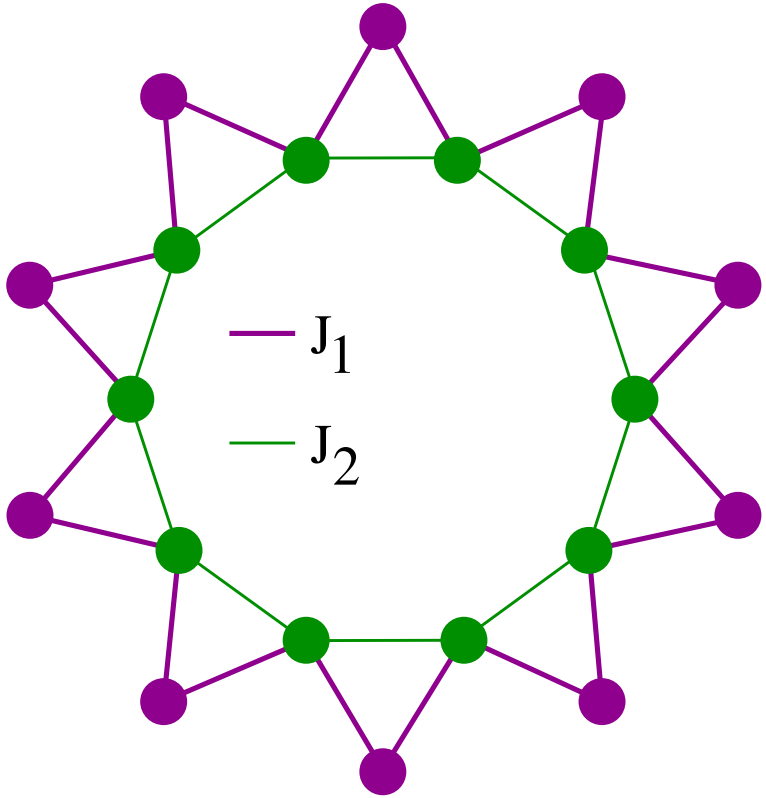
$Gd_{10}Fe_{10}$ – How to rationalize the experimental data?





$Gd_{10}Fe_{10}$ – structure = delta chain





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

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Model Hamiltonian

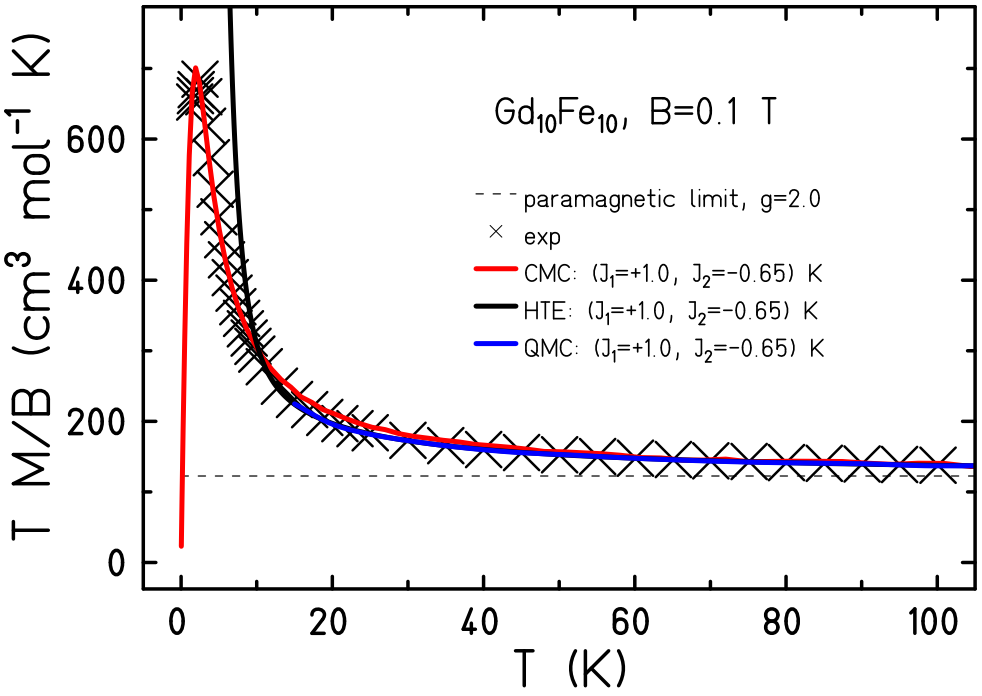
$$\begin{aligned} \underset{\sim}{H} &= -2J_1 \sum_i \vec{\underset{\sim}{s}}_{\mathsf{Gd},i} \cdot \left(\vec{\underset{\sim}{s}}_{\mathsf{Fe},i} + \vec{\underset{\sim}{s}}_{\mathsf{Fe},i+1} \right) \\ & \quad -2J_2 \sum_i \vec{\underset{\sim}{s}}_{\mathsf{Fe},i} \cdot \vec{\underset{\sim}{s}}_{\mathsf{Fe},i+1} + g\,\mu_B\,B \sum_i \left(\underset{\sim}{s}^z_{\mathsf{Gd},i} + \underset{\sim}{s}^z_{\mathsf{Fe},i} \right) \end{aligned}$$

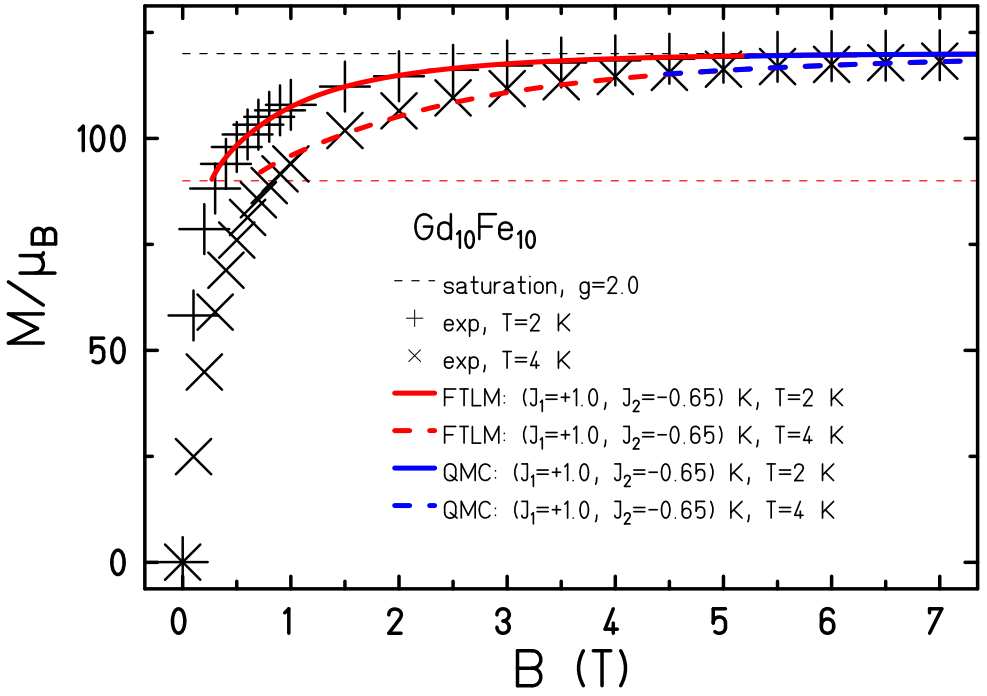
Dimension of Hilbert space

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

What would you do?

$Gd_{10}Fe_{10}$ – Methods





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

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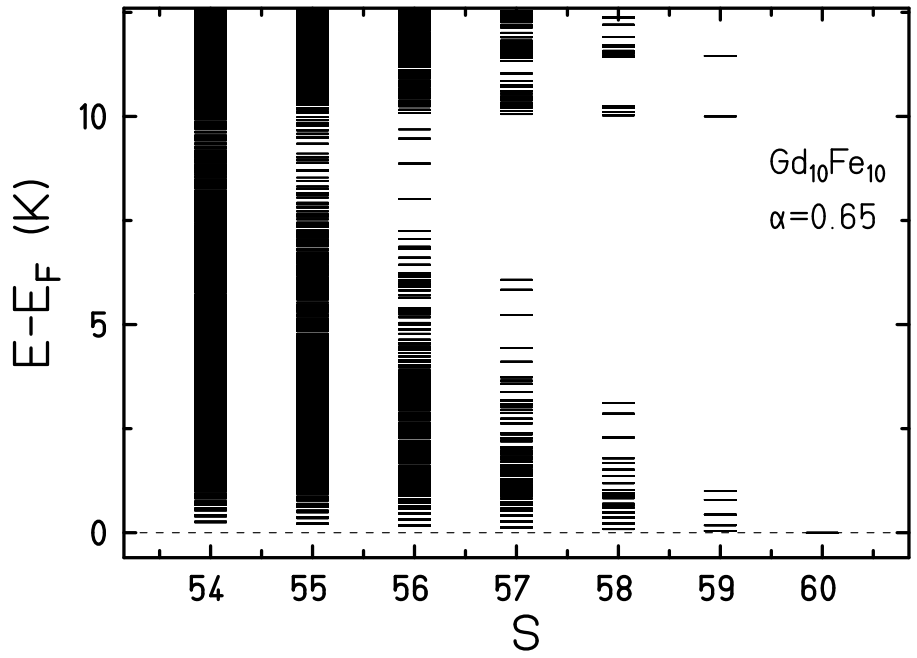
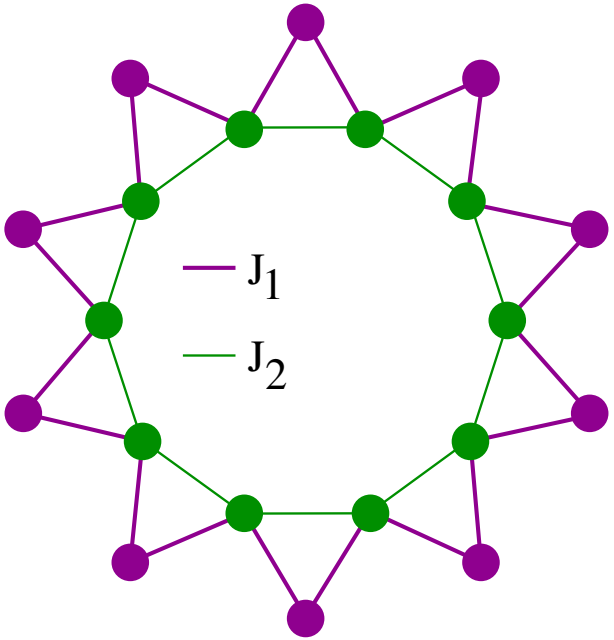
$Gd_{10}Fe_{10}$ – $S = 60$





