Magnon crystallization in the kagome lattice antiferromagnet

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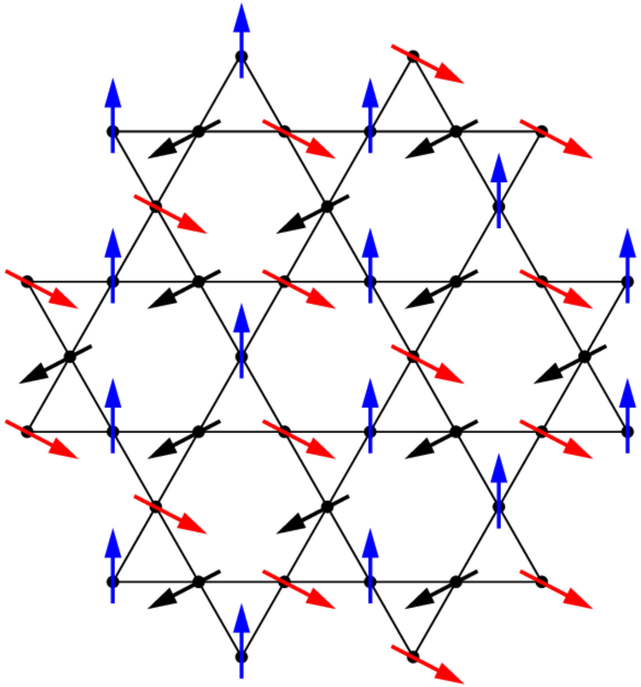
Kagome lattice antiferromagnet – scientific problems

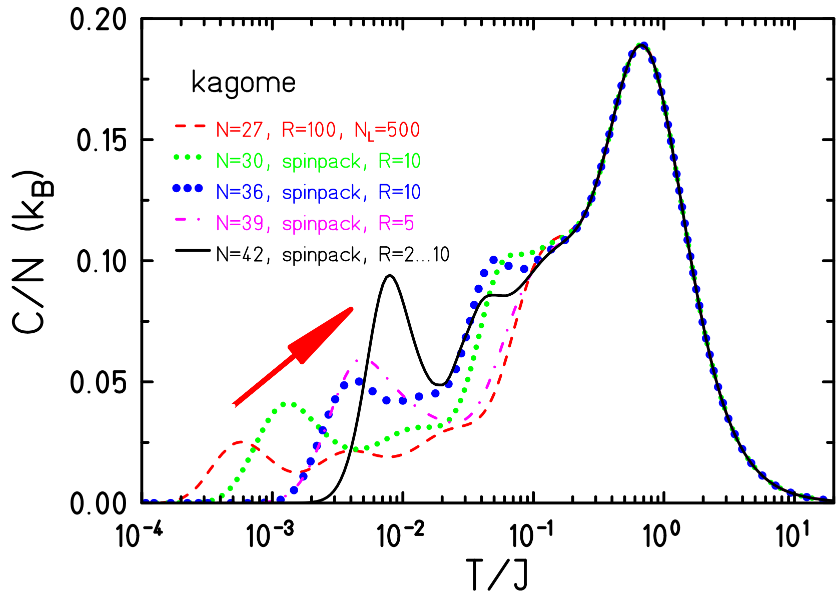


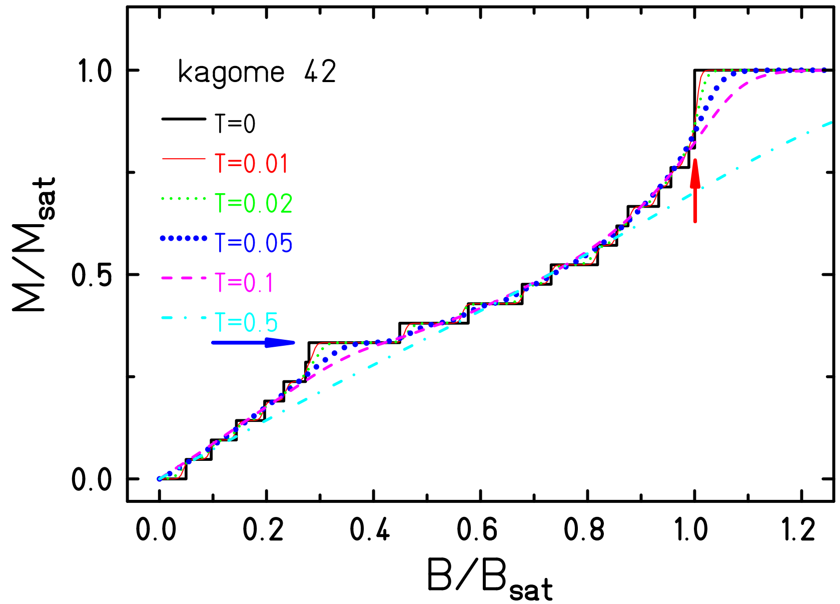
Kagome lattice antiferromagnet
(figure Mike Zhitomirsky)

