

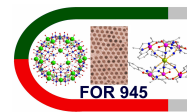
INFLUENCE OF INTERMOLECULAR INTERACTIONS ON MAGNETIC OBSERVABLES

Jürgen Schnack

Department of Physics – University of Bielefeld – Germany

<http://obelix.physik.uni-bielefeld.de/~schnack/>

DPG Spring Meeting
Dresden, 2017, March 21

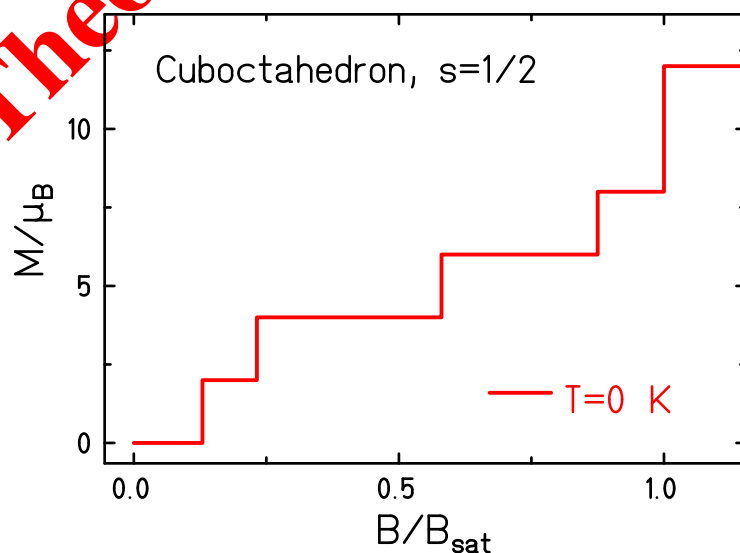


Problem:

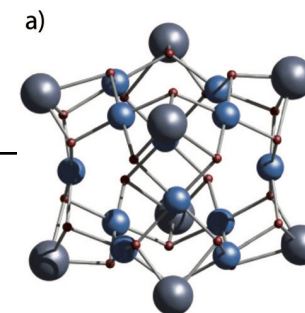
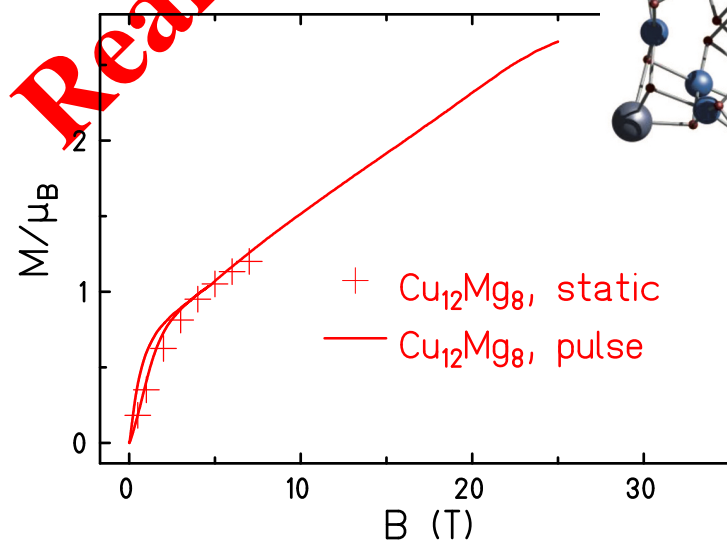
How robust are static molecular magnetic observables?

Example: magnetization steps are fingerprints

Theory



Reality



No magnetization steps! Reasons?

Your suggestions?

- (1) M. Palacios, E. Pineda, S. Sanz, R. Inglis, M. Pitak, S. Coles, M. Evangelisti, H. Nojiri, C. Heesing, E. Brechin, J. Schnack, R. Winpenney, ChemPhysChem **17**, 55 (2016);
- (2) and many more examples.

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. Anisotropic exchange
2. Randomness
3. Some basic theory
4. Intermolecular interactions

