Fluctuation induced ordering on the kagome lattice

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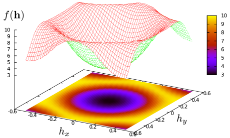


arxiv: 1207.4752

Outline

Order by disorder

- degeneracy and frustration
- zero, soft and hard modes

Phase diagram of KHAFM

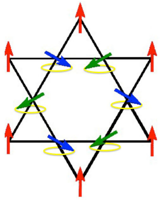
- coplanar order by disorder and dynamical symmetry
- numerical freezing

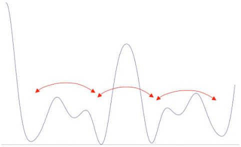
New algorithm

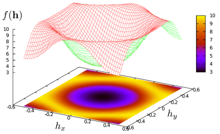
- stable low-T regime

Effective descriptions

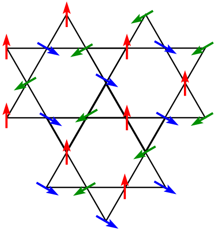
- effective Potts model
- two-component height model
  - ⇒ dipolar ordering via KT transition





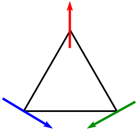


Frustration leads to degeneracy: kagome Heisenberg AFM



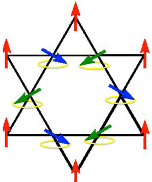
Kagome lattice = corner-sharing triangles

$$\mathcal{H} = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j = \frac{J}{2} \sum_{\alpha} \vec{\ell}_{\alpha}^{\,2}$$



$\Rightarrow$ Each triangle: $\vec{\ell}_{\alpha} = \vec{S}_{\alpha 1} + \vec{S}_{\alpha 2} + \vec{S}_{\alpha 3} = 0$

Triangle-based network: *local* "weathervane mode" at zero energy Chandra/Harris/Chalker et al. 1992



- local d.o.f.!
- extensive ground-state dimension of kagome magnet

Degeneracies are intrinsically unstable

Extensive ground-state degeneracy

- huge low-energy d.o.s.

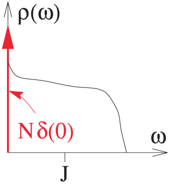
$\Rightarrow$any perturbation is strong!

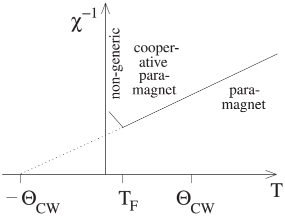
- subleading terms determine low-T behavior

Frustrated magnets have three regimes

- high-temperature paramagnet
- cooperative paramagnet ("universal")
- non-generic low-T

Θ_{cw}/T_F parametrises strength of frustration Obradors, Ramirez

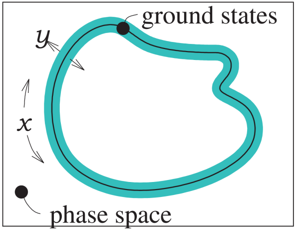


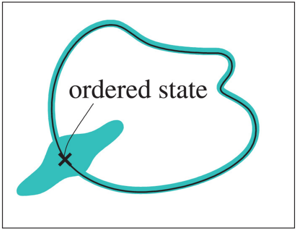


(Thermal) order by disorder

At $T > 0$, minimise $F = U - TS \approx -TS$

- maximise entropy!





Ordered states tend to have highest entropy!

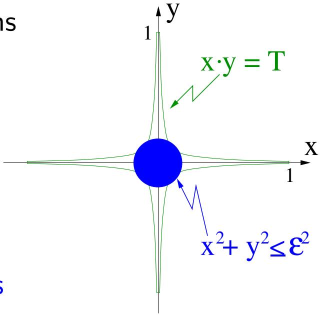
Example of obdo: $E = |x \cdot y|, \quad |x|, |y| \leq 1$

Ground states: $x = 0$ or $y = 0$

- can in principle explore both axes

Ground states weighted by fluctuations

$$\lim_{T \to 0} A_\epsilon / A_T \to 1!$$



$\Rightarrow$ System localised near origin

Mechanism: two 'soft' directions

- 'crossing' points of ground-states

Coplanar obdo in kagome Heisenberg AFM

All coplanar states have extensive number of soft (harmonic zero) modes! Chalker et al., 1992

