On the low-temperature behavior of a geometrically frustrated Heisenberg antiferromagnet

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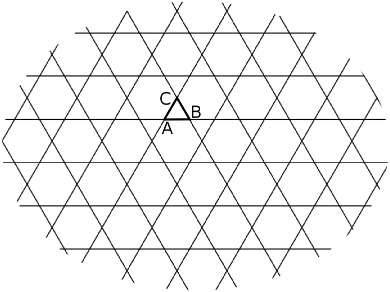
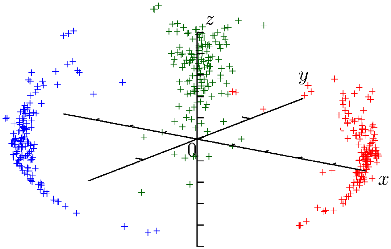
classical Heisenberg antiferromagnet

- $H = -J \sum_{\langle ij \rangle} \mathbf{S}_i \mathbf{S}_j$
- $J < 0$
- geometry induces frustration
- spin triangle has minimal energy if $\mathbf{S}_A + \mathbf{S}_B + \mathbf{S}_C = \mathbf{0}$ $(H_\Delta = \frac{1}{2}|\mathbf{S}_A + \mathbf{S}_B + \mathbf{S}_C|^2 - \frac{3}{2})$
- highly degenerate ground state



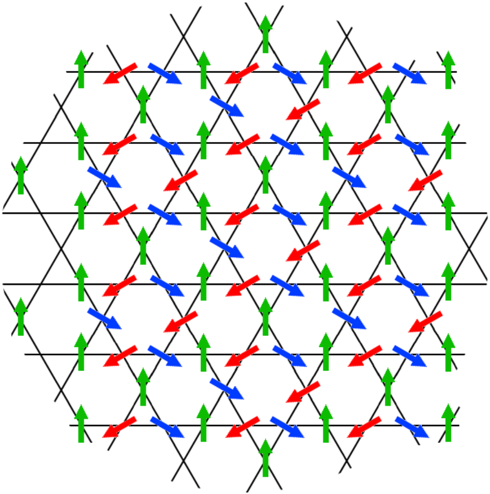
order by disorder

- at finite temperature coplanar state emerges, strong out-of-plane excitations possible $\rightarrow$ high entropy
- three basic spin directions
- similarity to three state Potts model
- further order?

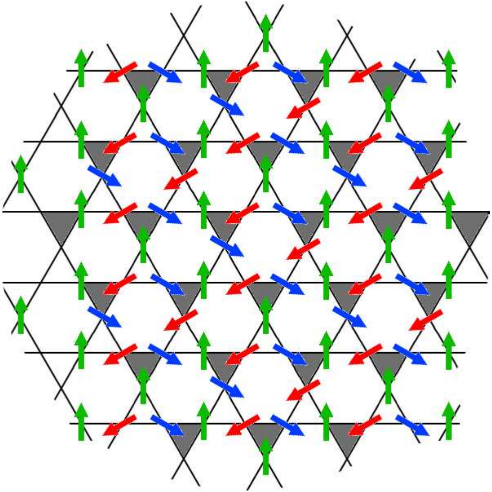


$\sqrt{3} \times \sqrt{3}$–state

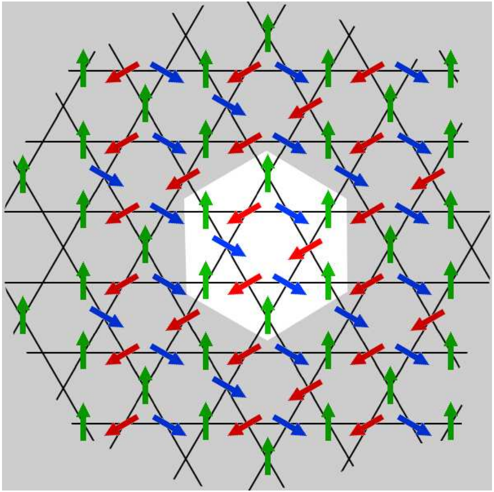
each hexagon a Weathervane loop



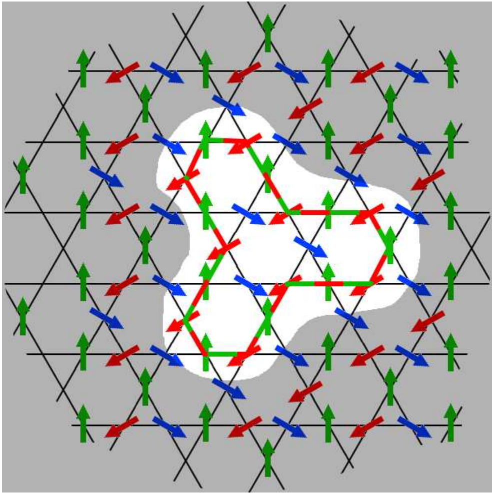
$\sqrt{3} \times \sqrt{3}$–state, chirality