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

$\Rightarrow$ $\alpha_{Gd_{10}Fe_{10}} = |J_2|/J_1 = 0.65$ What if J_2 stronger?

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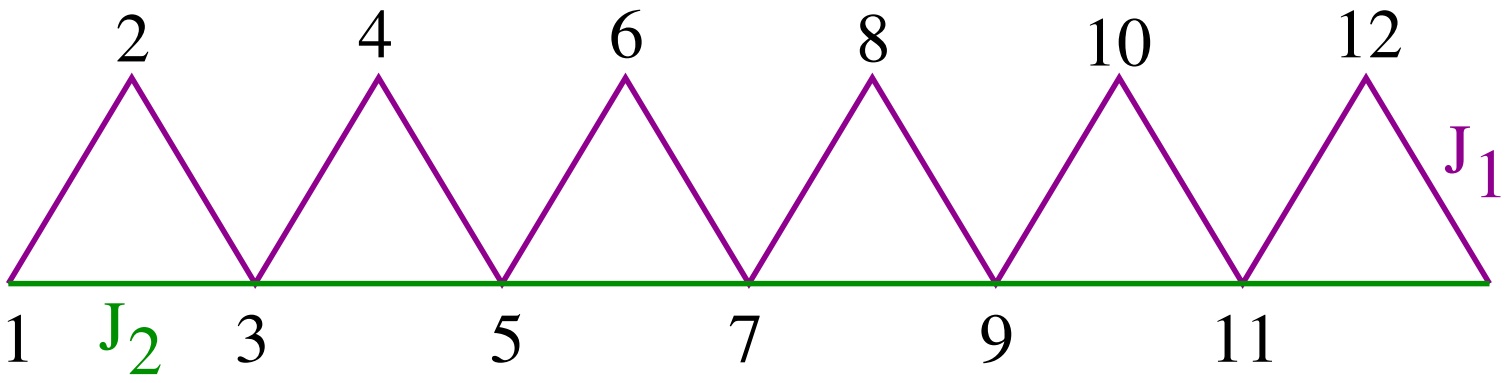
Excursus: sawtooth (delta) chain



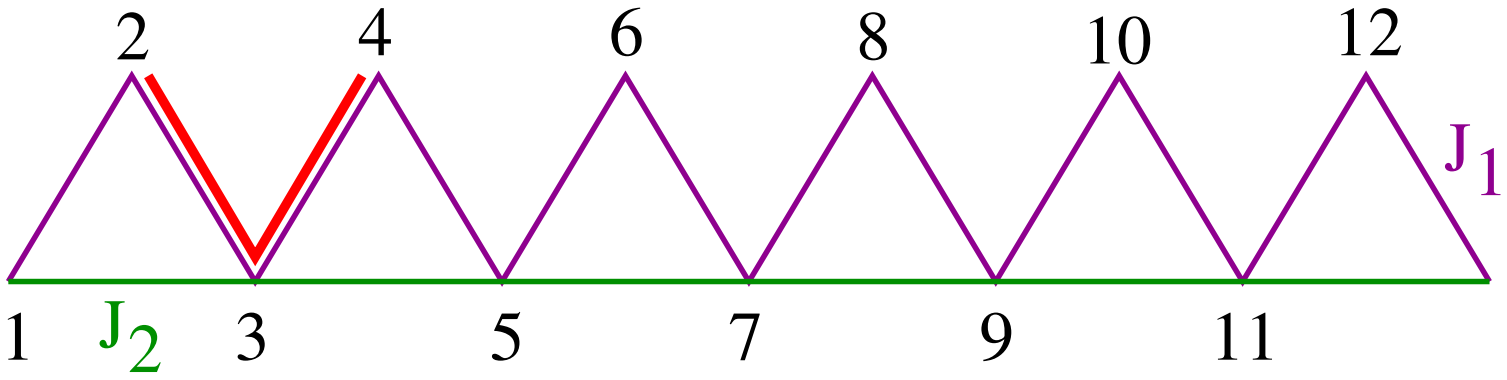
$\Rightarrow$ special properties for $J_1 > 0$ (ferro) and $J_2 < 0$ (af) at certain α_c

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

$\Rightarrow$ 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

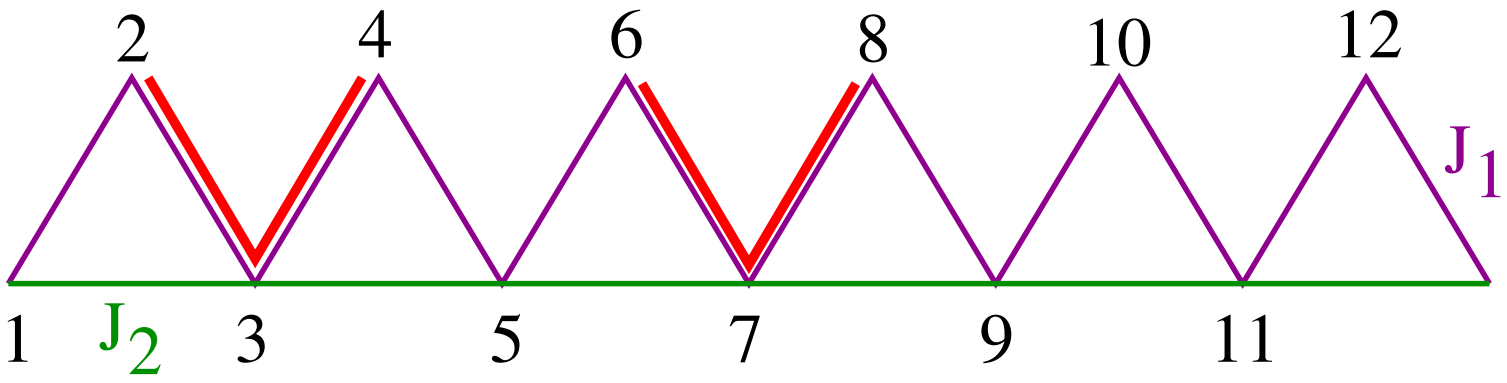
$\Rightarrow$ $|\,$1 localized magnon at (2,3,4)$\,\rangle = (\underset{\sim}{s}_2^- + \underset{\sim}{s}_4^- + 2\underset{\sim}{s}_3^-)\,|\,F\,\rangle$;

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

$\Rightarrow$ 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

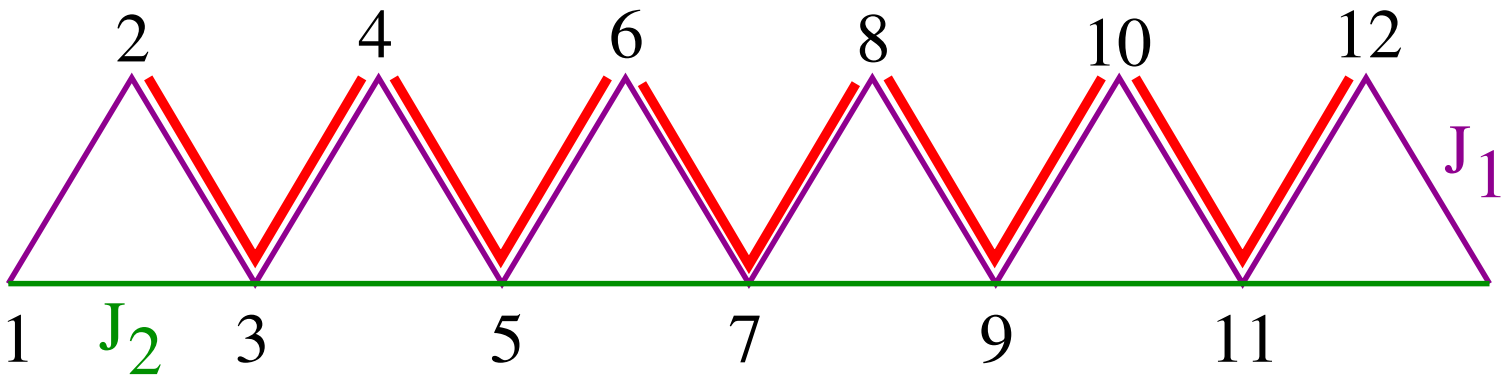


$\Rightarrow$ $|$ 2 localized magnons $\rangle$; $E = E_F, M = S_{\text{max}} - 2$