- 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

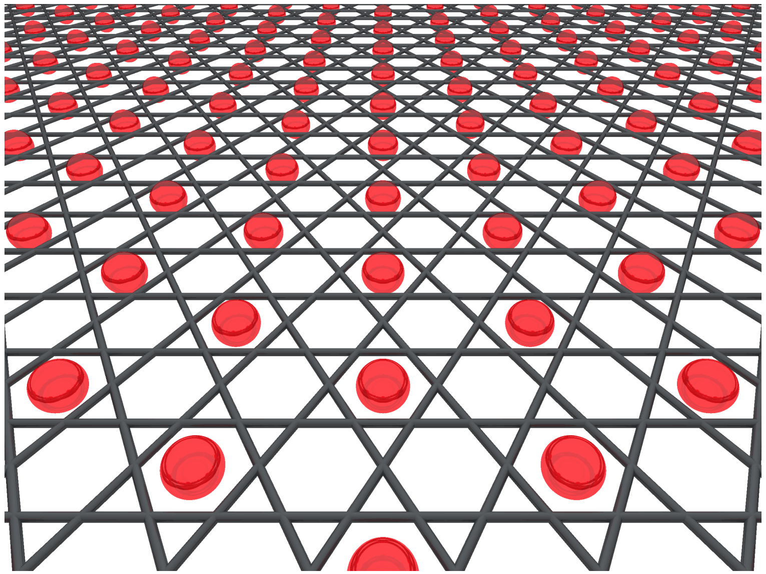


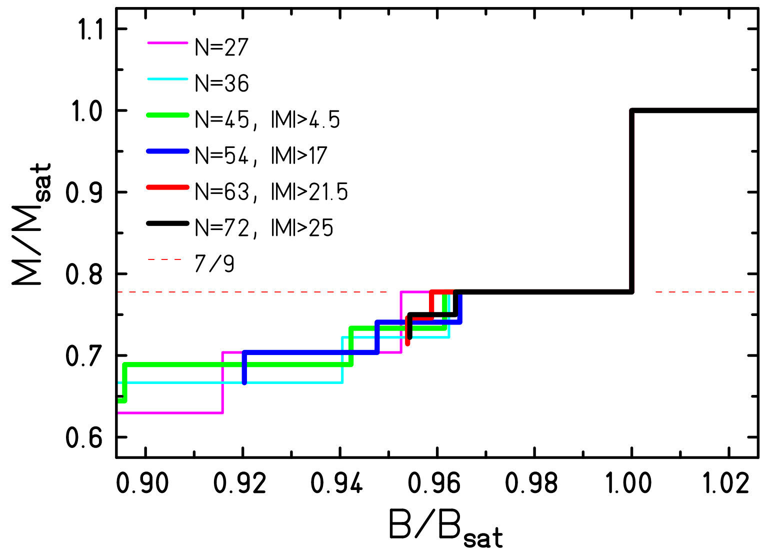


- Low-T peak moves to higher T with increasing N, maybe to form shoulder (2).
- Density of low-lying singlets seems to move to higher excitation energies!
- Magnetization exhibits plateaus and giant jump to saturation.

