Magnetism of the $N = 42$ kagome lattice antiferromagnet

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Workshop on quantum magnetism
Kosice, Slovakia, 5+6 July 2019

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The Bielefeld conspiracy

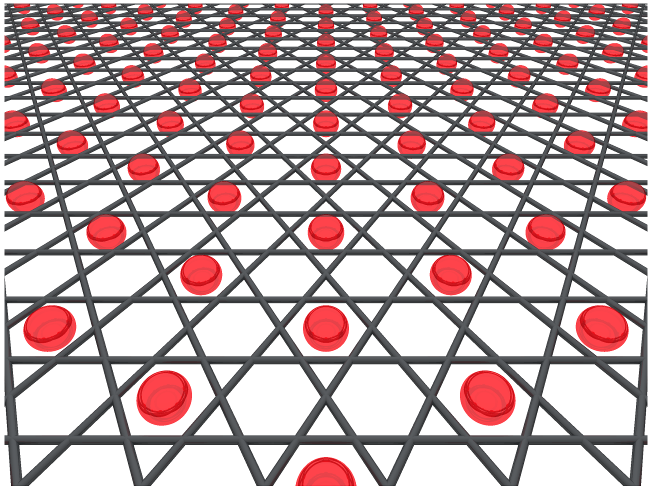
The story goes that the city of **BIELEFELD** in the German state of North Rhine-Westphalia **DOES NOT** actually **EXIST**. Rather, its existence is merely propagated by an entity known only as THEM, which has conspired with the authorities to create the illusion of the city's existence.

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

Kagome lattice antiferromagnet – the problem



- Thermodynamic functions, in particular heat capacity and susceptibility.
- Magnetization curve, in particular thermal stability of plateau at $\mathcal{M}_{\text{sat}}/3$.
- Method: Finite-temperature Lanczos.
- Comparison with tensor-network calculations.

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

Model Hamiltonian

$$\underset{\sim}{H} \;=\; J \sum_{i<j} \underset{\sim}{\vec{s}}_i \cdot \underset{\sim}{\vec{s}}_j \qquad + \qquad g\,\mu_B\,B \sum_{i}^{N} \underset{\sim}{s}_i^z$$

Heisenberg Zeeman

Finite-temperature Lanczos Method I

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

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

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

- $|\, n(\nu) \,\rangle$ 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).

