Magnetism of the $N = 42$ kagome lattice antiferromagnet

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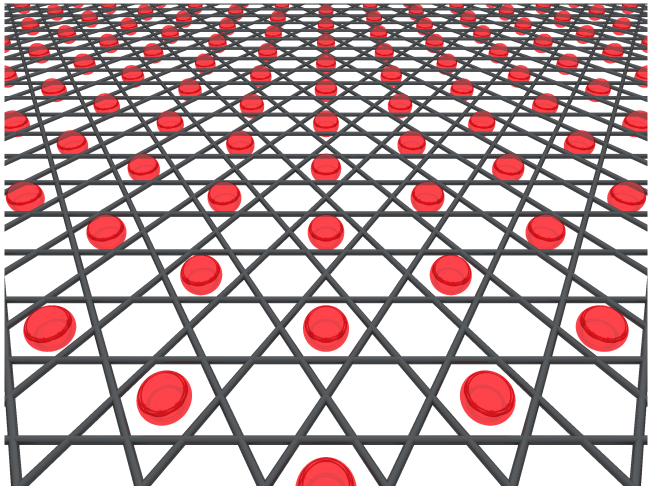
Regensburg, 02. 04. 2019

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: $R = 1 \ldots 10, N_L \approx 100$.

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

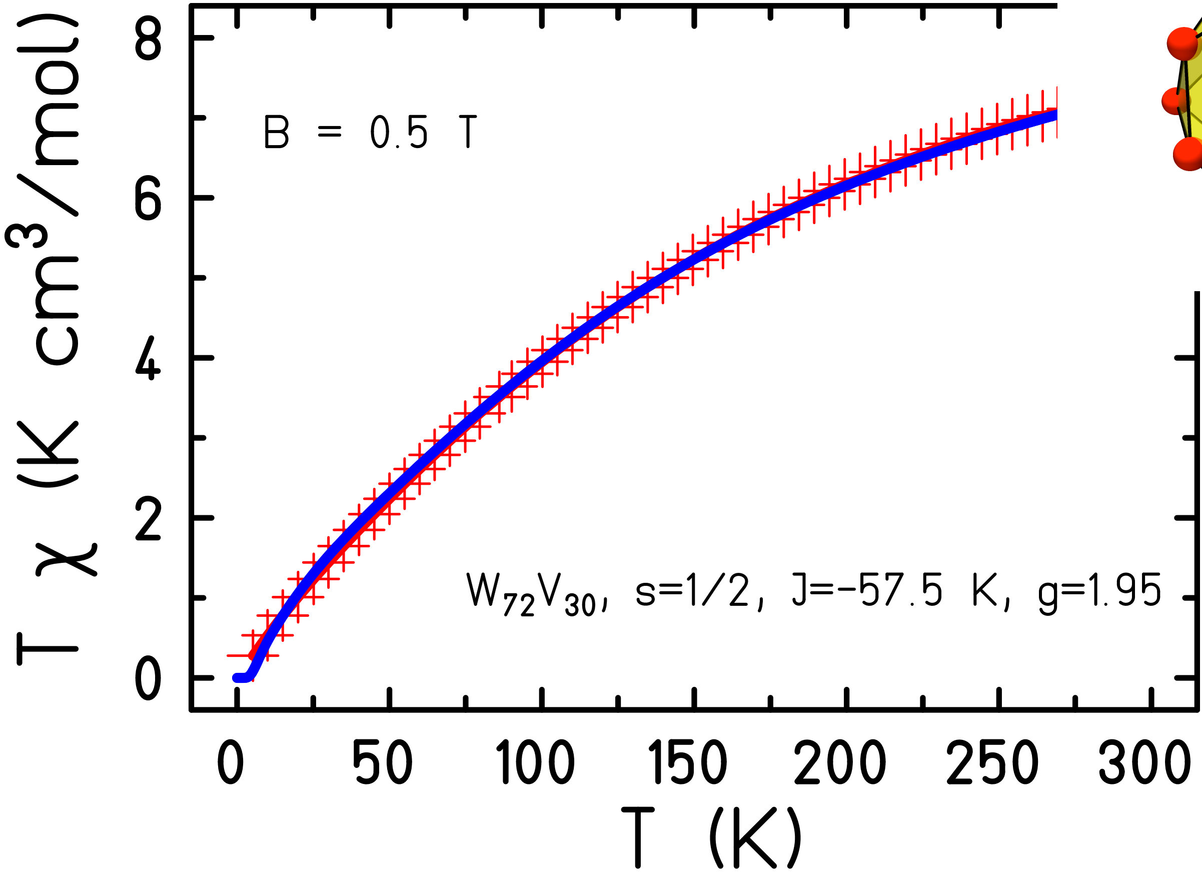
Finite-temperature Lanczos Method II

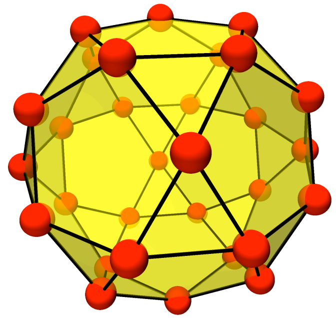
$$Z(T,B) \approx \sum_{\Gamma} \frac{\dim(\mathcal{H}(\Gamma))}{R_\Gamma} \sum_{\nu=1}^{R_\Gamma} \sum_{n=1}^{N_L} \exp\{-\beta\epsilon_n\} |\langle\, n(\nu,\Gamma)\,|\,\nu,\Gamma\,\rangle|^2$$

