Magnon Crystallization in the Kagome Lattice Antiferromagnet

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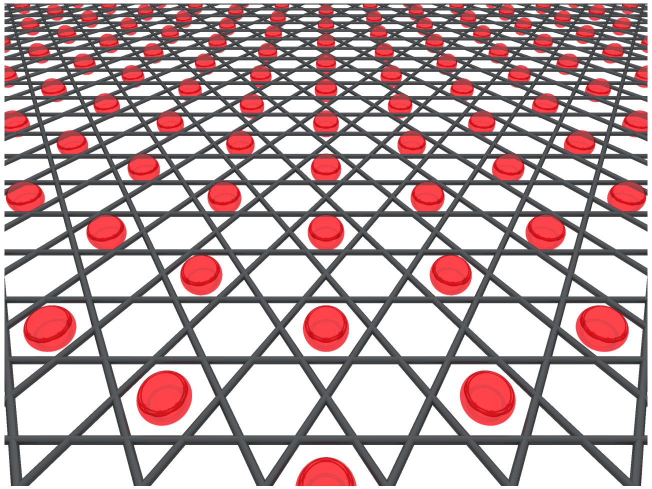
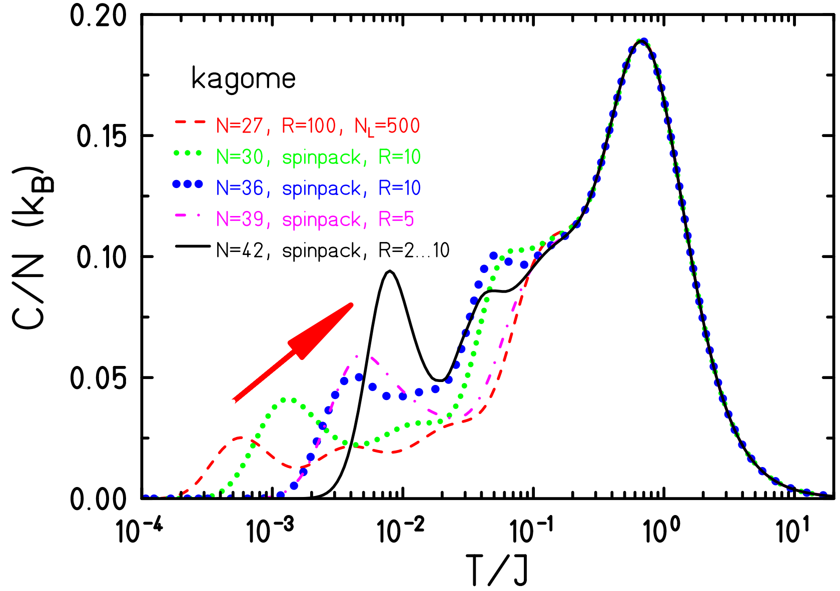
Kagome lattice antiferromagnet – scientific problems

