Advanced numerical methods for spin systems

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Schauinsland
Oberkirch/Marienfeld, 12.-14. 10. 2016

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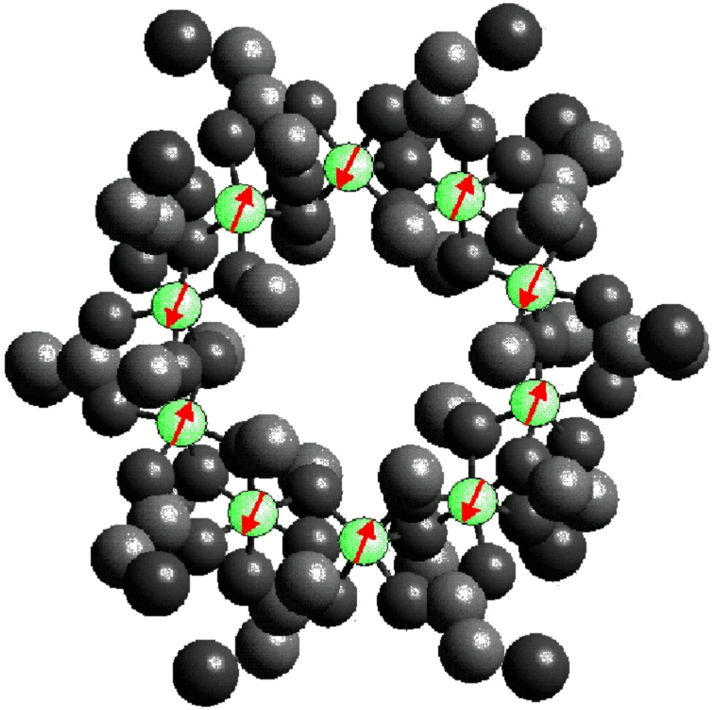
The problem

You have got a molecule!

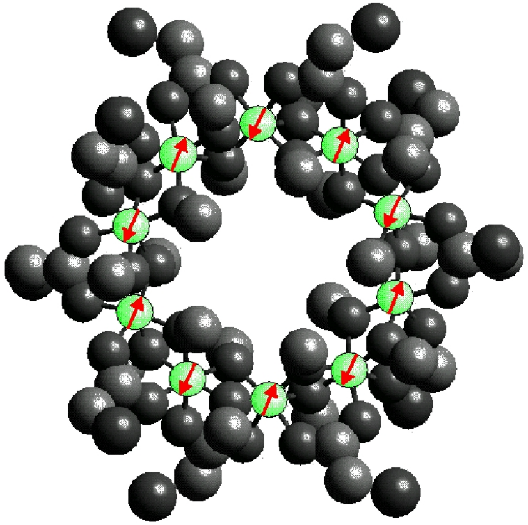


Congratulations!

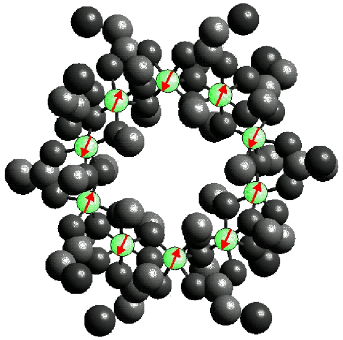
You have got an idea about the modeling!

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

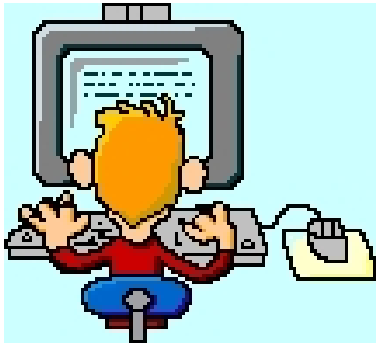
Heisenberg Zeeman



In the end it's always a big matrix!



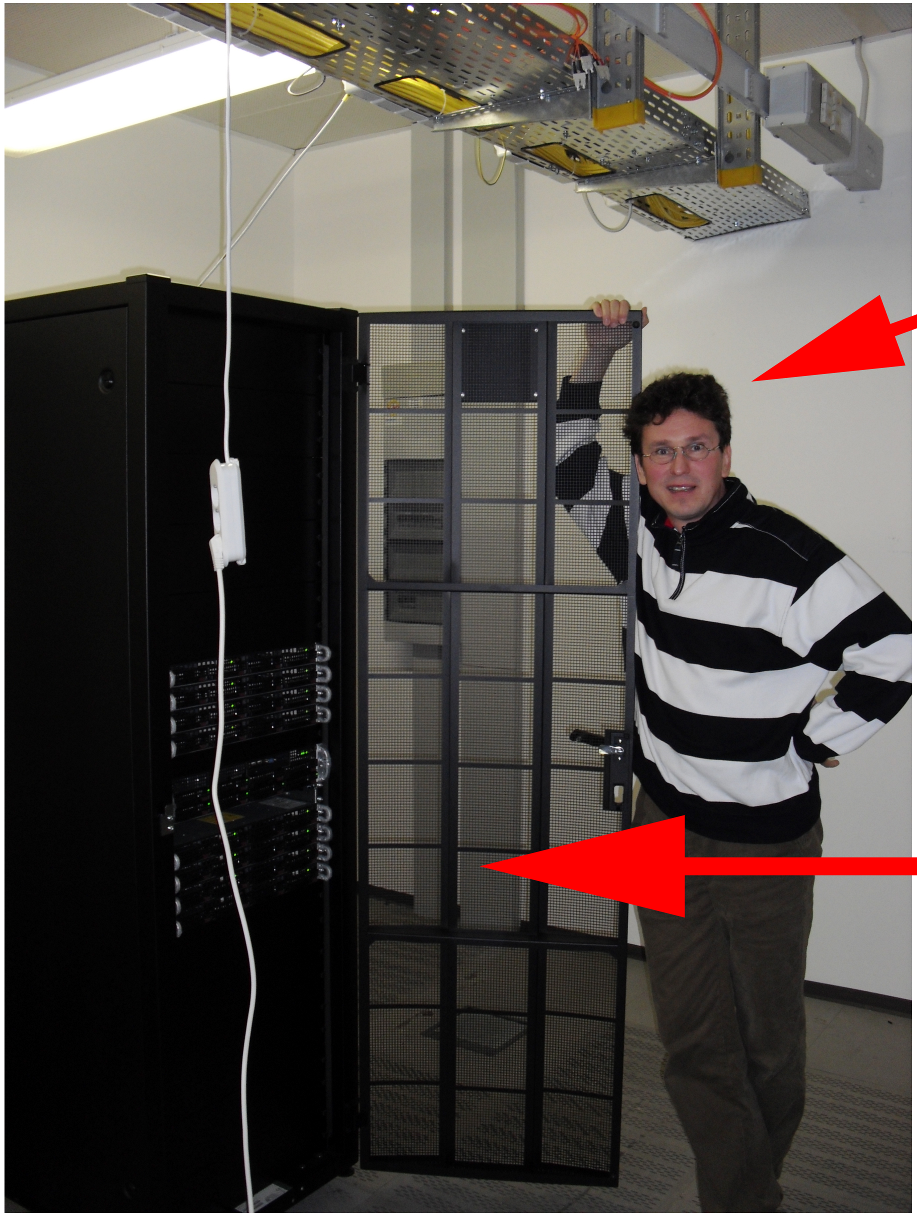
$$\Rightarrow \begin{pmatrix} -27.8 & 3.46 & 0.18 & \cdots \\ 3.46 & -2.35 & -1.7 & \cdots \\ 0.18 & -1.7 & 5.64 & \cdots \\ \vdots & \vdots & \vdots & \cdots \end{pmatrix} \Rightarrow$$



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

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

Thank God, we have computers



“Espresso-doped multi-core”

128 cores, 384 GB RAM

. . . but that’s not enough!

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. Complete diagonalization (easy)
2. Complete diagonalization (SU(2) & point group)
3. Finite-Temperature Lanczos
4. DMRG
5. QMC

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

How can one calculate such things?

(Partition function, observables in the canonical ensemble)

Complete diagonalization:
The easy version

Most physicists do this!

Model Hamiltonian – Heisenberg and more

$$\underset{\sim}{H} \;=\; -2\sum_{i<j} J_{ij}\,\underset{\sim}{\vec{s}}_i\cdot\underset{\sim}{\vec{s}}_j + \sum_{i,j}\underset{\sim}{\vec{s}}_i\cdot\mathbf{D}_{ij}\cdot\underset{\sim}{\vec{s}}_j + \mu_B\,B\sum_{i}^{N} g_i\,\underset{\sim}{s}_i^z$$

Heisenberg Anisotropy, . . . Zeeman

The Heisenberg model including anisotropy, and dipol-dipol interaction if necessary, as well as a Zeeman term describes the magnetic spectrum of many molecules with high accuracy.

Reason: Ions of the iron group have quenched angular momentum $\langle\, \underset{\sim}{l} \,\rangle \approx 0$ due to chemical binding, remaining spin-orbit coupling treated perturbatively with the help of anisotropy terms. This is different for rare earth ions!

Since the dimension of Hilbert space equals $(2s+1)^N$ the Hamiltonian can be diagonalized completely for small molecules. For larger ones approximate methods are used.

Product basis and symmtries

Product basis, total dimension: dim $(\mathcal{H}) = (2s+1)^N$

$$\underset{\sim}{s}_u^z \,|\, m_1, \dots, m_u, \dots, m_N \,\rangle = m_u \,|\, m_1, \dots, m_u, \dots, m_N \,\rangle$$

These states span the Hilbert space and are used to construct symmetry-related basis states. Use $a_u = s_u - m_u$ for computation (integer).

Symmetries of the Heisenberg model without anisotropy

$$\left[\underset{\sim}{H}, \underset{\sim}{\vec{S}}^2\right] = 0 \quad , \qquad \left[\underset{\sim}{H}, \underset{\sim}{S}_z\right] = 0$$

Additional (point group) symmetries are possible, e.g. shifts on a ring molecule.

Decomposition into mutually orthogonal subspaces

If $\left[\underset{\sim}{H}, \underset{\sim}{S}_z\right] = 0$, the Hilbert space $\mathcal{H}$ can be decomposed into mutually orthogonal subspaces $\mathcal{H}(M)$ (M is the quantum number belonging to $\underset{\sim}{S}_z$)

$$\left[\underset{\sim}{H}, \underset{\sim}{S}_z\right] = 0 \quad : \quad \mathcal{H} = \bigoplus_{M=-S_{\text{max}}}^{+S_{\text{max}}} \mathcal{H}(M) \ , \qquad S_{\text{max}} = Ns$$

$\mathcal{H}(M)$ containes all states $\left|\, m_1, \dots, m_u, \dots, m_N \,\right\rangle$ with $\sum_i m_i = M$.