- 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

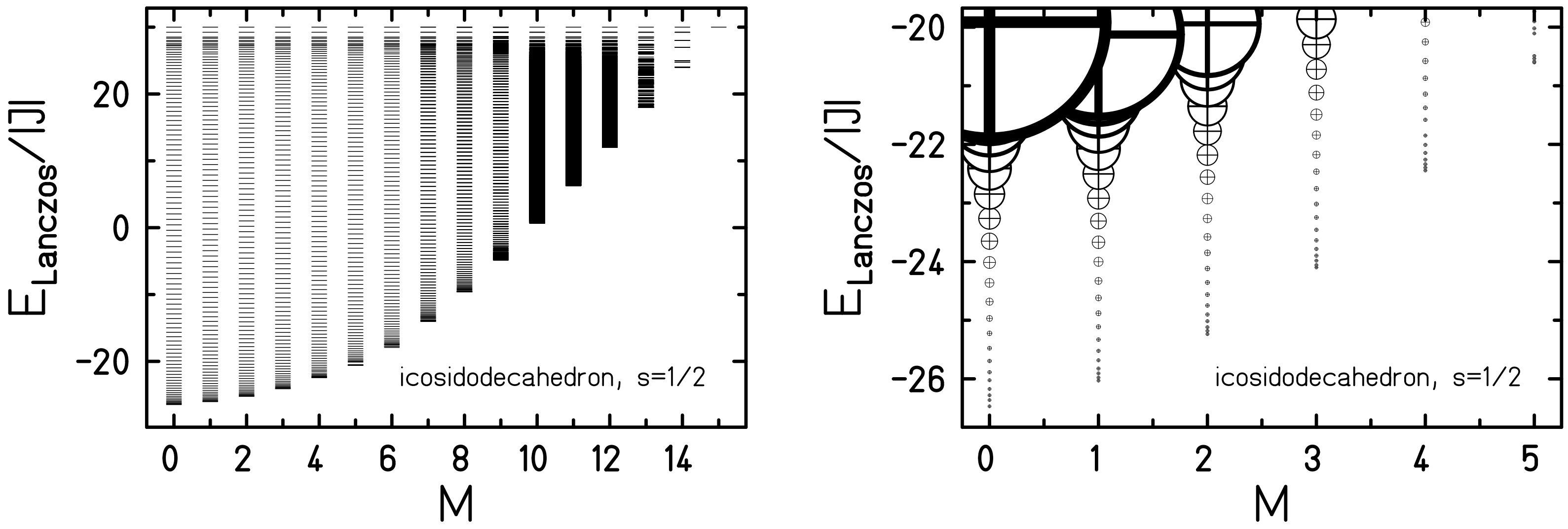
Icosidodecahedron $s = 1/2$





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

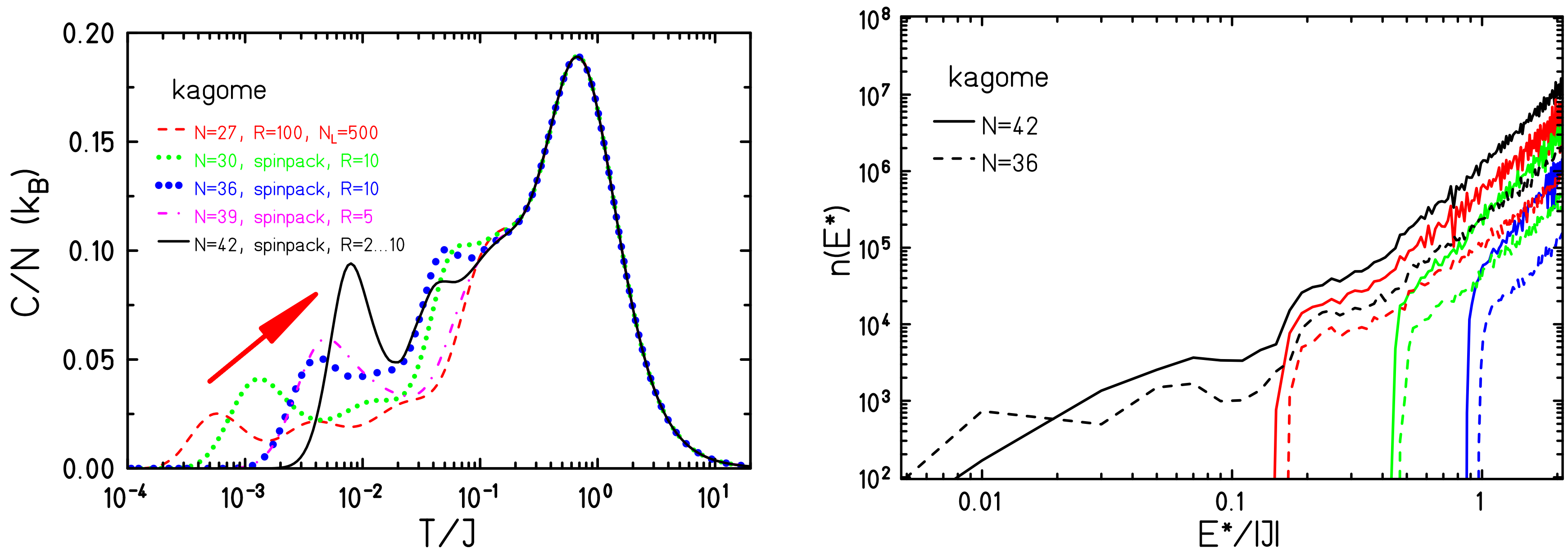