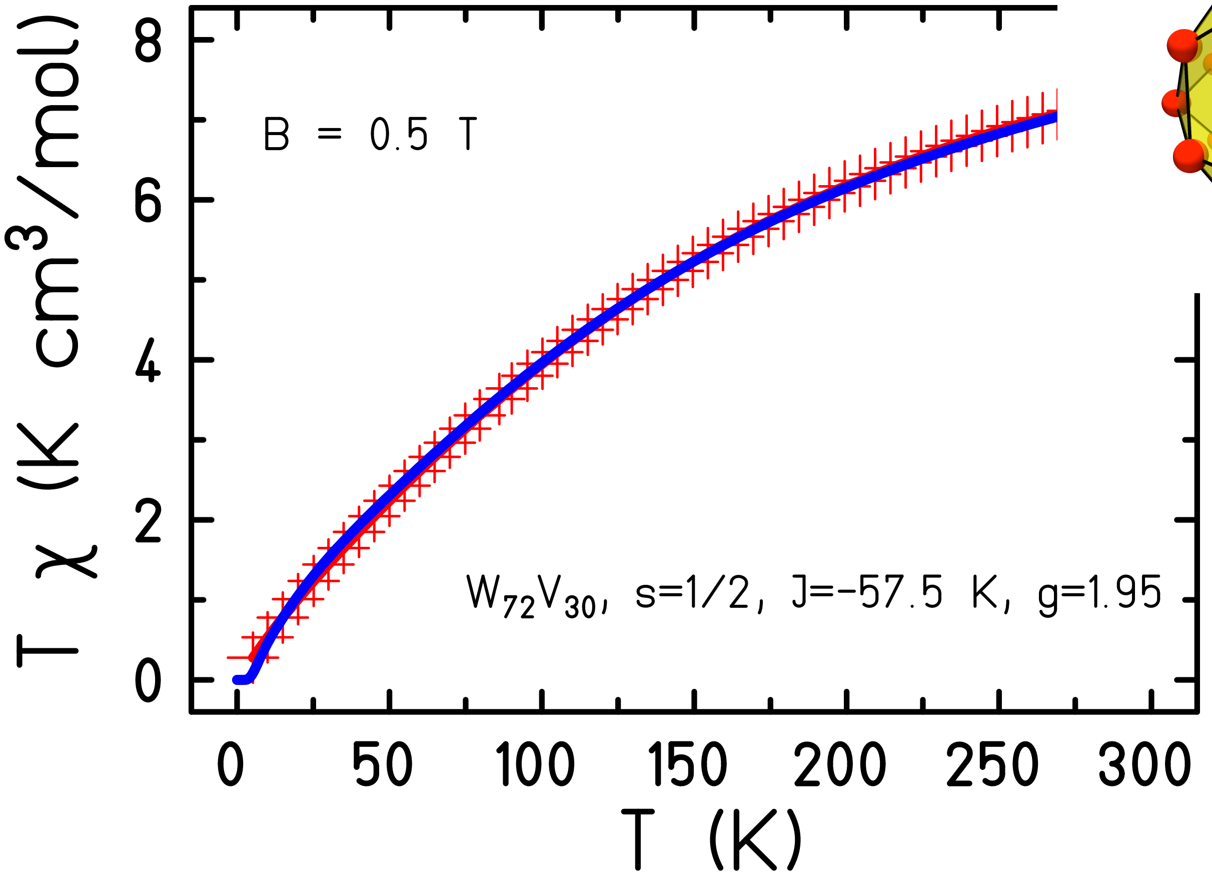
Finite-temperature Lanczos Method II

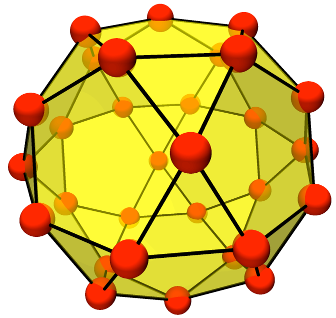
$$Z(T,B) \approx \sum_{\Gamma} \frac{\text{dim}(\mathcal{H}(\Gamma))}{R_\Gamma} \sum_{\nu=1}^{R_\Gamma} \sum_{n=1}^{N_L} \exp\{-\beta\epsilon_n\} \, |\langle \, n(\nu,\Gamma) \, | \, \nu,\Gamma \, \rangle|^2$$

- Approximation better if symmetries taken into account.
- Γ denotes the used irreducible representations;
  often this is just the $\underset{\sim}{S}^z$ symmetry, i.e. $\Gamma \equiv M$