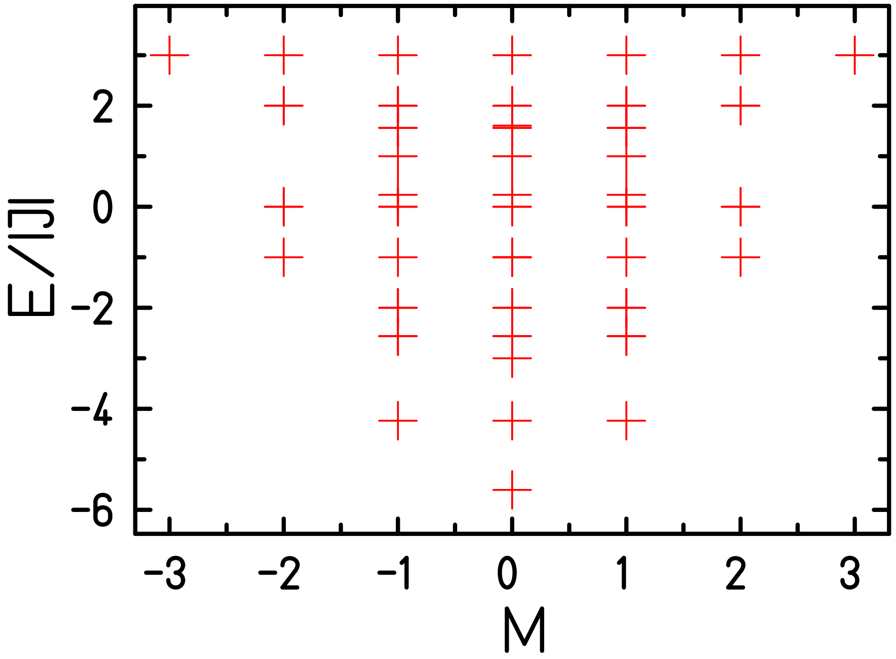
The Hamiltonian is diagonalized in all subspaces separately. The dimension of the largest subspace determines whether a Hamiltonian can diagonalized completely. If further symmetries apply this dimension will be further reduced.

For practical purposes $\underset{\sim}{\vec{s}}_i \cdot \underset{\sim}{\vec{s}}_j = \underset{\sim}{s}_i^z \underset{\sim}{s}_j^z + \frac{1}{2}\left[\underset{\sim}{s}_i^+ \underset{\sim}{s}_j^- + \underset{\sim}{s}_i^- \underset{\sim}{s}_j^+\right]$.

Example: spin ring with $N = 6, s = 1/2$

- Total dimension of $\mathcal{H}$: $Dim(\mathcal{H}) = (2 \times 1/2 + 1)^6 = 64$;
- $M = 3$: $|\,\Omega\,\rangle = |+++++\,+\rangle$; $Dim(\mathcal{H}(M)) = 1$;
- $M = 2$: $|-++++\,+\rangle$ and cyclic shifts; $Dim(\mathcal{H}(M)) = 6$;
- $M = 1$: $|--+++\,+\rangle, |-+-++\,+\rangle, |-++-+\,+\rangle$ and cyclic shifts; $Dim(\mathcal{H}(M)) = 15$;
- $M = 0$: $|---++\,+\rangle, |--+-+\,+\rangle, |-+--+\,+\rangle, |-+-+-\,+\rangle$ and cyclic shifts; $Dim(\mathcal{H}(M)) = 20$;
- Dimensional check: $64 = 1 + 6 + 15 + 20 + 15 + 6 + 1$ $\surd$
- Inclusion of translational symmetry leads to orthogonal subspaces $\mathcal{H}(M, k)$ with $k = 0, \ldots, 5$. Then the largest dimension is 4.

Exact diagonalization



- Numerically exact diagonalization feasible up to RAM size;
- Example: 10,000x10,000 complex*16, 1.6 GB RAM needed;
- Not much we can do at this point, wait for more RAM 😉

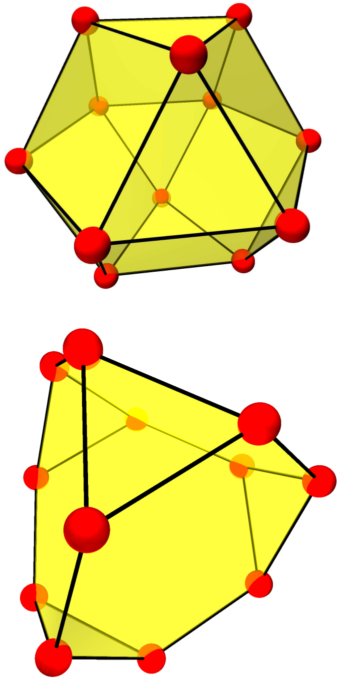
Complete diagonalization:

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).

Idea of ITO

$$\begin{aligned}\underset{\sim}{H}_{\text{Heisenberg}} &= -2\sum_{i<j} J_{ij}\ \underset{\sim}{\vec{s}}_i \cdot \underset{\sim}{\vec{s}}_j \\ &= 2\sqrt{3}\sum_{i<j} J_{ij}\,\underset{\sim}{T}^{(0)}(\{k_i\},\{\bar{k}_i\}|k_i = k_j = 1)\end{aligned}$$

Irreducible Tensor Operator approach

- Express spin operators and functions thereof as ITOs;
- Use vector coupling basis $|\,\alpha\ S\ M\,\rangle$ and recursive recoupling.

(1) Gatteschi, Tsukerblat, Coronado, Waldmann, . . .
(2) R. Schnalle, Ph.D. thesis, Osnabrück University (2009)

Point Group Symmetry

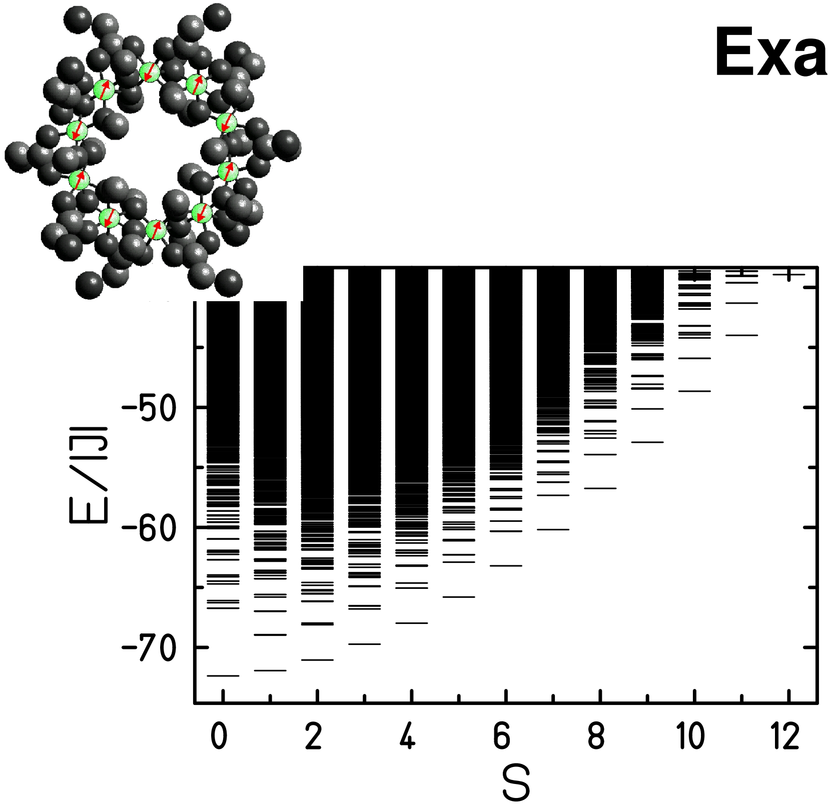
$$|\,\alpha'\,S\,M\,\Gamma\,\rangle = \mathcal{P}^{(\Gamma)}\,|\,\alpha\,S\,M\,\rangle = \left(\frac{l_\Gamma}{h}\sum_R \left(\chi^{(\Gamma)}(R)\right)^*\,\underset{\sim}{G}(R)\right)\,|\,\alpha\,S\,M\,\rangle$$

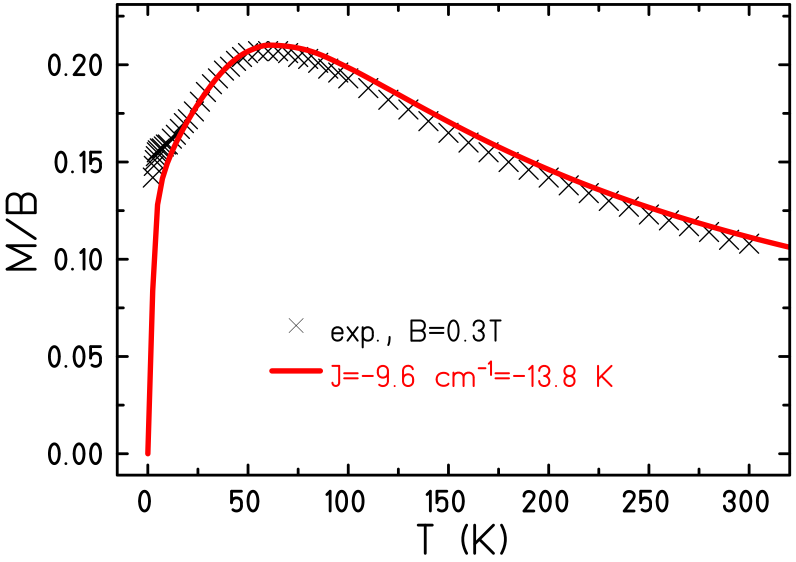
Method:

- 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) ⇐ contains EVERYTHING.

Example: Fe$_{10}$





Spin ring, $N = 10$, $s = 5/2$, Hilbert space dimension 60,466,176; symmetry D_2 (1).

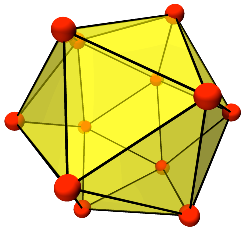
(1) R. Schnalle and J. Schnack, Int. Rev. Phys. Chem. **29**, 403-452 (2010).
(2) C. Delfs *et al.*, Inorg. Chem. **32**, 3099 (1993).