Icosidodecahedron $s = 1/2$



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

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

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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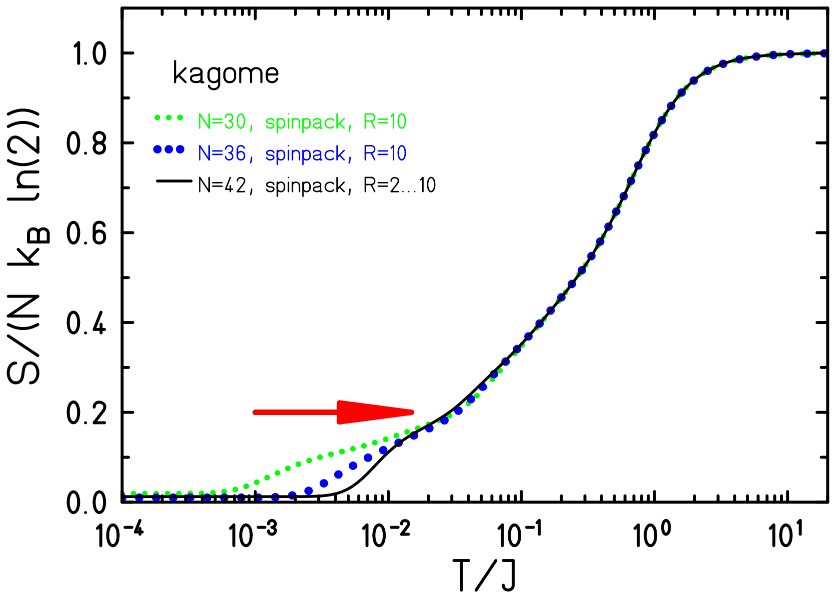
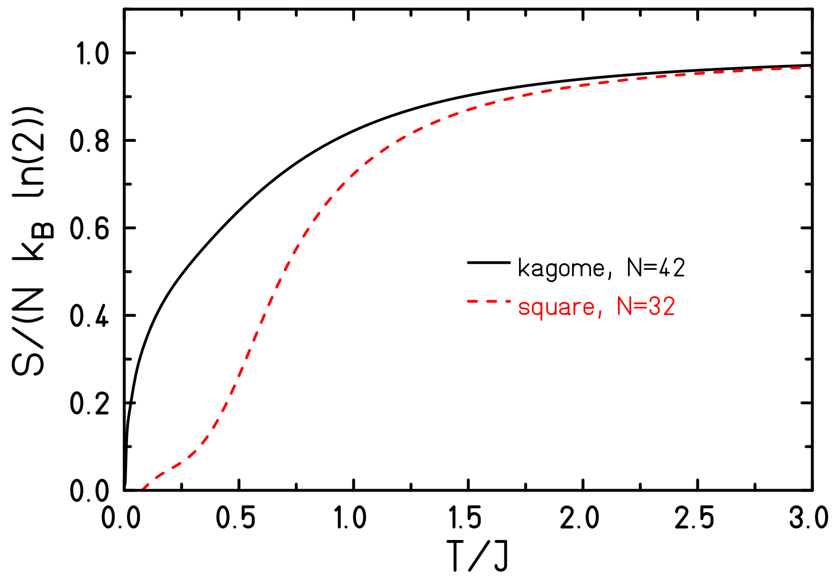
Kagome 42 – entropy

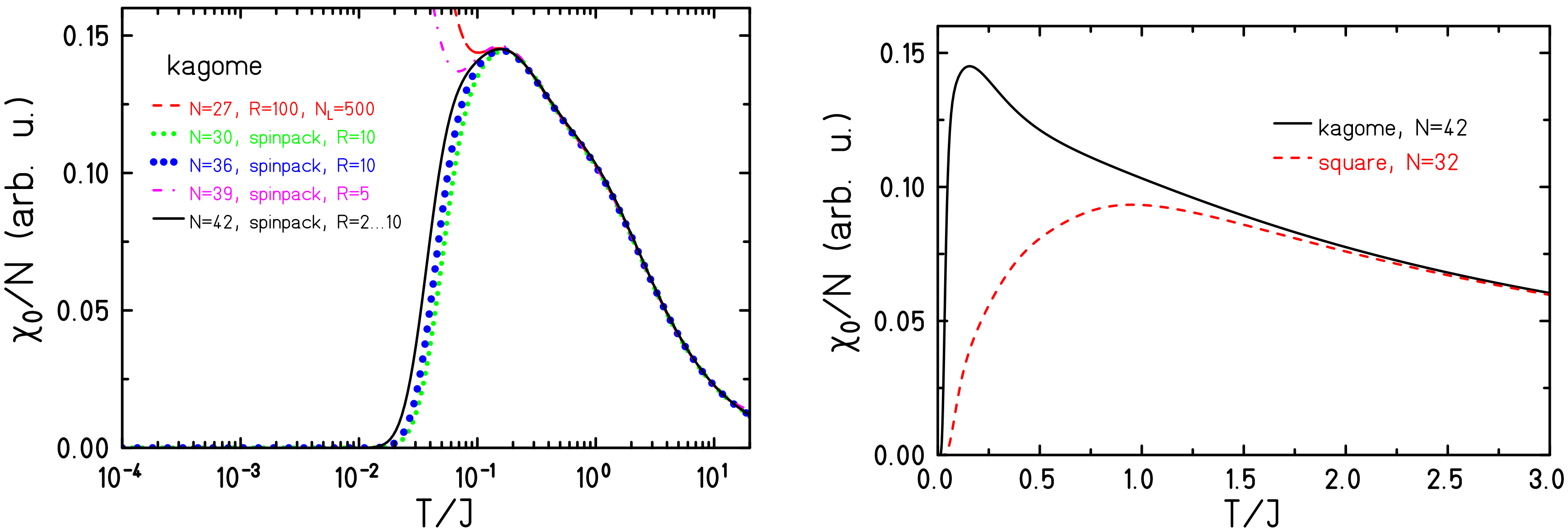




- Rise of entropy for higher T with increasing N.