(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)

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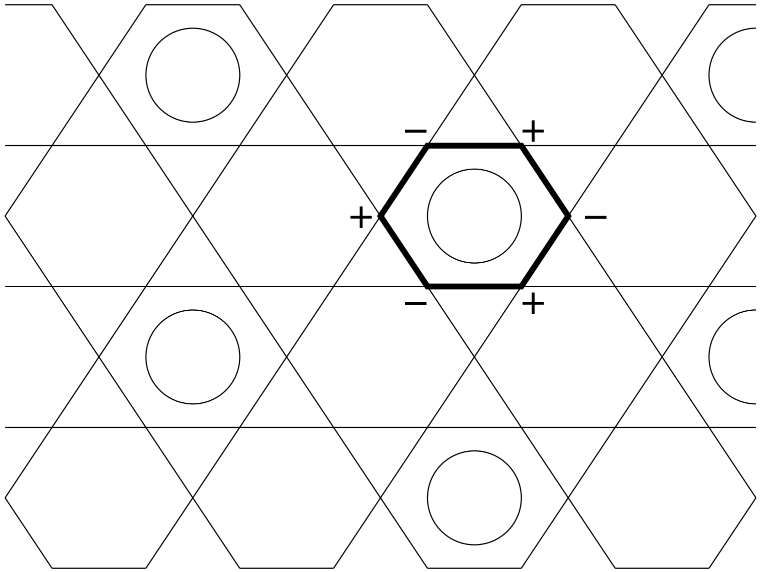

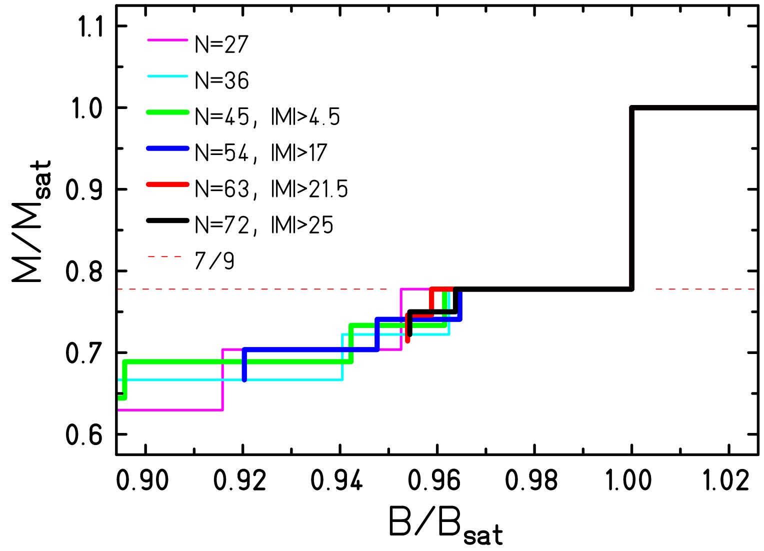

- Nearest-neighbor Heisenberg model: independent one-magnon states are eigenstates and ground states below the saturation field:
  $|\,\text{localized magnon}\,\rangle \propto (\underset{\sim}{s}_1^- - \underset{\sim}{s}_2^- + \underset{\sim}{s}_3^- - \underset{\sim}{s}_4^- + \underset{\sim}{s}_5^- - \underset{\sim}{s}_6^-)\,|\,\text{all spins}\uparrow\rangle$

- They lead to flat energy bands and can be localized as well.