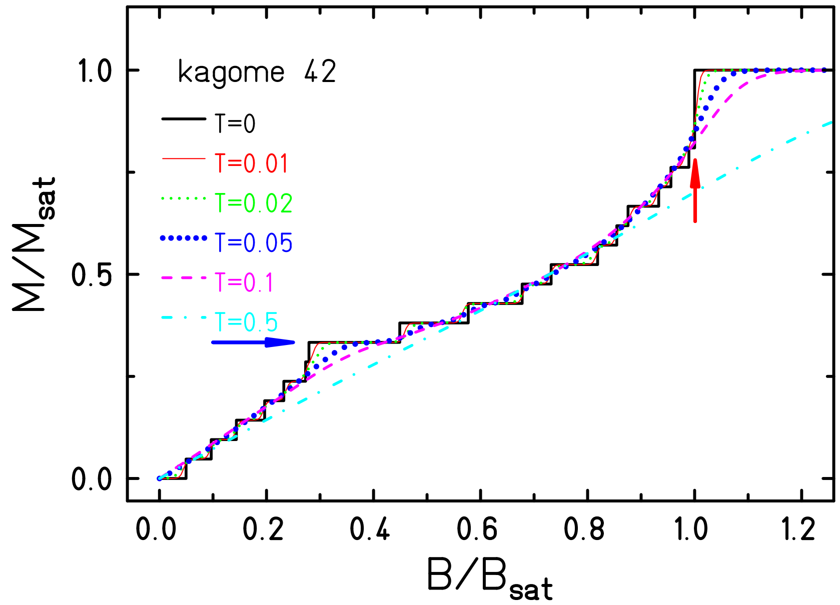


- $\underset{\sim}{H} = J \sum_{<i,j>} \underset{\sim}{\vec{s}}_i \cdot \underset{\sim}{\vec{s}}_j + g\mu_B B \underset{\sim}{S}^z$
- Thermodynamic functions (1)
- "Condensation" of low-lying singlets below the first triplet?
- Magnetization jump to saturation
- Thermal stability of magnetization plateaus
- 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)

Reminder: Kagome 42 – magnetic properties

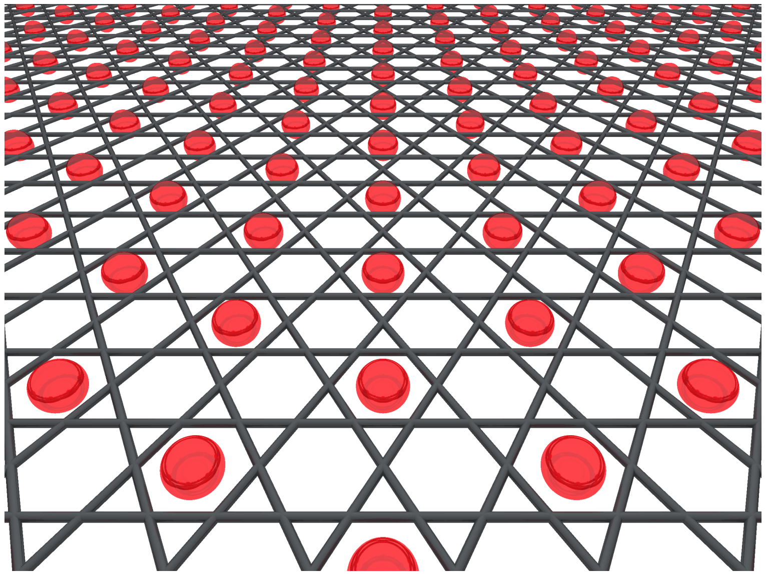


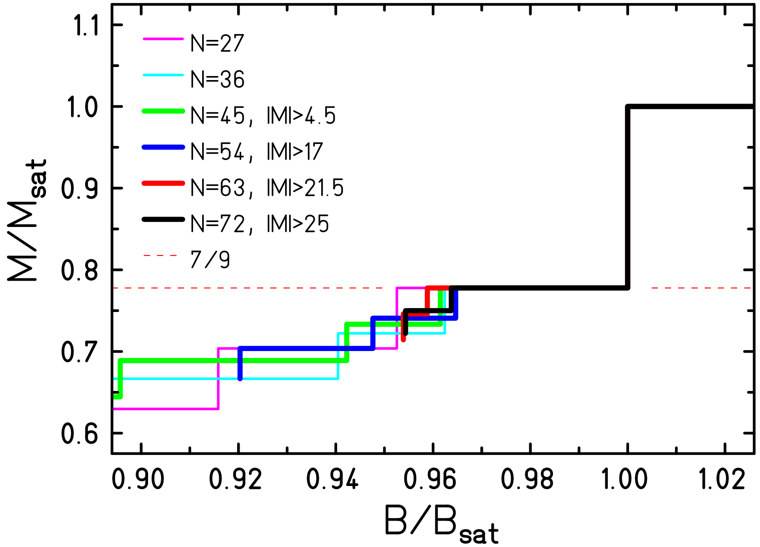


- Low-T peak moves to higher T with increasing N, maybe to form shoulder (2).
- Density of low-lying singlets seems to move to higher excitation energies!
- Magnetization exhibits plateaus and giant jump to saturation.