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

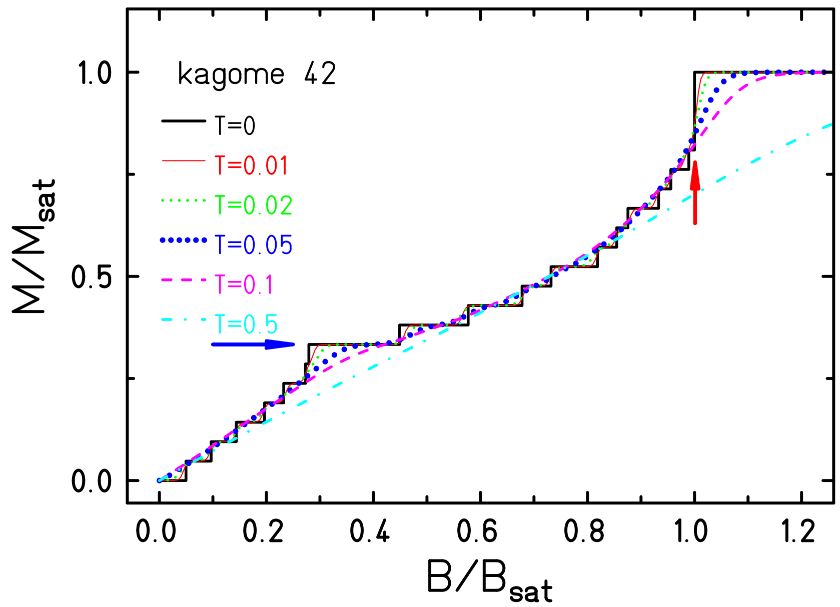
Kagome 42 – susceptibility

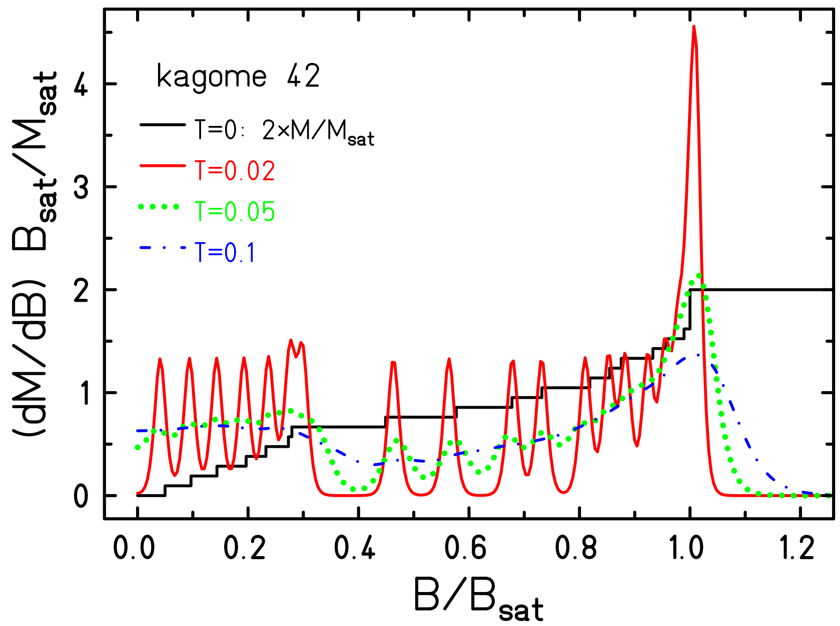


- Singlet-triplet gap shrinks very slowly with increasing N.

