Thermodynamics of the spin-half square kagome lattice antiferromagnet

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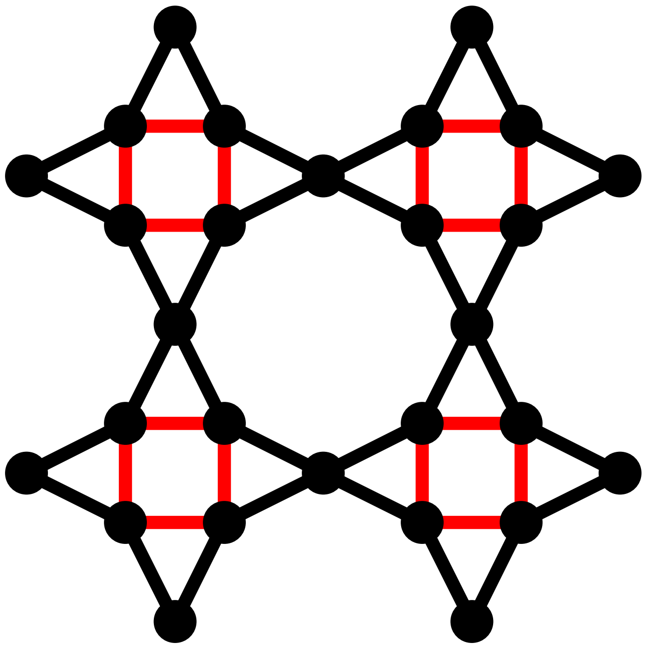
Square-Kagome lattice antiferromagnet – scientific problems

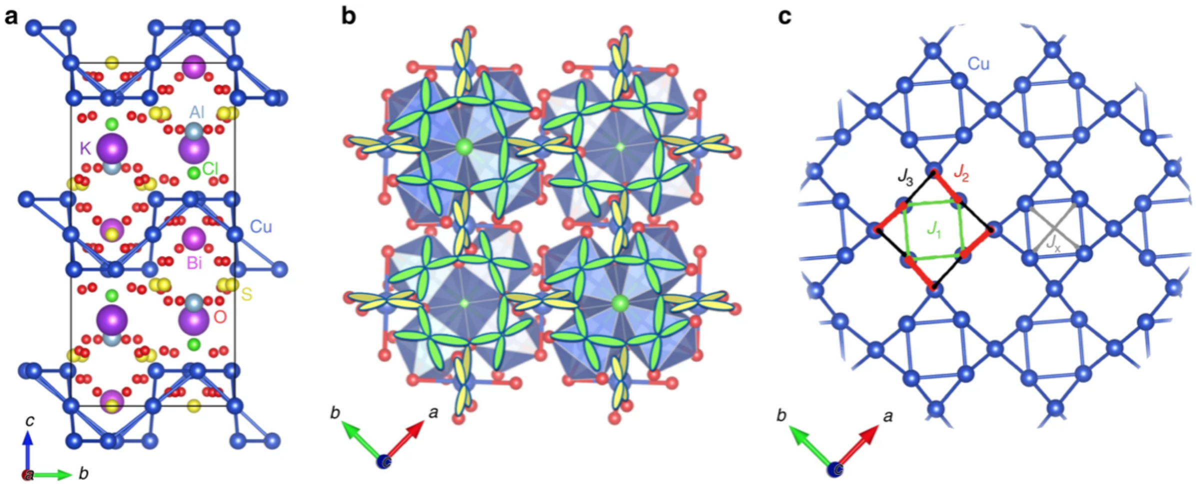


square kagome lattice
h.f. antiferromagnet

- $\underset{\sim}{H} = J \sum_{<i,j>} \underset{\sim}{\vec{s}}_i \cdot \underset{\sim}{\vec{s}}_j + g\mu_B B \sum_i \underset{\sim}{s}_i^z$
- Also termed shuriken lattice.
- Character of the ground state?
- Thermodynamic functions (1)
- Magnetization plateaus and thermal stability (TT 23.10)
- Magnetization jump to saturation (2)
- Relation to (more famous) kagome lattice?

(1) J. Richter, O. Derzhko, and J. Schnack, Phys. Rev. B **105**, 144427 (2022).
(2) J. Schnack, H.-J. Schmidt, J. Richter, and J. Schulenburg, Eur. Phys. J. B **24**, 475 (2001).

Square-Kagome lattice antiferromagnet – scientific problems



a Crystal structure of $KCu_6AlBiO_4(SO_4)_5Cl$ featuring a large interlayer spacing. **b** Arrangement of the Cu^{2+} orbitals in SKL. The $d_{x^2-y^2}$ orbitals carrying spin-1/2 are depicted on the Cu sites. **c** Square-kagome lattice of $KCu_6AlBiO_4(SO_4)_5Cl$ consisting of Cu^{2+} ions with nearest-neighbour exchange couplings J_1, J_2, J_3 and next-nearest-neighbour exchange coupling J_X.

Gapless spin liquid (1). Character of spin liquid not yet resolved (2).
For J_1–J_2 square-kagome lattice, see (3).

