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

Stefan Schnabel, David P. Landau

CompPhys 2010
classical Heisenberg antiferromagnet

- \[ H = -J \sum_{\langle ij \rangle} S_i S_j \]
- \( J < 0 \)
- geometry induces frustration
- spin triangle has minimal energy if
  \[ S_A + S_B + S_C = 0 \]
  \[ (H_\Delta = \frac{1}{2} |S_A + S_B + S_C|^2 - \frac{3}{2}) \]
- highly degenerate ground state
order by disorder

- at finite temperature coplanar state emerges, strong out-of-plane excitations possible → 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 $\mathbf{z}$:

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

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:

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

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

The probability of conformation $z$

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

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

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

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

$$P(E) \propto W(E)g(E),$$
$$g(E) \propto H(E)/W(E).$$
density of states $g(E)$

\[
\log_{10} g(E)
\]

$L=12, N=432$
$L=24, N=1728$
$L=36, N=3888$
density of states $g(E)$

\[ \log_{10} g(E) = \log_{10} \left(1 + \frac{E}{N} \right) \]

- $L=12, N=432$
- $L=24, N=1728$
- $L=36, N=3888$
specific heat

$L=12, N=432$
$L=24, N=1728$
$L=32, N=3072$
$L=36, N=3888$
angular excitations, $L = 12, N = 432$
$\sqrt{3} \times \sqrt{3}$ correlation

$$q_{\sqrt{3}} = \left( \frac{4}{3} \cdot 2\pi, 0, 0 \right)^T$$

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

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

$$C_{\sqrt{3}}(r) = \frac{\langle \gamma_{\sigma_0, \sigma_r} \rangle}{\cos(q_{\sqrt{3}} \cdot r)},$$

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

$L = 12, \, N = 432$

3-state Potts, $T = 0$

Heisenberg, $\frac{k_B T}{J} \approx 10^{-6}$
\( \sqrt{3} \times \sqrt{3} \) correlation, different temperatures

\[ L = 36, \quad N = 3888 \]

\[
\log_{10} \frac{k_B T}{J} = -3.03 \\
\log_{10} \frac{k_B T}{J} = -4.02 \\
\log_{10} \frac{k_B T}{J} = -5.01 \\
\log_{10} \frac{k_B T}{J} = -5.91
\]
\[ \log_{10} \frac{k_B T}{J} = -4.02 \]

- \( L = 12, N = 432 \)
- \( L = 24, N = 1728 \)
- \( L = 36, N = 3888 \)
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.