

Thermodynamics of the N=42 kagome lattice antiferromagnet and magnon crystallization in the kagome lattice antiferromagnet

Jürgen Schnack

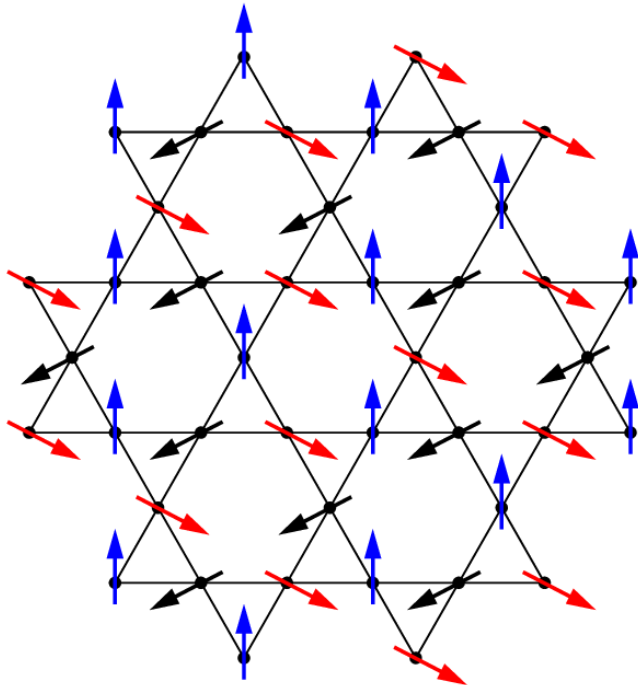
Department of Physics – University of Bielefeld – Germany

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

SUPERMUC-NG STATUS & RESULTS WORKSHOP

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Quantum magnetism: physics

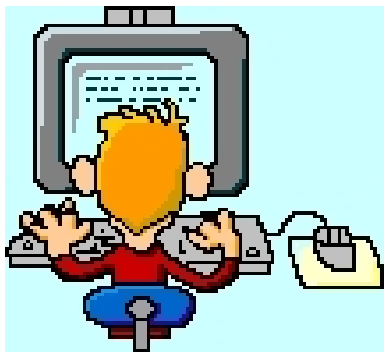


Kagome lattice
antiferromagnet
(figure Mike Zhitomirsky)

- Magnetic systems described by interacting moments (compass needles), e.g. spins.
- Magnetism of insulators, non-trivial properties, new phases, foundations of quantum computing.
- $$\underline{H} = \sum_{i < j} J_{ij} \underline{\tilde{s}}_i \cdot \underline{\tilde{s}}_j + g\mu_B B \sum_i \tilde{s}_i^z$$
- Effective models are used, e.g. Heisenberg model.

Quantum magnetism: math

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



- Eigenvalue problem of huge dimension.
- N spins s lead to a Hilbert space dimension of $(2s + 1)^N$, e.g. $N = 42$ spins $s = 1/2$ yield a dimension of 4,398,046,511,104.
- Even when using symmetries, the exponential growth renders an exact treatment of large systems impossible.
- Can we approximate the partition function $Z = \text{Tr}(\exp[-\beta \underline{H}])$ without solving the eigenvalue problem?

⇒ Trace estimators & Krylov space representation.

Solution I: trace estimators

$$\text{tr}(\tilde{Q}) \approx \langle r | \tilde{Q} | r \rangle = \sum_{\nu} \langle \nu | \tilde{Q} | \nu \rangle + \sum_{\nu \neq \mu} r_{\nu} r_{\mu} \langle \nu | \tilde{Q} | \mu \rangle$$

$$|r\rangle = \sum_{\nu} r_{\nu} |\nu\rangle, \quad r_{\nu} = \pm 1$$

- $|\nu\rangle$ some orthonormal basis of your choice; not the eigenbasis of \tilde{Q} , since we don't know it.
- $r_{\nu} = \pm 1$ random, equally distributed. Rademacher vectors.
- **Amazingly accurate, bigger (Hilbert space dimension) is better.**

