Phase transitions in long-range spin models
Transitions de phase dans les systèmes de spins régis par des interactions à longue portée

Sylvain Reynal
Laboratoire de Physique Théorique & Modélisation (UMR 8089)
CNRS/Université de Cergy-Pontoise
E.N.S.E.A.
Models: phase diagram of classical spin models with a long-range potential
- $Q$-state Potts model (controversies reexamined, crossovers)
- Random-Field Ising model (first numerical study)

Methods: multicanonical ensemble algorithms
- Multicanonical algorithm with single-spin updates (tailored to long-range potentials)
- Spinodal method (detection of the order of phase transitions)
- Breathing cluster method (extends the range of attainable lattice sizes)
I. Long-range Potts model: controversies and summary of the results of the thesis

II. The Multicanonical method

III. Spinodal method and phase diagram of the LR Potts model

IV. Breathing clusters: rationale, performance, and results
I. Long-range Potts chain
\begin{align*}
\mathbf{s}_i &= 1 \ldots q \\
H &= \sum_{i>j} J(|i-j|) \delta_{s_i, s_j}
\end{align*}

- Algebraically decaying ferromagnetic potential:

\[ J(|i-j|) = \frac{-1}{|i-j|^{1+\sigma}} \]

- \( \sigma \) is an adjustable decay parameter of the interaction, akin to an \textit{effective dimension}.

- Ordered phase: condensation in one of \( q \) phases.
In condensed matter physics:
- Systems with Van der Waals forces, Casimir effect.
- Kondo effect: $1/r^2$ interactions
- Spin glasses: RKKY interaction $r^{-D} \cos(k_0 r + \phi)$
- Thin magnetic films

In connected fields:
- Neural networks, small-world networks.
- Spreading epidemics and Lévy flights
- Tsallis generalized thermodynamics
I. LR Potts model
Modelling
Open questions
Addressed issues
Results

II. Multicanonical ensemble
Markov chains
Supercritical SD
Multicanonical weights
III. Spinodals
Spinodals points
Inverse-square interactions
Unusual FSS
IV. Breathing clusters
Single-spin vs clusters
Cluster construction
FFT
Accuracy
2D NN Potts
Surface tension
V. Conclusion

Phase transitions in long-range spin models
Sylvain Reynal

Phase diagram: open questions and controversies

- 1st order
- 2nd order
- short-range
- topological

Krech, Luijten
Glumac, Uzelac
Bayong et al.
Cardy
Phase diagram: addressed issues

Position of boundary $\sigma_c(q)$ between 1st and 2nd order regimes

- Krech/Luijten, Glumac/Uzelac: standard Monte Carlo (cluster, histogramming)
Nature of the transition at $\sigma = 1.0$: topological vs first-order?

- Cardy: topological transition
- Bayong et al.

- Cardy: renormalization of kink-gas model
- Bayong: single-histogram Monte Carlo
Phase diagram: addressed issues

Cross-over from LR to SR behavior

- Sak, Theumann/Gusmao: renormalization group ($\sigma_{co} = 1$)
Phase transitions in long-range spin models

Sylvain Reynal

Results

1. LR Potts model

Modelling

Open questions

Addressed issues

Results

II. Multicanonical ensemble

Markov chains

Supercritical SD

Multicanonical weights

III. Spinodals

Spinodals points

Inverse-square interactions

Unusual FSS

IV. Breathing clusters

Single-spin vs clusters

Cluster construction

FFT

Accuracy

2D NN Potts

Surface tension

V. Conclusion

Phase transitions in long-range spin models

- Phase diagram refined to two-digit accuracy
- Transition at $\sigma = 1.0$ is not of the first-order (unusual finite-size effect)
- Crossover SR/LR inside a narrow window $[1.0, 1.1]$.
- Methods: multicanonical ensemble + spinodal points.
II. Multicanonical ensemble
Markov chains and detailed balance

- Generate a Markov chain of configurations \( \{\sigma_1, \sigma_2, \ldots \} \) using a transition probability \( W(i \rightarrow f) \) from \( \sigma_i \) to \( \sigma_f \)
- Detailed balance for an equilibrium distribution \( w_i \):
  \[
  w_i W(i \rightarrow f) = w_f W(f \rightarrow i)
  \]

In the canonical ensemble:
  \[
  w_i = w(E_i) = e^{-\beta E_i}
  \]
  \[
  W(i \rightarrow f) = \min \left( 1, e^{\beta (E_i - E_f)} \right)
  \]

Limitations of canonical algorithms
- Supercritical slowing down at first-order transitions
- Reweighting procedure cumbersome.
Supercritical slowing down at first-order transitions

I. LR Potts model
   Modelling
   Open questions
   Addressed issues
   Results

II. Multicanonical ensemble
   Markov chains
   Supercritical SD
   Multicanonical weights
   III. Spinodals
   Spinodals points
   Inverse-square interactions
   Unusual FSS