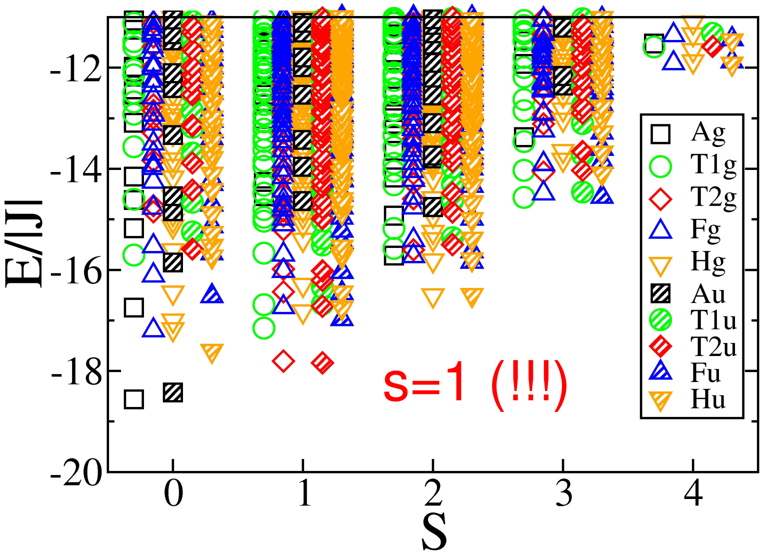
Point Group Symmetry II

$$\underset{\sim}{G}(R)\,|\,\alpha\,S\,M\,\rangle_a = |\,\alpha\,S\,M\,\rangle_b = \sum_{\alpha'} |\,\alpha'\,S\,M\,\rangle_a\;{}_a\langle\,\alpha'\,S\,M\,|\,\alpha\,S\,M\,\rangle_b$$

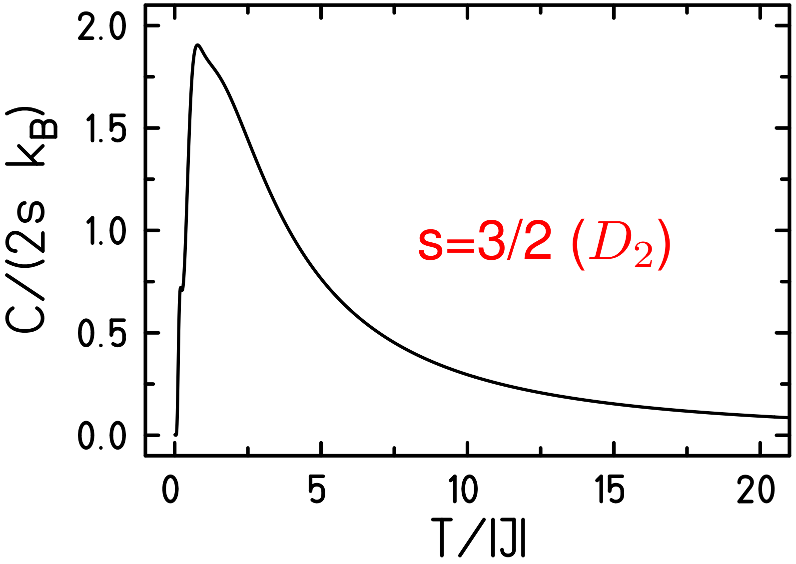
- Serious problem: application of $\underset{\sim}{G}(R)$, i.e. permutation of spins, leads to different coupling schemes: $a \Rightarrow b$;
- Solution: implementation of graph-theoretical results to evaluate recoupling coefficients ${}_a\langle\,\alpha'\,S\,M\,|\,\alpha\,S\,M\,\rangle_b$.

Example: Icosahedron





s=1 (!!!)



s=3/2 (D_2)

Icosahedron, $s = 3/2$, Hilbert space dimension 16,777,216; symmetry I_h;
Evaluation of recoupling coefficients for $s = 3/2$ in I_h **practically impossible** (1).

(1) R. Schnalle and J. Schnack, Int. Rev. Phys. Chem. **29**, 403-452 (2010).

World-leading, but . . .

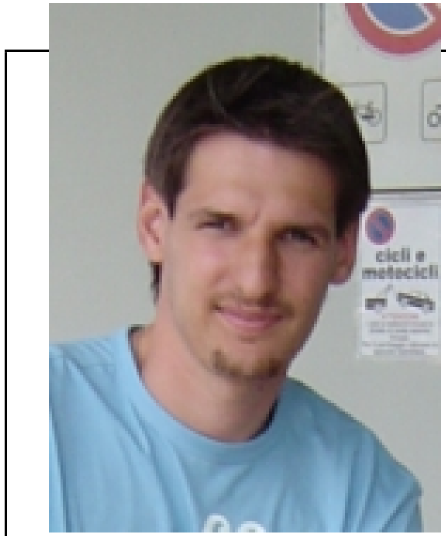
This world-leading method was developed in Osnabrück, unfortunately . . .

World-leading, but . . .

. . . too late!

There are more powerful and easy to program methods.

Nevertheless, matrix theory goes on . . .

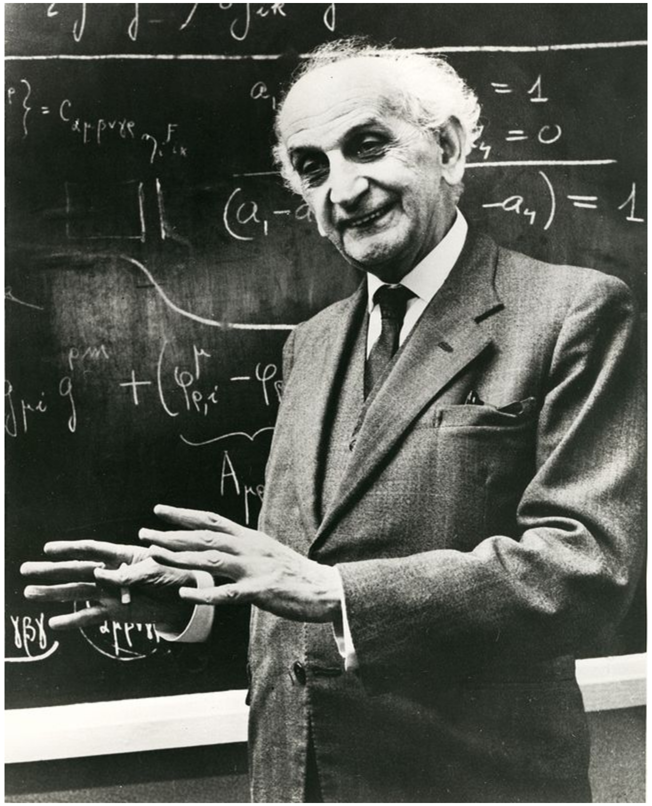


. . . at the Hessische Landesbank!

Finite-temperature Lanczos Method

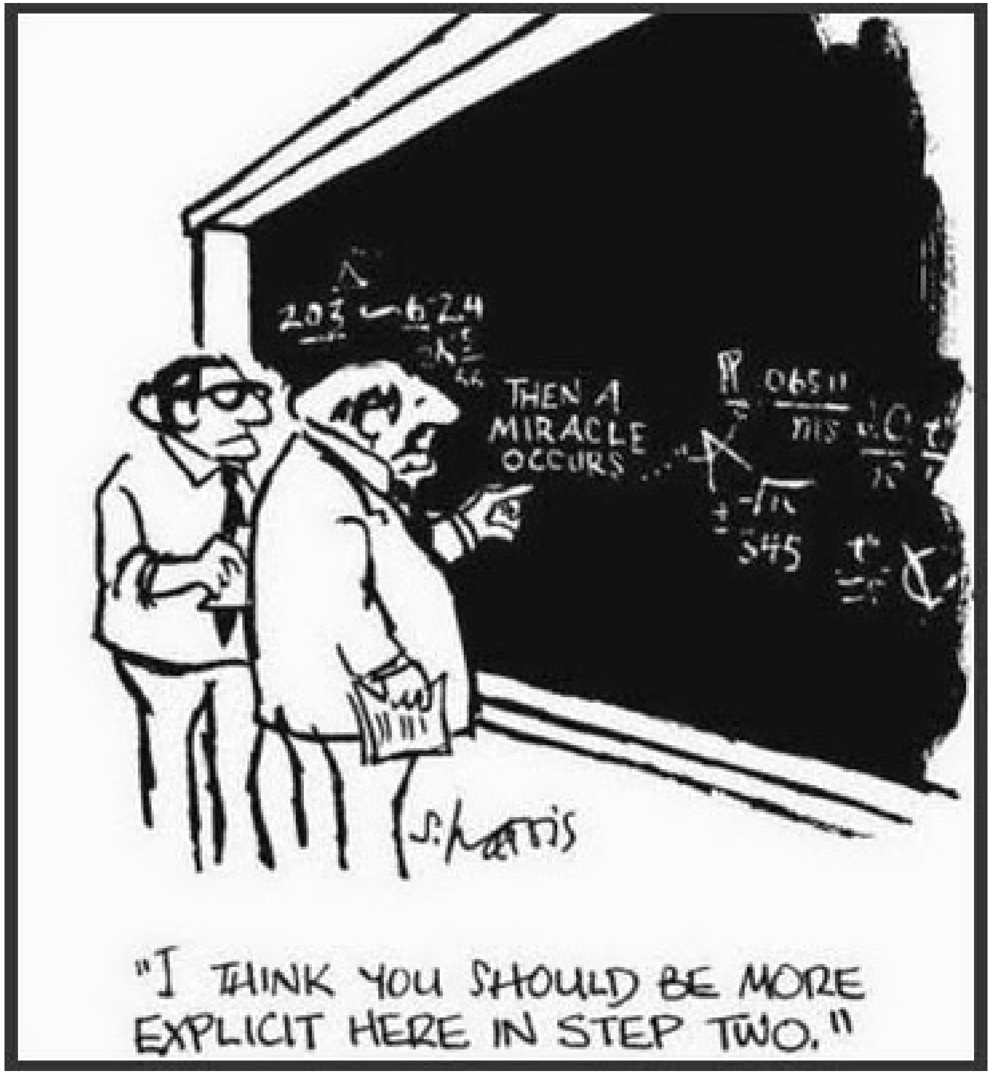
(Good for dimensions up to 10^{10}.)

Lanczos – a Krylov space method



- Idea: exact diagonalization in reduced basis sets.
- But which set to choose???
- Idea: generate the basis set with the operator you want to diagonalize: $\{\,|\,\phi\,\rangle, \underset{\sim}{H}\,|\,\phi\,\rangle, \underset{\sim}{H}^2\,|\,\phi\,\rangle, \underset{\sim}{H}^3\,|\,\phi\,\rangle, \dots\,\}$
- But which starting vector to choose???
- Idea: almost any will do!
- Cornelius Lanczos (Lánczos Kornél, 1893-1974)

(1) C. Lanczos, J. Res. Nat. Bur. Stand. **45**, 255 (1950).


THEN A MIRACLE OCCURS
S. Harris
"I THINK YOU SHOULD BE MORE EXPLICIT HERE IN STEP TWO."