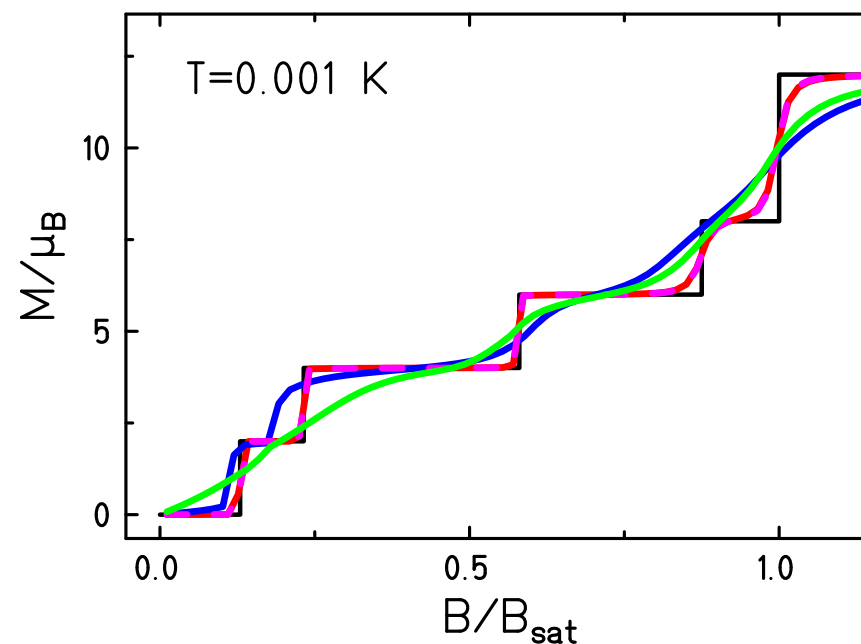
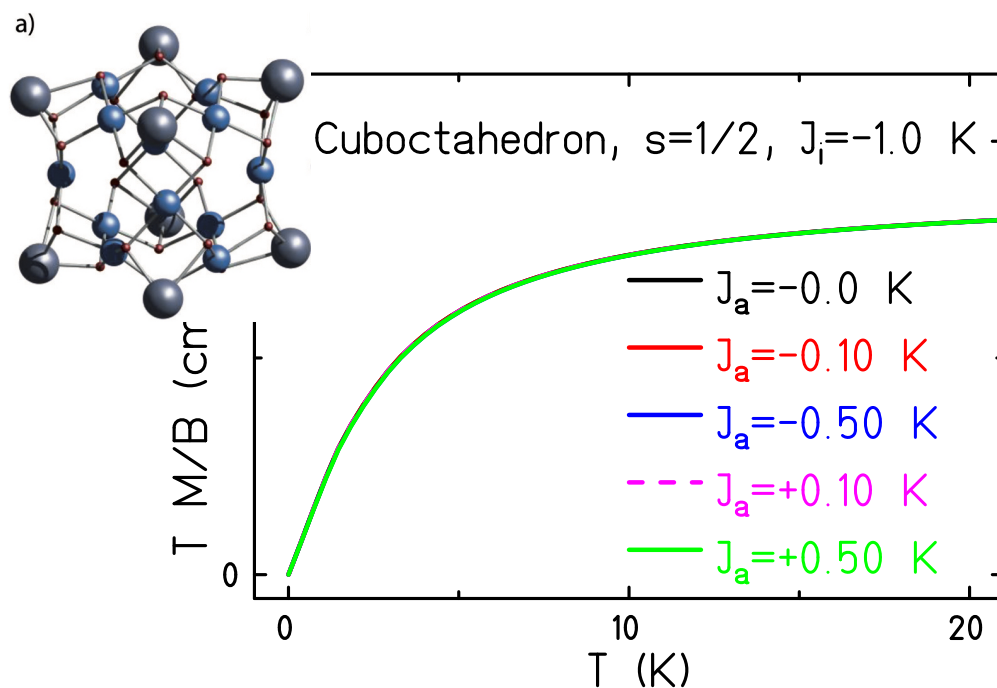
We are the sledgehammer team of matrix diagonalization.
Please send inquiries to jschnack@uni-bielefeld.de!

Anisotropic exchange

$$\underline{H} = -2 \sum_{i < j} \underline{\vec{s}}_i \cdot \mathbf{J}_{ij} \cdot \underline{\vec{s}}_j$$

Matrix $\mathbf{J}_{ij}$ contains isotropic Heisenberg exchange, anisotropic symmetric exchange as well as anisotropic antisymmetric exchange (Dzyaloshinskii-Moriya).