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

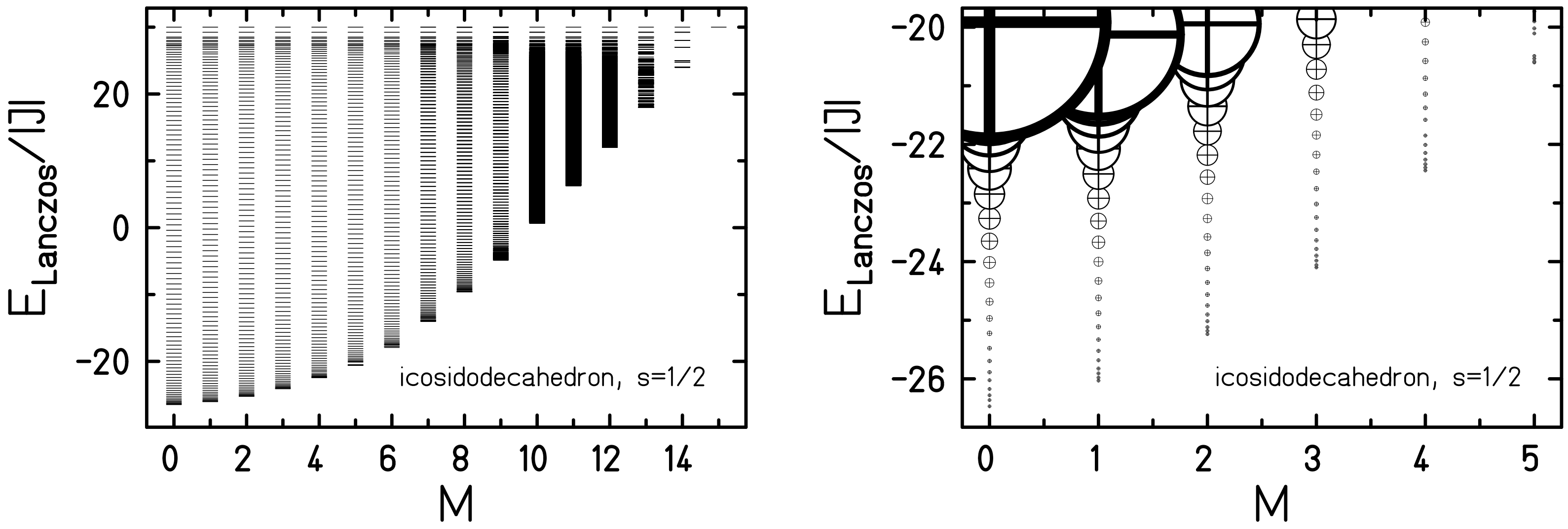
Icosidodecahedron $s = 1/2$





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

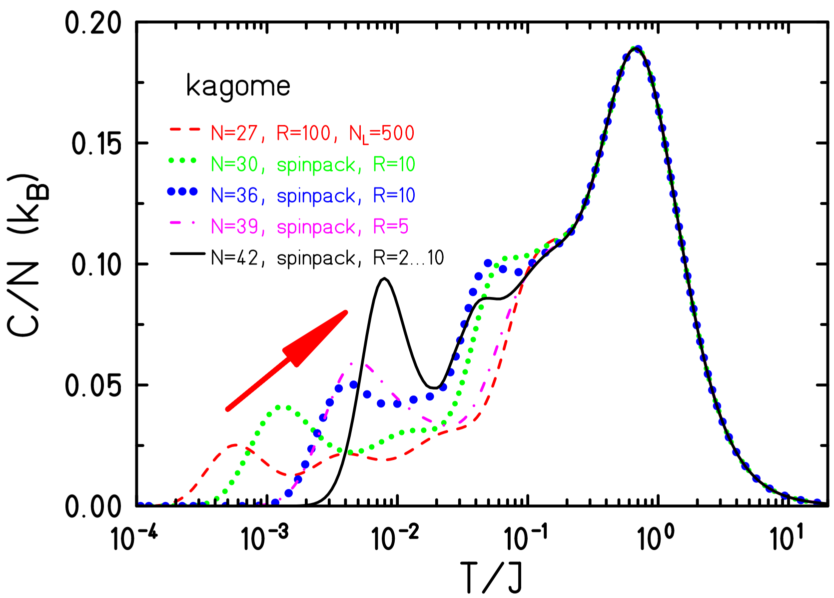
Icosidodecahedron $s = 1/2$

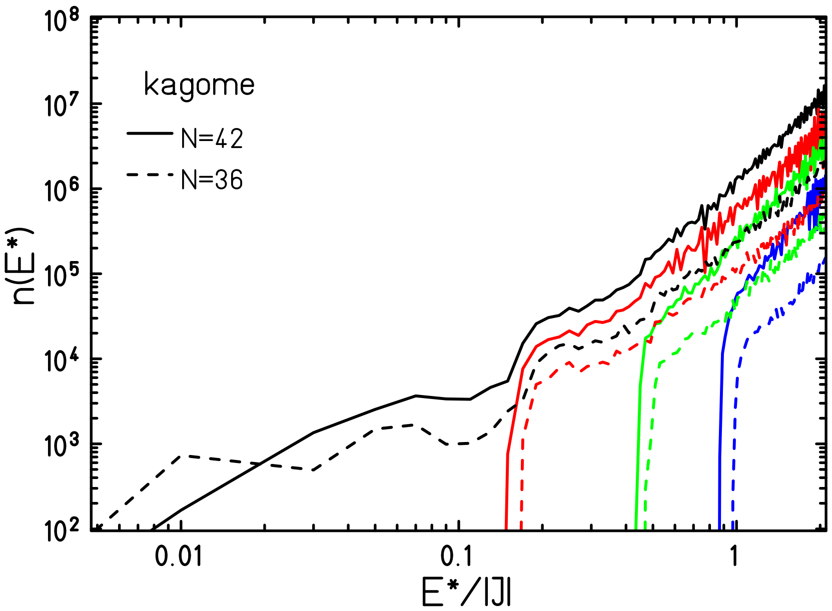


- The true spectrum will be much denser. This is miraculously compensated for by the weights.

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

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.