Finite-temperature Lanczos Method I

$$Z(T,B) = \sum_{\nu} \langle\, \nu \,|\, \exp\left\{-\beta \underset{\sim}{H}\right\} |\, \nu \,\rangle$$

$$\langle\, \nu \,|\, \exp\left\{-\beta \underset{\sim}{H}\right\} |\, \nu \,\rangle \approx \sum_{n} \langle\, \nu \,|\, n(\nu) \,\rangle \exp\left\{-\beta \epsilon_n\right\} \langle\, n(\nu) \,|\, \nu \,\rangle$$ (Step 2)

$$Z(T,B) \approx \frac{\text{dim}(\mathcal{H})}{R} \sum_{\nu=1}^{R} \sum_{n=1}^{N_L} \exp\left\{-\beta \epsilon_n\right\} |\langle\, n(\nu) \,|\, \nu \,\rangle|^2$$

- $|\, n(\nu) \,\rangle$ n-th Lanczos eigenvector starting from $|\, \nu \,\rangle$
- Partition function replaced by a small sum: $R = 1 \dots 10, N_L \approx 100$.

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

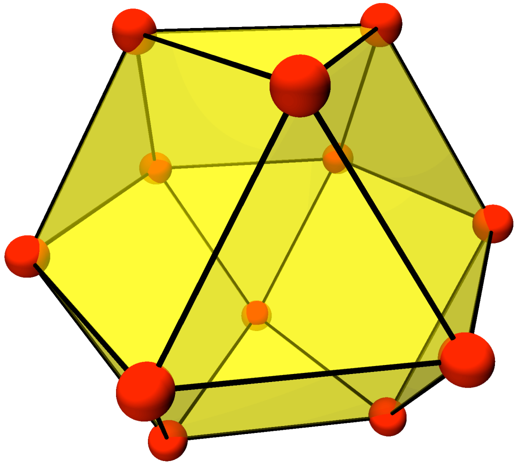
Finite-temperature Lanczos Method II

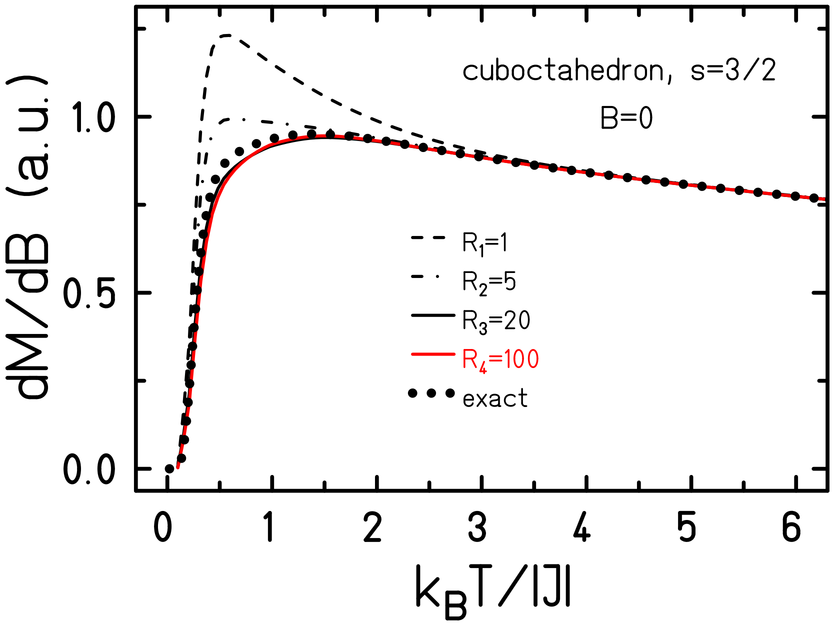
$$Z(T,B) \approx \sum_{\Gamma} \frac{\mathrm{dim}(\mathcal{H}(\Gamma))}{R_\Gamma} \sum_{\nu=1}^{R_\Gamma} \sum_{n=1}^{N_L} \exp\left\{-\beta\epsilon_n\right\} |\langle\, n(\nu,\Gamma) \,|\, \nu,\Gamma\,\rangle|^2$$

- Approximation better if symmetries taken into account.
- Γ denotes the used irreducible representations.

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

How good is finite-temperature Lanczos?

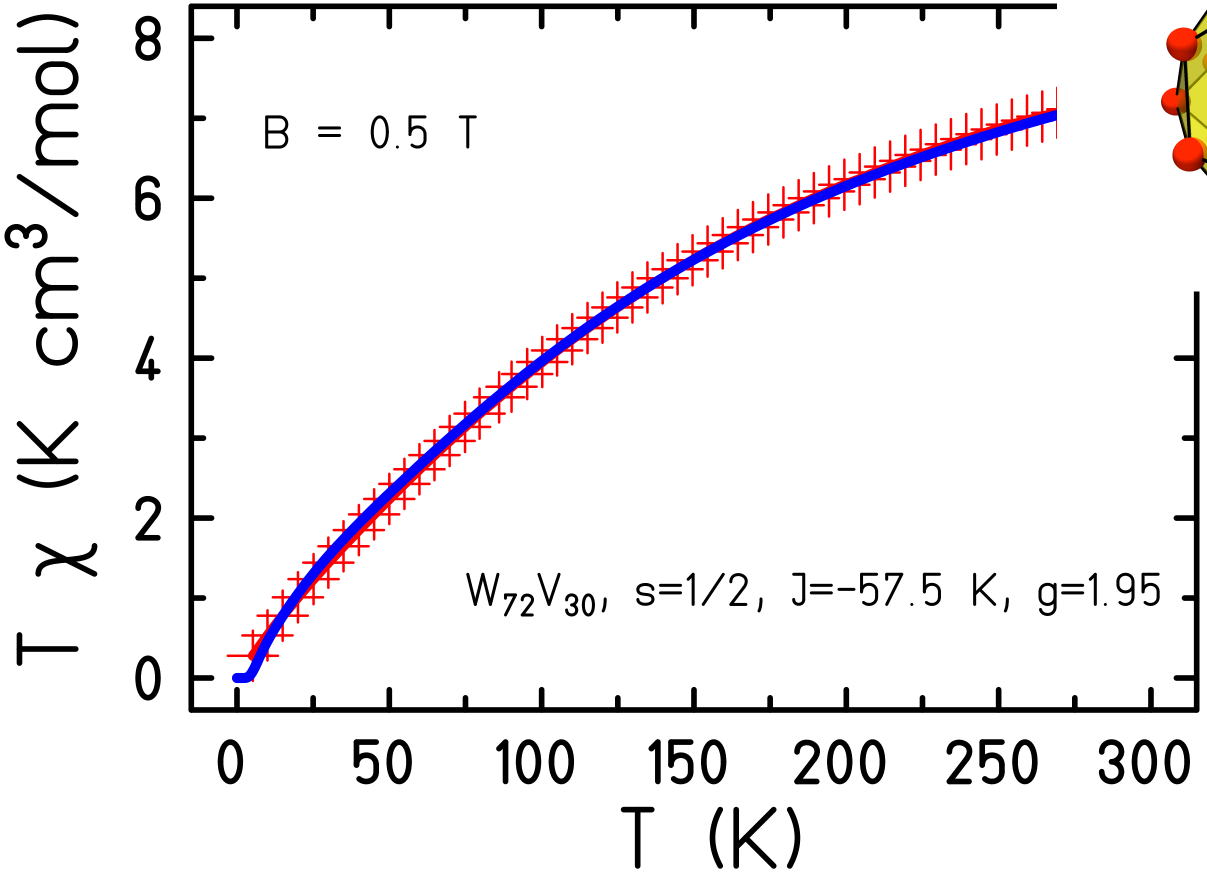


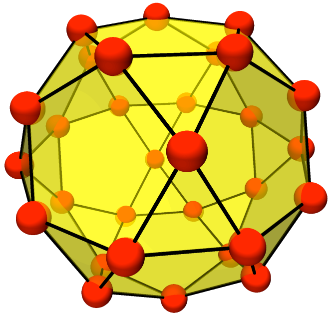


- Works very well: compare frustrated cuboctahedron.
- $N = 12, s = 3/2$: Considered $< 100,000$ states instead of 16,777,216.

Exact results: R. Schnalle and J. Schnack, Int. Rev. Phys. Chem. **29**, 403-452 (2010).
FTLM: J. Schnack and O. Wendland, Eur. Phys. J. B **78**, 535-541 (2010).

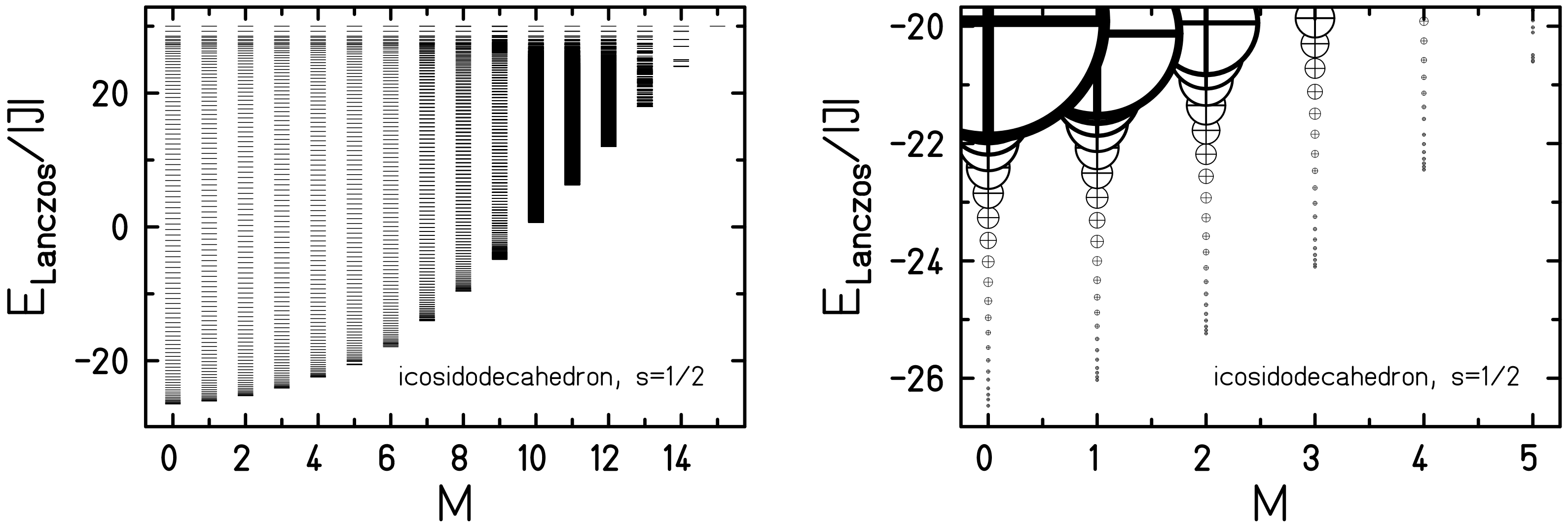
Icosidodecahedron $s = 1/2$





Exp. data: A. M. Todea, A. Merca, H. Bögge, T. Glaser, L. Engelhardt, R. Prozorov, M. Luban, A. Müller, Chem. Commun., 3351 (2009).