M. Hutchinson, Communications in Statistics - Simulation and Computation **18**, 1059 (1989).

Solution II: Krylov space representation

$$\exp \left[-\beta \underline{H} \right] \approx \underline{1} - \beta \underline{H} + \frac{\beta^2}{2!} \underline{H}^2 - \dots - \frac{\beta^{N_L-1}}{(N_L-1)!} \underline{H}^{N_L-1}$$

applied to a state $|r\rangle$ yields a superposition of

$$\underline{1}|r\rangle, \quad \underline{H}|r\rangle, \quad \underline{H}^2|r\rangle, \quad \dots \underline{H}^{N_L-1}|r\rangle.$$

These (linearly independent) vectors span a small space of dimension N_L ; it is called Krylov space.

Let's diagonalize \underline{H} in this space!

Partition function I: simple approximation

$$Z(T, B) \approx \langle r | e^{-\beta \tilde{H}} | r \rangle \approx \sum_{n=1}^{N_L} e^{-\beta \epsilon_n^{(r)}} |\langle n(r) | r \rangle|^2$$

$$O^r(T, B) \approx \frac{\langle r | \tilde{Q} e^{-\beta \tilde{H}} | r \rangle}{\langle r | e^{-\beta \tilde{H}} | r \rangle} = \frac{\langle r | e^{-\beta \tilde{H}/2} \tilde{Q} e^{-\beta \tilde{H}/2} | r \rangle}{\langle r | e^{-\beta \tilde{H}/2} e^{-\beta \tilde{H}/2} | r \rangle}$$

- Wow!!!
- One can replace a trace involving an intractable operator by an expectation value with respect to just ONE random vector evaluated by means of a Krylov space representation???
- Typicality = any random vector will do: $|r\rangle \equiv (T = \infty)$