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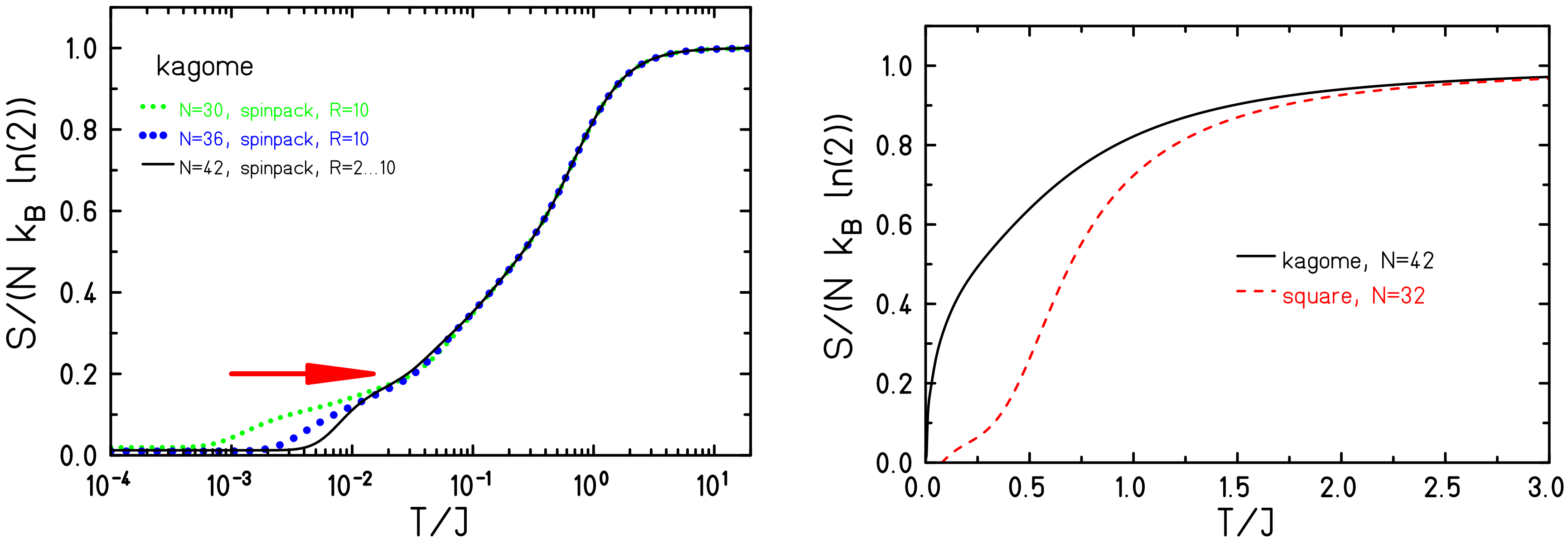
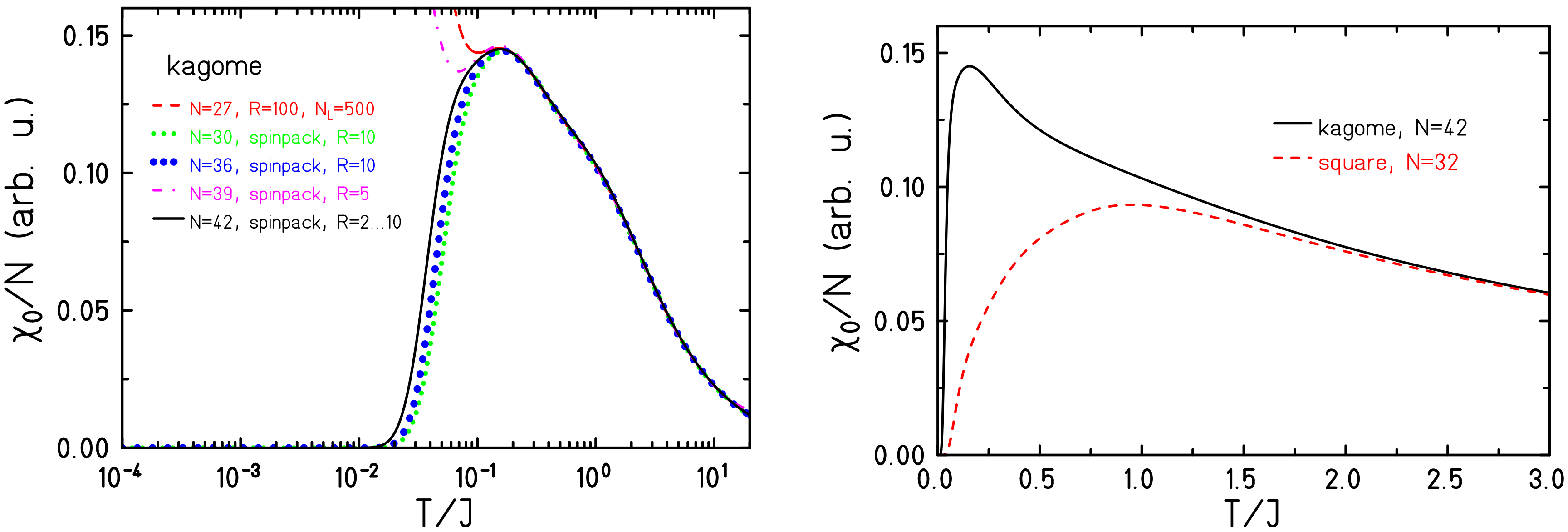
Kagome 42 – entropy



- Rise of entropy for higher T with increasing N.

