Properties of highly frustrated magnetic molecules studied by the finite-temperature Lanczos method

Jürgen Schnack and Oliver Wendland

Department of Physics – University of Bielefeld – Germany

http://obelix.physik.uni-bielefeld.de/$\sim$schnack/

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Model Hamiltonian (spin only)

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

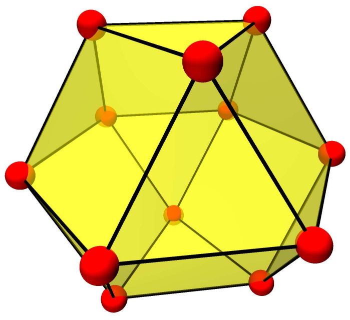
Exchange/Anisotropy Dzyaloshinskii-Moriya Zeeman

Isotropic Hamiltonian

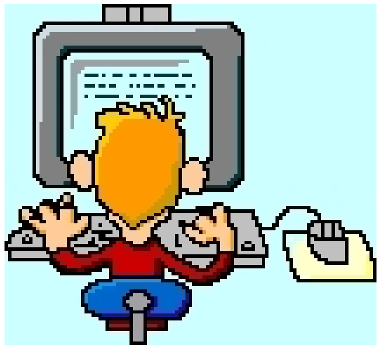
$$\underset{\sim}{H} = -2 \sum_{i<j} J_{ij} \underset{\sim}{\vec{s}}(i) \cdot \underset{\sim}{\vec{s}}(j) + g \mu_B B \sum_{i}^{N} \underset{\sim}{s}_z(i)$$

Heisenberg Zeeman

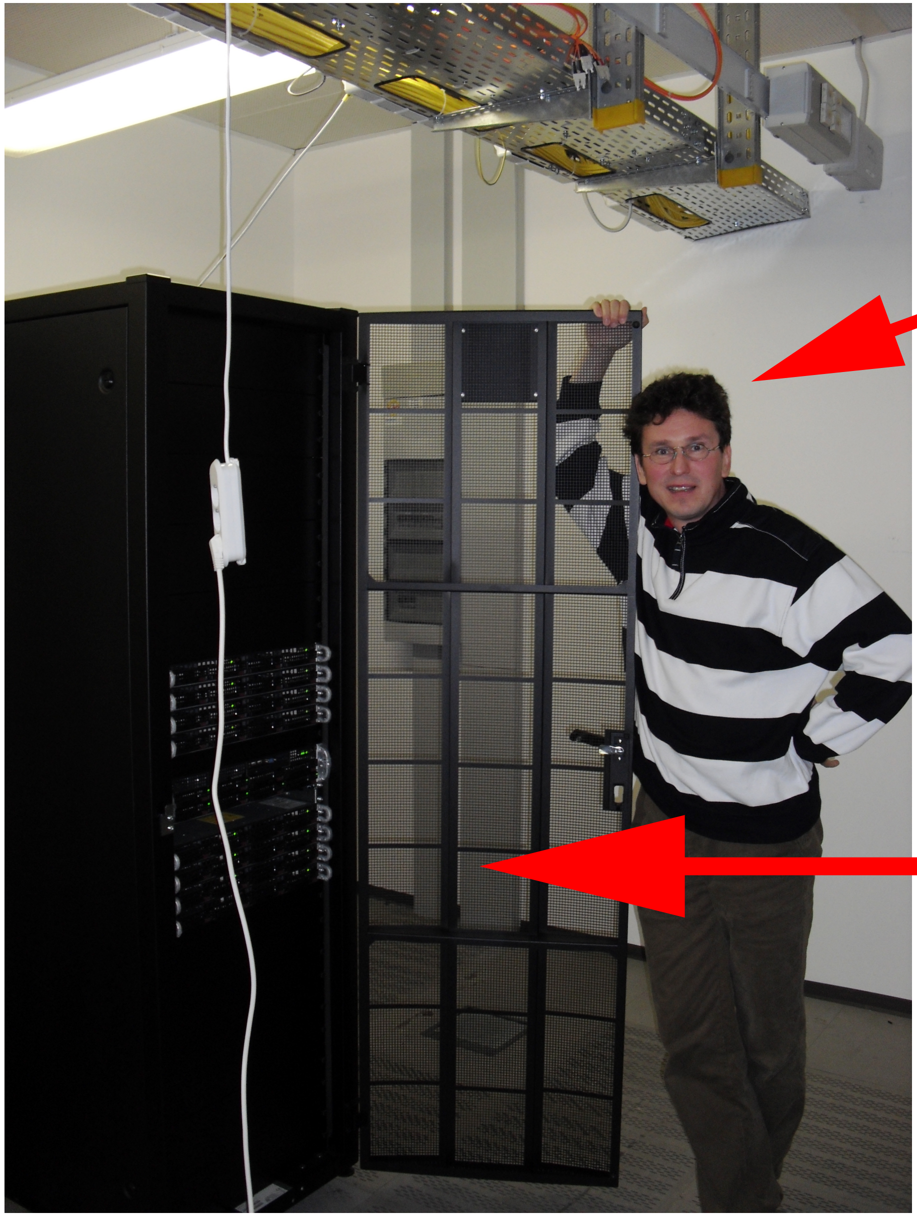
In the end it's always a big matrix!