IV. Breathing clusters
   Single-spin vs clusters
   Cluster construction
   FFT
   Accuracy
   2D NN Potts
   Surface tension
   V. Conclusion

Phase transitions in long-range spin models Sylvain Reynal
The surface tension $\Delta F$ increases with the lattice size $L$ and shows exponential suppression of mixed-phase configurations.
Multicanonical weights: algorithm

Overcome supercritical slowing down:
- Enhance rare events
- Reduce tunneling times from $\tau \sim e^{aL^b}$ to $\tau \sim L^z$ (Berg, Neuhaus)

Algorithm:
- Compute density of states $n(E)$ iteratively: Berg-Neuhaus’s, Wang-Landau’s or transition matrix schemes
- Feed the Markov chain with $w(E) \sim 1/n(E) = e^{-S(E)}$
- Thus sample a flat energy distribution: random walk in energy space
- Accept single-spin updates with a rate

$$W_{i \rightarrow f} = \min(1, e^{S(E_i) - S(E_f)})$$
Multicanonical weights: algorithm

\[ \beta(E) = \frac{dS(E)}{dE} \]

\[ \beta_c E \]

\[ E_i \quad E_f \]
Random walk in energy space

Canonical histogram @ $T = T_c$

Multicanonical histogram
Reweighting of thermodynamic averages

Goal: obtain thermodynamic averages as continuous functions of the temperature.

Energy distribution:

\[ N(E) \]

\( \beta_0 \) \hspace{1cm} \beta

reweighthed \hspace{1cm} sampled (multicanonical)

sampled (canonical at \( \beta \))
Compute free energy over a large range of energy and temperature, thus yielding reliable estimates of metastability temperatures.

- Temperatures of metastability form the basis of the spinodal method exposed in the following.
- We have $T_2 \rightarrow T_1$ as the first-order transition weakens.
III. Detecting the order of phase transitions: the spinodal method
Issue: weakening of the transition

- As boundary is approached \((\sigma \to \sigma_c^- (q))\), cluster sizes diverge: transition weakens.
- Traditional estimators \((\Delta F, \text{Binder cumulants})\) fail: tend too *smoothly* to their limit value
- Need distinct indicator: ratio of spinodals points
Weakening of the first-order transition

Assume FSS holds also for metastability temperatures:

$$T_2(L) - T_2(\infty) \propto 1/L + O(1/L^2).$$

Metastability temperatures $T_1$ and $T_2$ (spinodal points) merge into $T_c$ as $\sigma \to \sigma_c$

Yet $T_2 - T_1$ is not a good estimator.
A polynomial fit to infinite-size temperatures yields $\sigma_c(3) = 0.72(1)$.

- Ratio $T_2/T_c$ has a negative curvature
- Higher slope at $\sigma_c$ yields higher precision
\( \sigma = 1.0 \): controversy over the nature of the transition

- Topological transitions on the whole line (Cardy)
- \( \sigma_c(q) \) crosses at \( q = 8 \) (Bayong)
- Transition at \( \sigma = 1.0 \) is not of the first-order by virtue of an unusual finite-size effect.
\( \sigma = 1.0: \) unusual finite-size effect

- Transition appears discontinuous already for \( L < 400 \).
- FSS shows that it is continuous in the thermodynamic limit.
Interpretation in terms of the **truncation** of the LR potential due to the finite lattice size:

- **Artificially** enhances the rigidity of the spin array at small lattice sizes.
- "Pulls" the model towards the boundary line $\sigma_c(q)$

\[ J(r) \]

\[ r \]

\[ L_1 \]

\[ L_2 \]

\[ \sigma = 1.0: \text{unusual finite-size effect} \]
Spinodal points method offers a drastic refinement of the position of the boundary line an unprecedented range of $q$ and $\sigma$ values.

Detailed FSS analysis at $\sigma = 1.0$ lends support to Cardy’s scenario (topological transitions along the whole line).

Crossover SR/LR over a narrow window $[1.0, 1.1]$
IV. Breathing clusters
Multicanonical single-spin update implementations suffer from:

- in the case of LR models, an additional $O(N^2)$ complexity stemming from the (mandatory) computation of the energy at each MC step.
- non-optimal dynamic exponents $z$.

Why is it interesting to combine clusters and multicanonical?

- Clusters: improved dynamic performance
- We will show: cuts down the algorithmic complexity
**Goals:** Cut down algorithm complexity from $O(N^2)$ to $O(N \log N)$ for Long-Ranged (LR) spin models.
**Goals:** Cut down algorithm complexity from $O(N^2)$ to $O(N \log N)$ for Long-Ranged (LR) spin models.