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

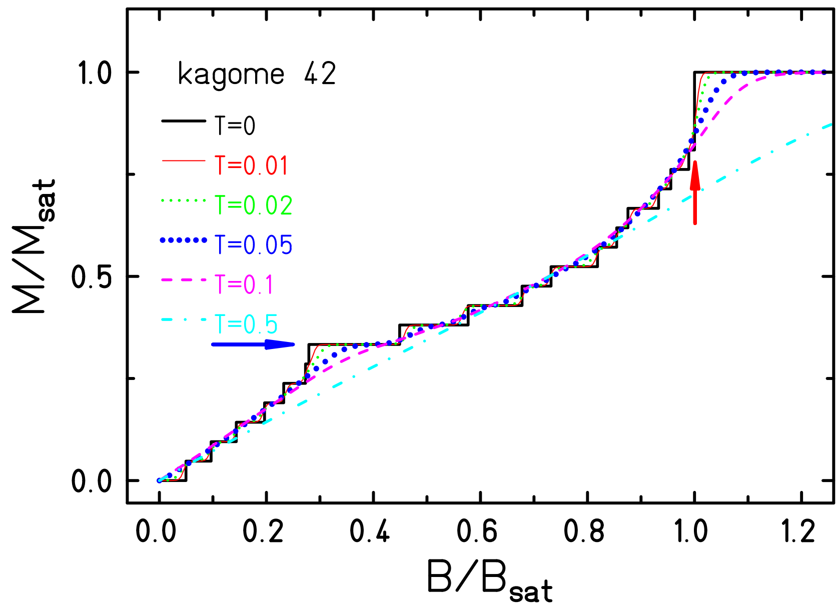
Kagome 42 – susceptibility

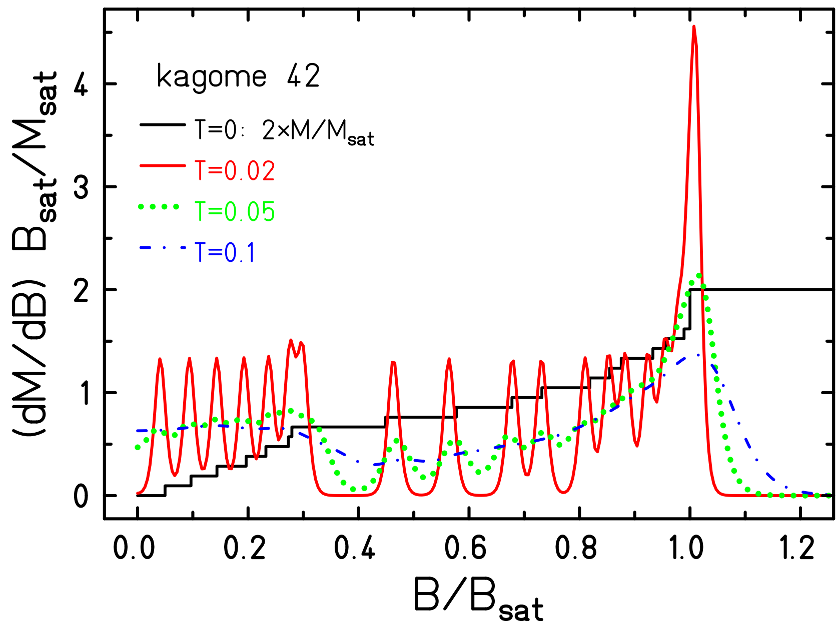


- Singlet-triplet gap shrinks very slowly with increasing N.

(1) A. Laeuchli, J. Sudan, and R. Moessner, arXiv:1611.06990.
(2) J. Schnack, J. Schulenburg, J. Richter, Phys. Rev. B **98** (2018) 094423