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



Thank God, we have computers



"cell professor"

128 cores, 384 GB RAM

. . . but that's not enough!

The idea of thermal Lanczos

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

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

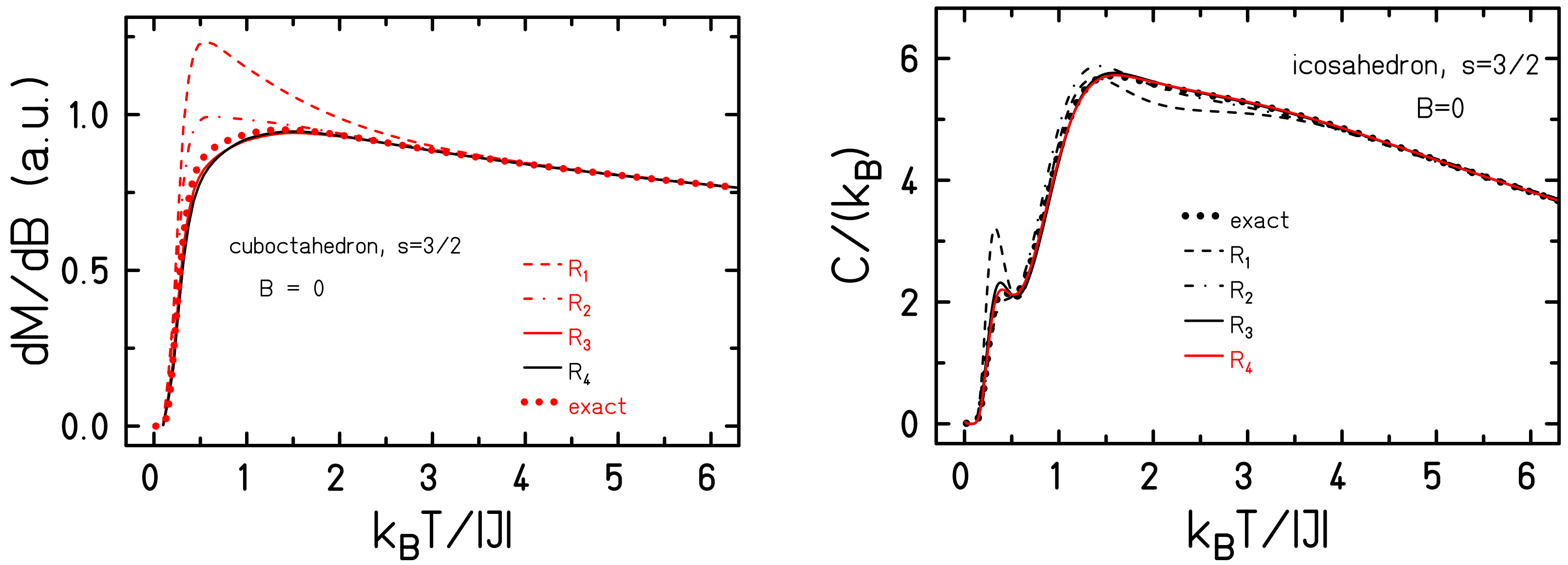
J. Jaklic and P. Prelovsek, Phys. Rev. B **49**, 5065 (1994).