(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

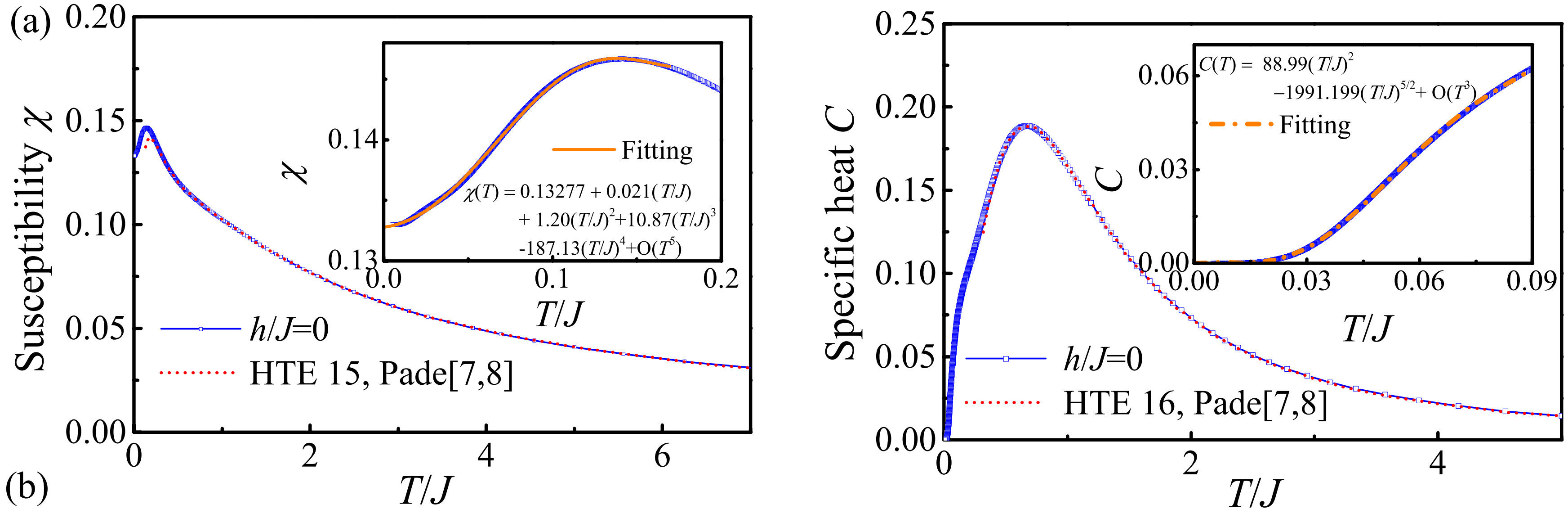




- Plateaus and jump; asymmetric melting of the plateau at $\mathcal{M}_{\text{sat}}/3$.

(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).

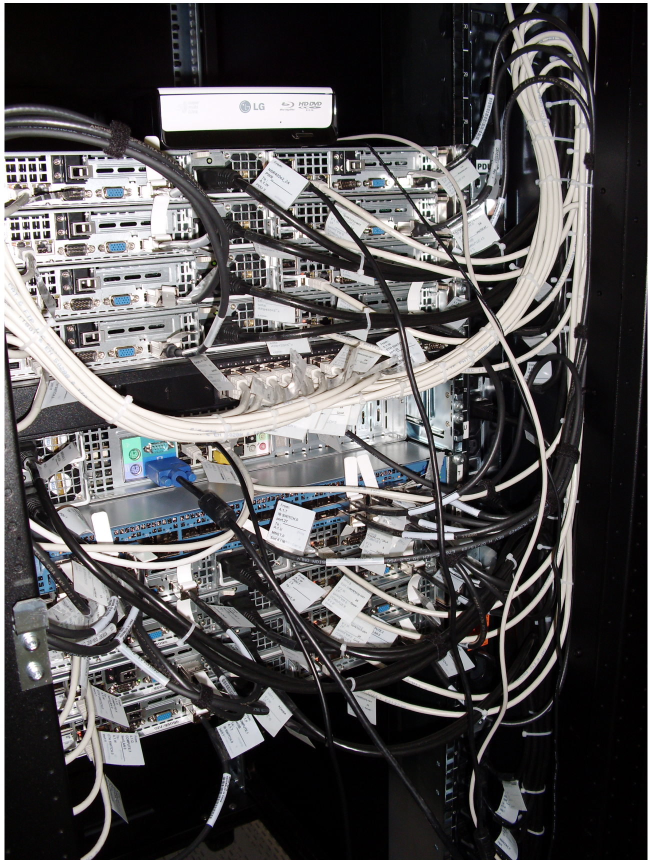
Kagome – tensor network calculations



- 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).

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.

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Thank you very much for your attention.

The end.

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