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

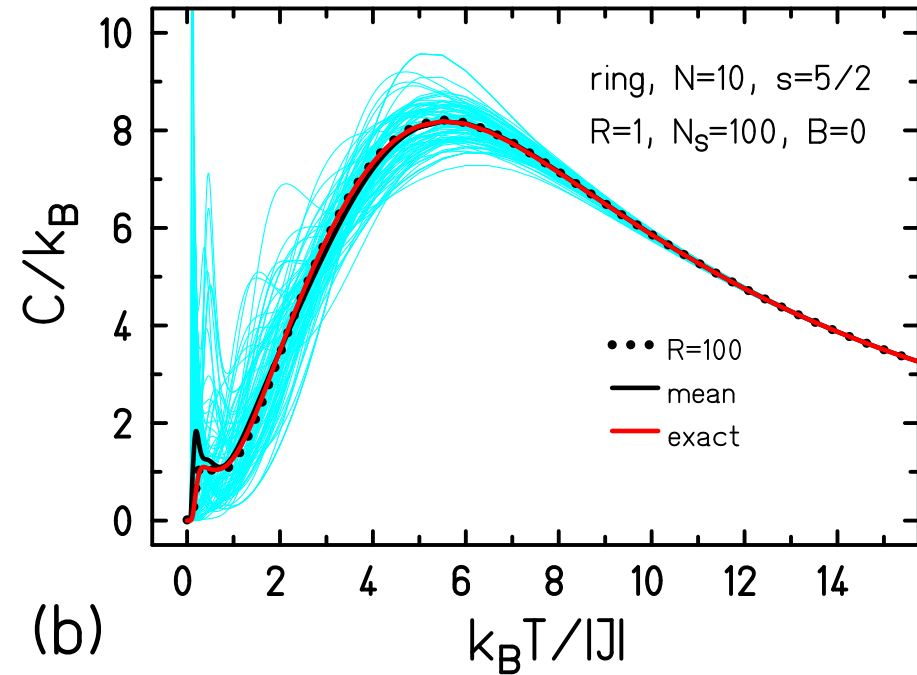
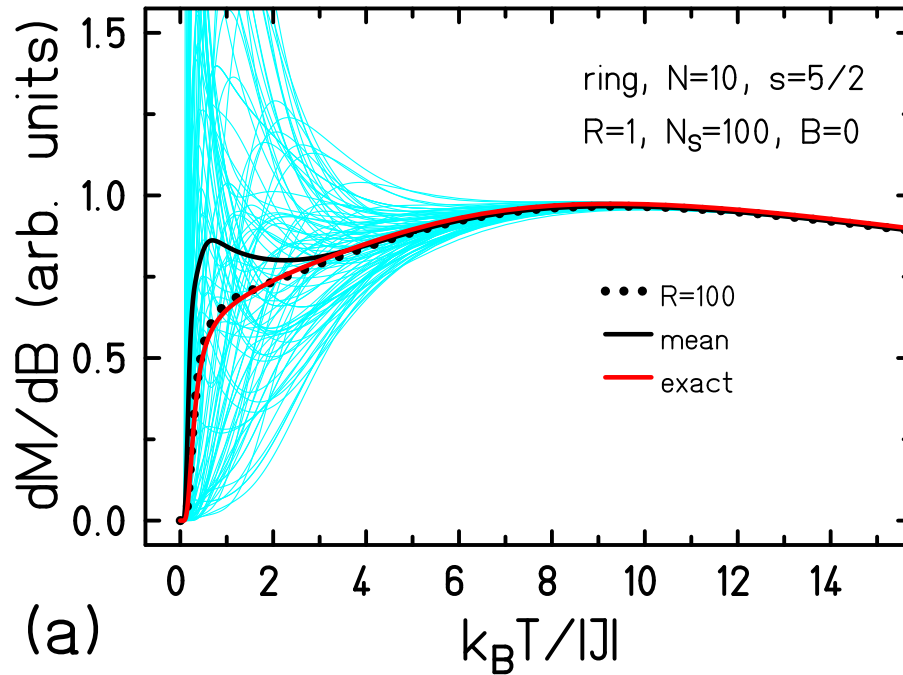
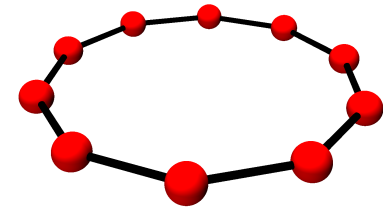
Partition function II: Finite-temperature Lanczos Method

$$Z^{\text{FTLM}}(T, B) \approx \frac{1}{R} \sum_{r=1}^R \sum_{n=1}^{N_L} e^{-\beta \epsilon_n^{(r)}} |\langle n(r) | r \rangle|^2$$

- Averaging over R random vectors is better.
- $|n(r)\rangle$ n -th Lanczos eigenvector starting from $|r\rangle$.
- **Partition function replaced by a small sum: $R = 1 \dots 100, N_L \approx 100$.**
- Implemented in `spinpack` by Jörg Schulenburg (URZ Magdeburg); MPI and openMP parallelized, used up to 3072 nodes.