(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



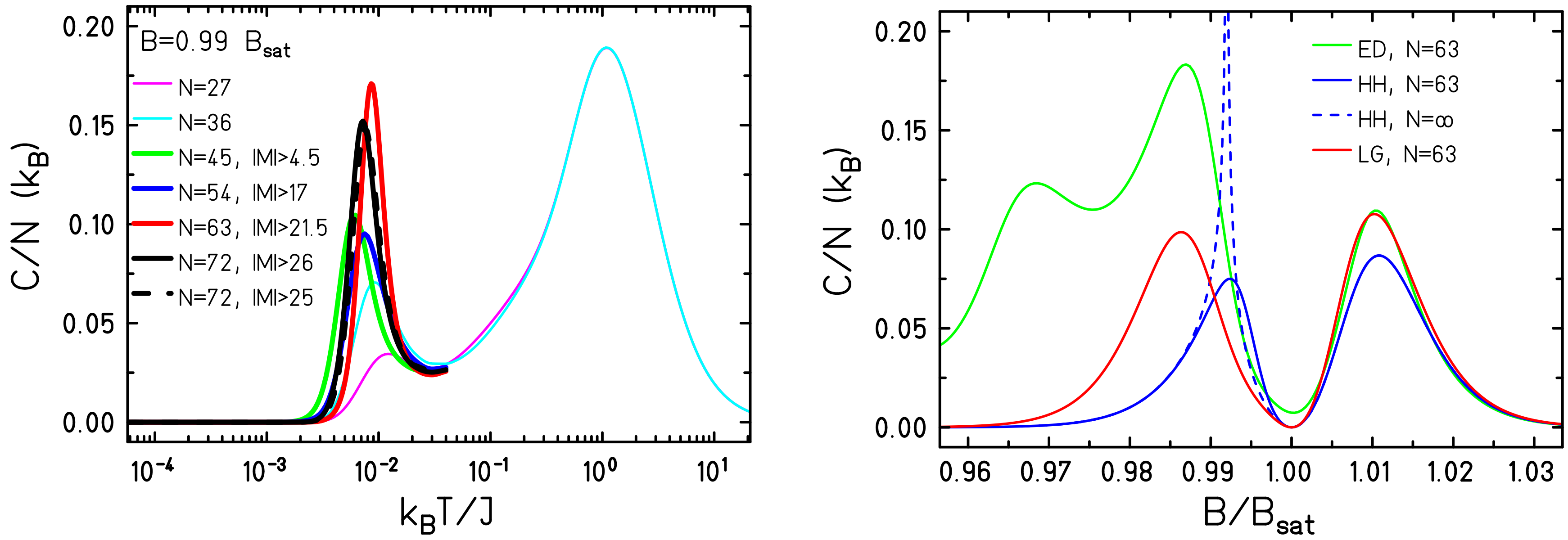


- Nearest-neighbor Heisenberg model: independent one-magnon states are eigenstates and ground states below the saturation field.

- They lead to flat 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)