Icosidodecahedron $s = 1/2$



- The true spectrum will be much denser. This is miraculously compensated for by the weights.

$$Z(T,B) \approx \frac{\text{dim}(\mathcal{H})}{R} \sum_{\nu=1}^{R} \sum_{n=1}^{N_L} \exp\{-\beta\epsilon_n\} \left|\langle\, n(\nu,\Gamma)\,|\,\nu,\Gamma\,\rangle\right|^2$$

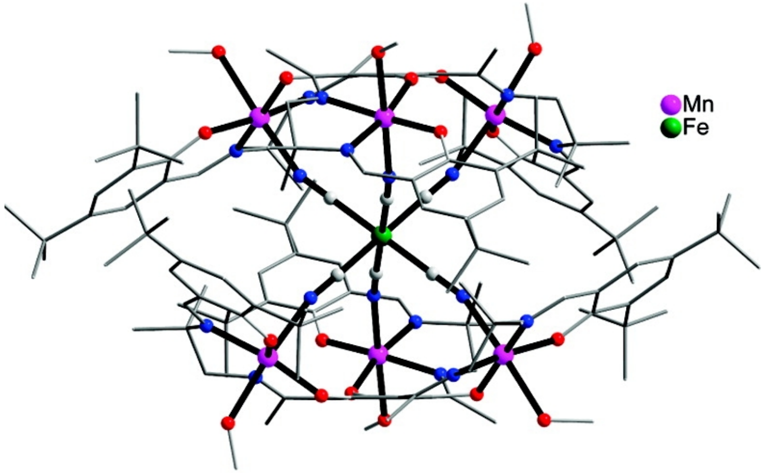
Anisotropic magnetic molecules I – Theory

$$\underset{\sim}{H}(\vec{B}) = -\sum_{i,j} J_{ij}\underset{\sim}{\vec{s}}(i)\cdot\underset{\sim}{\vec{s}}(j) + \sum_{i} d_i\left(\vec{e}_i\cdot\underset{\sim}{\vec{s}}(i)\right)^2 + \mu_B\,\vec{B}\cdot\sum_{i}^{N}\mathbf{g}_i\cdot\underset{\sim}{\vec{s}}(i)$$

- $\left[\underset{\sim}{H},\underset{\sim}{\vec{S}}^2\right]\neq 0$, $\left[\underset{\sim}{H},\underset{\sim}{S}_z\right]\neq 0$;
- You have to diagonalize $\underset{\sim}{H}(\vec{B})$ for every field (direction and strength)!
  $\Rightarrow$ Orientational average.
- If you are lucky, point group symmetries still exist. Use them!
- Easy: dim$(\mathcal{H}) < 30,000$; possible: $30,000 <$ dim$(\mathcal{H}) < 140,000$

T. Glaser *et al.* *et* J. Schnack, Inorg. Chem. **48**, 607 (2009).

Single Molecule Magnets V

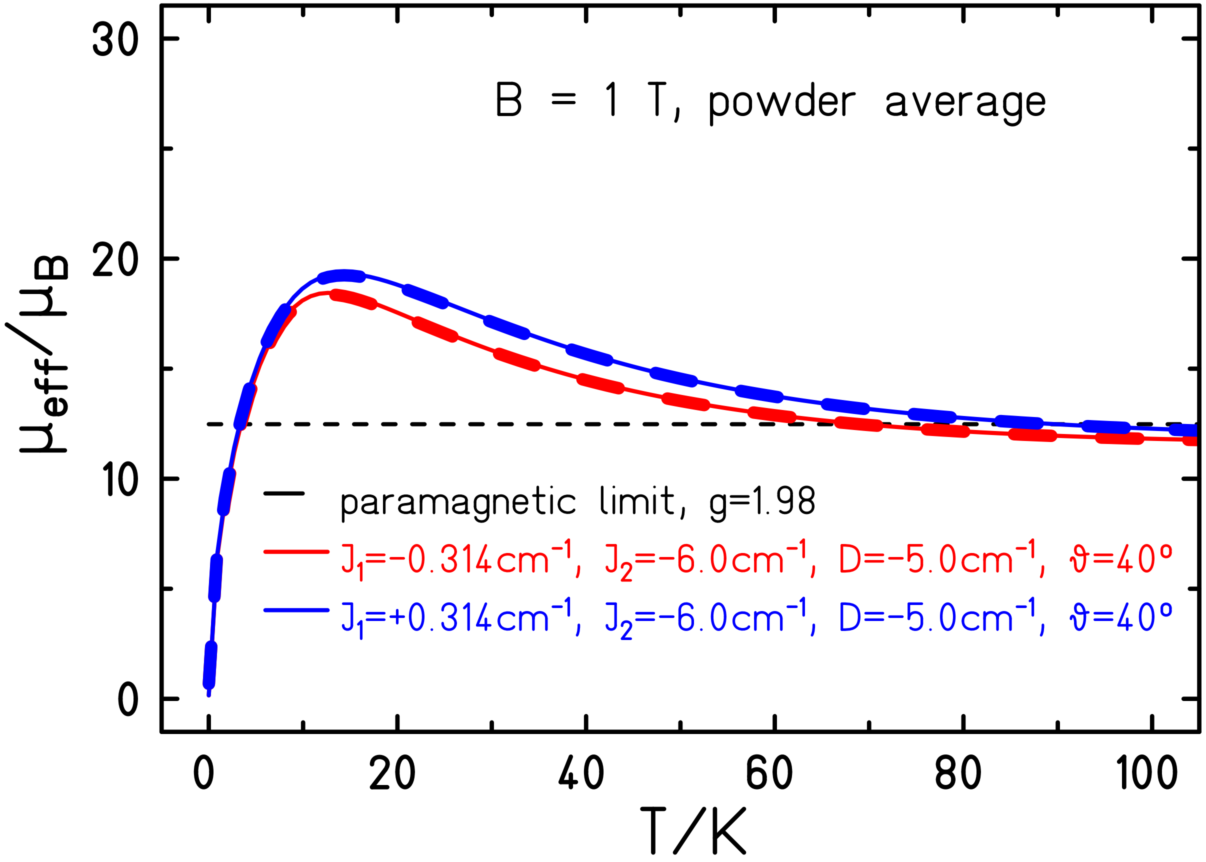


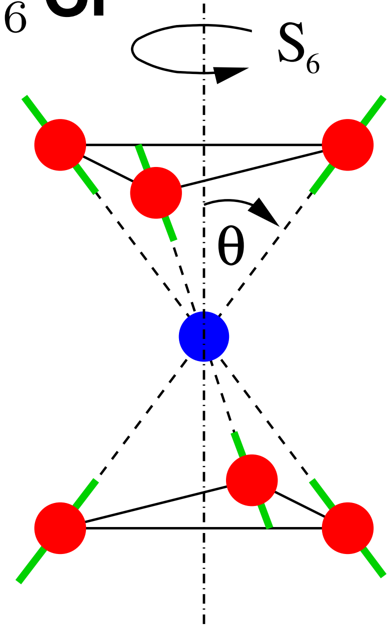
Rational design of strict C_3 symmetry:

- Idea of Thorsten Glaser (Bielefeld): C_3 symmetric alignment of local easy axes (easy axis $\equiv$ Jahn-Teller axis);
- Various ions could be used so far, e.g. Mn_6Cr (1), Mn_6Fe (2), . . .
- Advantage: no E-terms, i.e. no (less) tunneling;
- Problem: exchange interaction sometimes antiferromagnetic.

T. Glaser *et al.*, Angew. Chem.-Int. Edit. **45**, 6033 (2006).
T. Glaser *et al.*, Inorg. Chem. **48**, 607 (2009).

Glaser-type molecules: $\mathrm{Mn}_6^{\mathrm{III}}\mathrm{Cr}^{\mathrm{III}}$





$s = 2$, $s = 3/2$

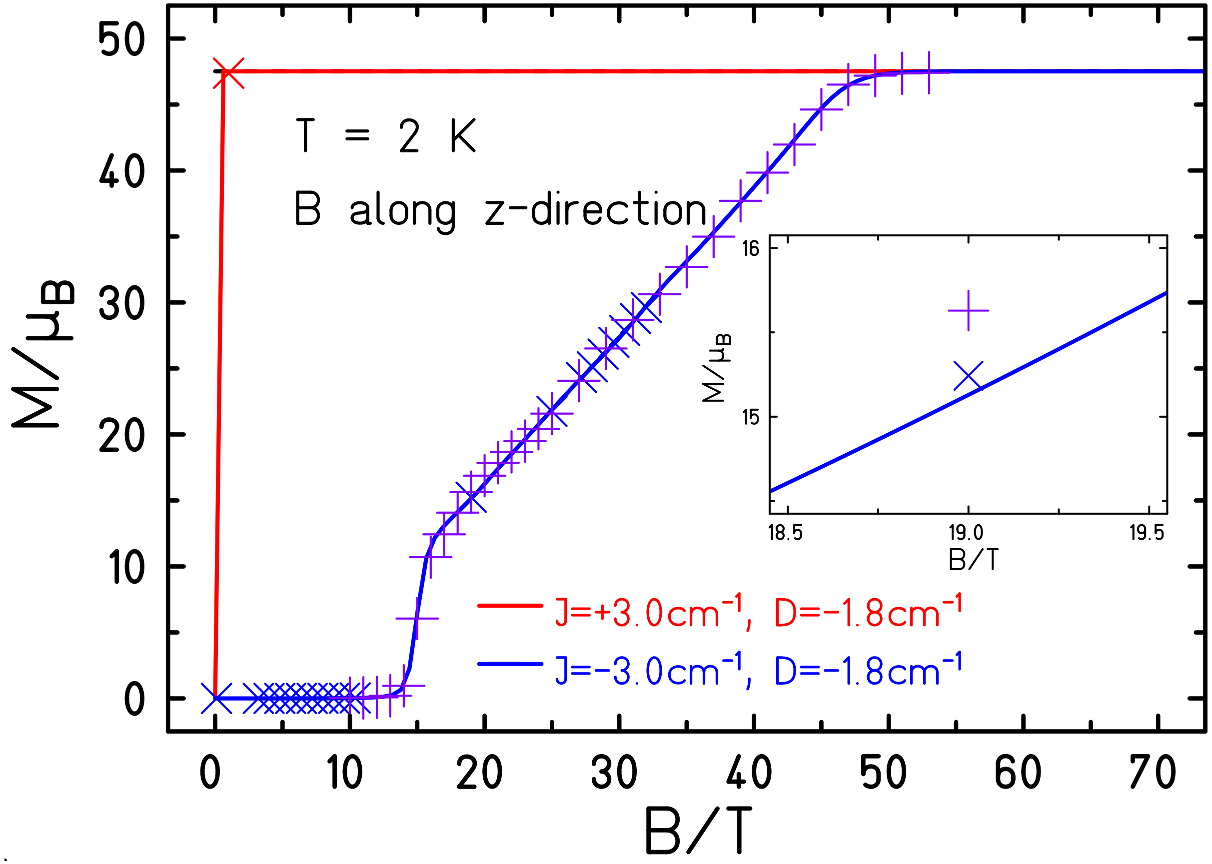
$\dim(\mathcal{H}) = 62,500$

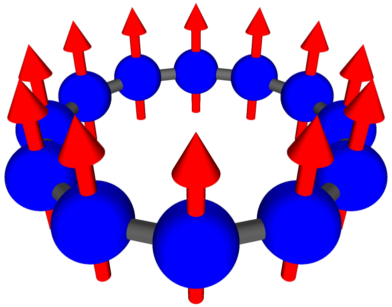
non-collinear easy axes

Hours compared to days, notebook compared to supercomputer!