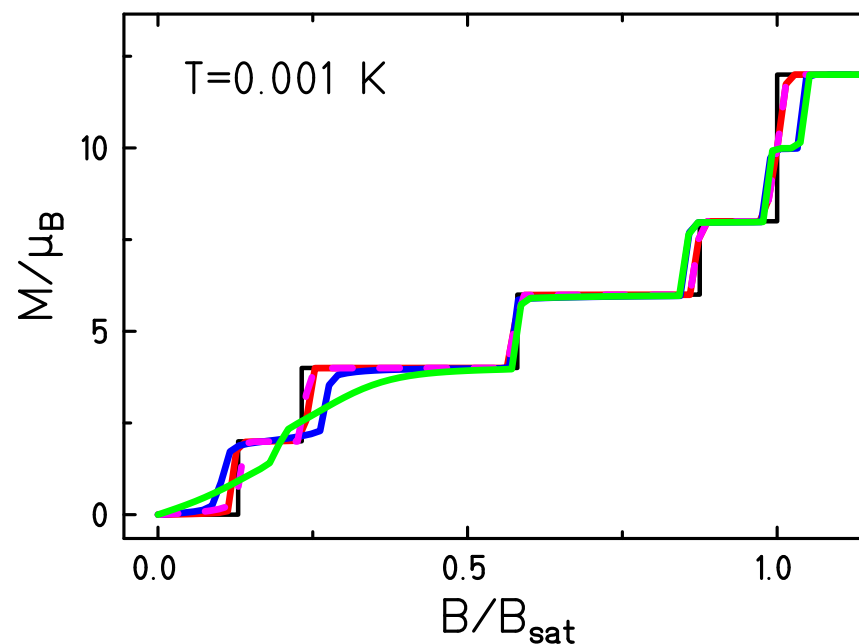
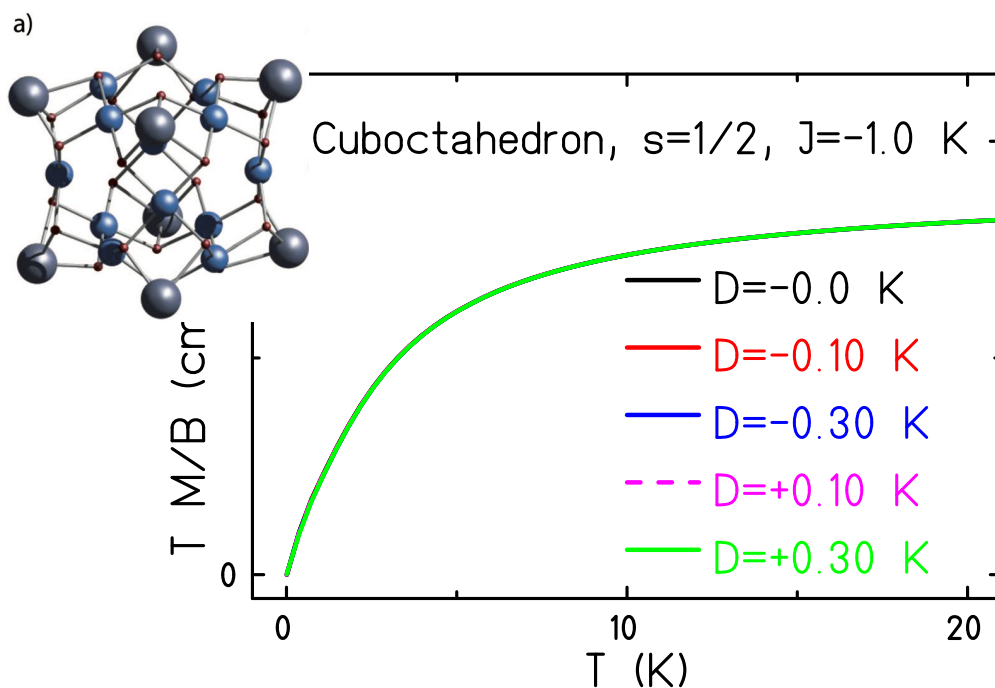
Anisotropic symmetric exchange



Needs about 50 % of symmetric exchange to wash out magnetization steps.

(1) M. Palacios, E. Pineda, S. Sanz, R. Inglis, M. Pitak, S. Coles, M. Evangelisti, H. Nojiri, C. Heesing, E. Brechin, J. Schnack, R. Winpenny, *ChemPhysChem* **17**, 55 (2016).

Anisotropic antisymmetric exchange



Needs about 50 % of antisymmetric exchange to wash out magnetization steps.

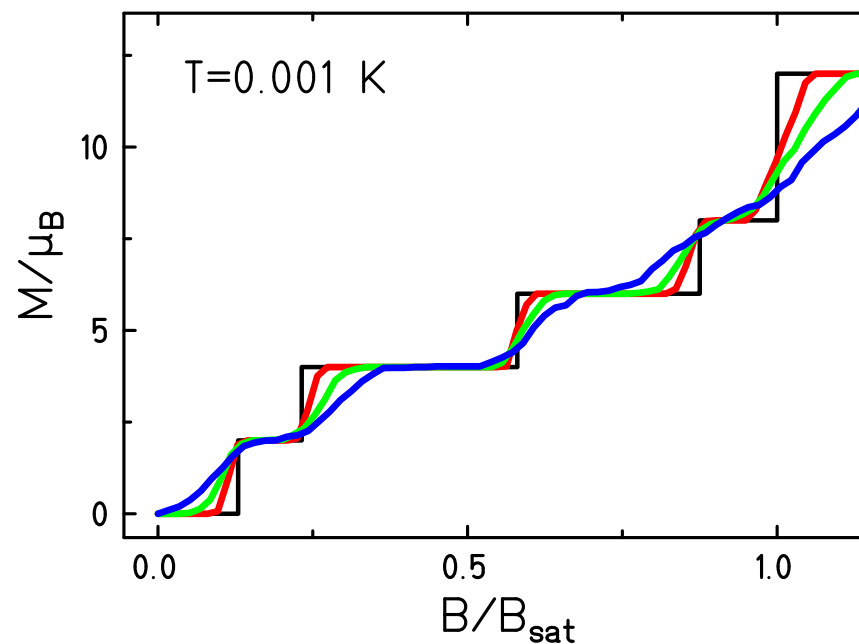
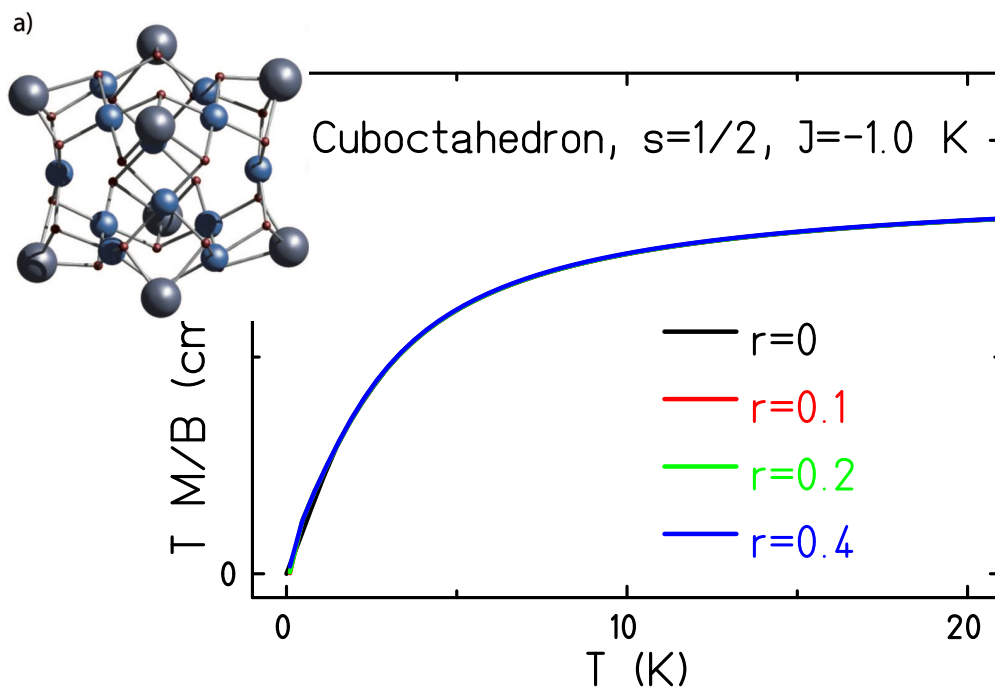
(1) M. Palacios, E. Pineda, S. Sanz, R. Inglis, M. Pitak, S. Coles, M. Evangelisti, H. Nojiri, C. Heesing, E. Brechin, J. Schnack, R. Winpenny, *ChemPhysChem* **17**, 55 (2016).

