Order by disorder and phase transitions in a highly frustrated spin model on the triangular lattice

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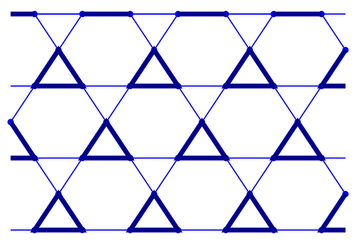
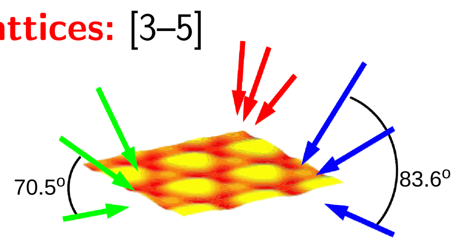
Motivation



1. **Spin-$1/2$ Heisenberg antiferromagnet on kagomé lattice: 1/3 plateau** [1]
   - approach from trimerized kagome lattice [2]:

$$H_{\text{eff.}} = \tilde{J} \sum_{\langle i,j \rangle} \vec{S}_i^t \cdot \vec{S}_j^t \left(C + \left(2\,\vec{e}_i \cdot \vec{\mathfrak{S}}_i\right)\left(2\,\vec{e}_j \cdot \vec{\mathfrak{S}}_j\right)\right)$$

   - pseudo-spin $\vec{\mathfrak{S}}_i$: chirality of triangle $\quad s = 1/2,\ J > 0$
   - 1/3 saturation: $\quad \vec{S}_i^t \to \frac{1}{2}$
2. **Ultracold quantum gases in optical lattices:** [3–5]
   - optical trimerized kagome lattice
   - 2/3 filling of spinless fermionic atoms
   - J tunable via Feshbach resonances



3. **Models of orbital frustration**

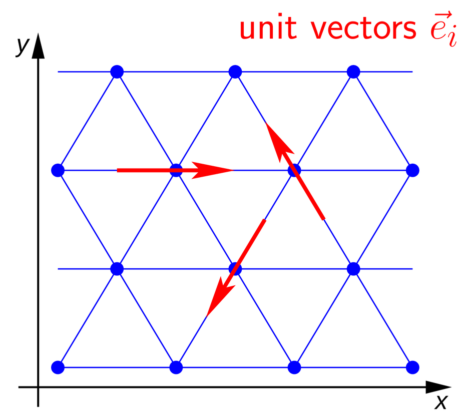
Model

Hamiltonian:

$$H = J \sum_{\langle i,j \rangle} \left(2\,\vec{e}_i \cdot \vec{\mathfrak{S}}_i\right)\left(2\,\vec{e}_j \cdot \vec{\mathfrak{S}}_j\right)$$