O. Hanebaum, J. Schnack, Eur. Phys. J. B **87**, 194 (2014)

A fictitious $\mathrm{Mn}_{12}^{\mathrm{III}}$ – M_z vs B_z





$s = 2$

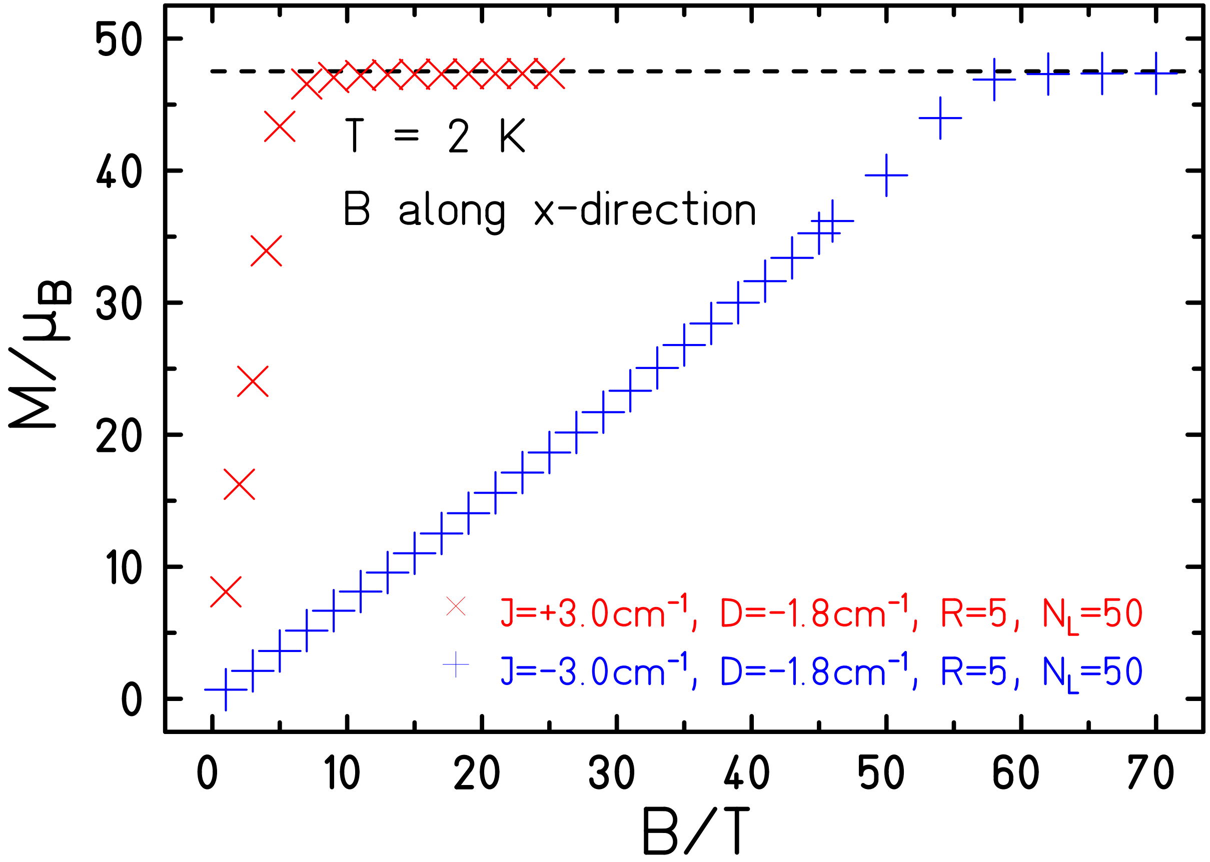
dim$(\mathcal{H}) = 244,140,625$

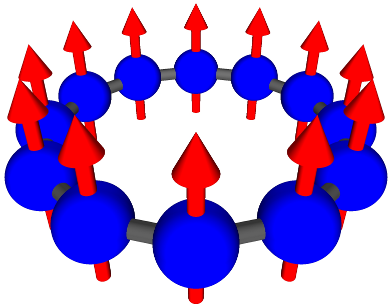
collinear easy axes

A few days compared to *impossible*!

O. Hanebaum, J. Schnack, Eur. Phys. J. B **87**, 194 (2014)

A fictitious $\mathrm{Mn}_{12}^{\mathrm{III}}$ – M_x vs B_x

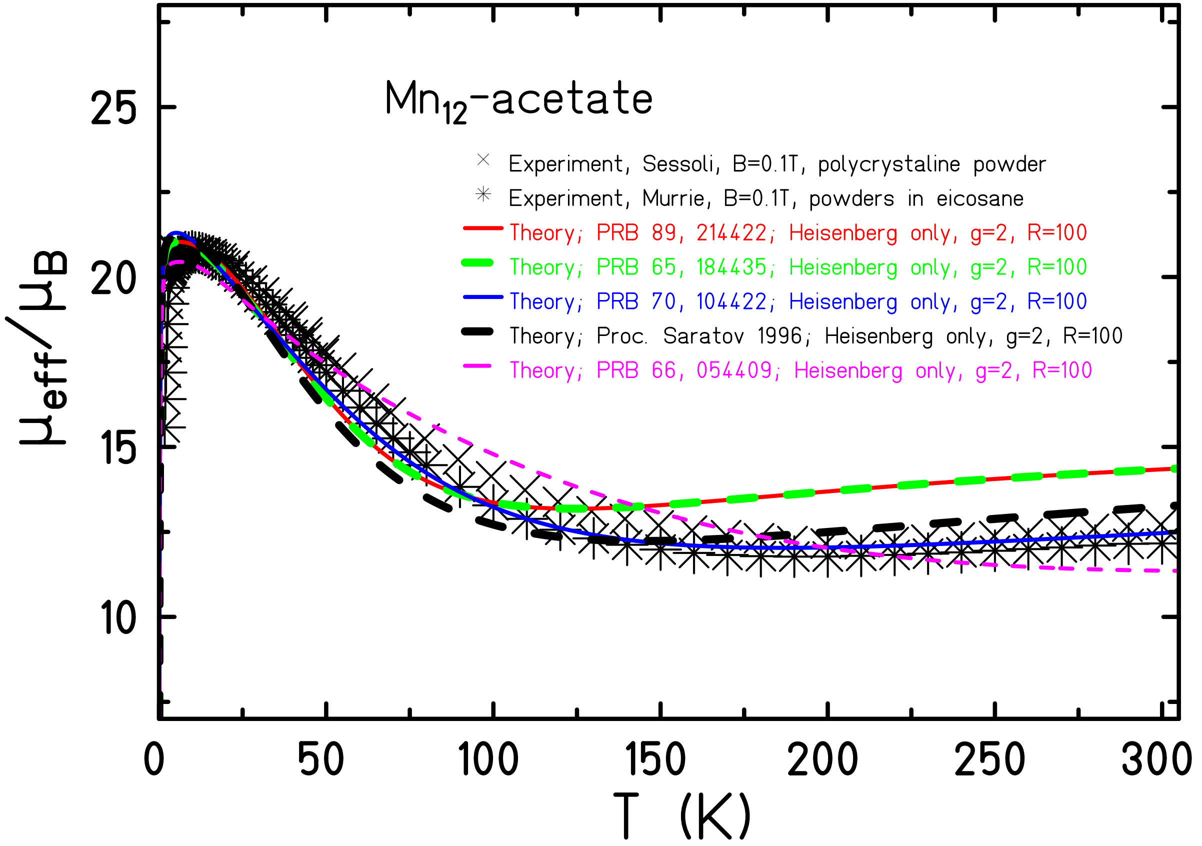




No other method can deliver these curves!

O. Hanebaum, J. Schnack, Eur. Phys. J. B **87**, 194 (2014)

Example FTLM: Mn_{12}-acetate with all spins



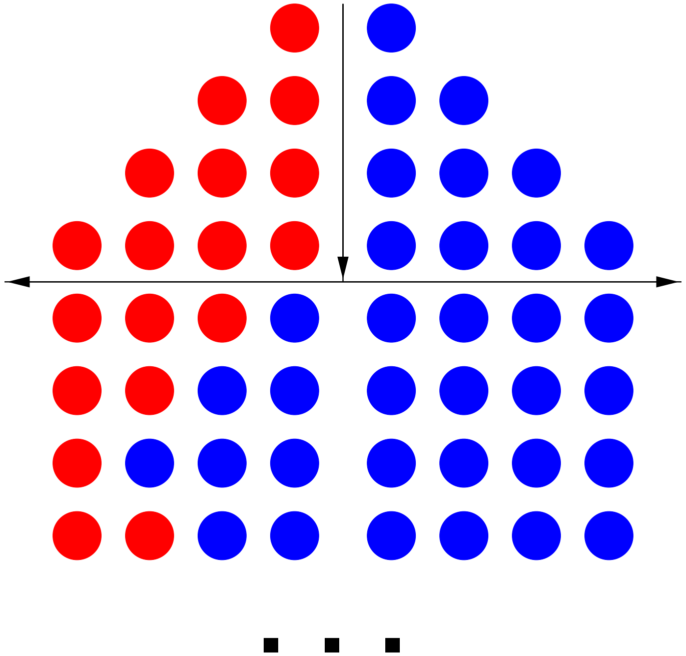
We can check DFT parameter predictions for large molecules (Mn_{12} – 100,000,000)!

(1) O. Hanebaum, J. Schnack, Phys. Rev. B **92**, 064424 (2015).

Density Matrix Renormalization Group

(Best for one-dimensional systems, even for huge sizes.)