Weathervane loop flips

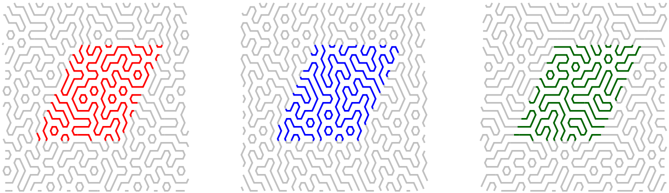


Weathervane loop flips

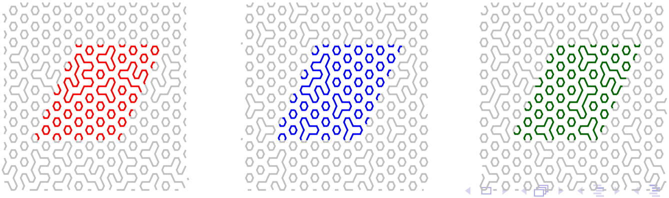


Weathervane loop structures

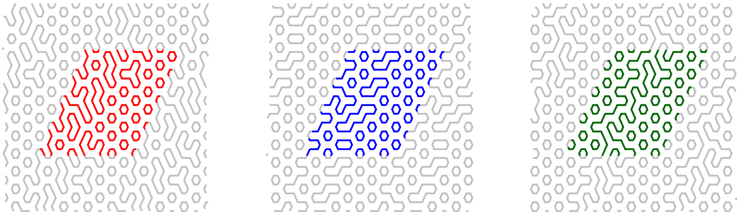
- smallest loop number (26):



- largest loop number (104):



infinite loop



simulated tempering

Combination of m canonical ensembles
Probability of conformation $\mathbf{z}$:

$$p(\mathbf{z}) = \frac{1}{m}\sum_{i=1}^{m} e^{f_i+c}\, e^{-\beta_i E(\mathbf{z})} \approx \frac{1}{m}\sum_{i=1}^{m} p_{\mathrm{can}}(\beta_i, \mathbf{z}).$$

Here, $m = 10000$ and $\log_{10}\beta_i$ are equally distributed in $[-3, 6]$.
Parameters f_i are tuned such that different temperatures are visited with equal frequency:

$$e^{-f_i-c} \approx Z(\beta_i) = \int_{\mathcal{Z}} d\mathbf{z}\, e^{-\beta_i E(\mathbf{z})},$$

$$\langle E\rangle(\beta) = \frac{df(\beta)}{d\beta} = -\frac{d\ln Z(\beta)}{d\beta}.$$

density of states $g(E)$

The probability of conformation $\mathbf{z}$

$$p(\mathbf{z}) \propto \sum_{i=1}^{m} e^{f_i} \, e^{-\beta_i E(\mathbf{z})},$$

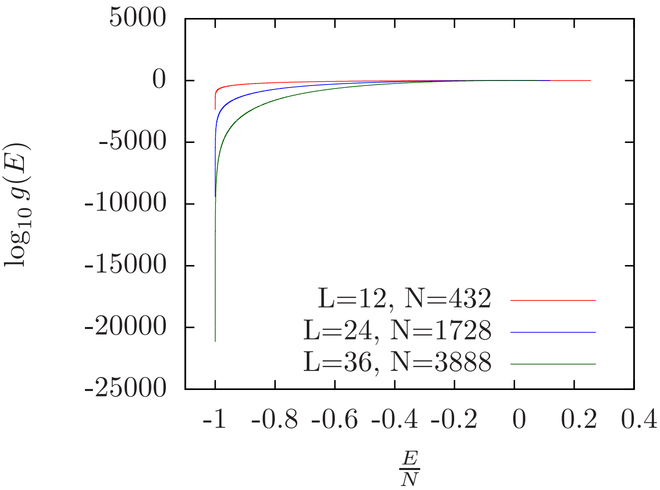
can be rewritten by replacing the sum with an energy dependent function $W(E)$,

$$p(\mathbf{z}) \propto W(E(\mathbf{z})), \qquad W(E) = \sum_{i=1}^{m} e^{f_i} \, e^{-\beta_i E},$$