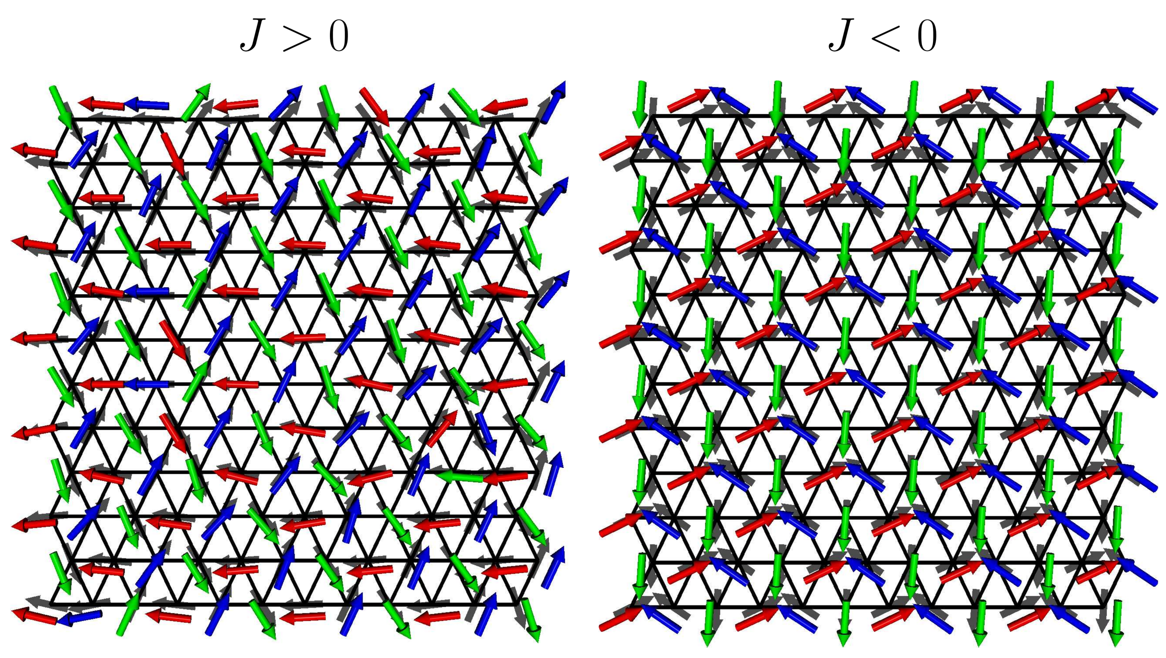
- $\vec{\mathfrak{S}}_i$: spin-s operator at site i
- classical limit for $\vec{\mathfrak{S}}_i$: unit vectors with 3 components

Triangular lattice



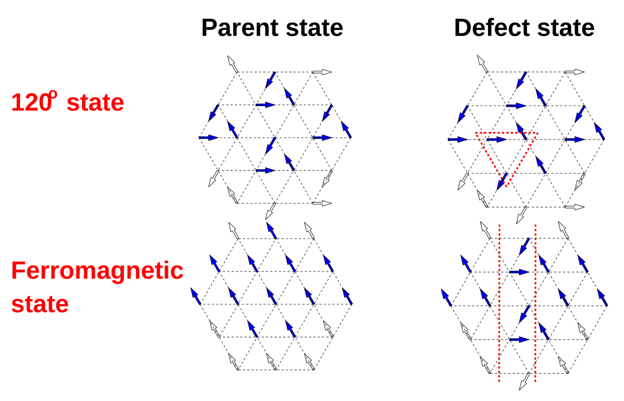
- **only discrete spin symmetry:** D_6 (symmetry group of a hexagon)
- **Mermin-Wagner theorem allows a finite transition temperature** for an ordered groundstate

Snapshots of configurations at $T = 10^{-3}\,|J|$



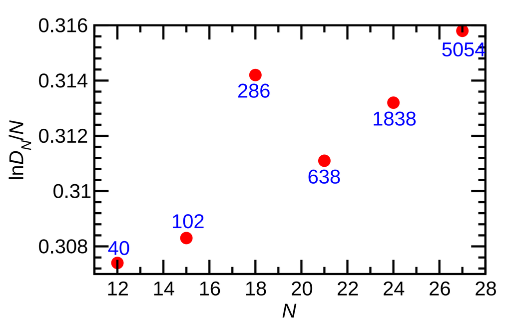
$J > 0$: Macroscopic groundstate degeneracy

Many groundstates [6]