Kagome 42 – magnetization

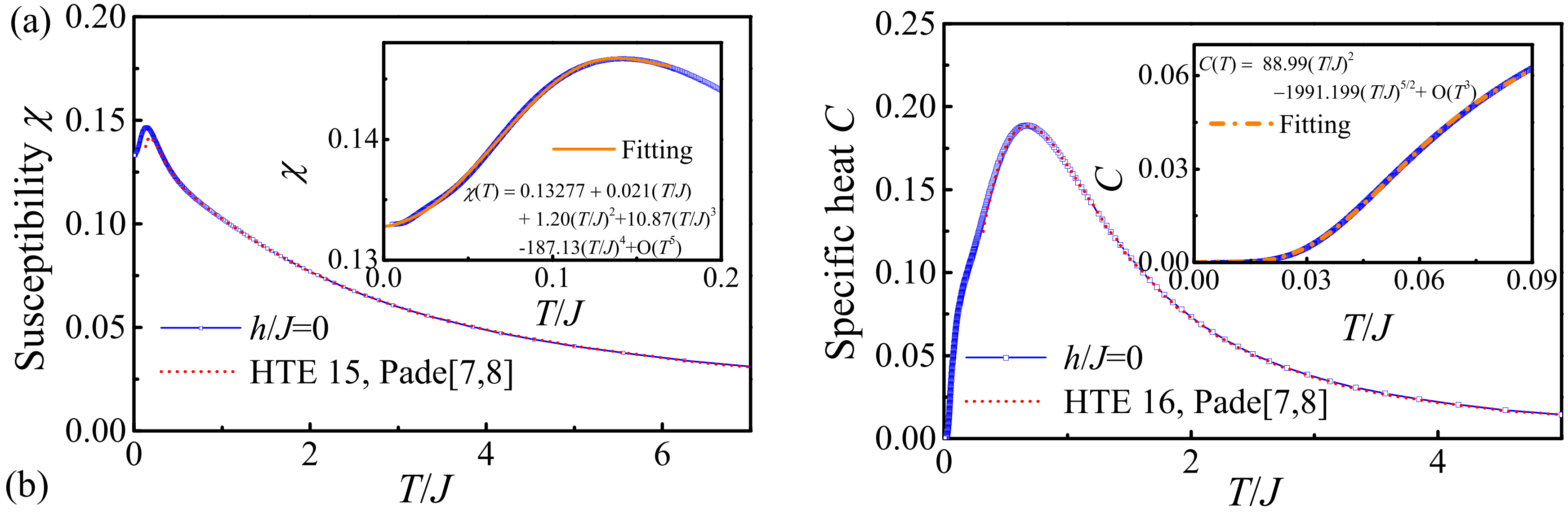




- Plateaus and jump; asymmetric melting of the plateau at $\mathcal{M}_{\text{sat}}/3$.

(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).