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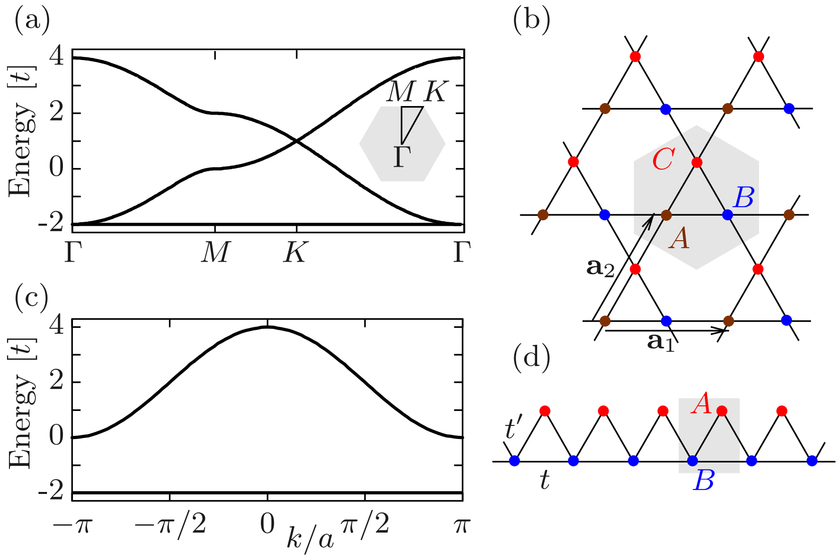
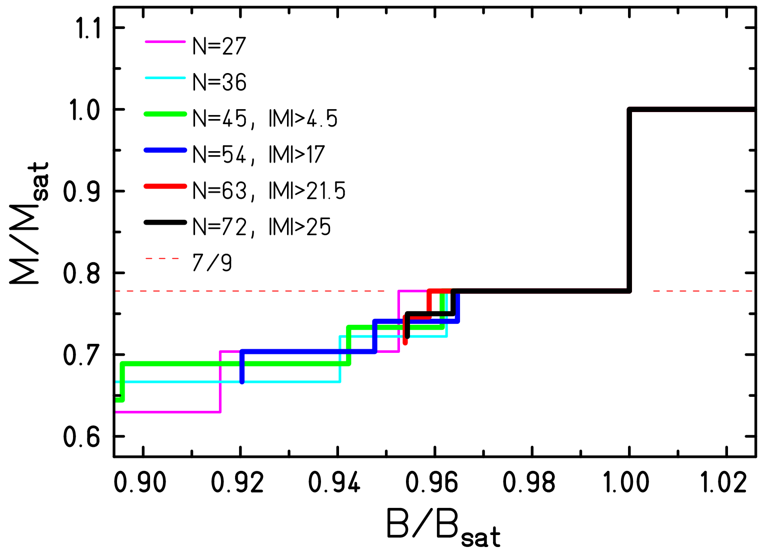


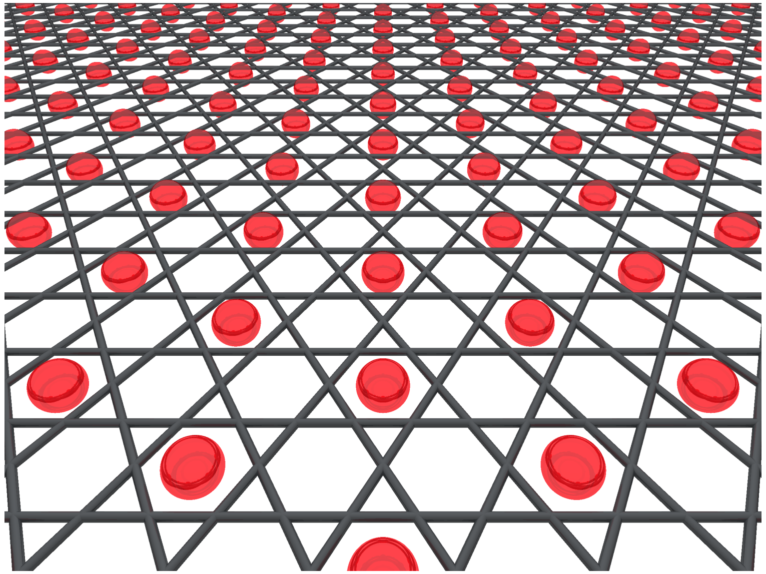


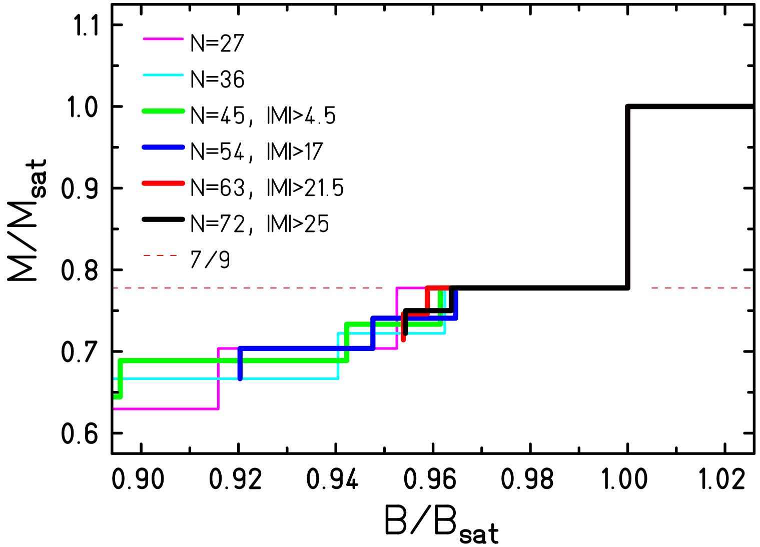
- Nearest-neighbor Heisenberg model: independent one-magnon states are eigenstates and ground states below the saturation field.