Final form of thermal Lanczos

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

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

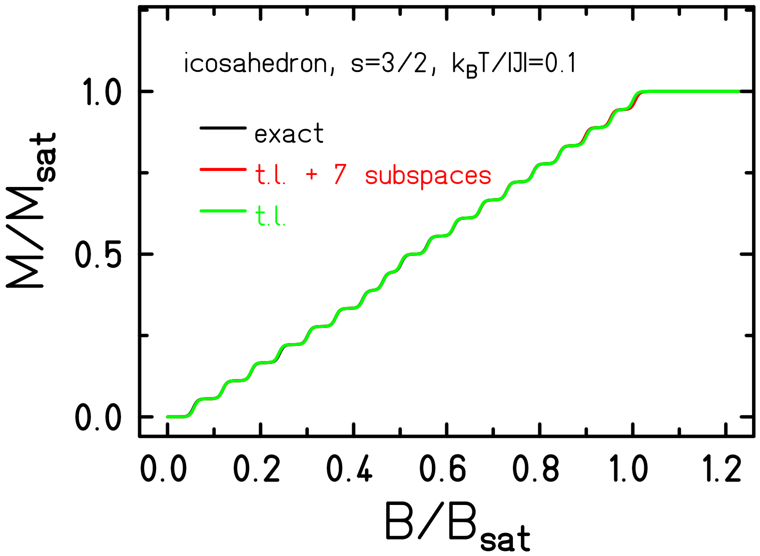
How good is thermal Lanczos?

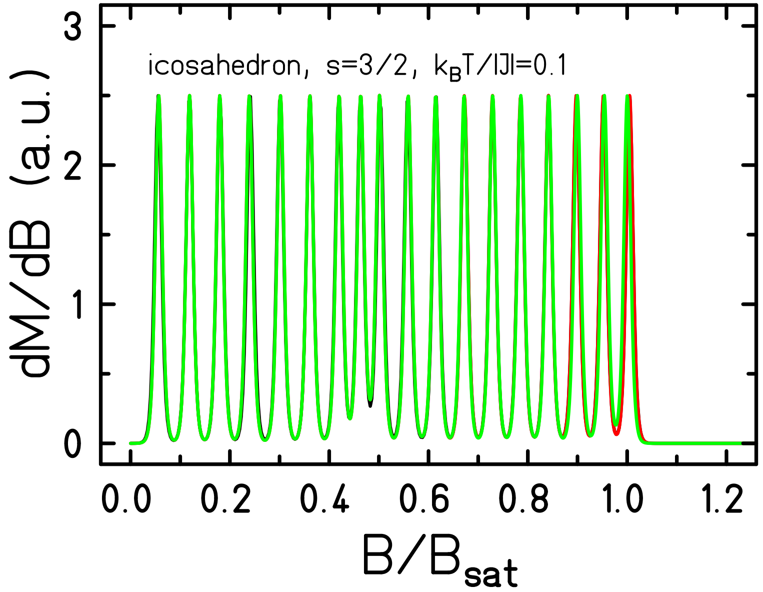


- Works very well, see e.g. cuboctahedron and icosahedron.
- $N = 12, s = 3/2$: Considered $< 100,000$ states instead of 16,777,216.

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

How good is thermal Lanczos?





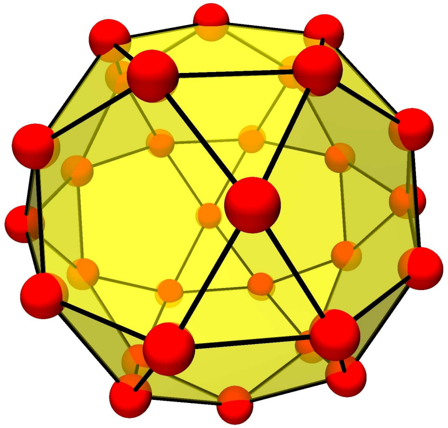
- Large degeneracies and small subspaces problematic.
- Small subspaces can be included exactly.