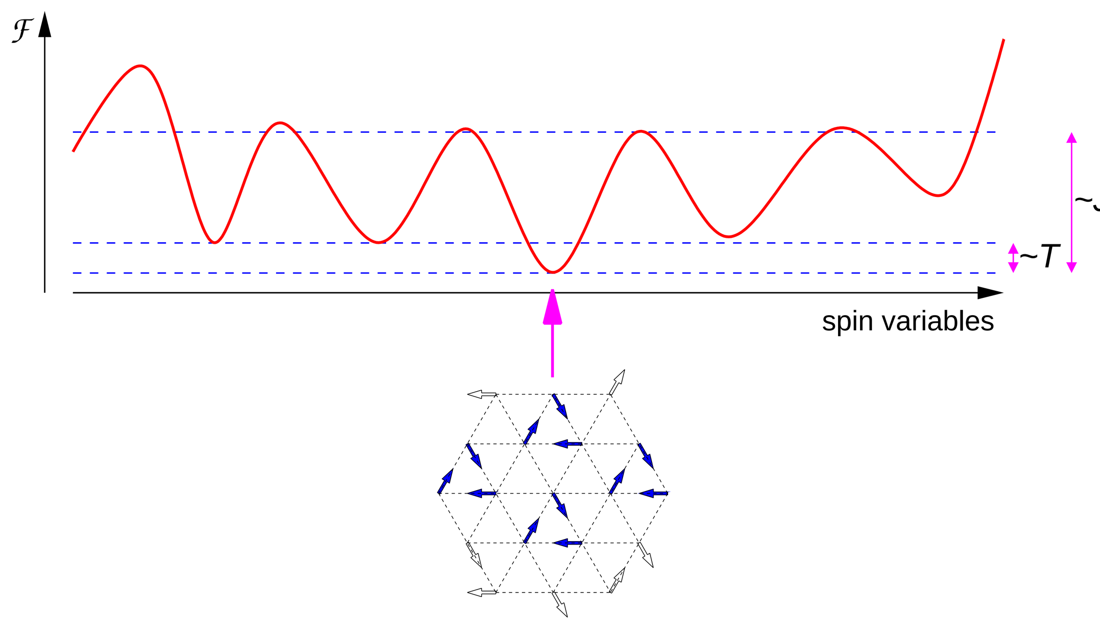
- many configurations with $E_{gs} = -3\,J\,N$
- $T = 0$: continuous global spin-rotation symmetry
- thermal fluctuations: lock-in at angles $n\frac{\pi}{3}$

Groundstate enumeration



- D_N: # groundstates at size N (one spin direction fixed)
- assumption: mutual angles $= n\frac{2\pi}{3}$
- 120° state: largest # 'soft' modes $\Rightarrow$ 'order-by-disorder' selection

$J > 0$: Free energy landscape



Free energy $\mathcal{F}$:
- many almost degenerate minima
- separated by energy barriers $\propto J$

$\Rightarrow$ similar to spin glasses
$\Rightarrow$ **use exchange Monte Carlo** ('parallel tempering') [7]

$J < 0$: Low-temperature state

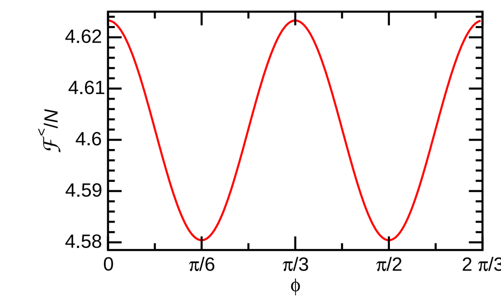
Groundstate

- Energetic selection of 120°-ordered state with $E_{gs} = 6\,J\,N$

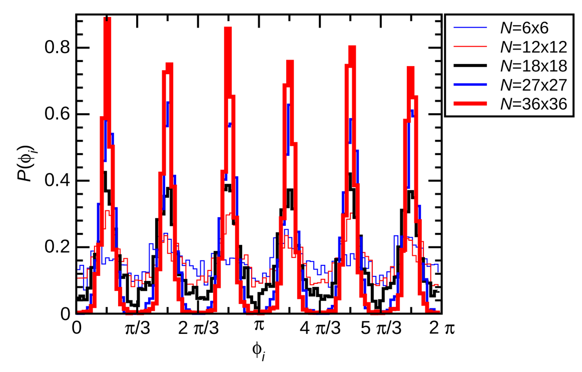
$\Rightarrow$ single-spin-flip Metropolis Monte Carlo sufficient

- $T = 0$: continuous global spin-rotation symmetry
- thermal fluctuations: lock-in at in-plane angles $\phi_i = n\,\pi/3 + \pi/6$