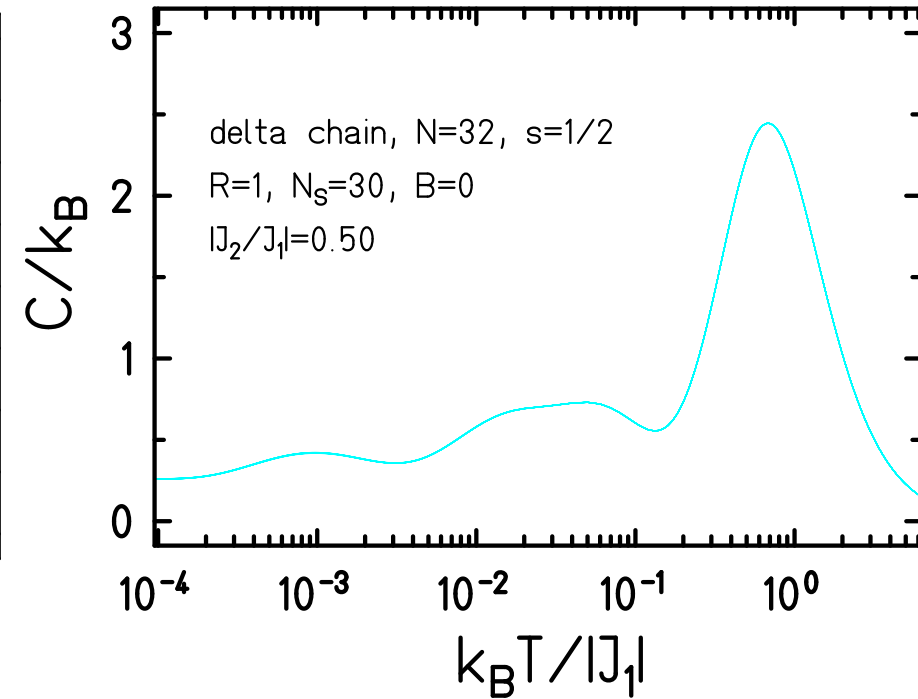
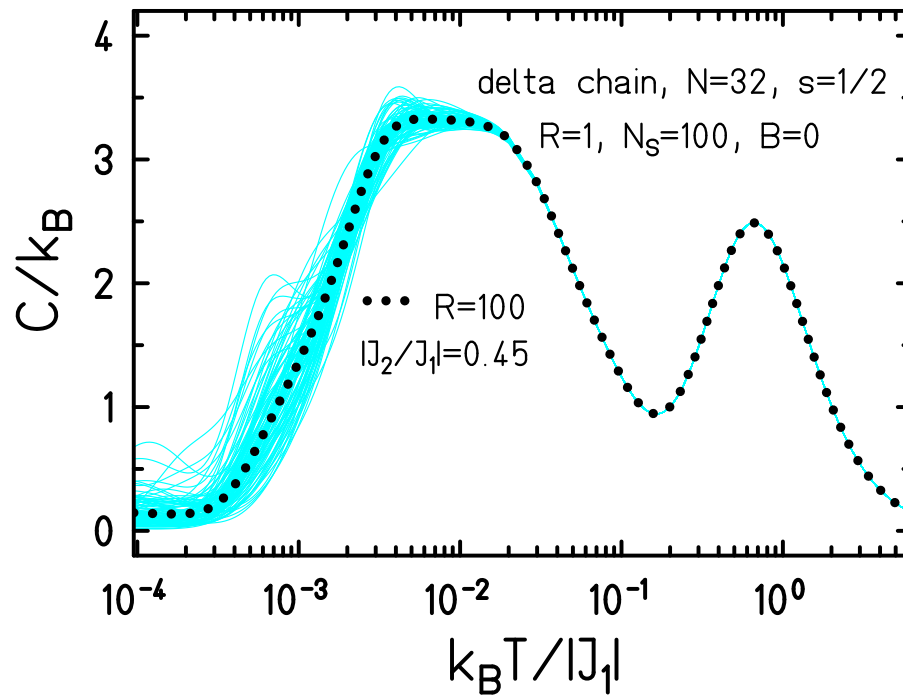
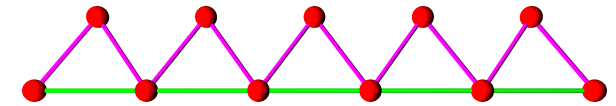
SPINPACK page: <https://www-e.uni-magdeburg.de/jschulen/spin/>

FTLM 1: ferric wheel



- (1) J. Schnack, J. Richter, R. Steinigeweg, Phys. Rev. Research **2**, 013186 (2020).
- (2) SU(2) & D₂: R. Schnalle and J. Schnack, Int. Rev. Phys. Chem. **29**, 403 (2010).
- (3) SU(2) & C_N: T. Heitmann, J. Schnack, Phys. Rev. B **99**, 134405 (2019)

FTLM 3: sawtooth chain



$|J_2/J_1| = 0.45$ – near critical, $|J_2/J_1| = 0.50$ – critical.