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

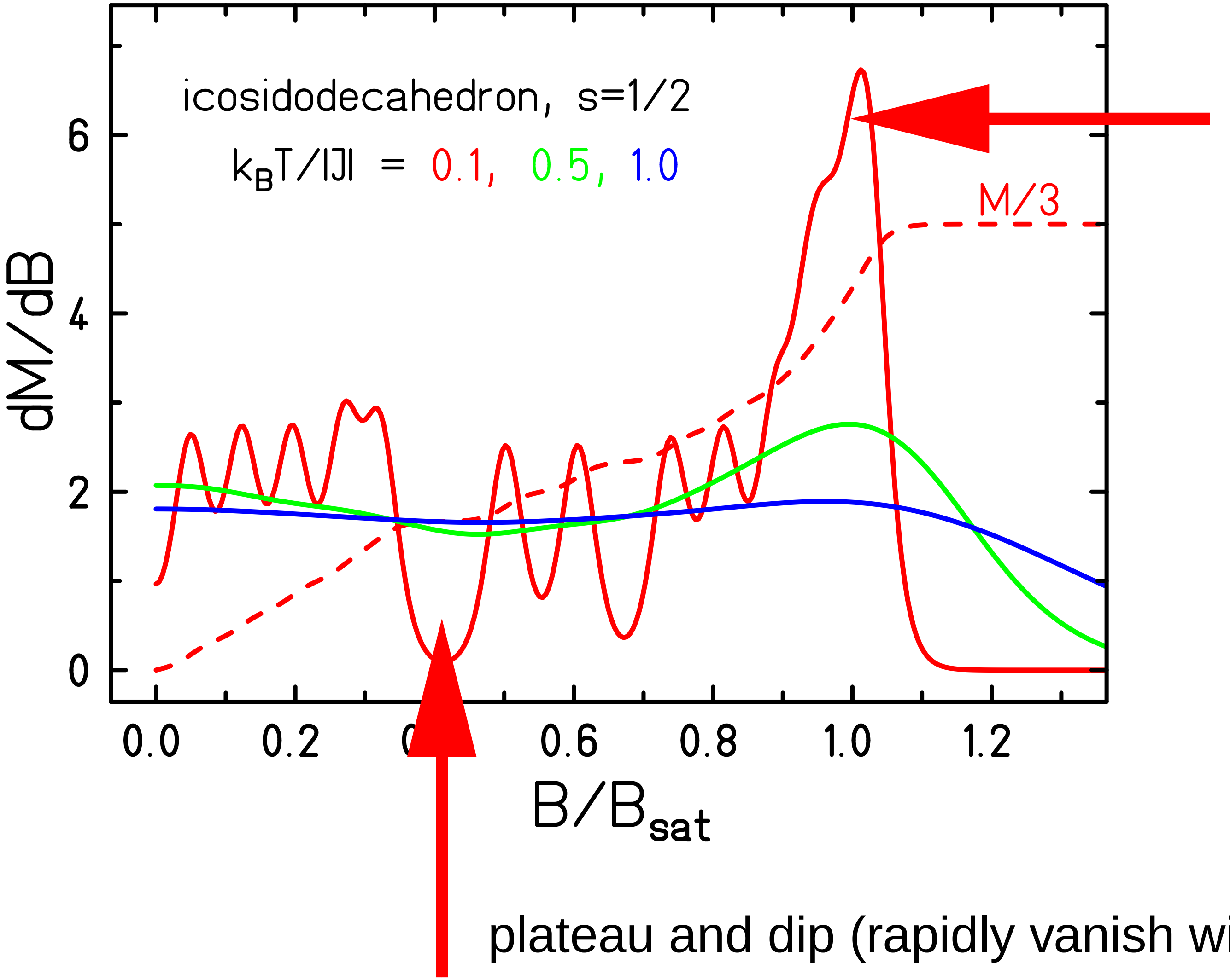
Finite-temperature Lanczos for

The icosidodecahedron $s = 1/2$

DIMENSION = 1,073,741,824



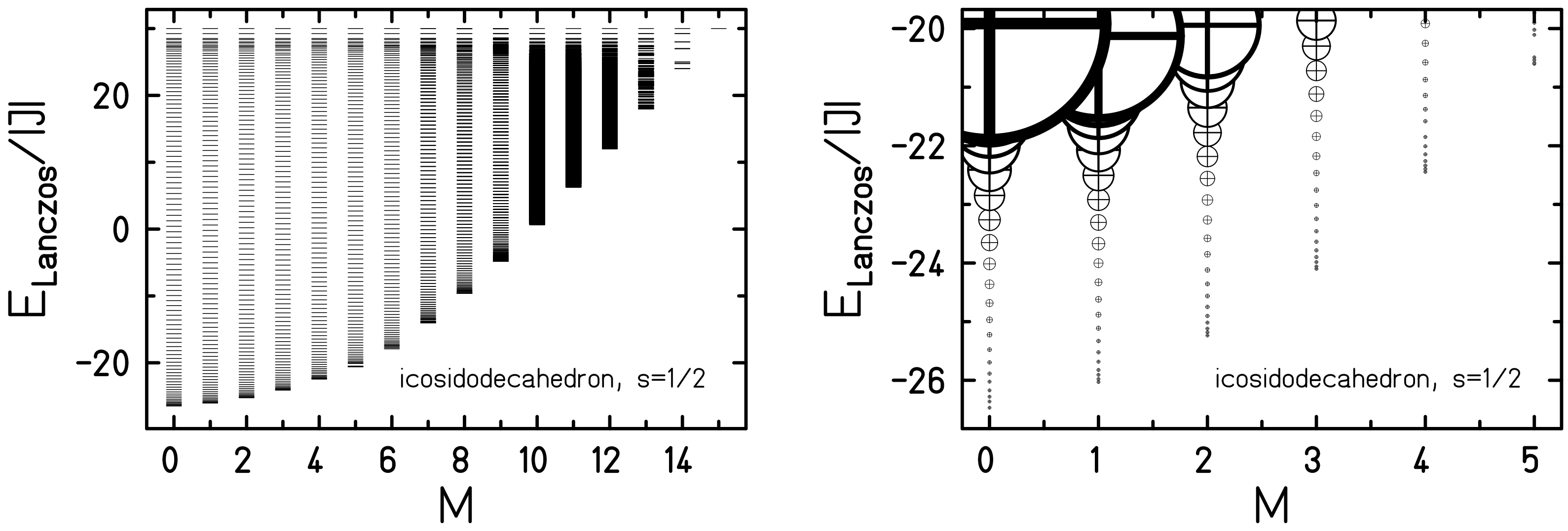
Icosidodecahedron $s = 1/2$



jump

plateau and dip (rapidly vanish with T)