$\Rightarrow$ 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



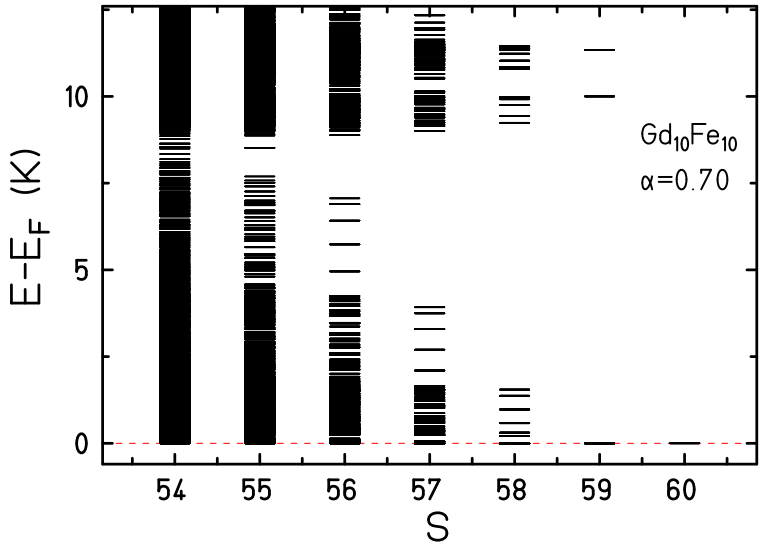
$\Rightarrow$ $|$ max. number of localized magnons $\rangle$; $E = E_F, M = S_{\text{max}} - N/2$

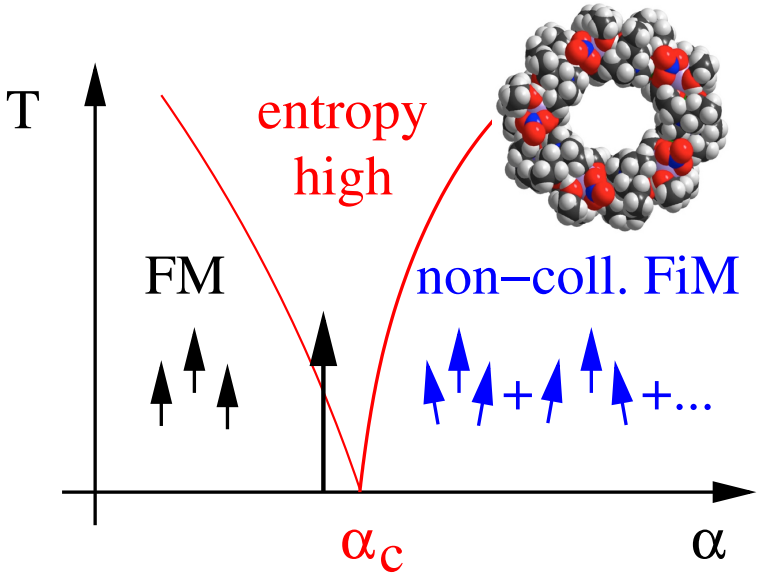
$\Rightarrow$ Macroscopic number of localized magnons. Degenerate with $|\, F \,\rangle$.

$\Rightarrow$ 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)

$Gd_{10}Fe_{10}$ – QCP





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

$\Rightarrow$ 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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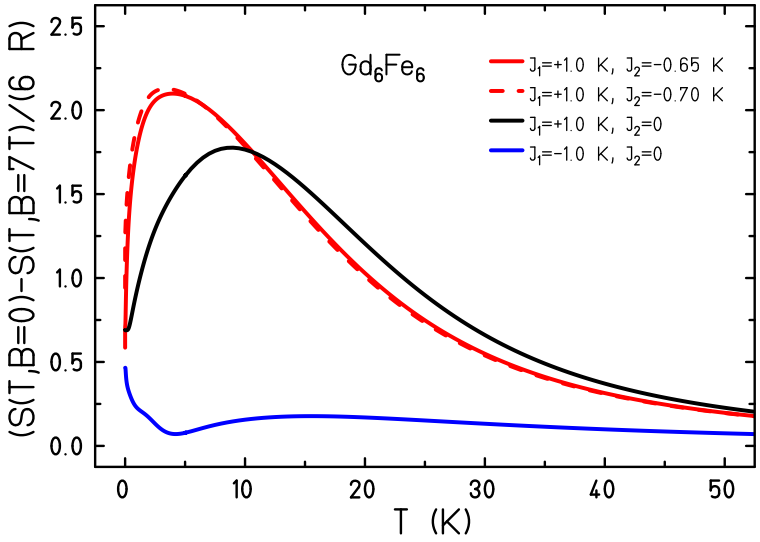
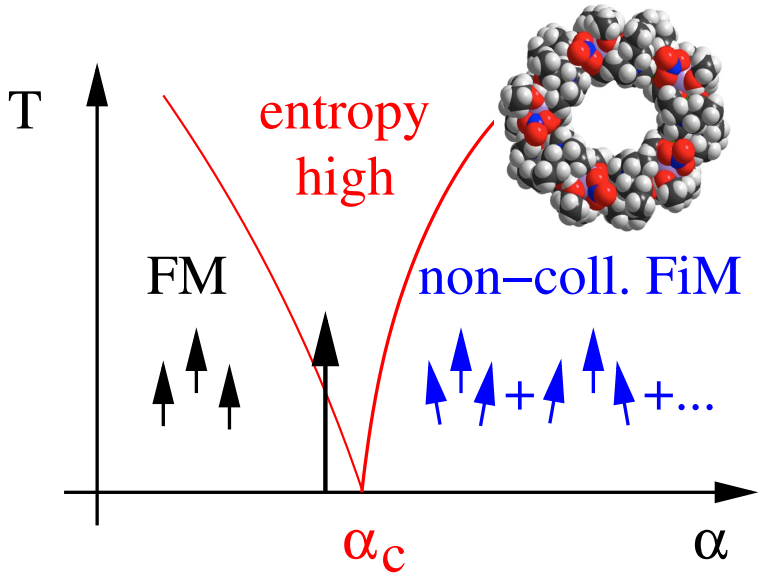
Quantum Phase Transition

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.

$Gd_{10}Fe_{10}$ – $T > 0$





$\Rightarrow$ although QPT and QCP at $T = 0$,

noticeable at elevated temperatures (arrow);

$\Rightarrow$ example isothermal entropy change:

little difference between $\alpha = 0.70$ and $\alpha = 0.65$.

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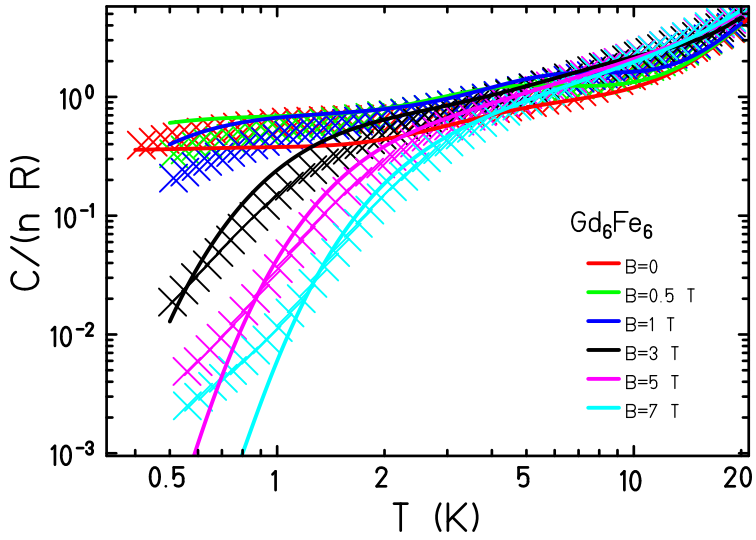
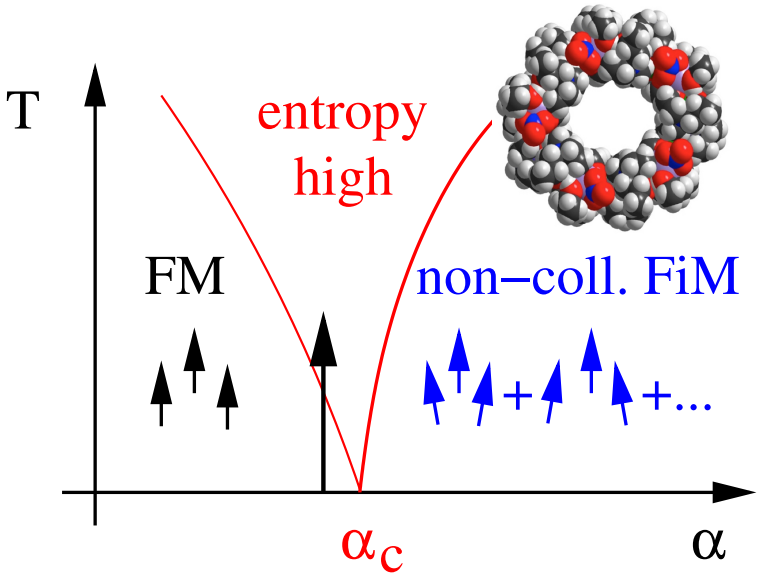
$Gd_{10}Fe_{10}$ – heat capacity





$\Rightarrow$ heat capacity assumes very large values

even down to lowest temperatures;

$\Rightarrow$ evaluated by means of FTLM for a smaller (hypothetical) system Gd_6Fe_6;

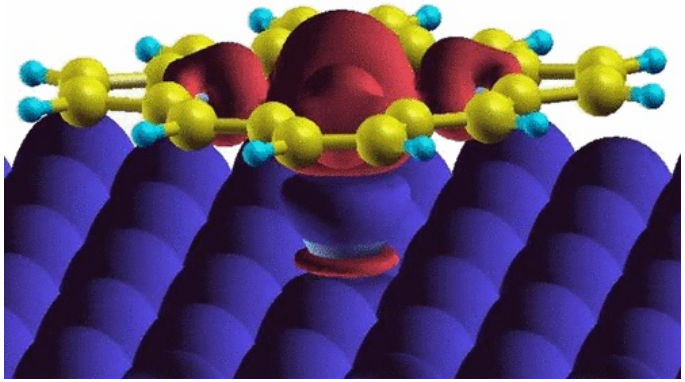
$\Rightarrow$ magnetic field separates $S = 60$ ground state, C drops.