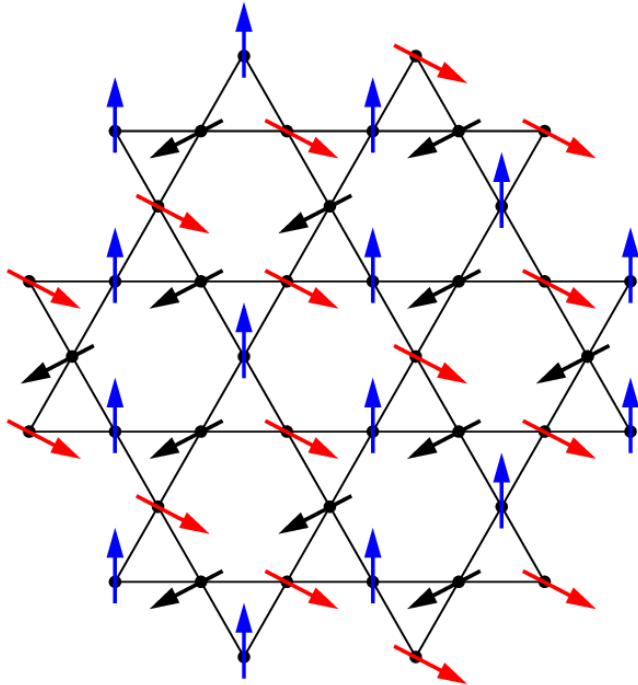
Frustration, technically speaking, works in your favour.

(1) J. Schnack, J. Richter, R. Steinigeweg, Phys. Rev. Research **2**, 013186 (2020)

(2) J. Schnack, J. Richter, T. Heitmann, J. Richter, R. Steinigeweg, Z. Naturforsch. A **75**, 465 (2020)

Physics of the kagome lattice antiferromagnet

Kagome lattice antiferromagnet – scientific problems

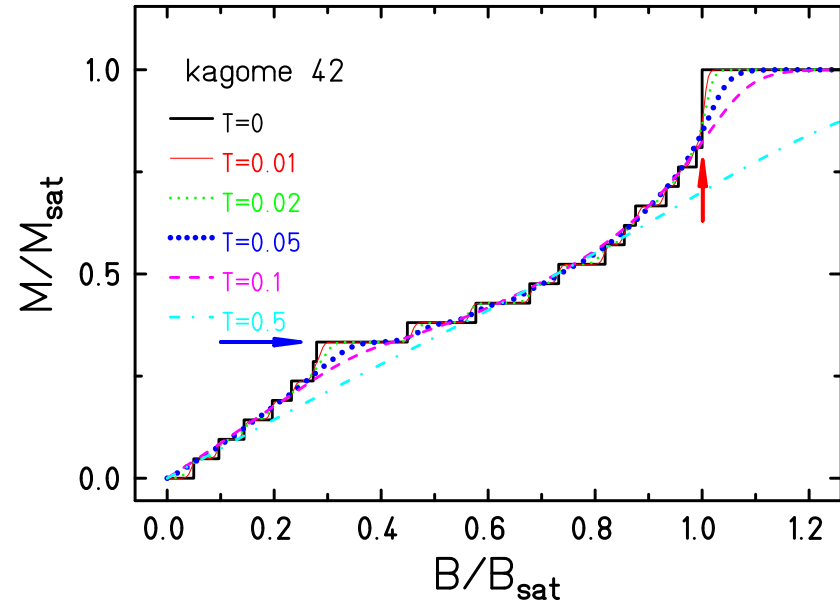
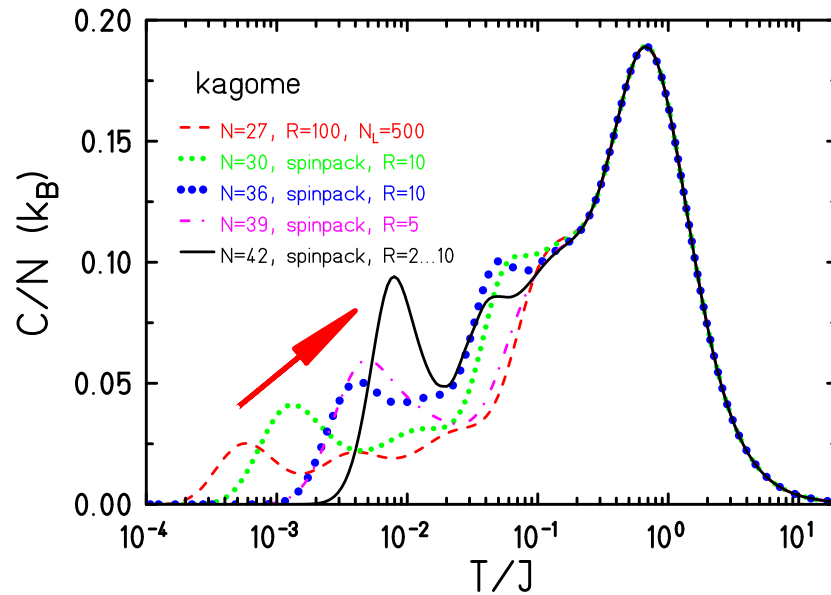