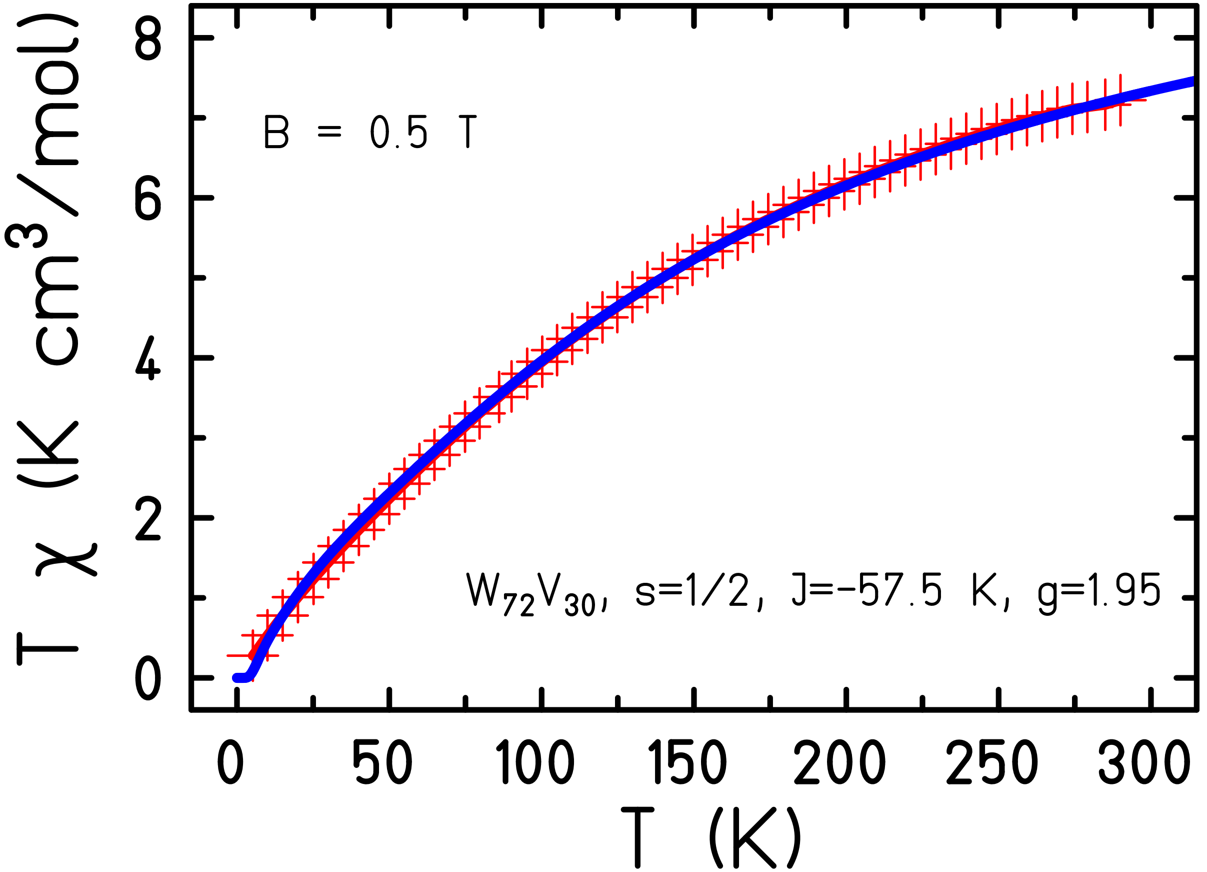
Icosidodecahedron $s = 1/2$



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

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

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. (2009) 3351.

Thank you very much for your attention.

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