Random exchange

$$\underline{H} = -2 \sum_{i < j} \vec{\underline{S}}_i J_{ij} \vec{\underline{S}}_j$$

$J_{ij} \in [(1 - r)J, (1 + r)J]$; random for each bond in each molecule, i.e. each molecule is different ($\rightarrow$ average over many molecules).

Random exchange



Needs about 50 % of antisymmetric exchange to wash out magnetization steps.

(1) M. Palacios, E. Pineda, S. Sanz, R. Inglis, M. Pitak, S. Coles, M. Evangelisti, H. Nojiri, C. Heesing, E. Brechin, J. Schnack, R. Winpenny, *ChemPhysChem* **17**, 55 (2016).

Take home:

50 % anisotropic interactions
or randomness is needed

(...to wash out e.g. magnetization steps.)

Before we proceed to intermolecular interactions . . .

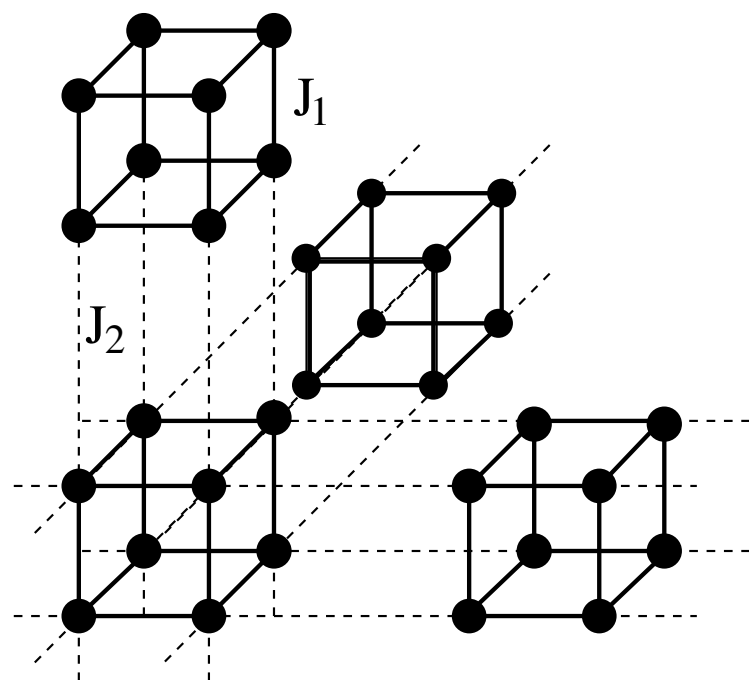
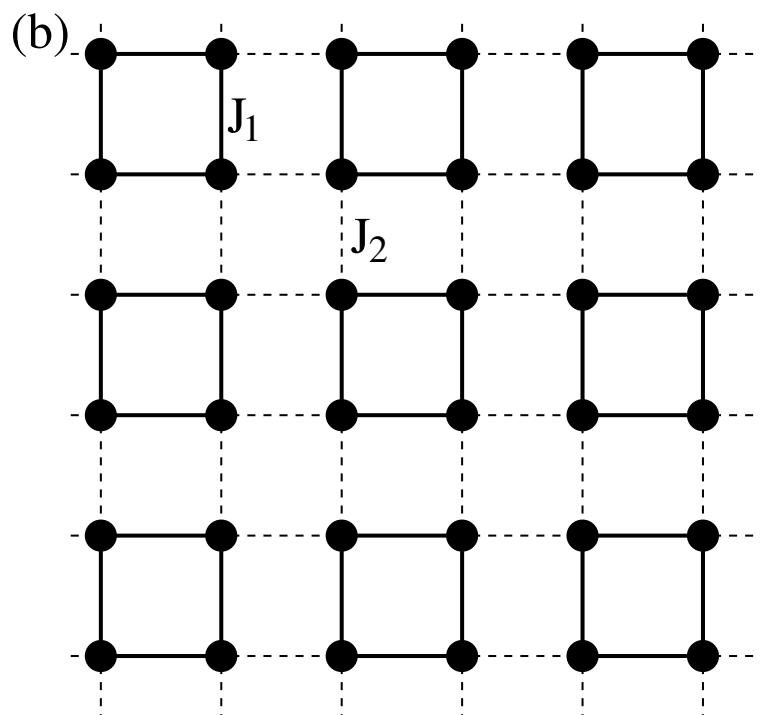
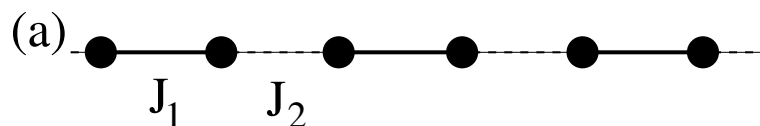
Some basic theory