(1) M. Fujihala *et al.*, Nat. Commun. **11**, 3429 (2020).
(2) R. Siddharthan and A. Georges, Phys. Rev. B **65**, 014417 (2001); J. Richter, J. Schulenburg, P. Tomczak, D. Schmalfuß, Condens. Matter Phys. **12**, 507 (2009); H. Nakano and T. Sakai, J. Phys. Soc. Jpn. **82**, 083709 (2013); I. Rousochatzakis, R. Moessner, and J. van den Brink, Phys. Rev. B **88**, 195109 (2013).
(3) J. Richter, J. Schnack, arXiv:2212.10838

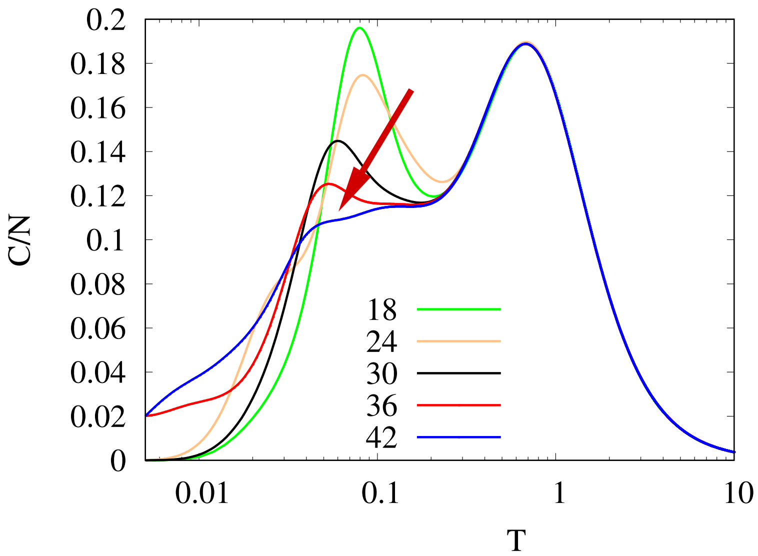
Square-Kagome lattice antiferromagnet – how to calculate?

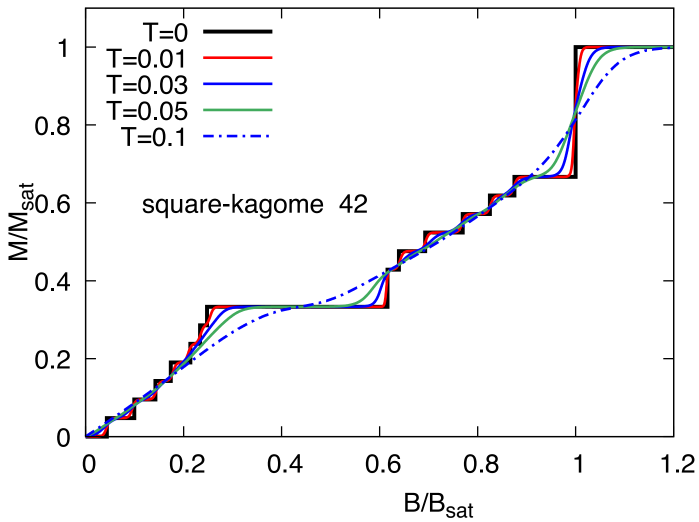
$$Z^{\text{FTLM}}(T,B) \approx \frac{1}{R}\sum_{r=1}^{R}\sum_{n=1}^{N_L} e^{-\beta\epsilon_n^{(r)}} |\langle\, n(r)\,|\,r\,\rangle|^2$$

- Finite-temperature Lanczos method (1):
  Partition function approximated by a small sum: $R = 1\dots100, N_L \approx 100$.
- Averaging over R random vectors $|\,r\,\rangle$; $|\,n(r)\,\rangle$ n-th Lanczos eigenvector starting from $|\,r\,\rangle$.
- Implemented in e.g. `spinpack` by Jörg Schulenburg (URZ Magdeburg);
  MPI and openMP parallelized, used up to 3072 nodes @LRZ for $N = 42$.

(1) J. Jaklic and P. Prelovsek, Phys. Rev. B **49**, 5065 (1994); J. Schnack, J. Richter, and R. Steinigeweg, Phys. Rev. Research **2**, 013186 (2020); J. Schnack, J. Richter, T. Heitmann, J. Richter, and R. Steinigeweg, Z. Naturforsch. A **75**, 465 (2020).
(2) SPINPACK page: https://www-e.uni-magdeburg.de/jschulen/spin/