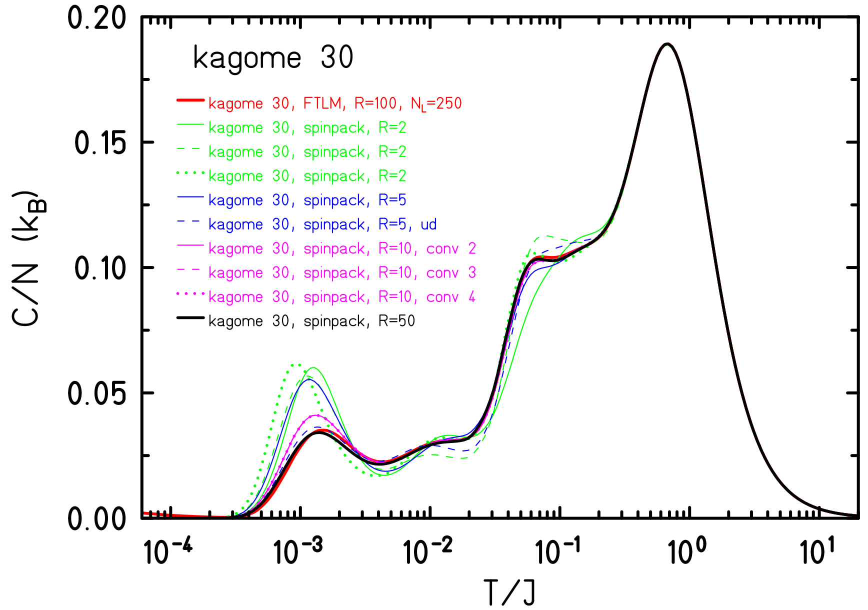
Kagome – tensor network calculations

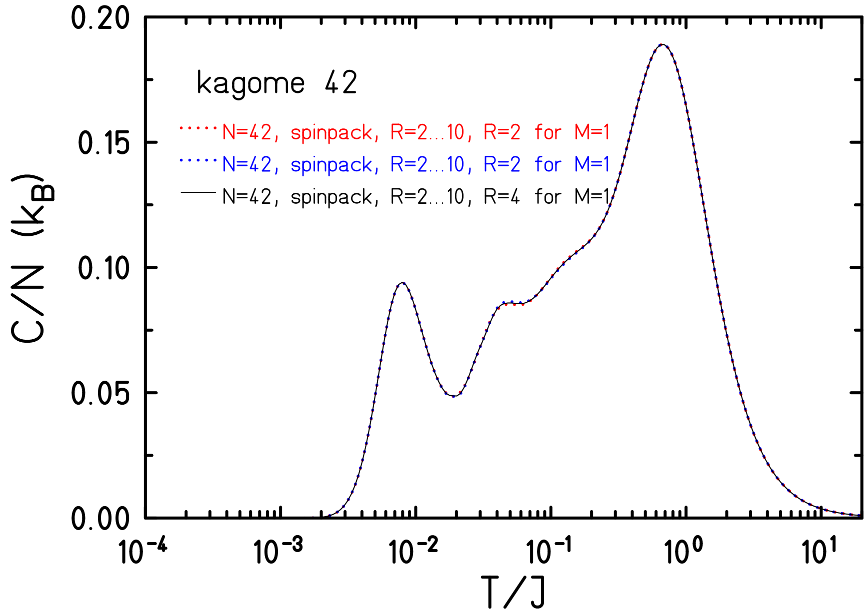


- Tensor network calculations for the infinite system (1).

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

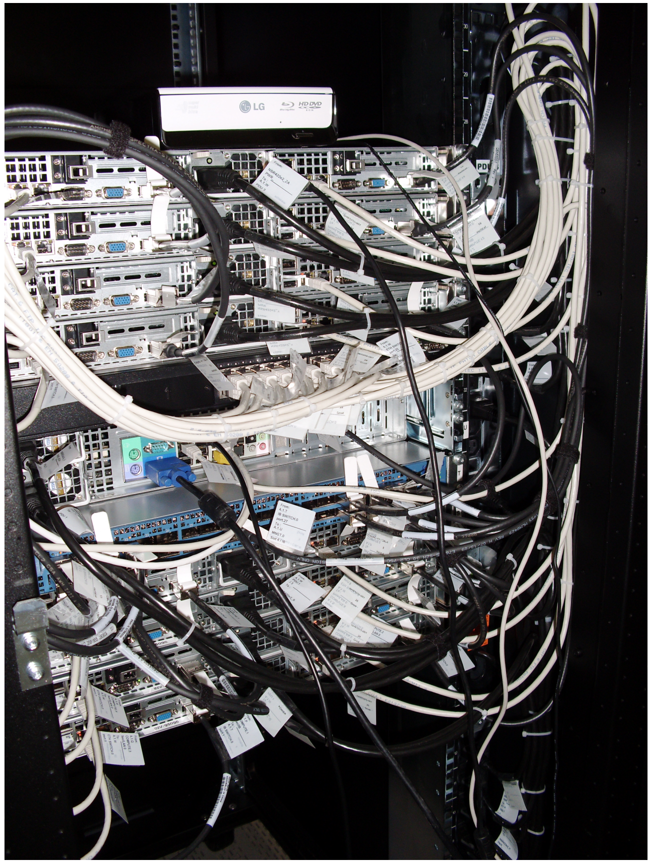
Error estimates of FTLM for the kagome calculations





FTLM more accurate for larger dimensions of Hilbert space.

Summary



- Largest FTLM calculation for a spin system so far (5 Mio. core hours).
- Unexpected N-dependence of low-T peak of heat capacity.
- B-dependence of density of states leads to asymmetric melting of plateaus.

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)
- M. Luban (Ames Lab); 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); M. Evangelisti (Zaragosa); A. Honecker (U de Cergy-Pontoise); E. Garlatti, S. Carretta, G. Amoretti, P. Santini (Parma); A. Tennant (ORNL); Gopalan Rajaraman (Mumbai); M. Affronte (Modena)
- **J. Richter**, **J. Schulenburg** (Magdeburg); B. Lake (HMI Berlin); B. Büchner, V. Kataev, H.-H. Klauß (Dresden); A. Powell, W. Wernsdorfer (Karlsruhe); E. Rentschler (Mainz); 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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