Summary: theory methods

- **Complete diagonalization:** exact; spectra, transitions, observables, time-evolution; Dimension of largest Hilbert space $< 10^5$.
- **Finite Temperature Lanczos Method (FTLM):** pseudo-spectrum, low-lying levels good, transitions, observables, time-evolution; DoH $< 10^{10}$.
- **Quantum Monte Carlo (QMC):** observables; bad/no convergence for competing interactions (frustration) due to negative sign problem; otherwise HUGE systems possible.
- **Density Matrix Renormalization Theory (DMRG):** low-lying target states, correlation functions, short time evolution, maybe thermodynamics; best for 1-d; HUGE systems possible.

Intermolecular interactions

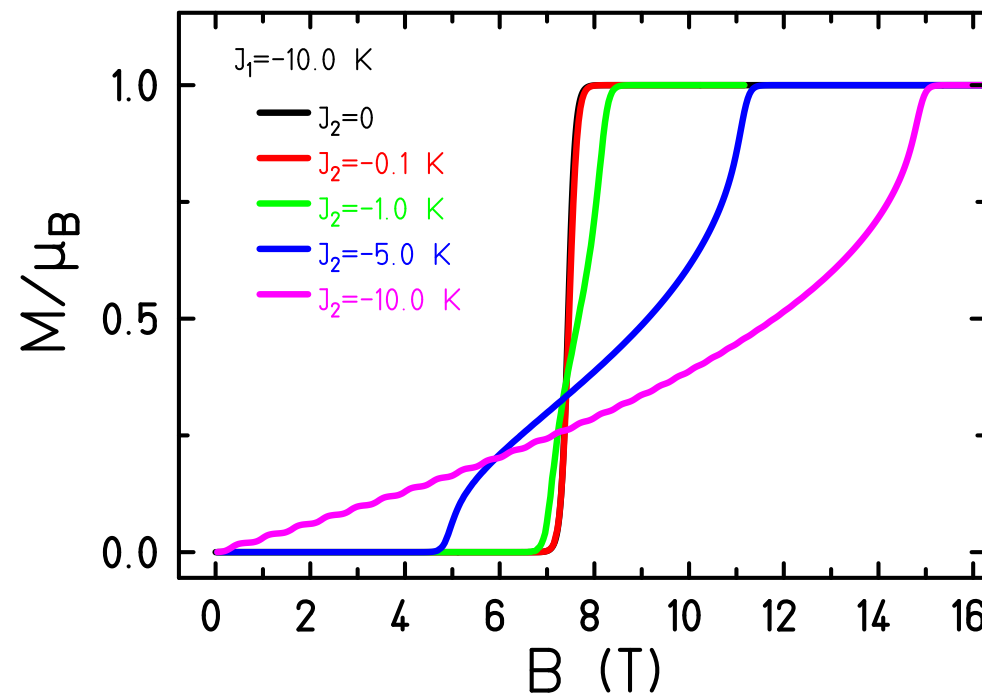
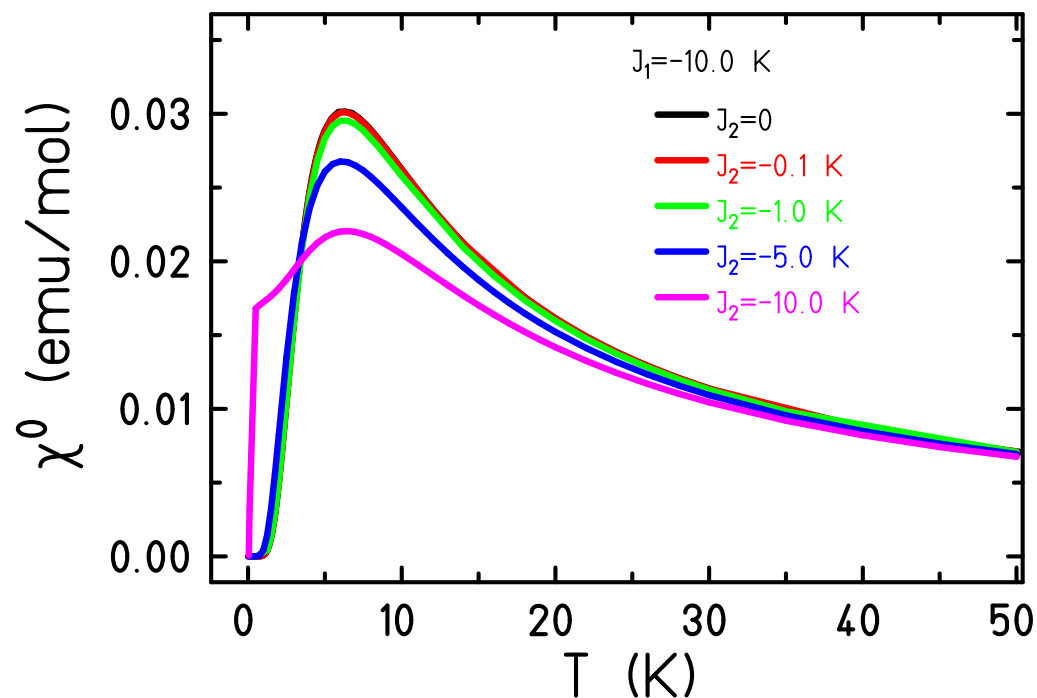
Intermolecular interactions – systems