Kagome lattice
antiferromagnet
(figure Mike Zhitomirsky)

- Thermodynamic functions (1)
- “Condensation” of low-lying singlets below the first triplet?
- Magnetization jump to saturation
- Thermal stability of magnetization plateaus
- Crystallization of localized magnons?
- Notoriously enigmatic (2)!

(1) J. Schnack, J. Schulenburg, J. Richter, Phys. Rev. B **98**, 094423 (2018)
 (2) A.M. Läuchli, J. Sudan, R. Moessner, Phys. Rev. B **100**, 155142 (2019)

Kagome $N = 42$ – magnetic properties

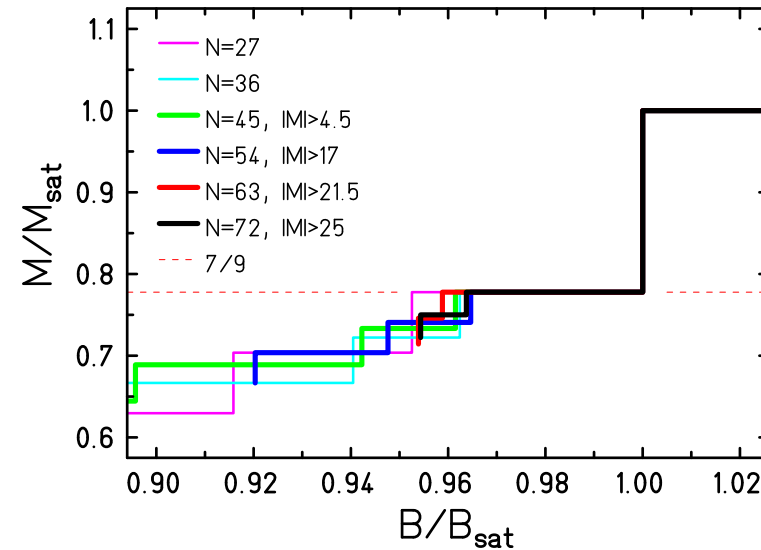
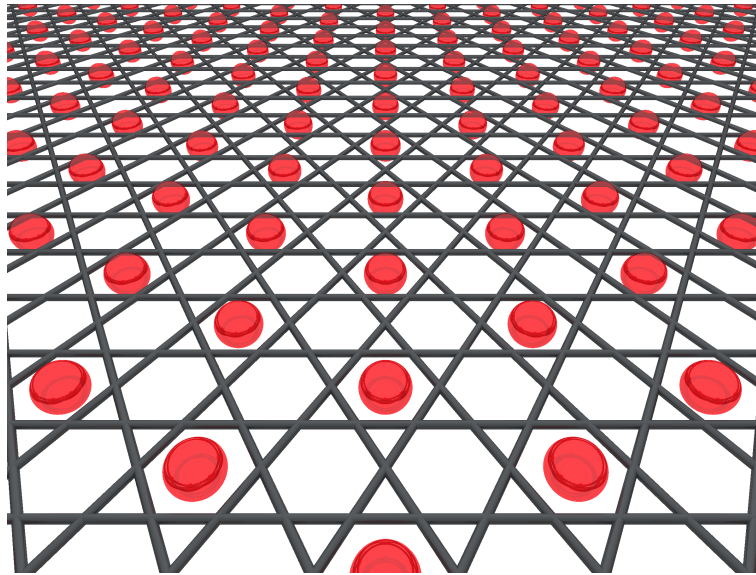