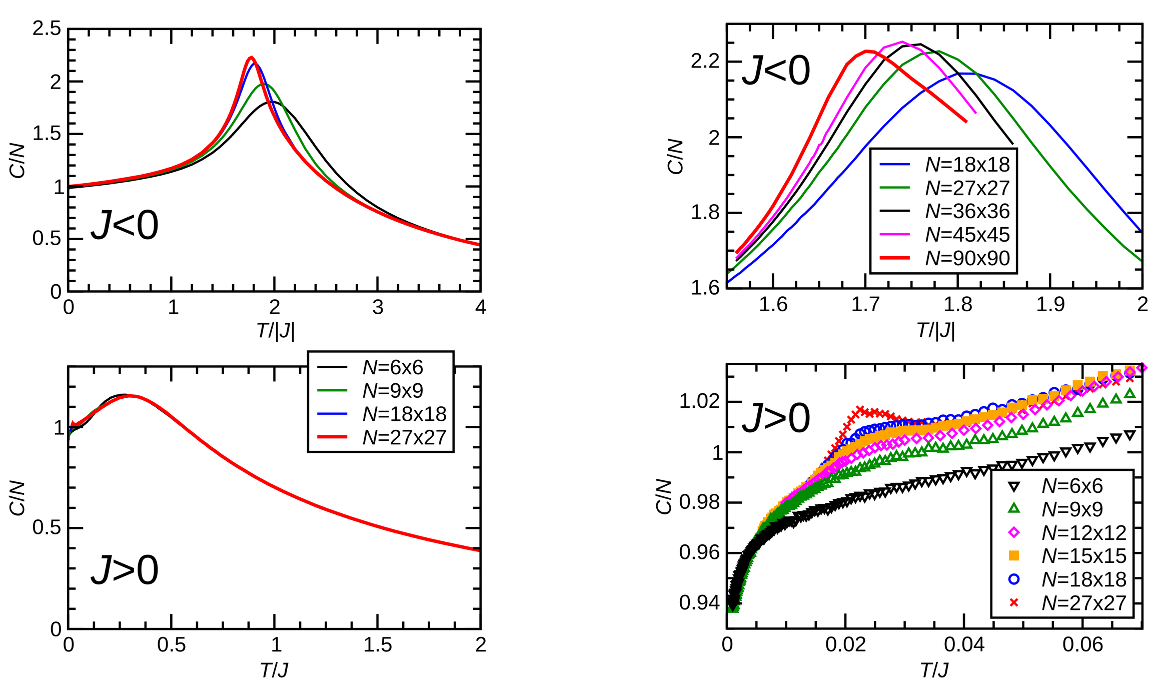
- Spin-wave contribution to free energy:



- Histogram angles at $T = 10^{-3}\,|J|$:



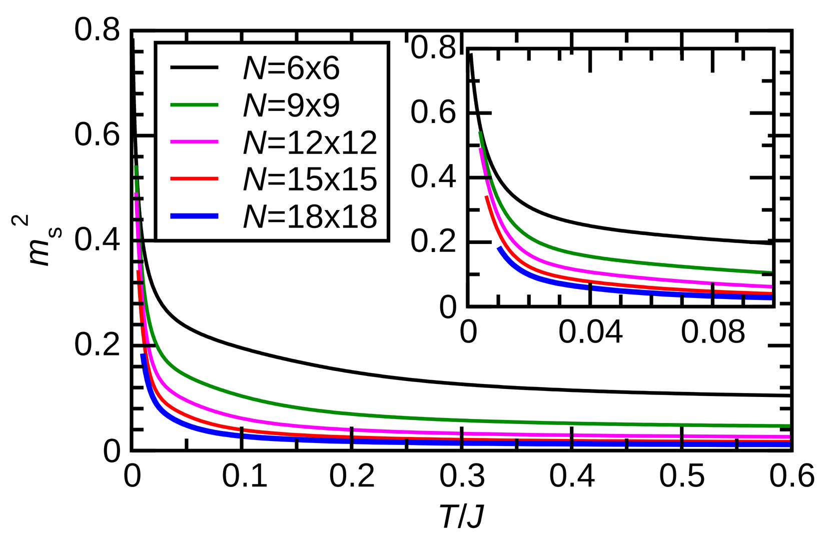
Specific heat



- $J < 0$: phase transition at $T \lesssim 1.7\,|J|$ (?) equipartition among quadratic modes $\Rightarrow$ $C/N \to 1$ for $T \to 0$
- $J > 0$: phase transition at $T \approx J/50$ (?) 120° state: one flat branch at harmonic level $\Rightarrow$ $\frac{C}{N} \to \frac{11}{12}$ for $T \to 0$