QMC investigation: Dimers in 1-d, squares in 2-d, cubes in 3-d.
All interactions antiferromagnetic, all spins $s = 1/2$. $N = 100 \dots 1000$. PBC.

(1) J. Schnack, Phys. Rev. B **93**, 054421 (2016).

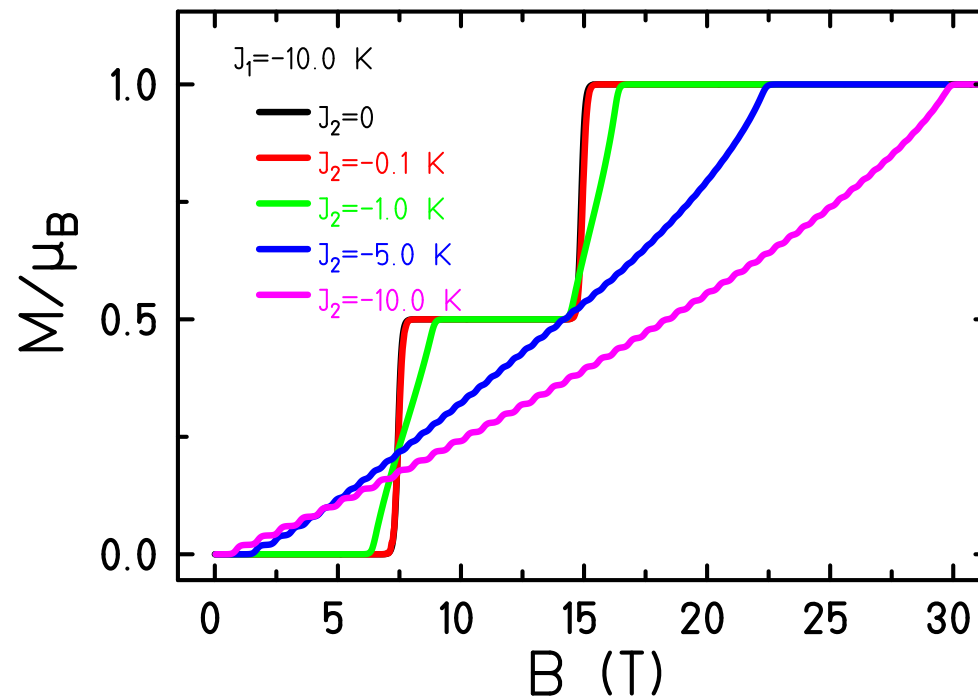
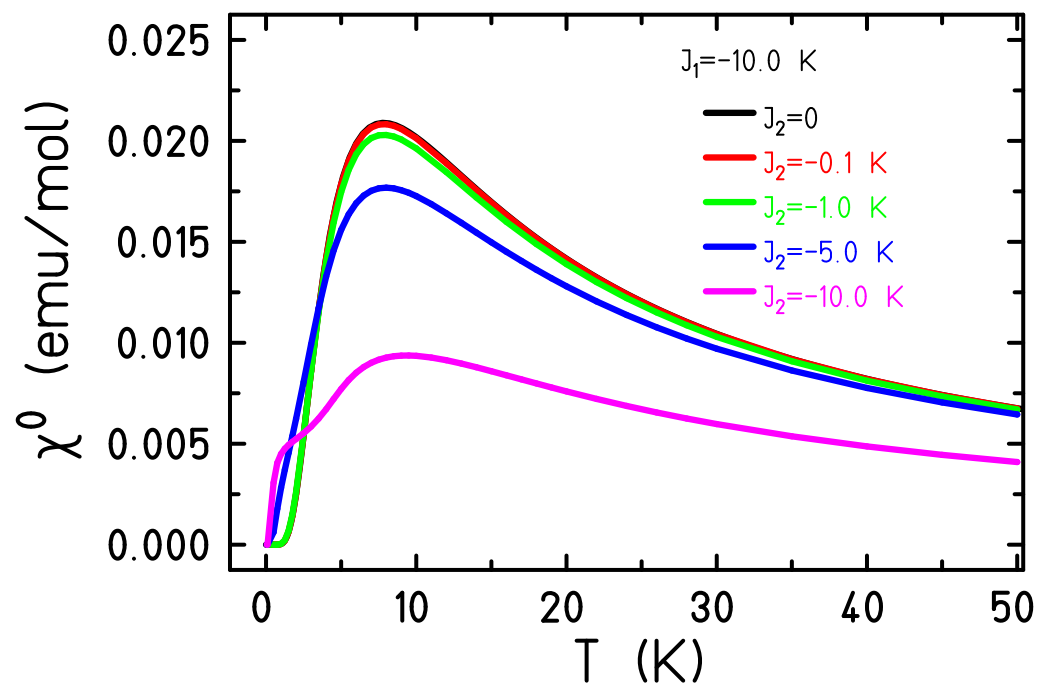
Intermolecular interactions – 1-d