Density Matrix Renormatization Group



Again: build your appropriate reduced basis set

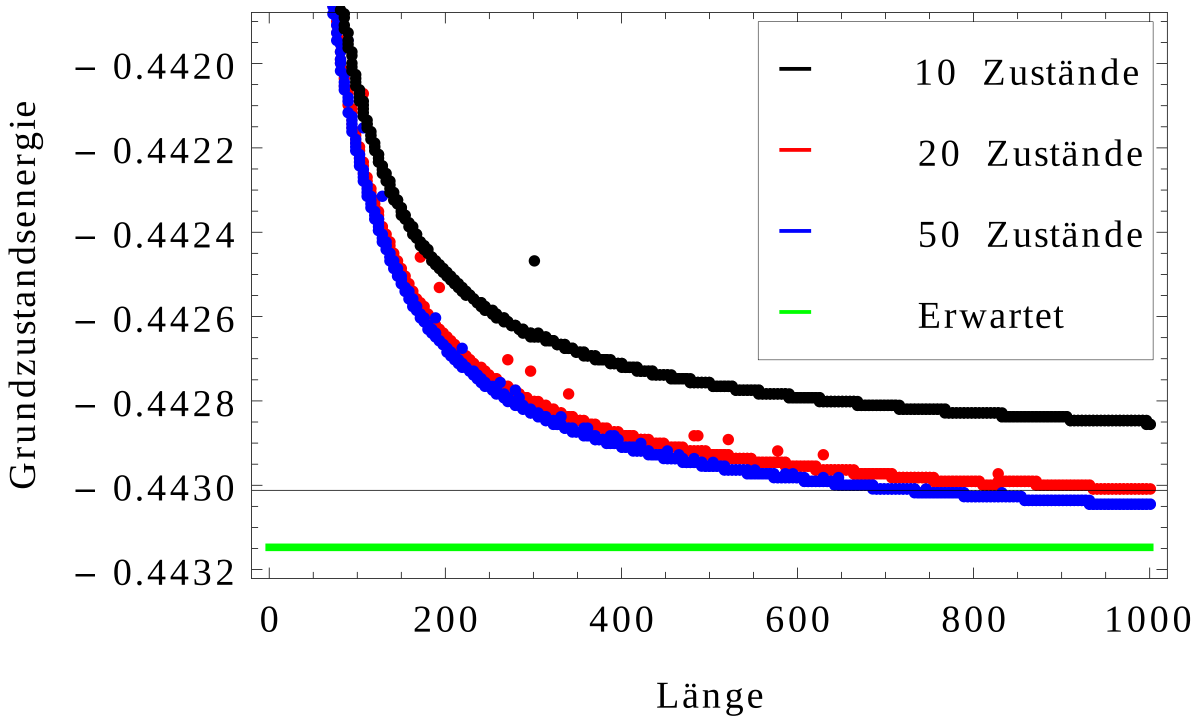
- Naive idea: start with small system, diagonalize $\underset{\sim}{H}$, keep only m lowest states, enlarge system, diagonalize $\underset{\sim}{H}$, keep only m lowest states, . . .

- Better: similar idea, use low-lying eigenstates of density matrix of part of system (1,2,3).

- Technical procedure: growth of system & sweeps.

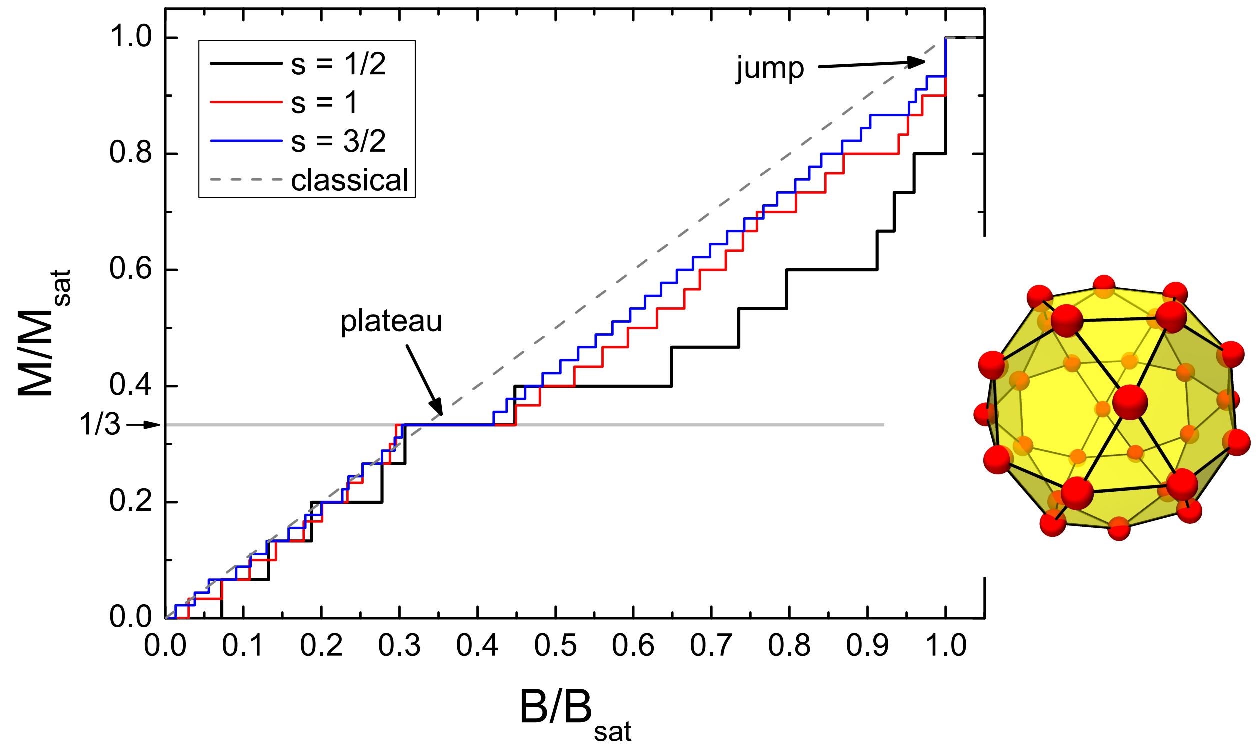
(1) S. R. White, Phys. Rev. Lett. **69**, 2863 (1992).
(2) S. R. White, Phys. Rev. B **48**, 10345 (1993).
(3) U. Schollwöck, Rev. Mod. Phys. **77**, 259 (2005).

DMRG spin chain $s = 1/2$



- Simple example: 1000 spins with $s = 1/2$; Hilbert space dimension $2^{1000} \approx 10^{301}$.
- Approaches result known from Bethe ansatz with matrices as small as 50×50!

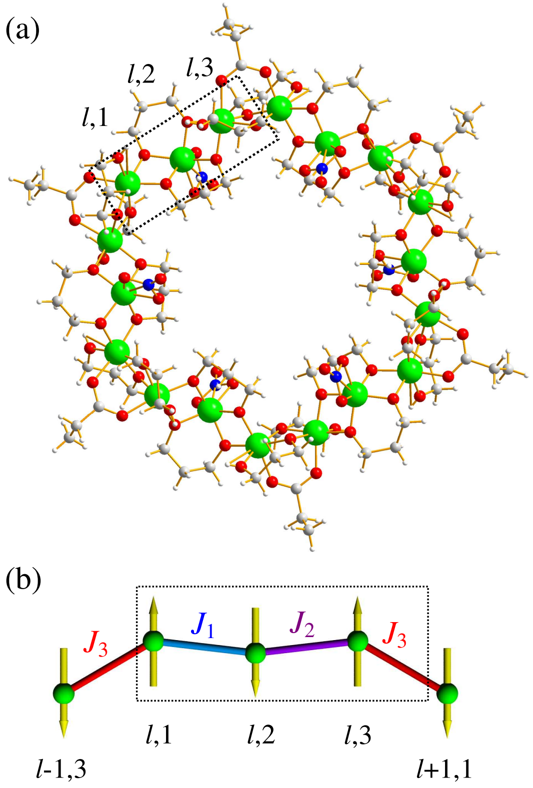
Density Matrix Renormatization Group



- DMRG yields ground states + very few low-lying states in orthogonal subspaces.
- Magnetization curve for $T = 0$, resonance energies for spectroscopy.

(1) J. Ummethum, J. Schnack, and A. Laeuchli, J. Magn. Magn. Mater. **327** (2013) 103

Dynamical Density Matrix Renormatization Group

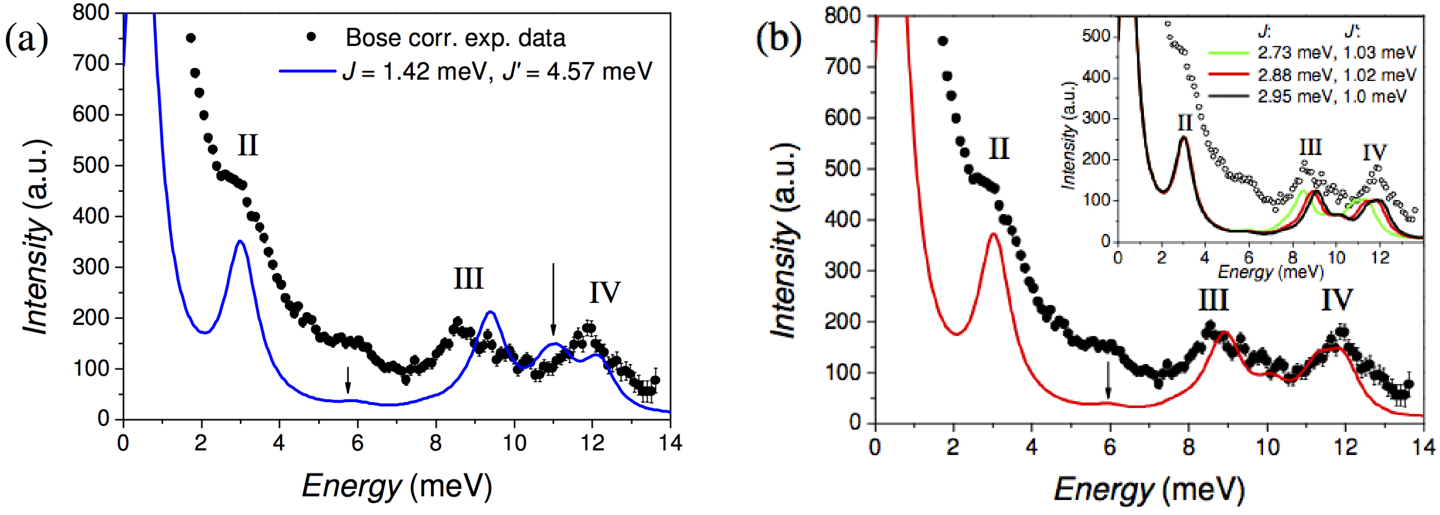


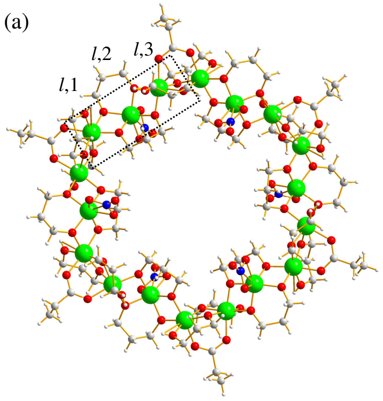
Evaluation of correlation functions, e.g. for INS:

- $S^{zz}_{jj'}(\omega) \equiv \sum_n \langle 0|\underset{\sim}{s}^{z}_{j}|n\rangle\langle n|\underset{\sim}{s}^{z}_{j'}|0\rangle\, \delta(\hbar\omega - E_n + E_0)$; transitions from the ground state;
- $S^{zz}_{jj'}(\omega) \approx \frac{1}{\pi}\langle 0|\underset{\sim}{s}^{z}_{j} \frac{\eta}{(E_0+\hbar\omega-\underset{\sim}{H})^2+\eta^2} \underset{\sim}{s}^{z}_{j'}|0\rangle$;
- Use DMRG ground state and DMRG representation of $\underset{\sim}{H}$ (1,2); η – finite broadening.