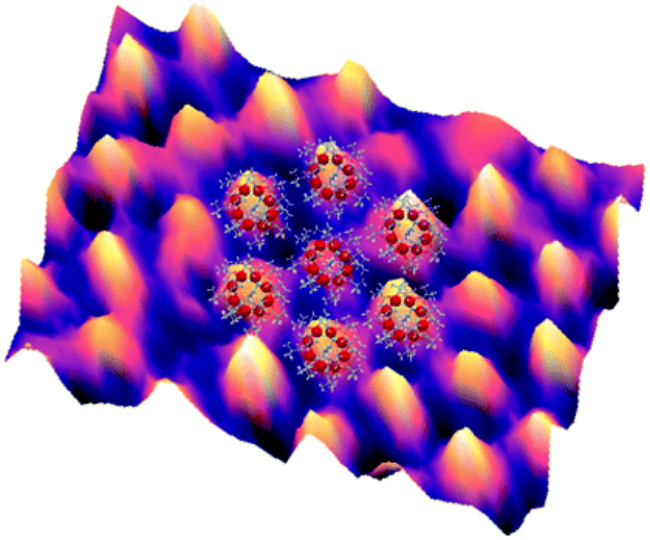
A. Baniodeh *et al., npj Quantum Materials* ***3****, 10 (2018)*

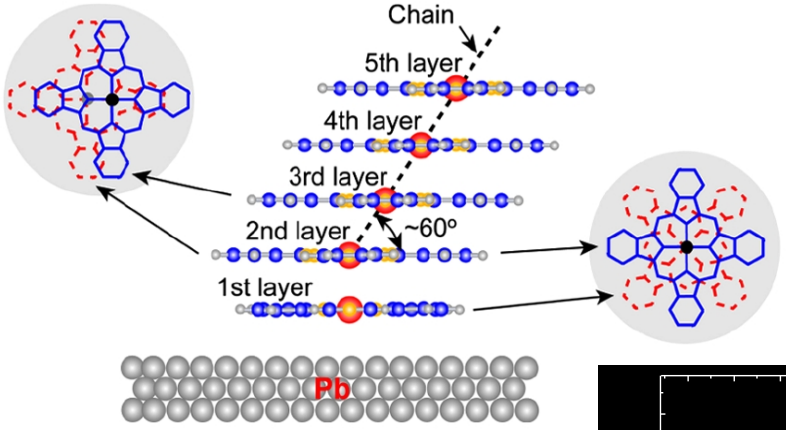
Numerical Renormalization Group calculations

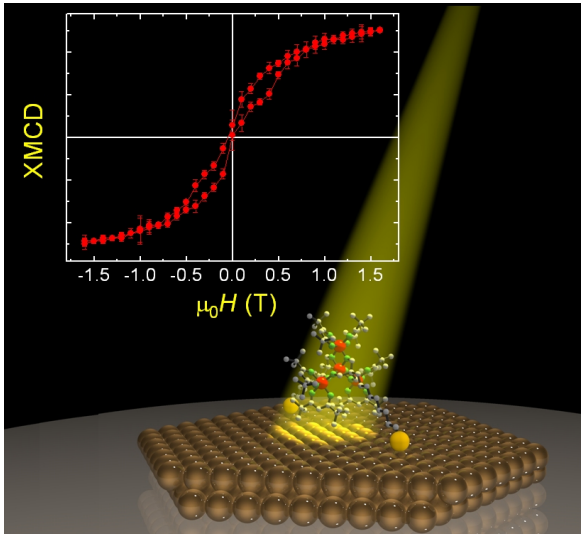
(Good for deposited molecules.)

You want to deposite a molecule



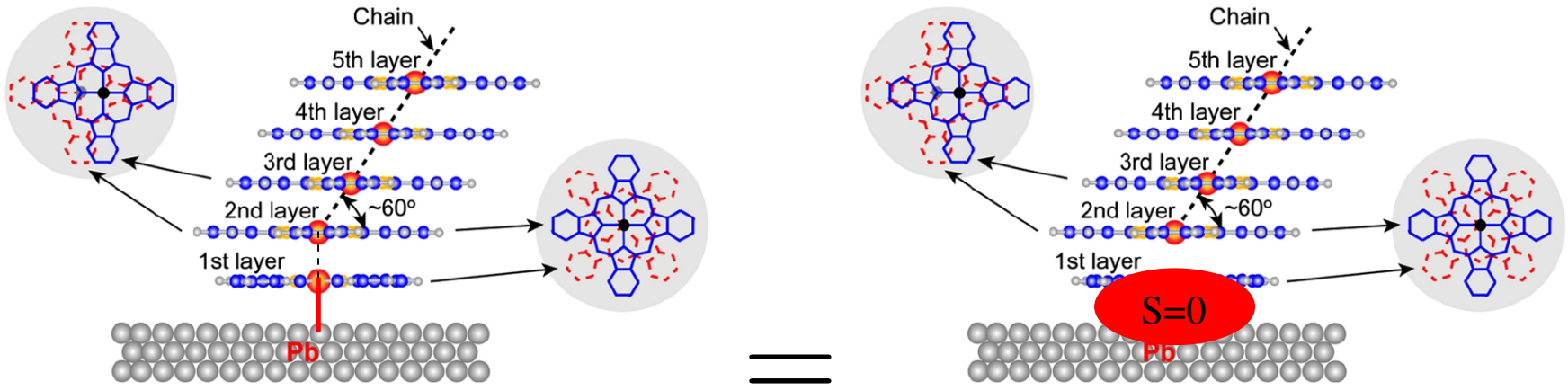






M. Bernien *et al.*, Phys. Rev. Lett. **102**, 047202 (2009); A. Ghirri*et al.*, ACS Nano, **5**, 7090-7099 (2011); X. Chen *et al.*, Phys. Rev. Lett. **101**, 197208 (2008); M. Mannini *et al.*, Nature Materials **8**, 194 - 197 (2009).

Physical example (ICMM 2010)

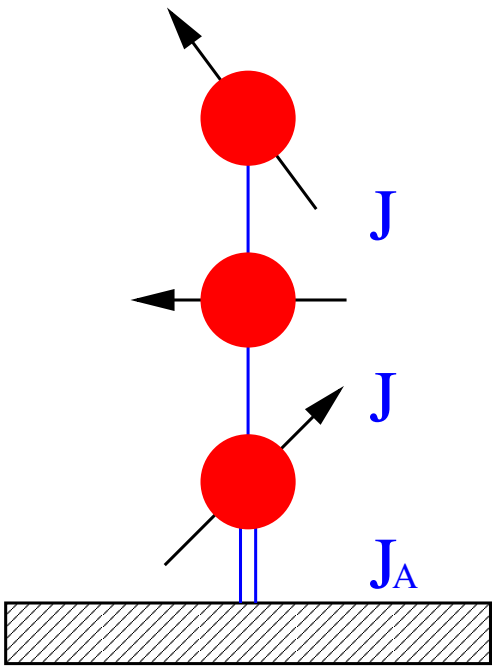


Stack of deposited Cobalt phthalocyanine (CoPc) molecules;
Co^{2+} with spin $s = 1/2$.

Under which circumstances is the picture of total screening correct?

X. Chen *et al.*, Phys. Rev. Lett. **101**, 197208 (2008).

NRG – minimal model (already an approximation!)