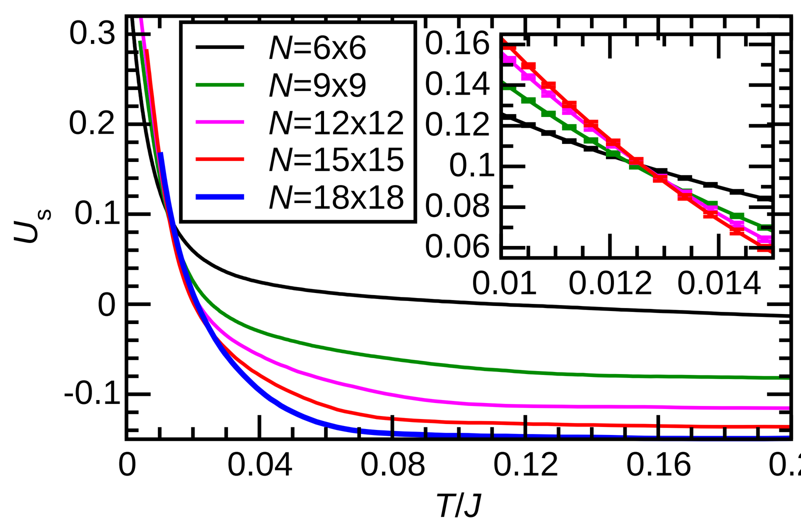
$J > 0$: Sublattice magnetization

$$\vec{M}_s = \frac{3}{N} \sum_{i \in \text{Sublattice } \mathcal{L}} \vec{\mathfrak{S}}_i\,, \qquad m_s^2 = \left\langle \vec{M}_s^2 \right\rangle$$



$J > 0$: Binder cumulant

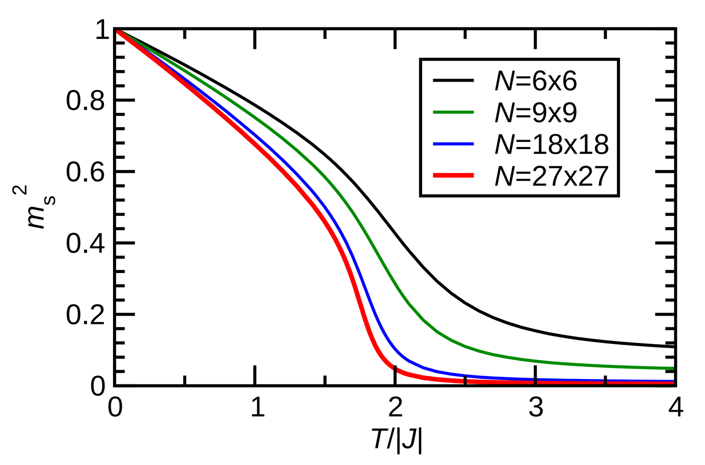
$$U_s = 1 - \frac{3\left\langle \vec{M}_s^4 \right\rangle}{5\left\langle \vec{M}_s^2 \right\rangle^2}$$



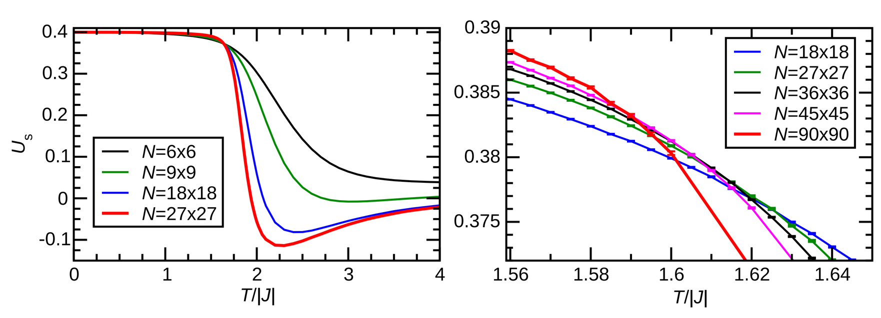
$\Rightarrow$ **Transition temperature:**