Gradually af dimers turn into gapless af chain.
Even at 50 % gap still large.

(1) J. Schnack, Phys. Rev. B **93**, 054421 (2016).

Intermolecular interactions – 2-d

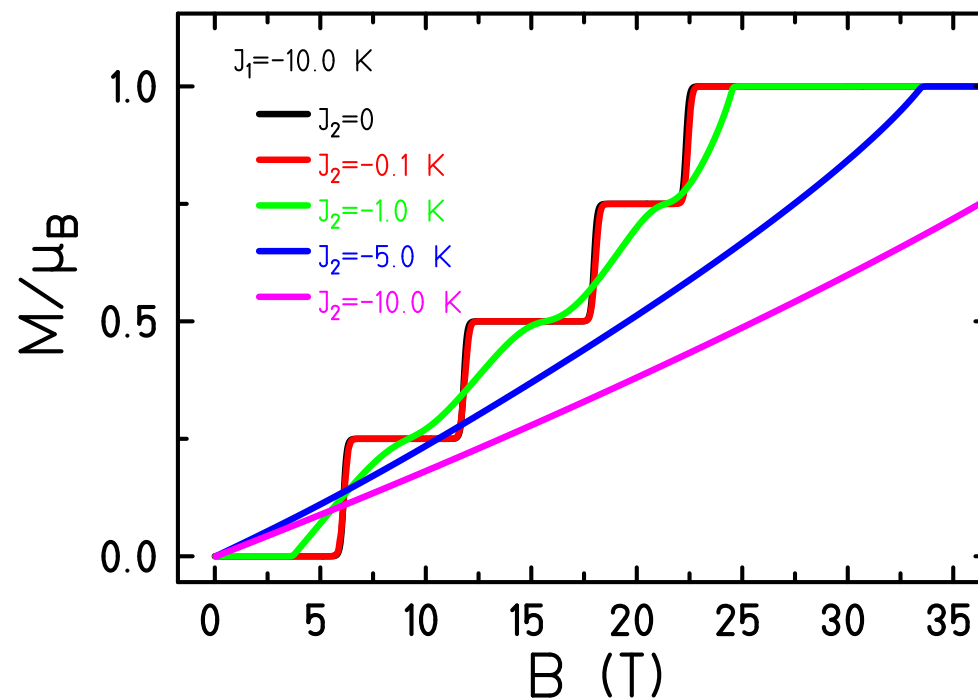
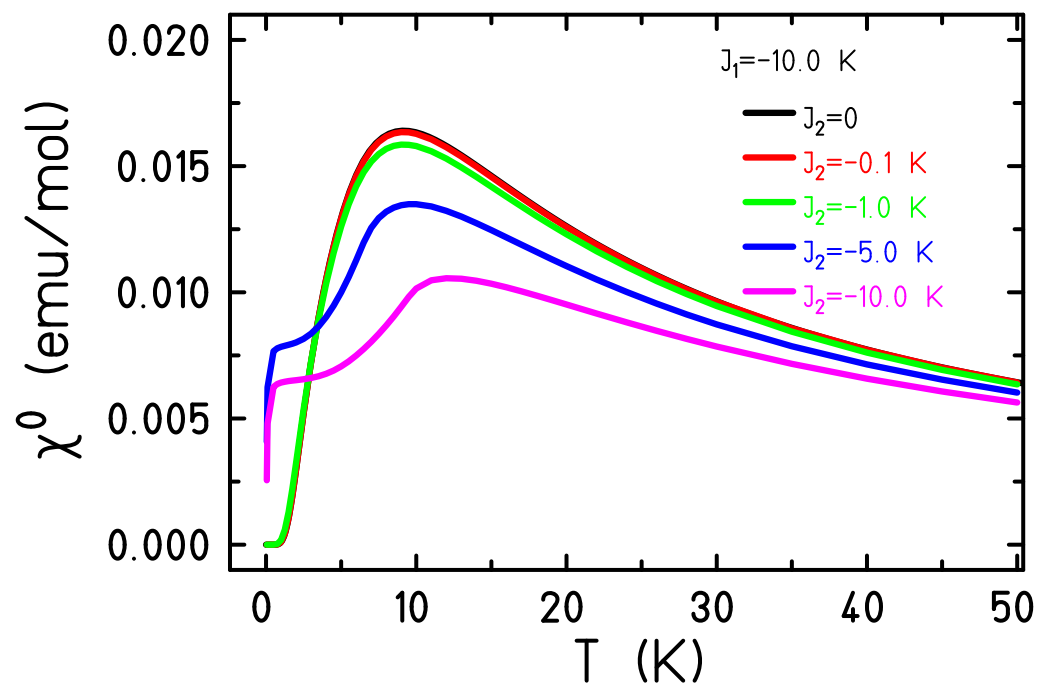