- $\underset{\sim}{H} = \underset{\sim}{H}_{\text{electrons}} + \underset{\sim}{H}_{\text{coupling}} + \underset{\sim}{H}_{\text{impurity}}$

  $\underset{\sim}{H}_{\text{electrons}} = \sum_{i \neq j,\,\sigma} t_{ij} \underset{\sim}{d}^{\dagger}_{i\sigma} \underset{\sim}{d}_{j\sigma} + g_e \mu_B B \underset{\sim}{\mathcal{S}}^z$

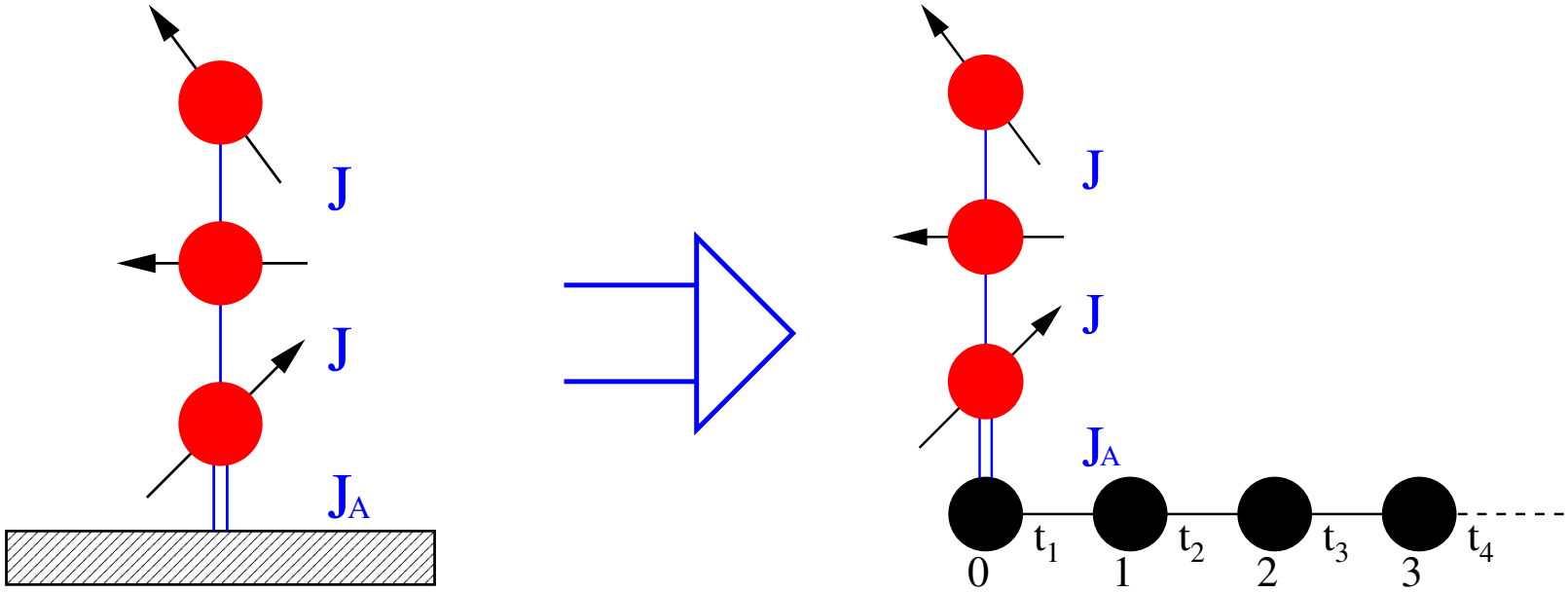
  $\underset{\sim}{H}_{\text{coupling}} = -2 J_A \underset{\sim}{\boldsymbol{S}} \cdot \underset{\sim}{\boldsymbol{s}}_0$, $\underset{\sim}{\boldsymbol{s}}_0$ – spin density at contact

- $\underset{\sim}{H}_{\text{impurity}}$ = Hamiltonian of your molecule!

- NRG ≡ construction of a small (!) effective model in order to evaluate properties of the deposited cluster, the impurity (3).

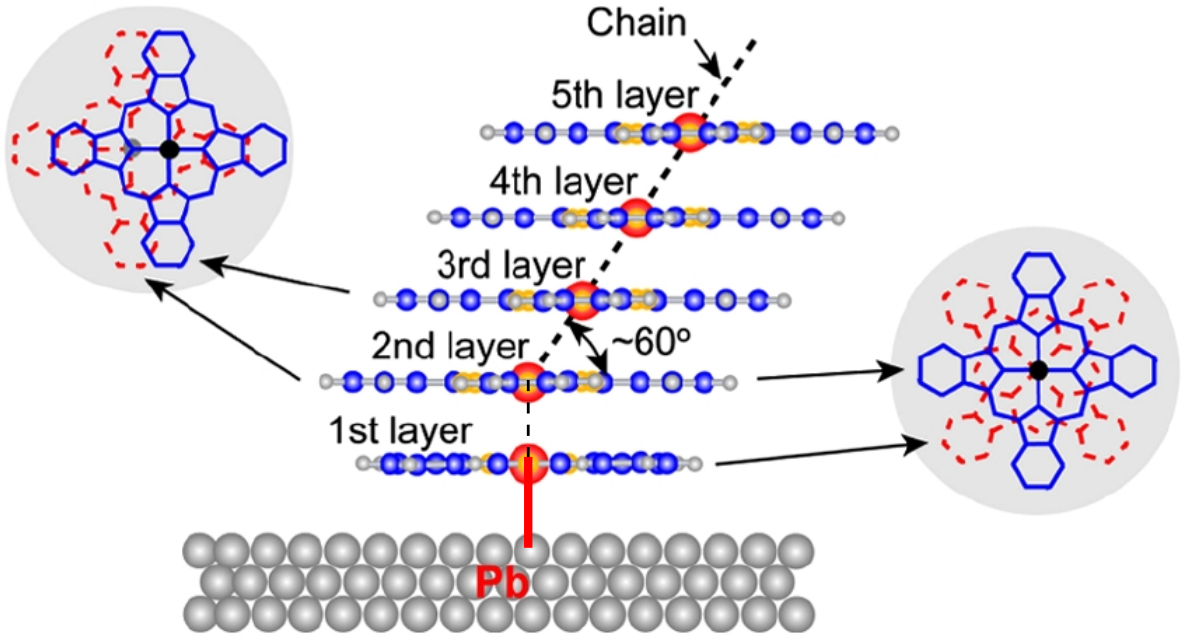
(1) K. G. Wilson, Rev. Mod. Phys. **47**, 773 (1975)
(2) M. Höck, J. Schnack, Phys. Rev. B **87**, 184408 (2013)
(3) *Impurity* is a technical term in this context and not an insult to chemists.

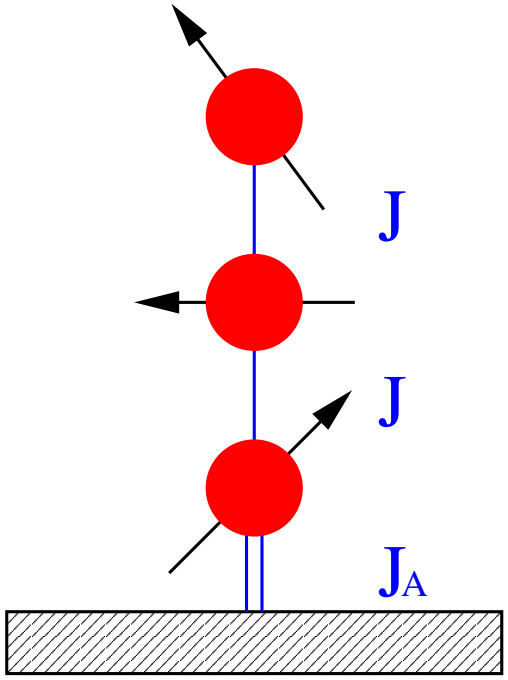
NRG in a cartoon



Metallic surface is replaced by semi-infinite Hubbard chain;
Parameters of the chain: hopping matrix elements and on-site energies;
Stepwise enlargement of the chain ($t_1 > t_2 > t_3 \ldots$);
Truncation of basis set when matrices grow too big.