- quadru-, octupolar order: $\langle e^{3i\Theta} \rangle$

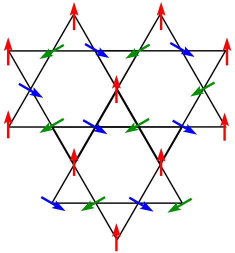
  Zhitomirsky 2008

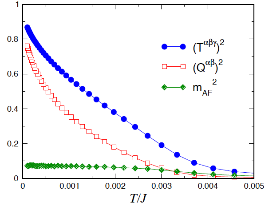
- perfect extensive degeneracy of free energy at harmonic level
- maps onto 3-state Potts model

  Huse + Rutenberg 90s

Order is cut off by T at exp. large distance

Mermin + Wagner





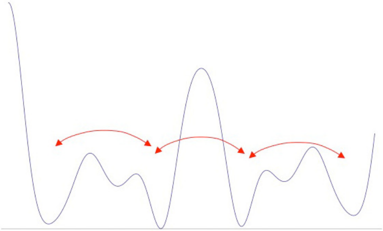
Any dipolar (spin) order at low T?

Analytics: unknown (purely anharmonic problem) Holdsworth + Shender

- unweighted coplanar Potts ensemble is critical Baxter

Numerics: unknown

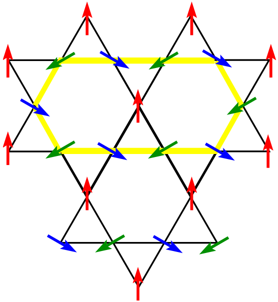
- algorithms freeze as coplanar obdo sets in Reimers, Huse+Rutenberg, . . . Zhitomirsky (1992-2012)
- not even small systems can be solved exactly



Cluster algorithm for Heisenberg model

Exploit dynamical symmetry: $\eta = \pm 1$ maps between coplanar states Hassan+R.M.

$$\begin{aligned} \dot{\ell}^1_\alpha + \dot{\ell}^2_\alpha &= \left(\eta S^2_{\alpha\beta}\right)\left(\eta \ell^3_\beta\right) - S^3_{\alpha\beta}\ell^2_\beta \quad , \\ \dot{\ell}^2_\alpha - \dot{\ell}^1_\alpha &= S^3_{\alpha\beta}\ell^1_\beta - \left(\eta S^1_{\alpha\beta}\right)\left(\eta \ell^3_\beta\right) \quad , \\ \left(\eta \dot{\ell}^3_\alpha\right) &= \left(\eta S^1_{\alpha\beta}\right)\ell^2_\beta - \left(\eta S^2_{\alpha\beta}\right)\ell^1_\beta \end{aligned}$$



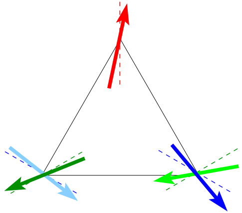
Conventional cluster algorithm fails

- small fluctuations around coplanar states

Write $\vec{S} = \vec{S}^{(0)} + \vec{s}$, cluster algo acts on $\vec{S}^{(0)}$: colour exchange around loop

- Boltzmann factor only for ‘anharmonic part’ $\vec{s}_i$

Can equilibrate systems with $O(10^3)$ spins for $T \to 0$.



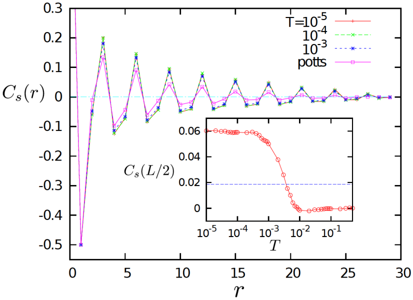
Low-T regime

Low-T regime reached for $T \lesssim 10^{-4} J$

- "entropic" Boltzmann factors: $\exp\left(-\frac{TS}{T}\right) = \exp(-S)$ is T-independent cf Henley

Enhanced correlations saturate

- thermodyn. limit still not reachable!

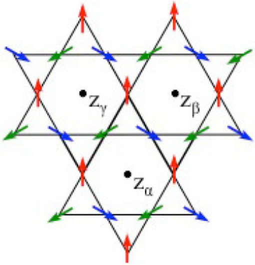


Effective model I: height model

Coplanar states map onto (2-component) Gaussian height model: Holdsworth + Shender

$$\vec{z}_\beta = \vec{z}_\alpha + \vec{S}_{\alpha\beta}$$

Harmonic (XY=Potts) problem at exactly solvable critical point Baxter; Huse+Rutenberg



Role of anharmonic fluctuations?