- They lead to flat energy bands and can be localized as well.

L.h. figure from S. D. Huber and E. Altman, Phys. Rev. B **82**, 184502 (2010).
J. Schulenburg, A. Honecker, J. Schnack, J. Richter, H.-J. Schmidt, Phys. Rev. Lett. **88**, 167207 (2002)

Kagome – magnetization jump due to independent magnons



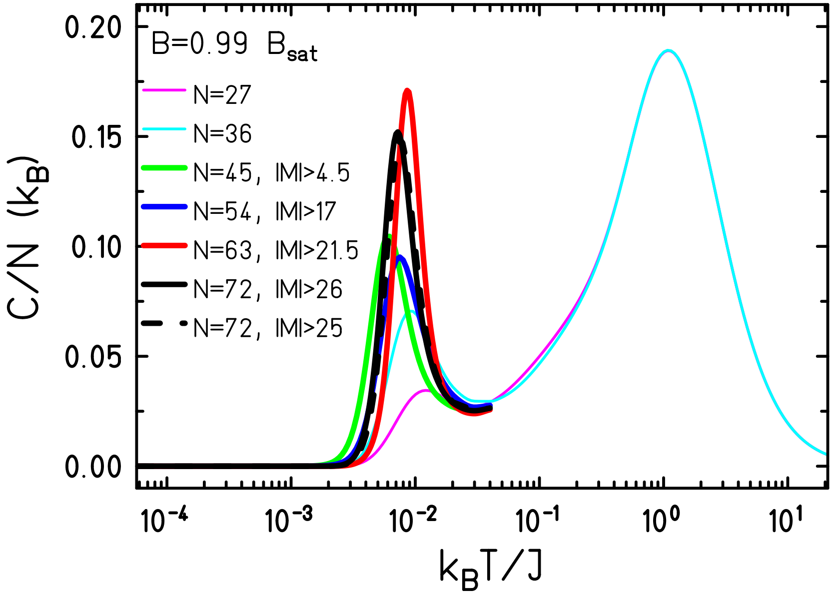


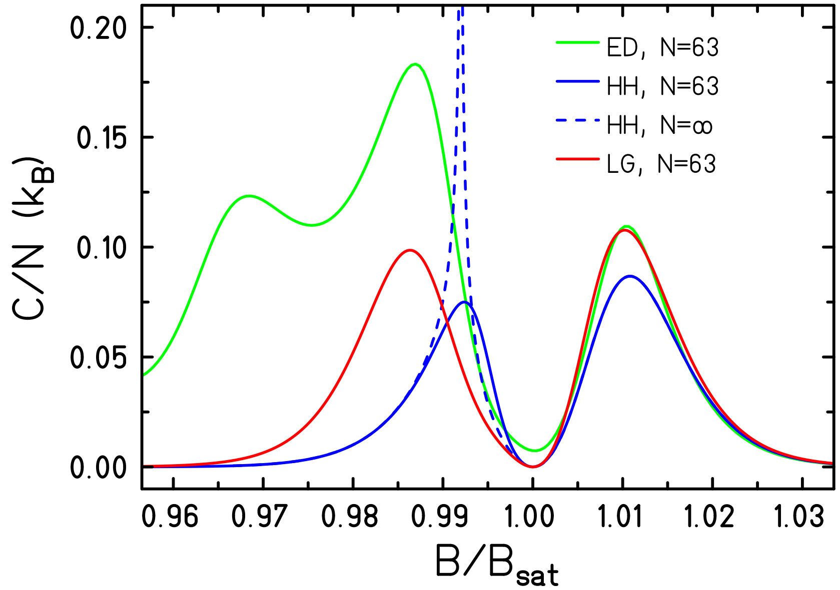
- Nearest-neighbor Heisenberg model: independent one-magnon states are eigen-states and ground states below the saturation field.