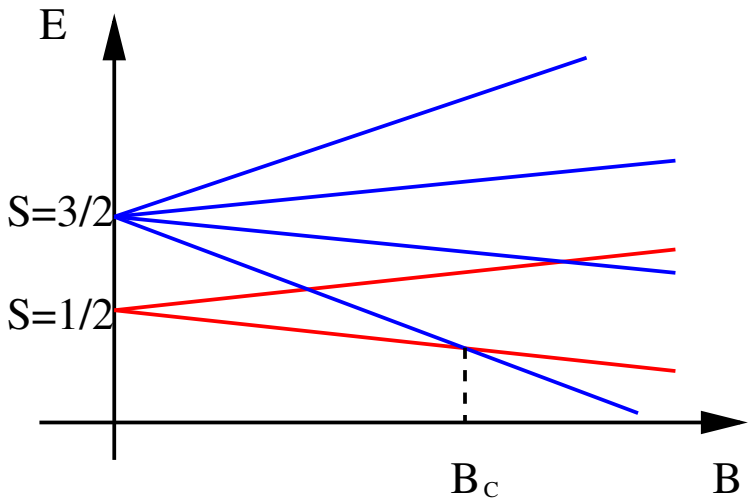
Once more: deposited chain



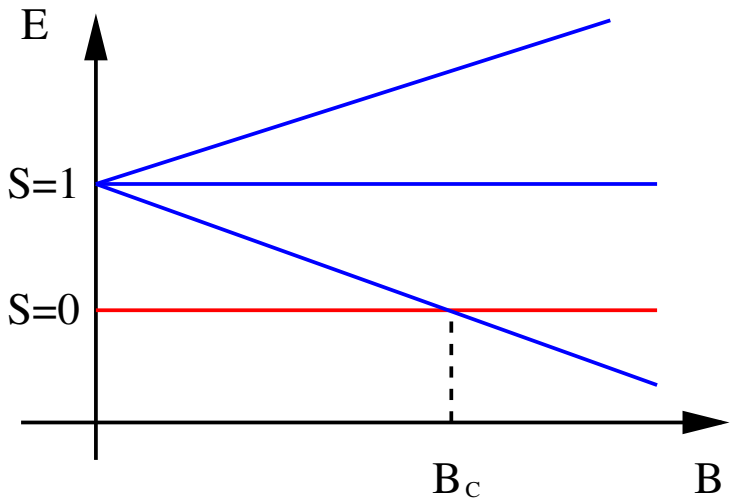


X. Chen *et al.*, Phys. Rev. Lett. **101**, 197208 (2008).

Energy levels of limiting cases for deposited trimer



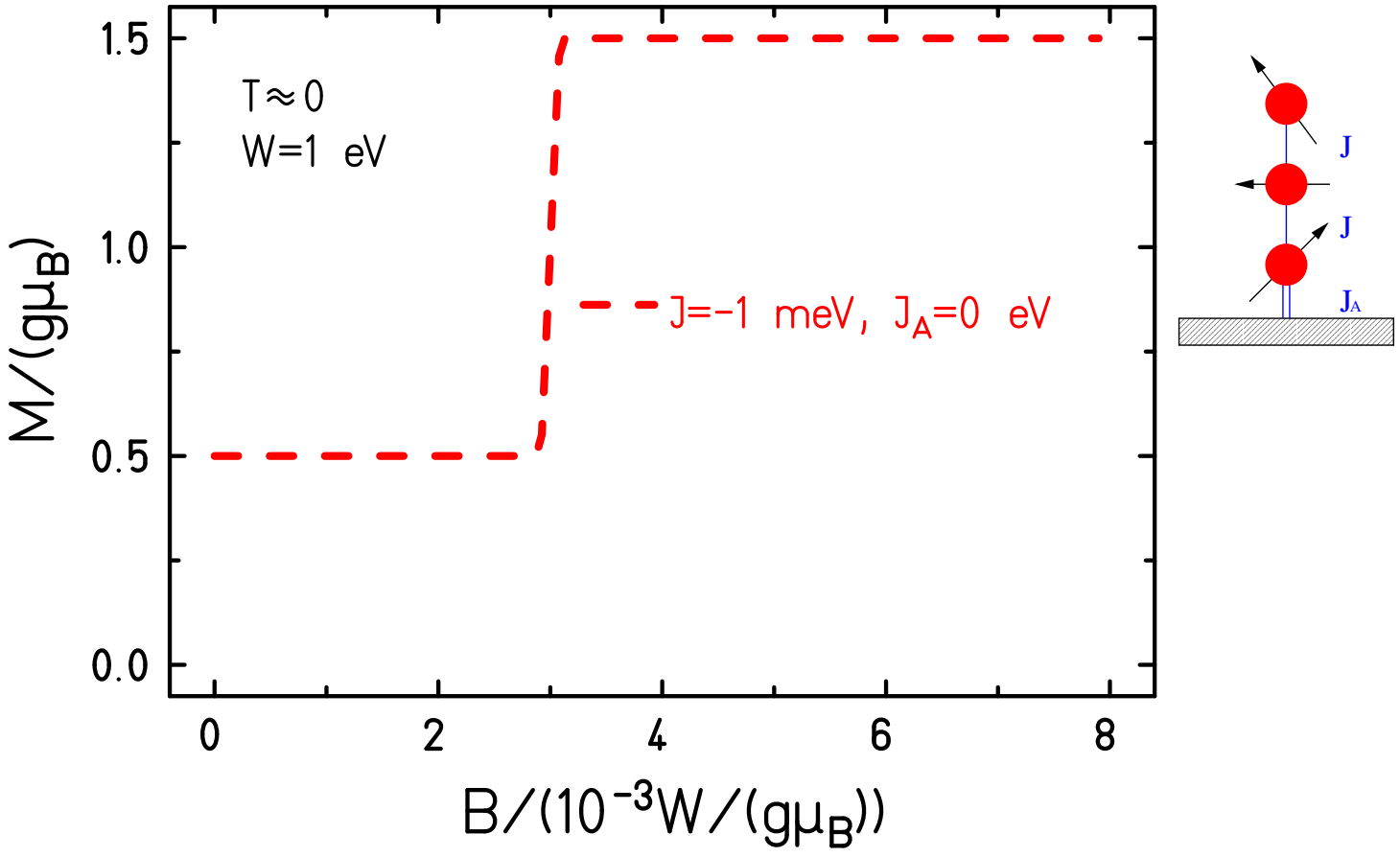
- energy levels of a trimer



- energy levels of a dimer

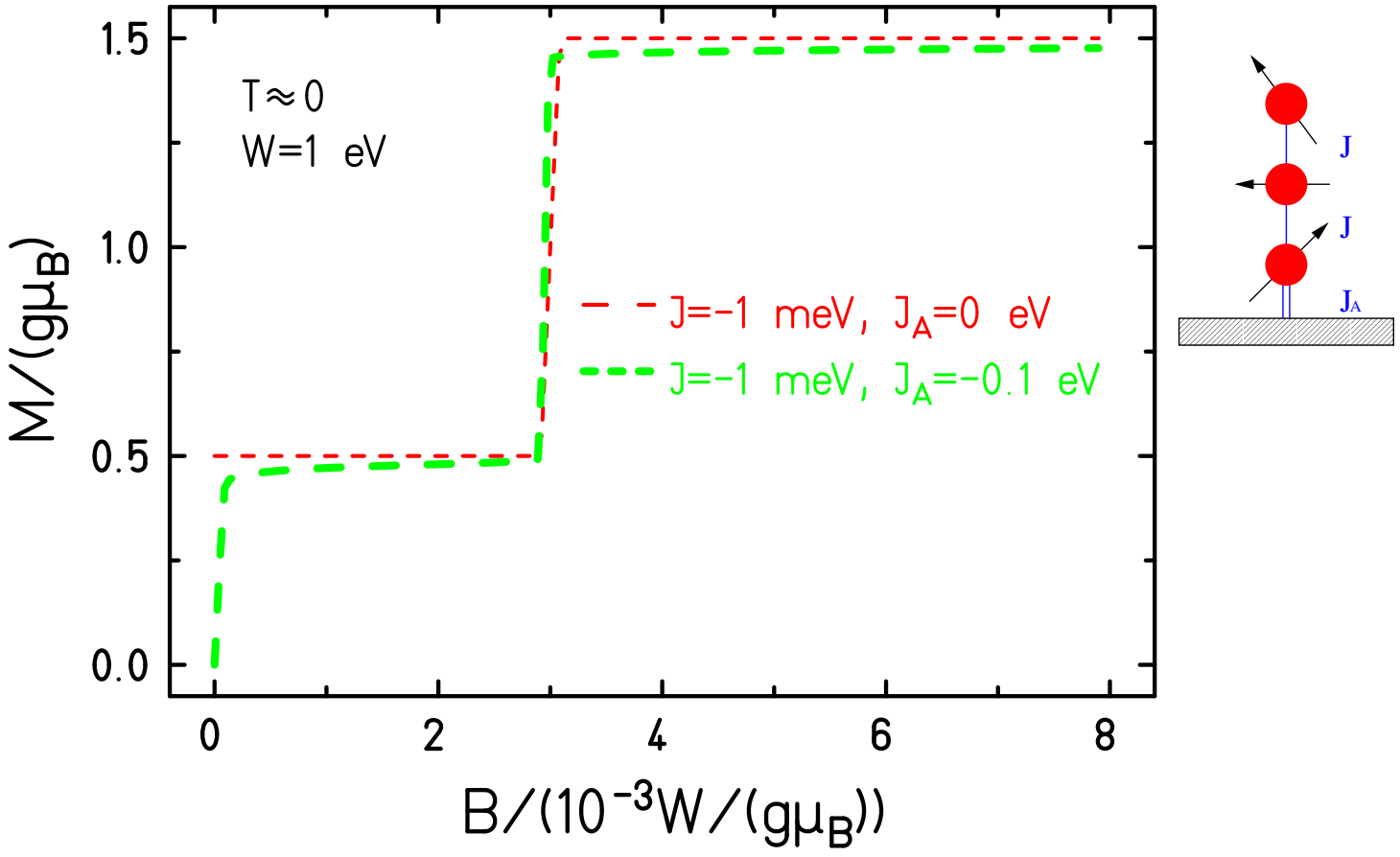
Magnetization curves different; could be seen in XMCD.
NRG calculates observables also between limiting cases
and can thus tell under which circumstances a limiting case applies.