- Low- T peak moves to higher T with increasing N , maybe to form shoulder (2).
- **Density of low-lying singlets seems to move to higher excitation energies!**
- Magnetization exhibits plateaus and giant jump to saturation.

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

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

Kagome – magnetization jump due to independent magnons

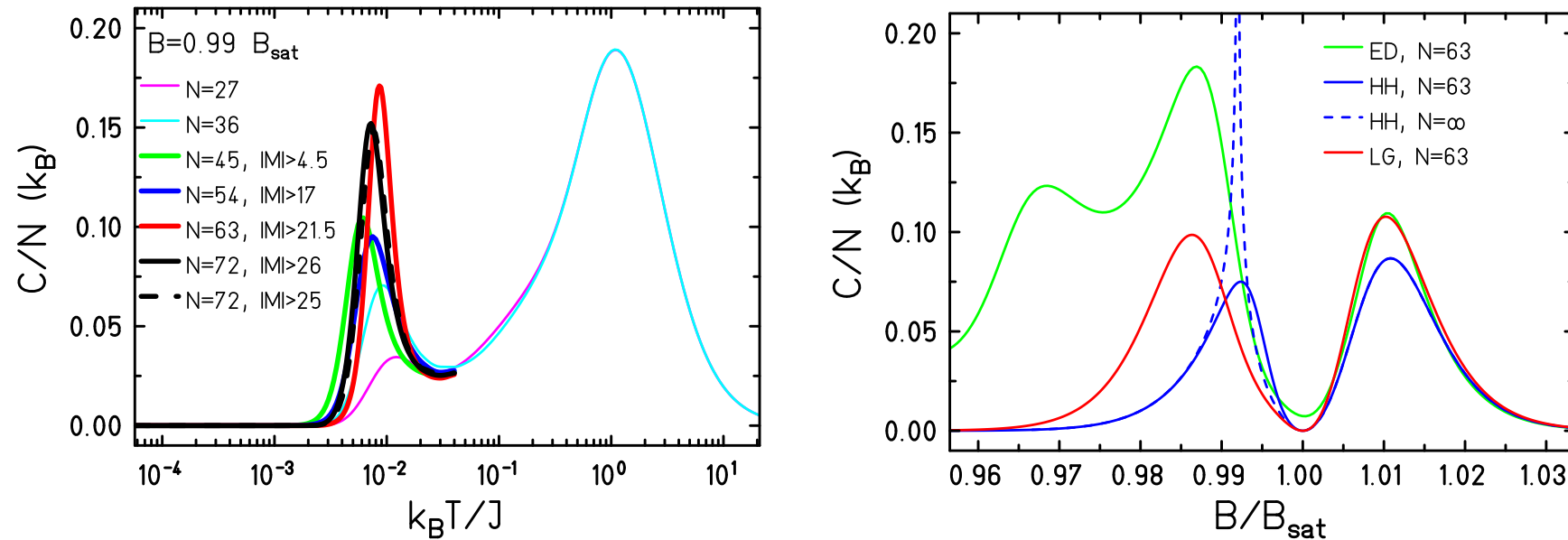


- Nearest-neighbor Heisenberg model: independent one-magnon states are eigenstates and ground states below the saturation field.
- They lead to flat energy bands and can be localized as well.