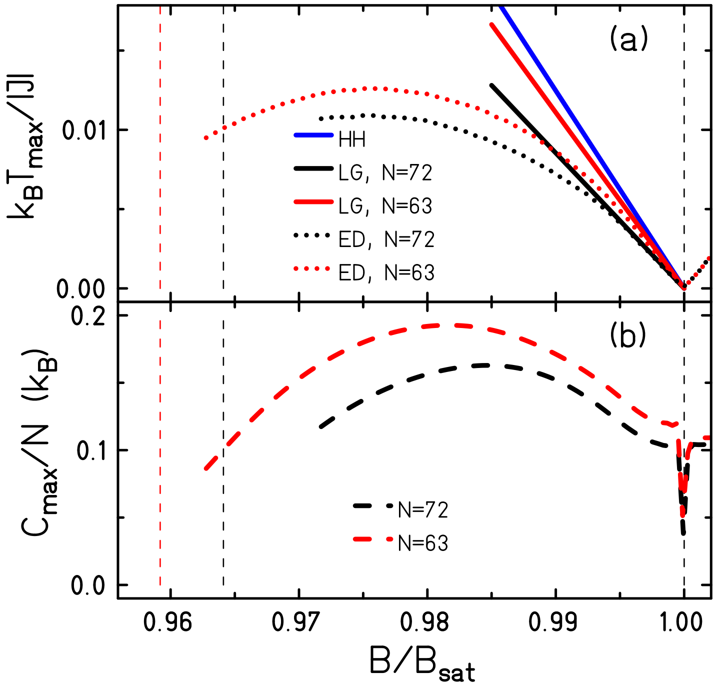
Kagome – crystallization of magnons



- 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

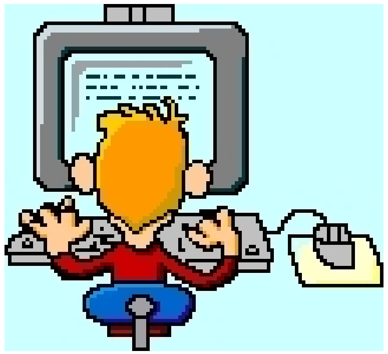


- Crystallization of localized magnons (1).
- T-B phase diagram for finite lattices.
- Extends limiting picture of hard hexagons.
- Loop gas provides good rationalization as long as other states can be neglected (2,3).
- Experimentally relevant for e.g. Cd-kapellasite (4).

(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)

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

  $Z = \text{Tr}\left(\exp[-\beta \underset{\sim}{H}]\right)$

  without solving the eigenvalue problem?

$\Rightarrow$ Trace estimators & Krylov space representation.

Solution I: trace estimators

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

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

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

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

Solution II: Krylov space representation

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

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

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

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).

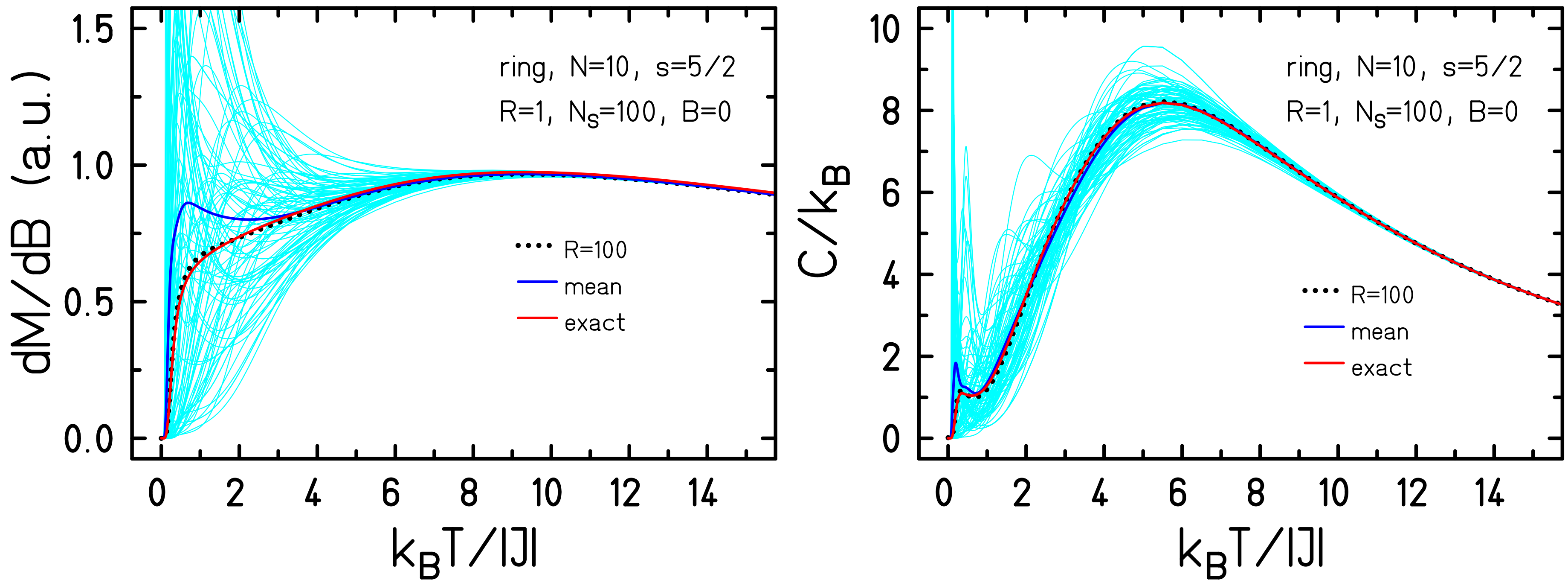
Partition function II: Finite-temperature Lanczos Method

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

- Averaging over R random vectors is better. Note, $\langle\, r\,|\, r\,\rangle = \text{dim}(\mathcal{H})$.
- $|\, n(r)\,\rangle$ 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.