Increasing coupling to the substrate



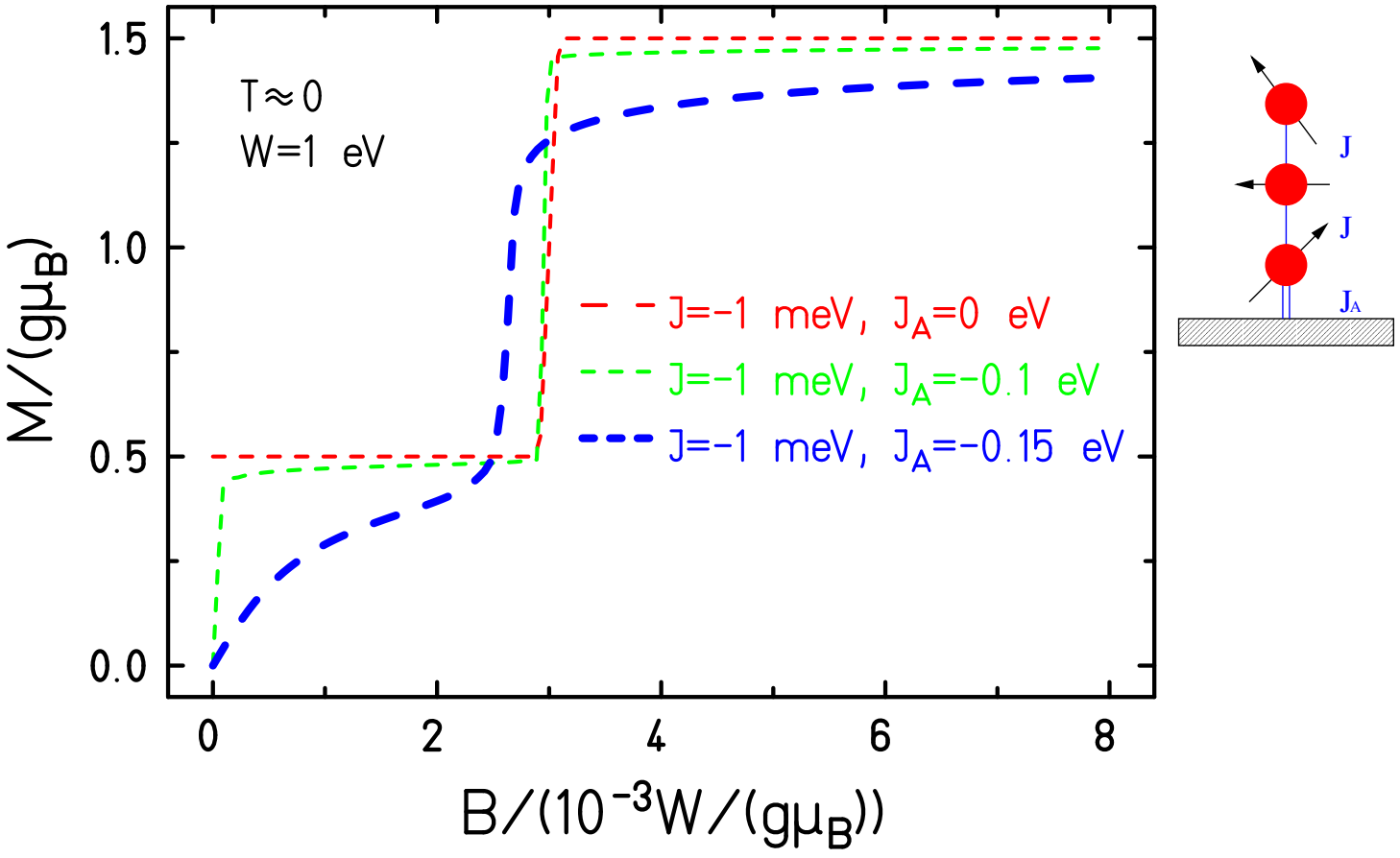
H.-T. Langwald, J. Schnack, Eur. Phys. J. B **92**, 56 (2019)

Increasing coupling to the substrate



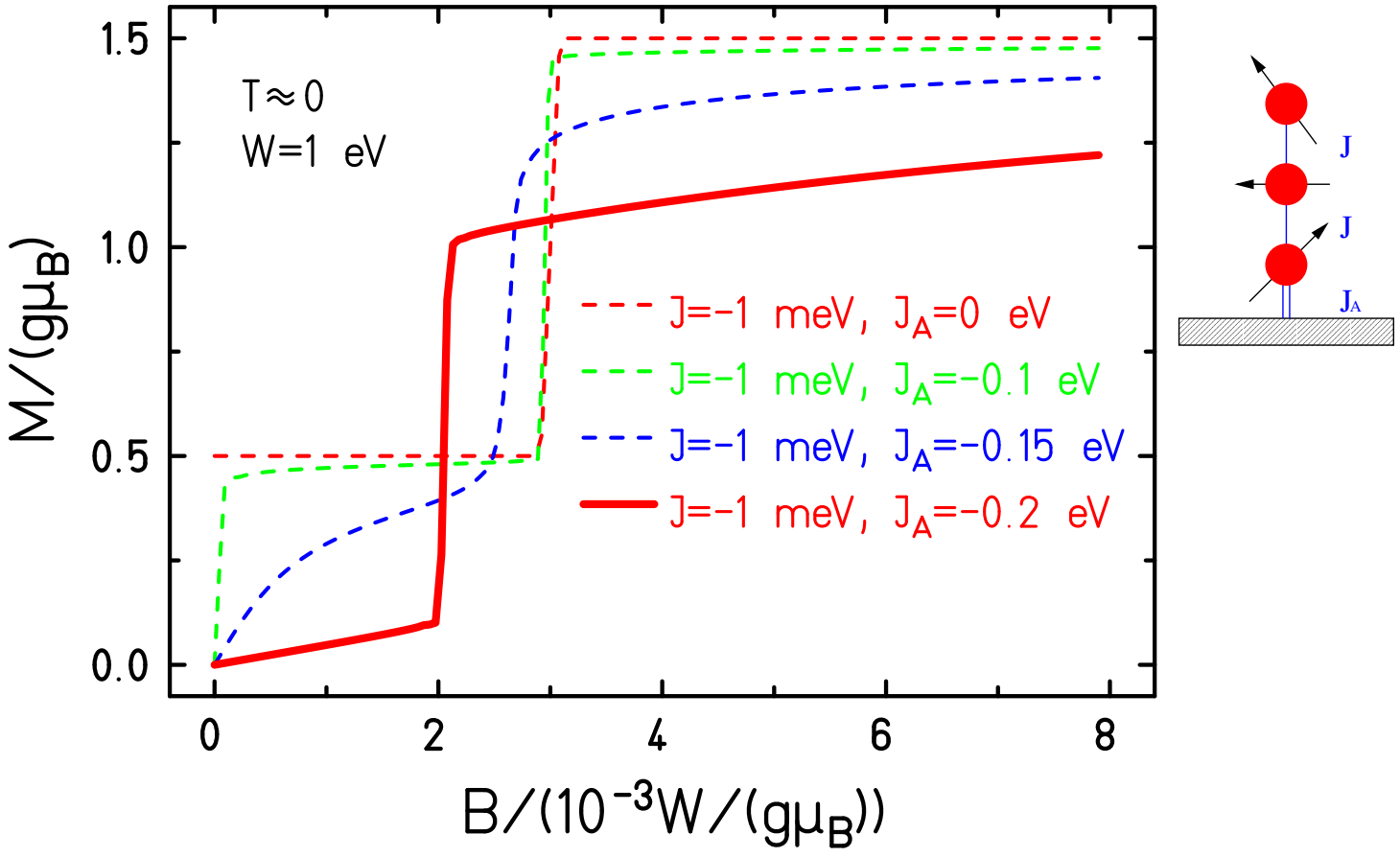
H.-T. Langwald, J. Schnack, Eur. Phys. J. B **92**, 56 (2019)

Increasing coupling to the substrate



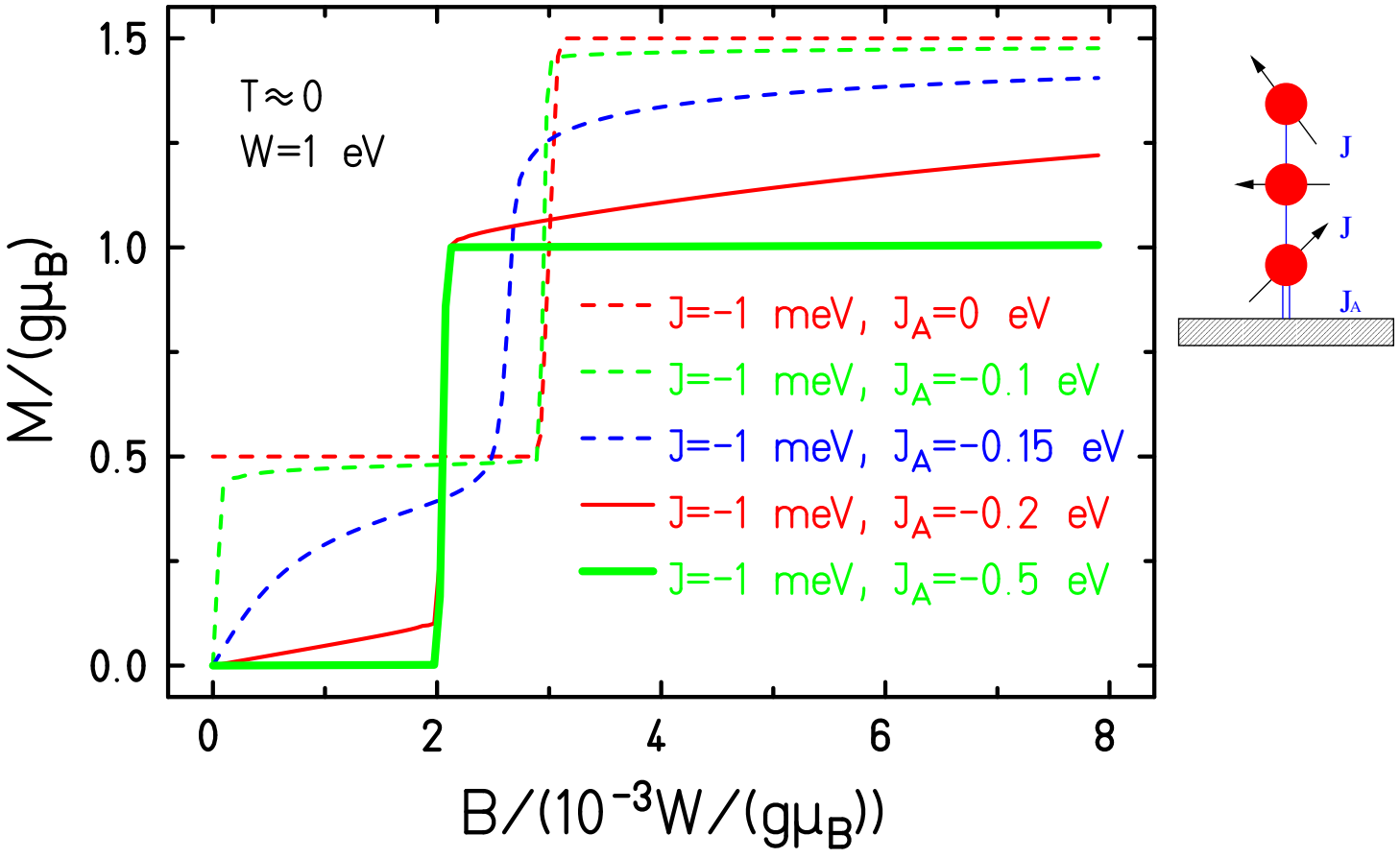
H.-T. Langwald, J. Schnack, Eur. Phys. J. B **92**, 56 (2019)