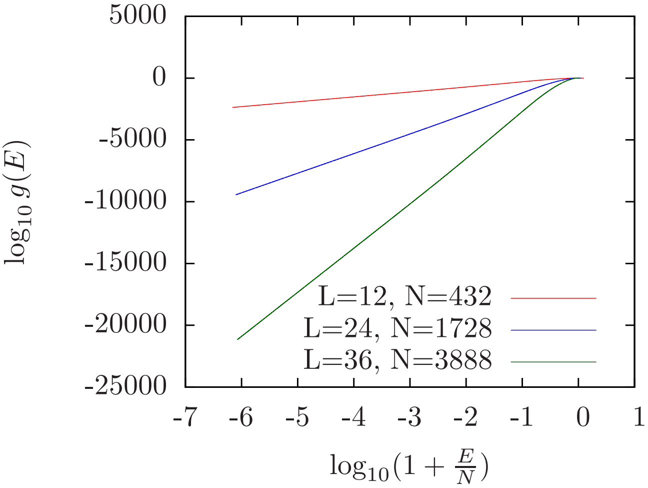
which allows access to density of states $g(E)$ via an overall histogram $H(E)$ (no multi-histogram reweighting):

$$\begin{aligned} P(E) &\propto W(E)g(E), \\ g(E) &\propto H(E)/W(E). \end{aligned}$$

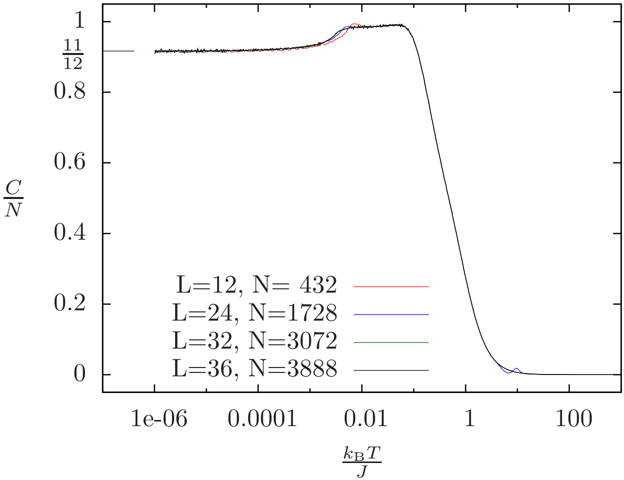
density of states $g(E)$



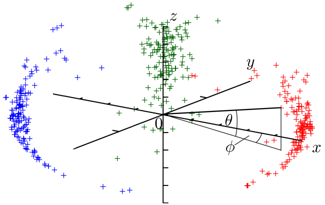
density of states $g(E)$

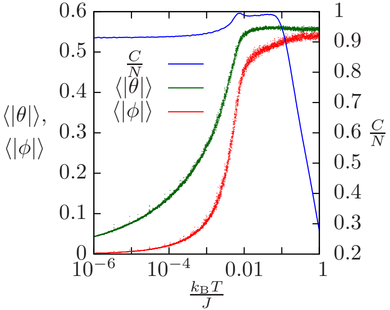


specific heat

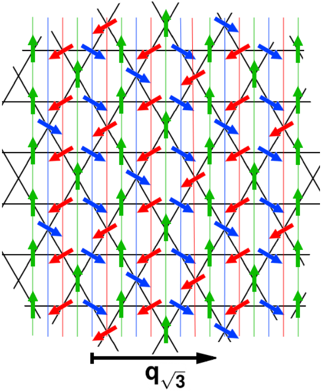


angular excitations, $L = 12$, $N = 432$





$\sqrt{3} \times \sqrt{3}$ correlation



$$\mathbf{q}_{\sqrt{3}} = (\frac{4}{3} \cdot 2\pi, 0, 0)^T$$

$$C'_{\sqrt{(3)}}(\mathbf{r}) = \frac{\langle \mathbf{S_0} \cdot \mathbf{S_r} \rangle}{\cos(\mathbf{q}_{\sqrt{3}} \cdot \mathbf{r})},$$