Square-Kagome lattice antiferromagnet – magnetic properties



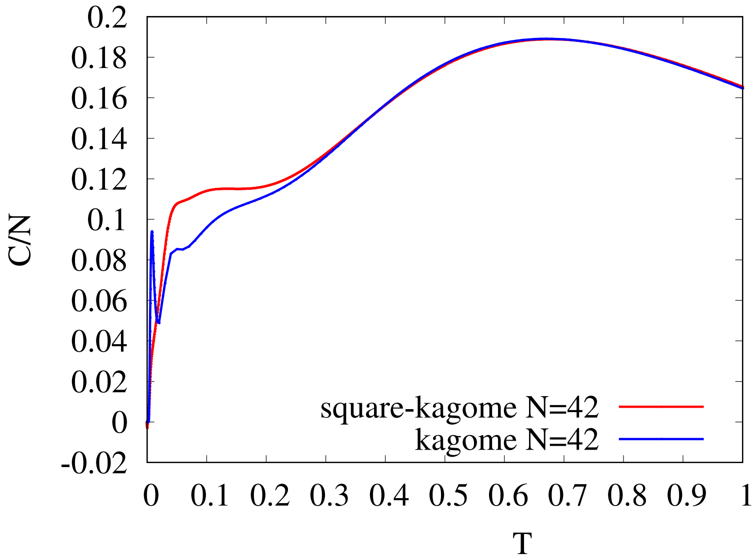


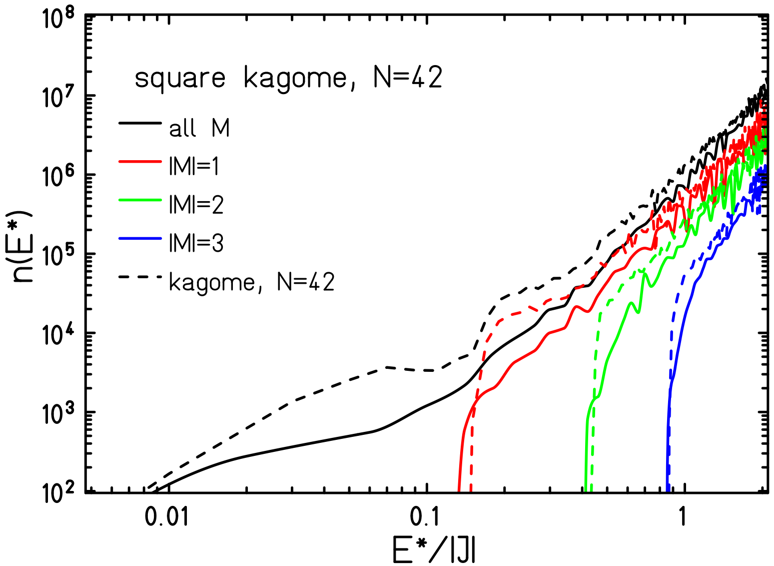
- C: Low-T peak moves to lower T with increasing N (1). Shoulder?

- M: Magnetization exhibits plateaus and giant jump to saturation. For thermal behaviour, see TT 23.10.

(1) J. Richter, O. Derzhko, and J. Schnack, Phys. Rev. B **105**, 144427 (2022).

Square-Kagome lattice antiferromagnet – relation to kagome



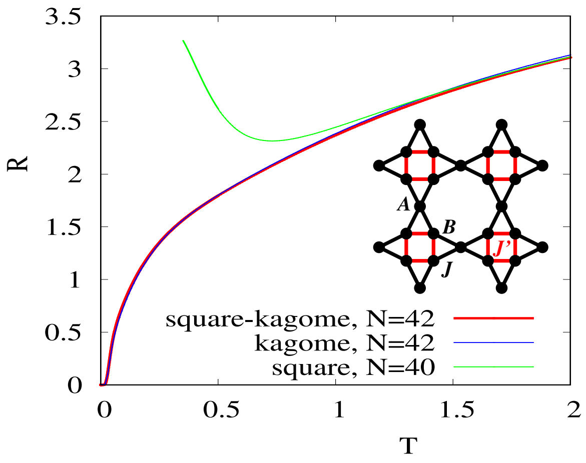


- C: heat capacity rather similar down to $T \sim 0.3$ (1).

- DOS: density of states very similar;
  low-T behavior dominated by singlet excitations.

(1) J. Richter, O. Derzhko, and J. Schnack, Phys. Rev. B **105**, 144427 (2022).

Summary



$R(T) = 4\pi^2 T\chi/(3S(T))$

- Square-Kagome antiferromagnet is highly frustrated and features flat bands, magnetization jump, and magnetization plateaus.
- Low-T physics dominated by singlet excitations very similar to kagome lattice antiferromagnet and very different to non-frustrated square lattice.
- Modified Wilson ratio (1) hints at quantum spin liquid similar to kagome lattice. This changes with J_1–J_2 Hamiltonian (2).

(1) P. Prelovsek, K. Morita, T. Tohyama, and J. Herbrych, Phys. Rev. Research **2**, 023024 (2020).
(2) J. Richter, J. Schnack, arXiv:2212.10838
(3) More exp.: O. V. Yakubovich *et al.*, Inorganic Chemistry **60**, 11450 (2021); B. Liu *et al.*, Phys. Rev. B **105**, 155153 (2022); M. Markina *et al.*, arXiv:2212.11623.
(4) More square-kagome physics: MA 40.24

Thank you very much for your attention.

 Oleg Derzhko

 Johannes Richer

 Jörg Schulenburg

 Jürgen Schnack

The end.

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