Increasing coupling to the substrate



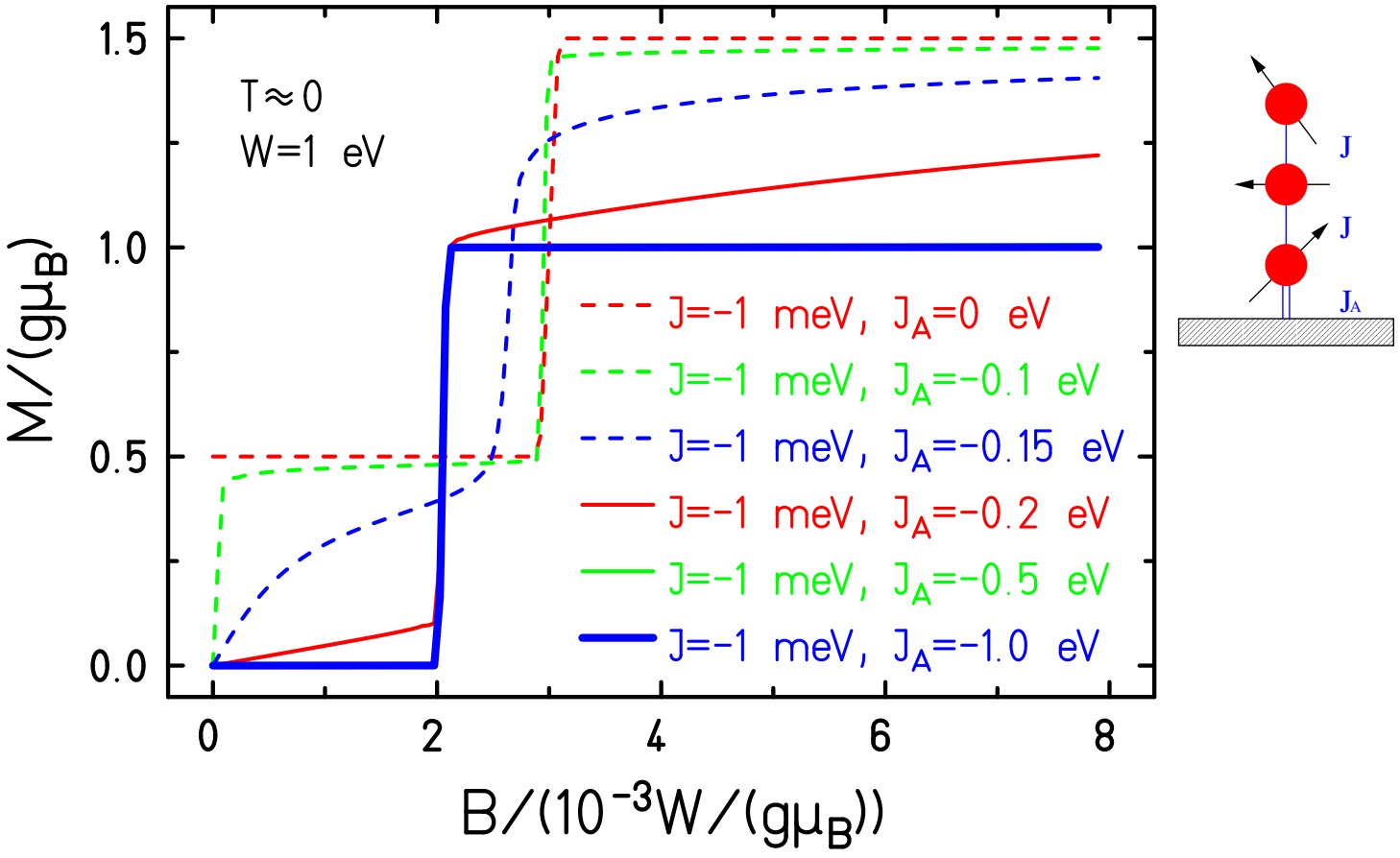
H.-T. Langwald, J. Schnack, Eur. Phys. J. B **92**, 56 (2019)

Increasing coupling to the substrate



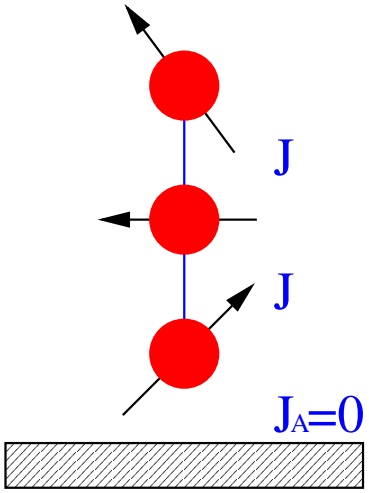
H.-T. Langwald, J. Schnack, Eur. Phys. J. B **92**, 56 (2019)

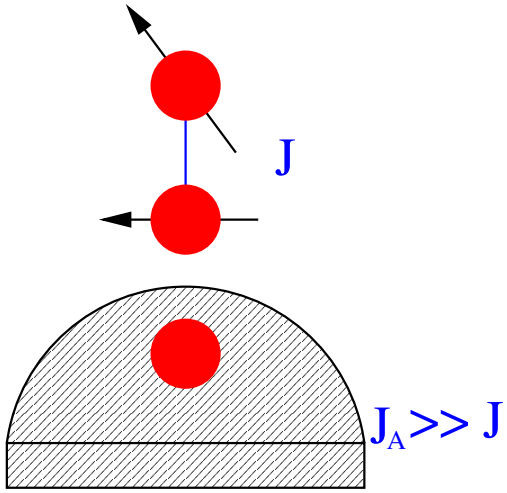
Increasing coupling to the substrate



H.-T. Langwald, J. Schnack, Eur. Phys. J. B **92**, 56 (2019)

Weak vs. strong coupling

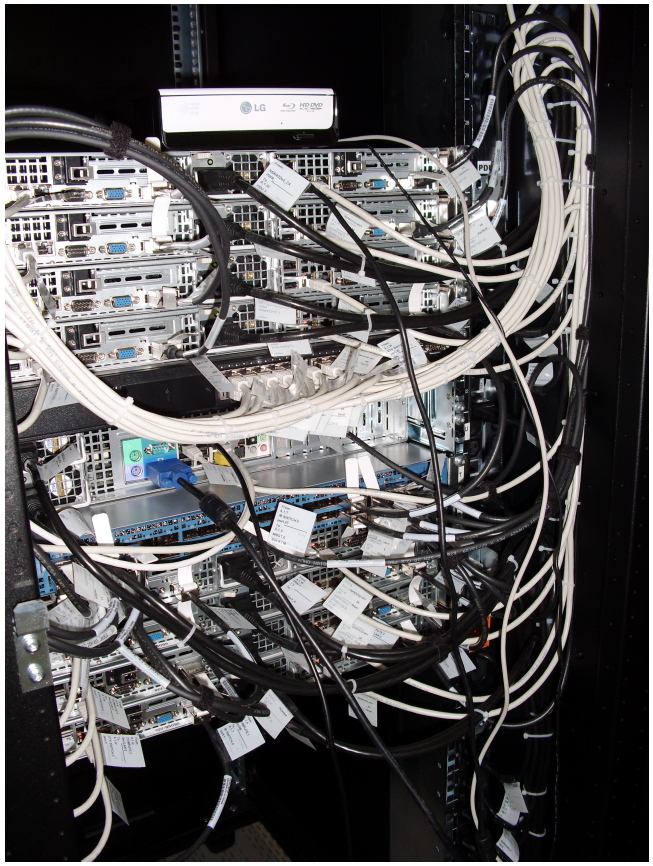




- weak coupling limit: unperturbed molecule (trimer)
- $|J_A| \lessapprox 0.1W$
- strong coupling limit: effective remainder (dimer)
- $|J_A| \gtrapprox 0.5W$

Inbetween: no simple characterization + further sequential screening possible

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 $(T = 0, B = 0)$.
- Screening can lead to interesting limiting cases, which might show different (worse/better) behavior compared to the free molecule.
- ED, HTE, CMC, QMC, FTLM, DMRG, DDMRG, thDMRG for magnetic molecules.

Many thanks to my collaborators





- C. Beckmann, M. Czopnik, T. Glaser, O. Hanebaum, Chr. Heesing, M. Höck, N.B. Ivanov, H.-T. Langwald, A. Müller, R. Schnalle, Chr. Schröder, J. Ummethum (Bielefeld)
- **K. Bärwinkel**, **H.-J. Schmidt**, M. Neumann (Osnabrück)
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The end.

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