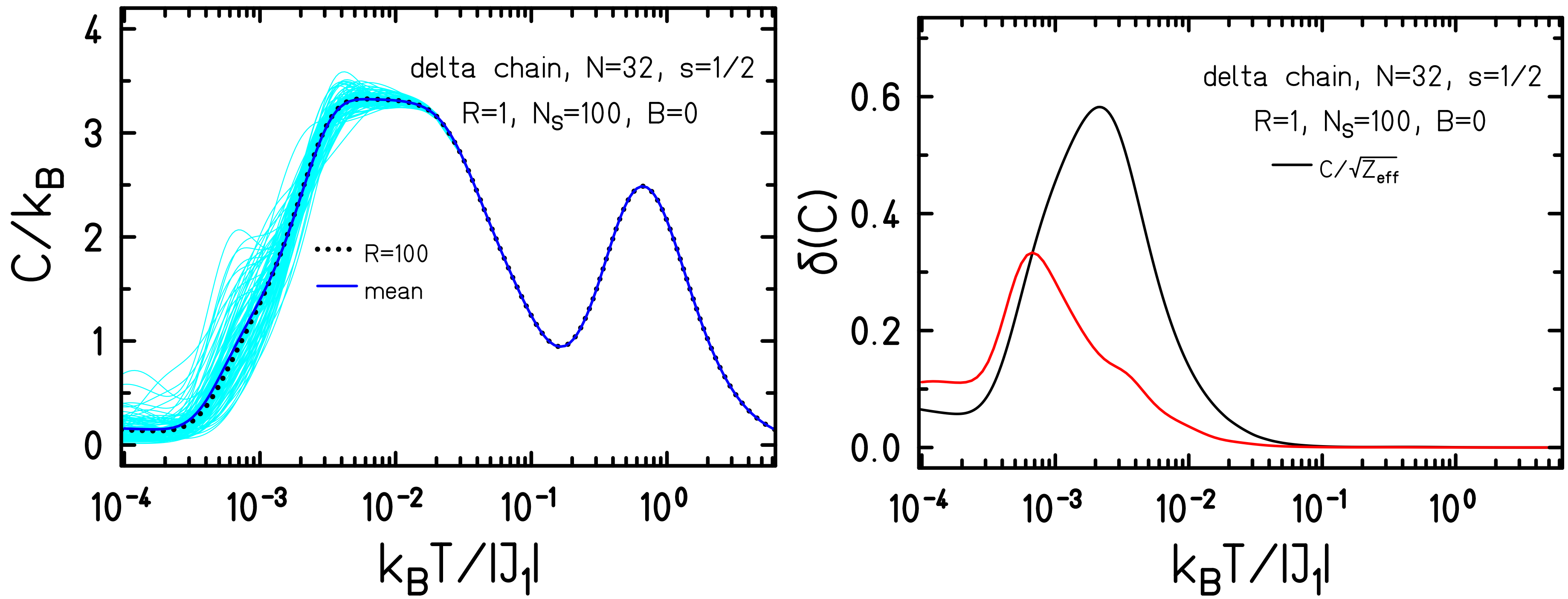
SPINPACK page: https://www-e.uni-magdeburg.de/jschulen/spin/

FTLM 1: ferric wheel



J. Schnack, J. Richter, R. Steinigeweg, arXiv:1911.08838

FTLM 3: sawtooth chain



This is how one calculates Fe_6Gd_6 as approximation for $Fe_{10}Gd_{10}$.

Frustration, technically speaking, works in your favour.

J. Schnack, J. Richter, R. Steinigeweg, arXiv:1911.08838

Thank you very much for your attention.


Andreas Honecker


Johannes Richer


Jörg Schulenburg


Jürgen Schnack

The end.