The two magnetization steps vanish more rapidly with intermolecular interactions in 2-d.

(1) J. Schnack, Phys. Rev. B **93**, 054421 (2016).

(2) O. Götze, S. E. Krüger, F. Fleck, J. Schulenburg, and J. Richter, Phys. Rev. B **85**, 224424 (2012).

Intermolecular interactions – 3-d



In 3-d 10 % intermolecular interactions sufficient to wash out magnetization steps.

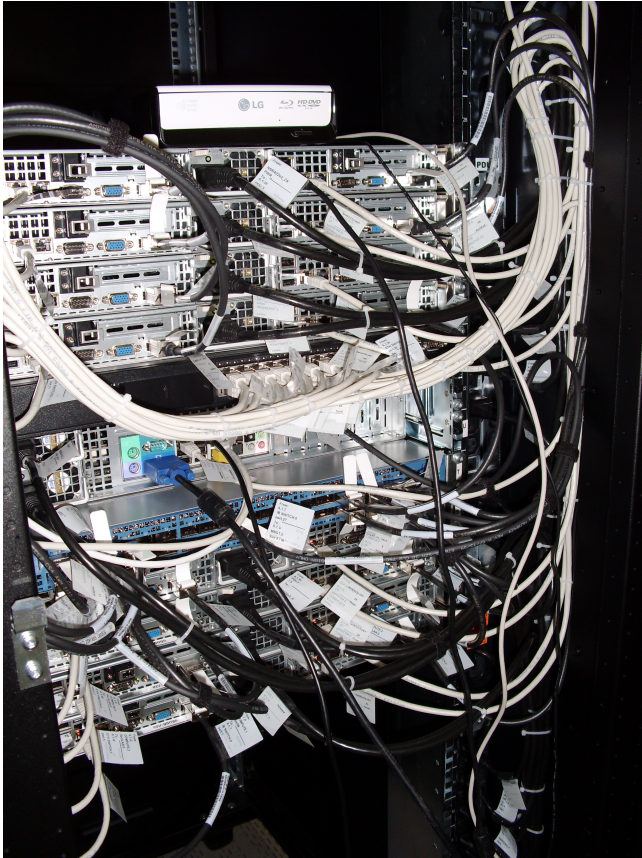
(1) J. Schnack, Phys. Rev. B **93**, 054421 (2016).

Take home:

10 % intermolecular interactions
in 3-d is enough

(...to spoil static molecular magnetic observables.)

Summary



- Magnetic molecules for storage, q-bits, MCE, and since they are nice.
- Quantum Monte Carlo can treat huge **bipartite** systems quasi exactly.
- In 3-d intermolecular interactions of 10 % strength wash out magnetization features.
- To spoil controlled time-evolution much less is needed, since influence of intermolecular interactions accumulates in the course of time.

Many thanks to my collaborators worldwide

- 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)
- M. Luban (Ames Lab, USA); P. Kögerler (Aachen, Jülich, Ames); D. Collison, R.E.P. Winpenny, E.J.L. McInnes, F. Tuna (Man U); L. Cronin, M. Murrie (Glasgow); E. Brechin (Edinburgh); H. Nojiri (Sendai, Japan); A. Postnikov (Metz); W. Wernsdorfer (Grenoble); M. Evangelisti (Zaragoza); E. Garlatti, S. Carretta, G. Amoretti, P. Santini (Parma); Gopalan Rajaraman (Mumbai)
- J. Richter, J. Schulenburg (Magdeburg); A. Honecker (Göttingen); U. Kortz (Bremen); A. Tennant, B. Lake (HMI Berlin); B. Büchner, V. Kataev, H.-H. Klauß (Dresden); P. Chaudhuri (Mühlheim); J. Wosnitza (Dresden-Rossendorf); J. van Slageren (Stuttgart); R. Klingeler (Heidelberg); O. Waldmann (Freiburg)

Thank you very much for your
attention.

The end.

Molecular Magnetism Web

www.molmag.de

Highlights. Tutorials. Who is who. Conferences.