(1) T. D. Kühner and S. R. White, Phys. Rev. B **60**, 335 (1999).
(2) E. Jeckelmann, Phys. Rev. B **66**, 045114 (2002).
(3) P. King, T. C. Stamatatos, K. A. Abboud, and G. Christou, Angew. Chem. Int. Ed. **45**, 7379 (2006).
(4) O. Waldmann *et al.*, Phys. Rev. Lett. **102**, 157202 (2009).

Dynmical Density Matrix Renormatization Group





- Accurate description of low-lying excitations for the giant ferric wheel Fe_{18}. Hilbert space dimension 10^{14}.

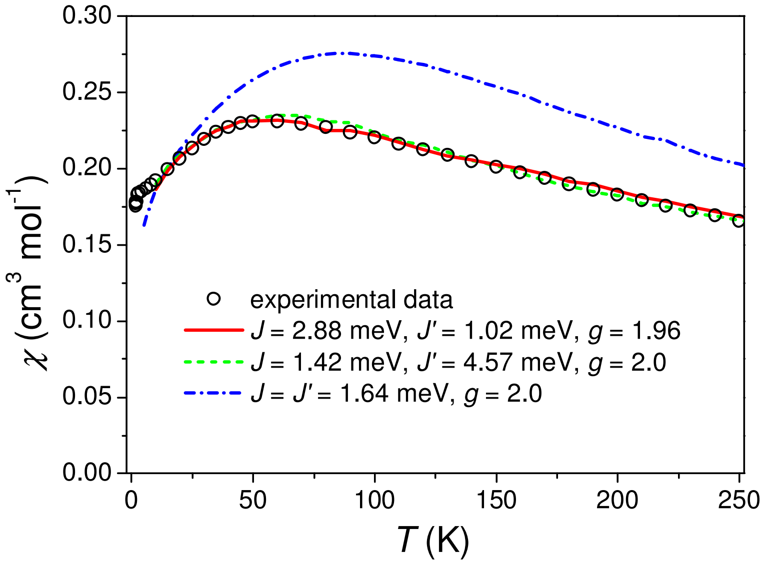
- Determination of model parameters.

(1) J. Ummethum, J. Nehrkorn, S. Mukherjee, N. B. Ivanov, S. Stuiber, Th. Strässle, P. L. W. Tregenna-Piggott, H. Mutka, G. Christou, O. Waldmann, J. Schnack, Phys. Rev. B **86**, 104403 (2012).

Quantum Monte Carlo

(Very good for non-frustrated systems, even for huge sizes.)

Quantum Monte Carlo

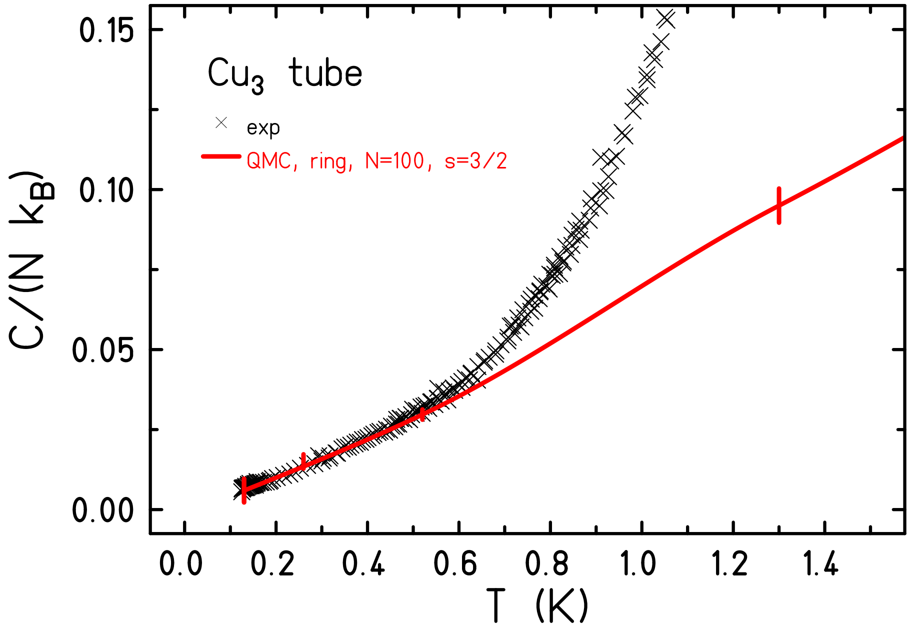


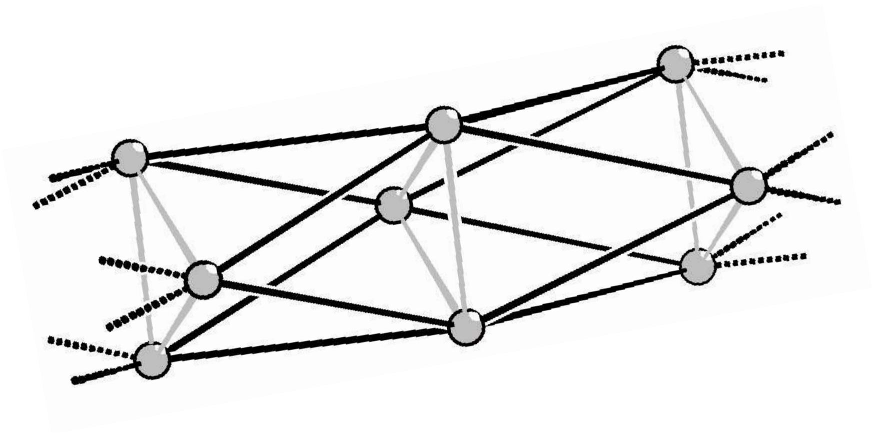
Chopped (sliced) partition function:

- $$\begin{aligned} Z(T,B) &= \sum_\nu \langle\,\nu\,|\,\exp\left\{-\beta \underset{\sim}{H}\right\}\,|\,\nu\,\rangle \\ &= \sum_\nu \langle\,\nu\,|\,\left[\exp\left\{-\beta \underset{\sim}{H}/m\right\}\right]^m\,|\,\nu\,\rangle \\ &= \sum_{\nu,\alpha,\beta,\dots} \langle\,\nu\,|\,\exp\left\{-\beta \underset{\sim}{H}/m\right\}\,|\,\alpha\,\rangle\langle\,\alpha\,|\,\cdots \\ &\approx \sum_{\nu,\alpha,\beta,\dots} \langle\,\nu\,|\,\left\{1-\beta \underset{\sim}{H}/m\right\}\,|\,\alpha\,\rangle\langle\,\alpha\,|\,\cdots \end{aligned}$$
- Bad/no convergence for frustrated systems (negative sign problem).

(1) A. W. Sandvik and J. Kurkijärvi, Phys. Rev. B **43**, 5950 (1991).
(2) A. W. Sandvik, Phys. Rev. B **59**, R14157 (1999).
(3) L. Engelhardt and M. Luban, Phys. Rev. B **73**, 054430 (2006); L. Engelhardt *et al.*, Phys. Rev. B **79**, 014404 (2009).
(4) J. Ummethum *et al.*, Phys. Rev. B **86**, 104403 (2012).

Quantum Monte Carlo



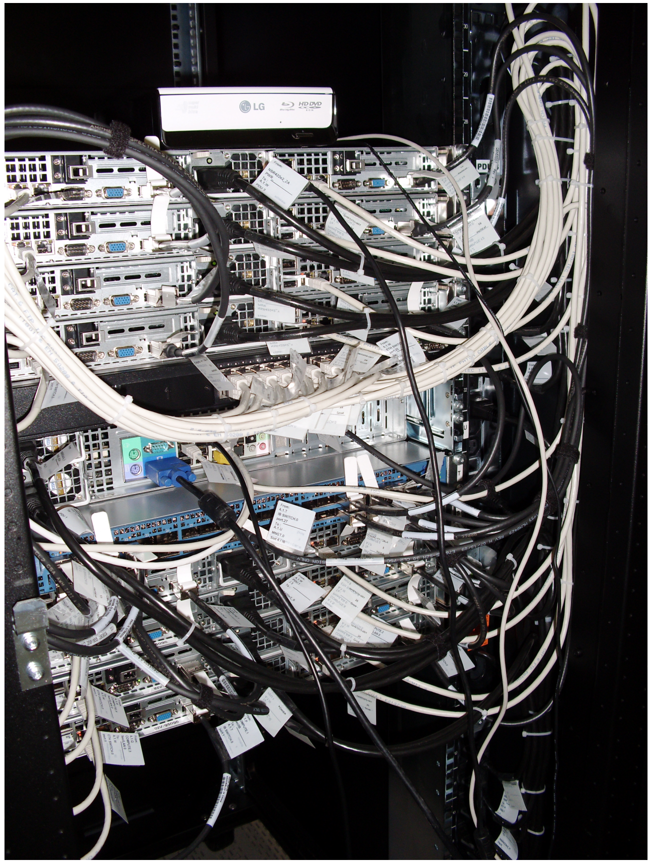


- [(CuCl$_2$tachH)$_3$Cl]Cl$_2$: spins on triangles effectively coupled to $s = 3/2$, treatment as chain $\Rightarrow$ Luttinger liquid behavior, i.e. $C \propto T$.

- 100 spins $s = 3/2$ are no problem for QMC.

(1) N. B. Ivanov, J. Schnack, R. Schnalle, J. Richter, P. Kögerler, G.N. Newton, L. Cronin, Y. Oshima, Hiroyuki Nojiri, Phys. Rev. Lett. **105**, 037206 (2010).

Summary



- Exact diagonalization is great but limited.
- Finite-temperature Lanczos is a good approximate method for Hilbert space dimensions smaller than 10^{10}. DMRG for big 1-d systems. QMC for non-frustrated systems. ALPS!
- Magnetic molecules for storage, q-bits, MCE, and since they are nice.
- Often, the juice is in the anisotropic terms.

(1) A. Albuquerque *et al.*, J. Magn. Magn. Mater. **310**, 1187 (2007).
(2) http://alps.comp-phys.org (English, Japanese, Chinese)

Many thanks to my collaborators worldwide

- M. Czopnik, T. Glaser, O. Hanebaum, Chr. Heesing, M. Höck, N.B. Ivanov, F. Kaiser, H.-T. Langwald, S. Leiding, 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 (Zaragosa); 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.

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