$T_c = (0.0125 \pm 0.0009)\ J$

$J < 0$: Sublattice magnetization



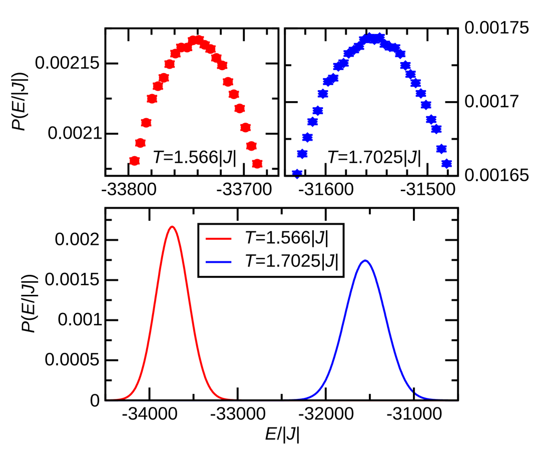
$J < 0$: Binder cumulant



$\Rightarrow$ **Transition temperature:**

$T_c = (1.566 \pm 0.005)\ J$

$J < 0$: Energy histogram



$\Rightarrow$ **second order**

$J < 0$: Critical exponents

$N = L \times L$

$$\left.\frac{\partial U_s}{\partial T}\right|_{T=T_c} \approx a\,L^{1/\nu} \quad \Rightarrow \quad 1/\nu = 0.24 \pm 0.02$$

$$\left.m_s^2\right|_{T=T_c} \approx \mathcal{M}\,L^{-2\beta/\nu} \quad \Rightarrow \quad 2\beta/\nu = 0.257 \pm 0.006$$

$$\left.C\right|_{T=T_c} \approx \mathcal{C}\,L^{\alpha/\nu} \quad \Rightarrow \quad \alpha/\nu = 0.016 \pm 0.003$$

- Hyperscaling $\quad d\,\nu = 2 - \alpha \quad (d = 2) \quad$ strongly violated ???

Summary

- $J < 0$:
  - 120°-ordered low-temperature phase, $T_c = \mathcal{O}(|J|)$
  - hyperscaling strongly violated ???
- $J > 0$:
  - macroscopic classical groundstate degeneracy
  - order-by-disorder selection of another 120° state

References

[1] D.C. Cabra, M.D. Grynberg, P.C.W. Holdsworth, A. Honecker, P. Pujol, J. Richter, D. Schmalfuß, J. Schulenburg, Phys. Rev. B **71** (2005) 144420

[2] V. Subrahmanyam, Phys. Rev. B **52** (1995) 1133

[3] L. Santos, M.A. Baranov, J.I. Cirac, H.-U. Everts, H. Fehrmann, M. Lewenstein, Phys. Rev. Lett. **93** (2004) 030601

[4] B. Damski, H. Fehrmann, H.-U. Everts, M.A. Baranov, L. Santos, M. Lewenstein, Phys. Rev. A **72** (2005) 053612

[5] G.-B. Jo, J. Guzman, C.K. Thomas, P. Hosur, A. Vishwanath, D.M. Stamper-Kurn, Phys. Rev. Lett. **108** (2012) 045305

[6] B. Damski, H.-U. Everts, A. Honecker, H. Fehrmann, L. Santos, M. Lewenstein, Phys. Rev. Lett. **95** (2005) 060403

[7] K. Hukushima, K. Nemoto, J. Phys. Soc. Jpn. **65** (1996) 1604

[8] A. Honecker, D.C. Cabra, H.-U. Everts, P. Pujol, F. Stauffer, Phys. Rev. B **84** (2011) 224410

Acknowledgments

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