- Maximal filling with localized independent magnons of minimal size. Crystal?

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

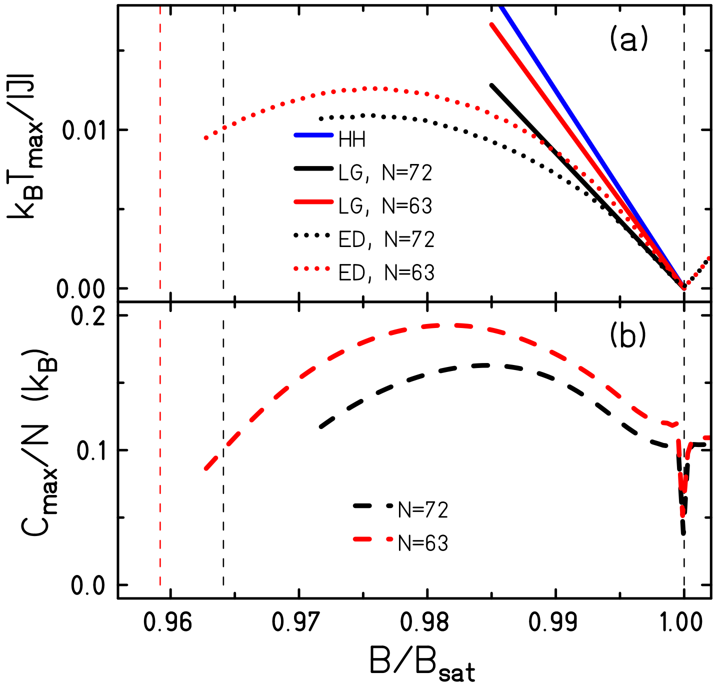




- Finite-temperature continuous transition to a magnon crystal (universality class of the two-dimensional three-state Potts model).
- Numerical investigation with FTLM up to $N = 72$: rounded peaks in C vs T (1).
- Qualitative agreement with loop gas model as well as hard hexagon model (2).

(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)

Thank you very much for your attention.


Andreas Honecker


Johannes Richer


Jörg Schulenburg


Jürgen Schnack

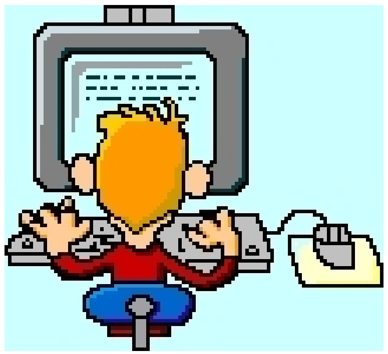
The end.

Magnon crystallization in the kagome lattice antiferromagnet

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

Quantum magnetism: math

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



- 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
  $Z = \mathrm{Tr}\big(\exp[-\beta \underset{\sim}{H}]\big)$
  without solving the eigenvalue problem?

$\Rightarrow$ Trace estimators & Krylov space representation.

Solution I: trace estimators

$$\text{tr}\left(\underset{\sim}{O}\right) \approx \langle\, r\,|\,\underset{\sim}{O}\,|\,r\,\rangle = \sum_{\nu}\langle\,\nu\,|\,\underset{\sim}{O}\,|\,\nu\,\rangle + \sum_{\nu\neq\mu} r_\nu r_\mu \langle\,\nu\,|\,\underset{\sim}{O}\,|\,\mu\,\rangle$$

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

- $|\,\nu\,\rangle$ some orthonormal basis of your choice;
  not the eigenbasis of $\underset{\sim}{O}$, 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

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

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

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

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

Let's diagonalize $\underset{\sim}{H}$ in this space!