J. Schnack, H.-J. Schmidt, J. Richter, J. Schulenburg, Eur. Phys. J. B **24**, 475 (2001)

J. Schulenburg, A. Honecker, J. Schnack, J. Richter, H.-J. Schmidt, Phys. Rev. Lett. **88**, 167207 (2002)

Kagome – crystallization of magnons

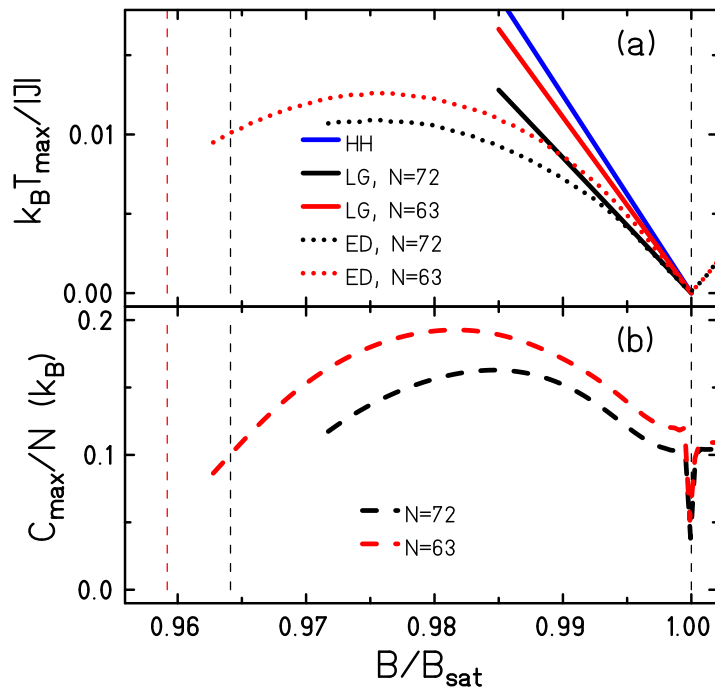


- Finite-temperature continuous transition to a magnon crystal (universality class of the two-dimensional three-state Potts model).
- Numerical investigation with FTLM up to $N = 72$: rounded peaks in C vs T (1).
- Qualitative agreement with loop gas model as well as hard hexagon model (2).

(1) J. Schnack, J. Schulenburg, A. Honecker, J. Richter, Phys. Rev. Lett. **125**, 117207 (2020)

(2) M. E. Zhitomirsky and Hirokazu Tsunetsugu, Phys. Rev. B **70**, 100403(R) (2004)

Kagome – crystallization of magnons



- Crystallization of localized magnons (1).
- T - B phase diagram for finite lattices.
- Extends limiting picture of hard hexagons.
- Loop gas provides good rationalization as long as other states can be neglected (2,3).
- Experimentally relevant for e.g. Cd-kapellasite (4).

(1) J. Schnack, J. Schulenburg, A. Honecker, J. Richter, Phys. Rev. Lett. **125**, 117207 (2020)

(2) A. Honecker, J. Richter, J. Schnack, A. Wietek, Cond. Matter Phys. **23**, 43712 (2020)

(3) <https://perso.u-cergy.fr/~ahonecker/talks/kagomeLoop15december2020.pdf>

(4) R. Okuma, D. Nakamura, T. Okubo, A. Miyake, A. Matsuo, K. Kindo, M. Tokunaga, N. Kawashima, S. Takeyama, and Z. Hiroi, Nat. Commun. **10**, 1229 (2019)

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Thank you very much for your attention.



Andreas Honecker



Johannes Richer



Jörg Schulenburg



Jürgen Schnack

The end.