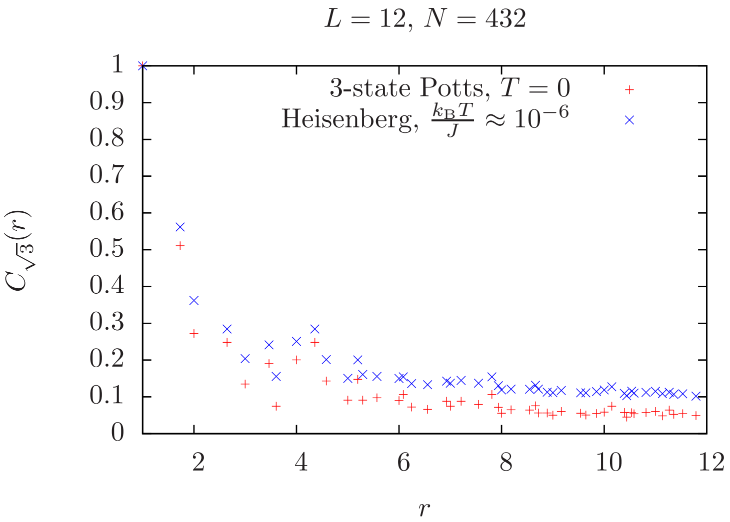
using directions $\sigma_{\mathbf{r}} \in \{1, 2, 3\}$ (projection on Potts-state):

$$C_{\sqrt{(3)}}(\mathbf{r}) = \frac{\langle \gamma_{\sigma_{\mathbf{0}}, \sigma_{\mathbf{r}}} \rangle}{\cos(\mathbf{q}_{\sqrt{3}} \cdot \mathbf{r})},$$

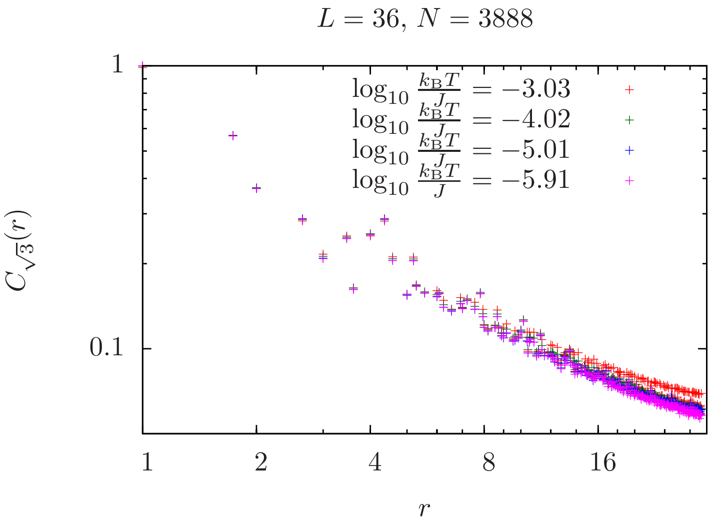
with

$$\gamma_{i,j} = \begin{cases} 1 & \text{if} \quad i = j, \\ -\frac{1}{2} & \text{else.} \end{cases}$$

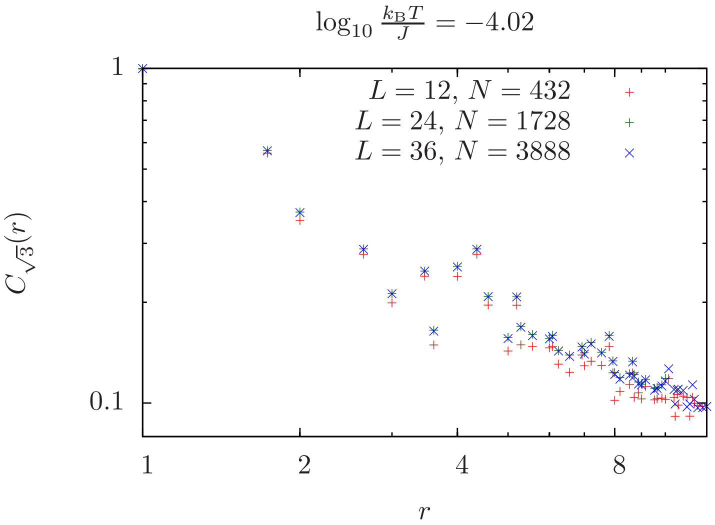
$\sqrt{3} \times \sqrt{3}$ correlation, Potts vs Heisenberg



$\sqrt{3} \times \sqrt{3}$ correlation, different temperatures



$\sqrt{3} \times \sqrt{3}$ correlation, different system sizes



conclusion

- In the coplanar state, the $\sqrt{3} \times \sqrt{3}$ correlations are widely independent of temperature and system size.
- The system will not attain the $\sqrt{3} \times \sqrt{3}$ state.

I thank you for the attention and the NSF for funding.