Partition function I: simple approximation

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

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

- 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: $|\, r \,\rangle \equiv (T = \infty)$

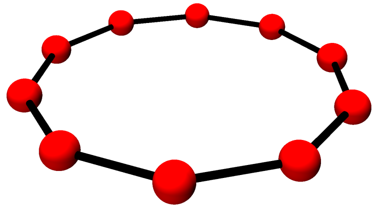
J. Jaklic and P. Prelovsek, Phys. Rev. B **49**, 5065 (1994).

Partition function II: Finite-temperature Lanczos Method

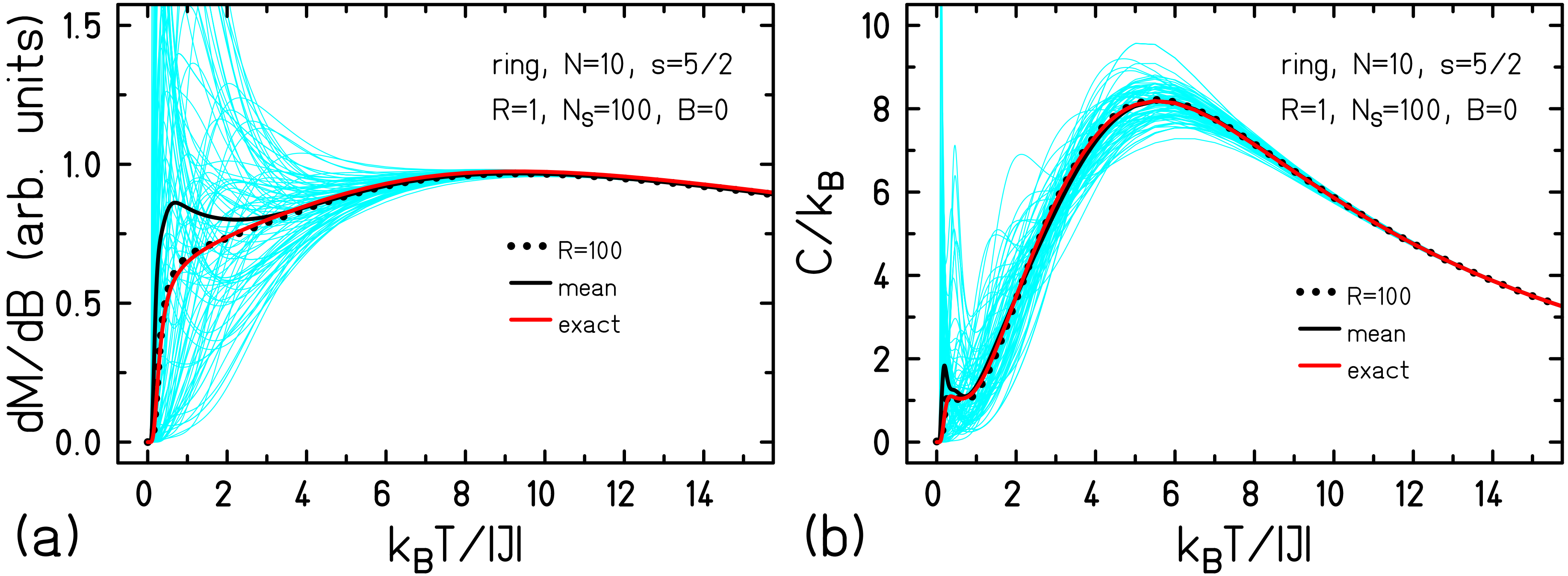
$$Z^{\text{FTLM}}(T,B) \approx \frac{1}{R}\sum_{r=1}^{R}\sum_{n=1}^{N_L} e^{-\beta\epsilon_n^{(r)}} |\langle\, n(r)\,|\, r\,\rangle|^2$$

- 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: $R = 1\dots100, N_L \approx 100$.
- 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