Height model basics

Rough phase ⇒ algebraic spin correlations

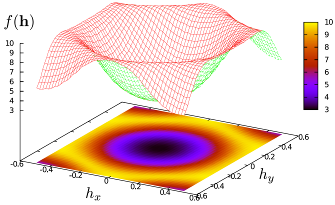
- Kosterlitz-Thouless physics

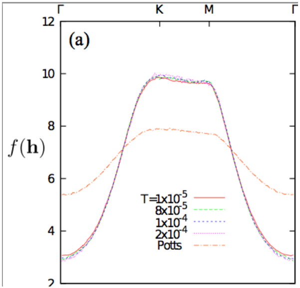
Flat phase ⇒ long-range order

- can classify all candidate orders

Height-space is periodic

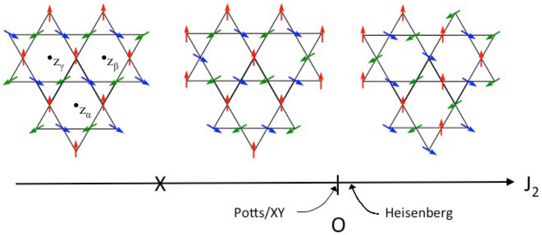
- histogram in unit cell ⇒ nature of ordering

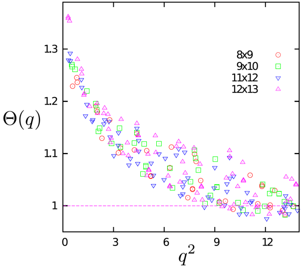




Enhanced stiffness $\Longrightarrow$ dipolar order

Gaussian model: $\mathcal{S} = \frac{K}{2} \int |\nabla z|^2 d^2 r$



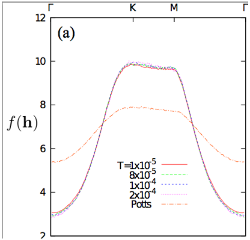


K grows upon inclusion of fluctuations? Yes!

$$\Theta(q) = \mathrm{K}_{\mathrm{H'berg}}/\mathrm{K}_{\mathrm{potts}} = \left|z_{\mathrm{potts}}(q)/z_{\mathrm{H'berg}}(q)\right|^2$$

Enhanced but weak maximum at Γ point suggests $\sqrt{3} \times \sqrt{3}$ order

- thermodynamic limit?

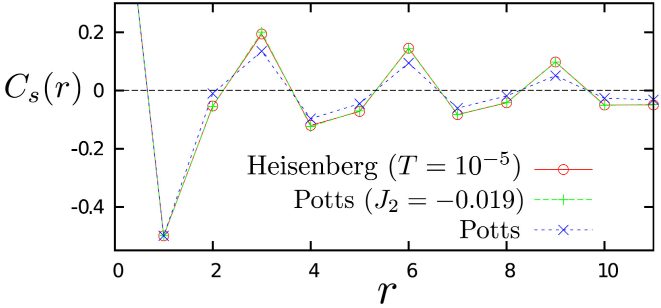


Effective model II: extended Potts model

Try to fit entropic weights by additional interaction

- simulate effective model

Single parameter $\mathcal{J}_2$ suffices: n.n.n. interactions only



$\mathcal{J}_2 \approx 0.019$ is quite small

Data collapse and KT transition

Can simulate up to 10^6 spins

- consider broader phase diagram

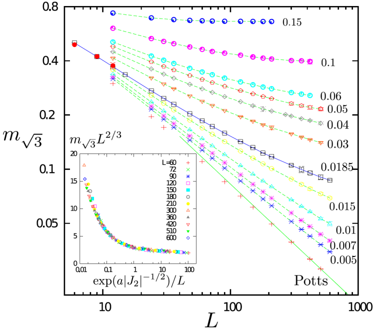
Data collapse for KT transition with $\mathcal{J}_2^c = 0$

- small ordered moment, $< 10\% m_{\mathrm{SAT}}$

Hard to discern because of long correlation length

- rather than smallness: cf. chirality
- further phase transitions?

Castelnovo *et al.*



The Heisenberg kagome afm

Complex instance of obdo

- harmonic: coplanar ('octupolar') order
- anharmonic: ('dipolar') spin order
- ordering is delicate
  - small $T = 0$ order parameter (classically!)
  - large crossover length

New efficient algorithm cf. Schnabel+Landau

- can access low-T regime

Effective field theory + Potts model

- access long wavelengths+large-scales

Beyond n.n. Heisenberg model

- semiclassics Henley; perturbations
- connection to experiment

Also: pyro. XY; hyperkagome/garnet; . . .