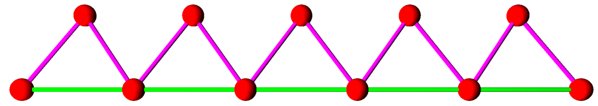


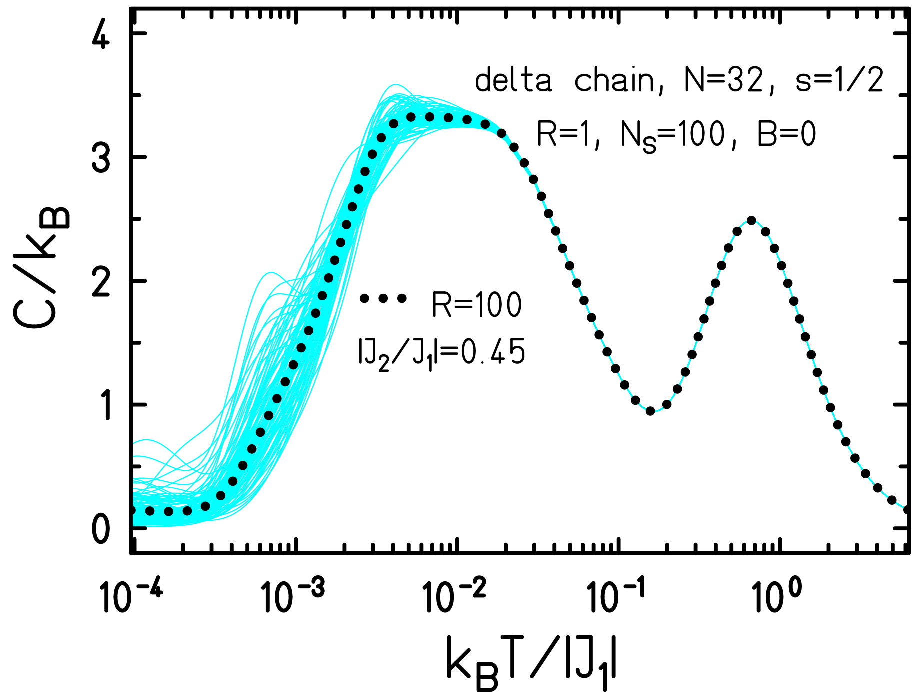
(1) J. Schnack, J. Richter, R. Steinigeweg, Phys. Rev. Research **2**, 013186 (2020).

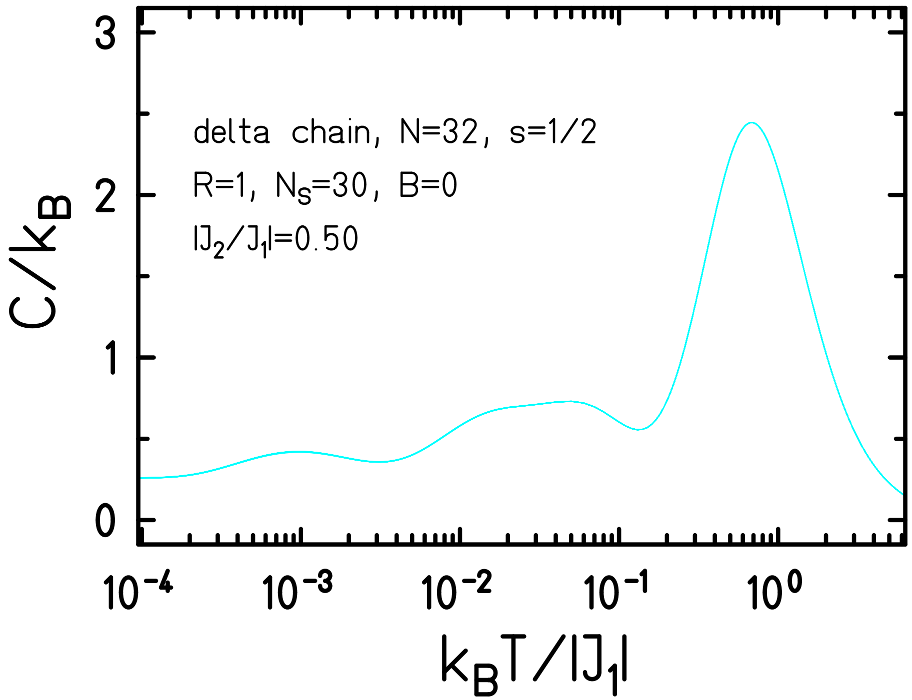
(2) SU(2) & D_2: R. Schnalle and J. Schnack, Int. Rev. Phys. Chem. **29**, 403 (2010).

(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)