**Diagram:**
- $t_{CPU}(\mu s)$ vs $\log_2(L)$
- Lines for $q = 12$, $q = 6$, and $q = 3$
- Local-update and collect-update markers

**Graph:**
- Axes: $\log_2(L)$ on the x-axis, $t_{CPU}(\mu s)$ on the y-axis
- Data points for different $q$ values and update methods

**Text:**
- **Goals**: Cut down algorithm complexity from $O(N^2)$ to $O(N \log N)$ for Long-Ranged (LR) spin models.
- **Diagram**: Shows the CPU time ($t_{CPU}$) in microseconds ($\mu s$) as a function of the logarithm of the system size ($\log_2(L)$). The graph includes lines for different interaction strengths ($q$) and markers for local-update and collect-update methods.
Breathing clusters: dynamic characteristics

Reduce dynamic exponents to their ideal value $\tau \sim D$.

<table>
<thead>
<tr>
<th>$q$</th>
<th>6</th>
<th>$\sigma$</th>
<th>0.7</th>
<th>$z_{\text{loc}}$</th>
<th>1.35(3)</th>
<th>$z_{\text{col}}$</th>
<th>1.05(1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>0.4</td>
<td></td>
<td></td>
<td>1.13(2)</td>
<td></td>
<td>0.89(1)</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>0.6</td>
<td></td>
<td></td>
<td>1.48(2)</td>
<td></td>
<td>1.11(1)</td>
<td></td>
</tr>
</tbody>
</table>

![Graph showing tunneling times and dynamic exponents](image_url)

- $q = 6$, $\sigma = 0.7$
- $q = 3$, $\sigma = 0.4$
- $q = 3$, $\sigma = 0.6$

- local-update
- collec.-update
Main impediment to a combination of both algorithm:
- Clusters need (i) symmetries in $H$ (ii) a temperature;
- Multicanonical weights lose track of both: $w(E) = 1 / n(E)$

How do we meet the issue?
- Cluster construction driven by the microcanonical temperature
- Rewrite the multicanonical weight as $w(E) = \phi(E)e^{-\beta(E)E}$
- Yet acceptance rate no longer equal to 1!
Invoke the Fortuin-Kasteleyn representation and rewrite \( w(E) \) as

\[
    w(E) = \phi(E) \sum_{\substack{\sigma_i, \sigma_j \in \{0,1\} \ \delta_{b_{ij},1} + \delta_{b_{ij},0}}}
    \prod_{i<j} p_{ij}(E) \delta_{\sigma_i,\sigma_j}.
\]

with \( p_{ij}(E) = e^{\beta(E)J(|i-j|)} - 1 \).
Cluster construction

**Algorithm**

1. Activate a bond with probability
   \[ \pi_a(i, j) = 1 - e^{-\beta(E_a) J(|i-j|)}. \]

2. Identify clusters of connected spins, and draw a new spin value at random for each cluster.

3. Accept the attempted cluster flips with probability
   \[ W_{flip}(a \rightarrow b) = \min \left( 1, \frac{\phi(E_b)}{\phi(E_a)} \prod_{l>1} \left[ \frac{p_l(E_b)}{p_l(E_a)} \right]^{B(l)} \right), \]
   where \( B(l) = \text{number of bonds of length } l = |j-i|. \)

**Note:** there exists an efficient algorithm for building clusters in \( O(N) \) operations (Luijten-Blöte): still usable here!
At first order in $\epsilon = E_b - E_a$, we have

$$1 - \langle W_{flip} \rangle (E_a) \sim |\beta'(E_a)| \epsilon$$

→ high acceptance rate in the region of phase coexistence.
Efficient computation of the lattice energy

- Computing $E_b$ represents another $O(N^2)$ burden
- This is reduced to $O(N \ln N)$ using an FFT implementation of the convolution theorem
  \[ H = -\frac{1}{2N} \sum_{k=0}^{N-1} \tilde{J}(k) \tilde{S}(k) \cdot \tilde{S}(-k) \]
- With a cluster-update scheme, only $O(N \ln N)$ operations are needed to update the whole lattice (as against $O(N^2)$ for single-spin updates)
Breathing clusters: accuracy

Lower statistical error on the computation of the density of states
Tunneling times and dynamic exponents

<table>
<thead>
<tr>
<th>$Q$</th>
<th>$z_{\text{loc}}$</th>
<th>$z_{\text{col}}$</th>
<th>$z_{\text{mubo}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>2.60(4)</td>
<td>1.82(2)</td>
<td>1.84</td>
</tr>
<tr>
<td>10</td>
<td>2.87(4)</td>
<td>2.23(1)</td>
<td>2.1</td>
</tr>
</tbody>
</table>

Finite-size temperatures:

For $Q = 10$, $T_c(\infty) = 0.70123(6)$

For $Q = 7$, $T_c(\infty) = 0.701232 \ldots$
Numerical results for the LR Potts chain

Finite-size temperatures

- $kT_1 = 1.6769(4)$
- $kT_c = 1.6877(2)$
- $kT_2 = 1.6926(2)$

$T_c(C_v) = 1.68764(1)$
$T_c(\chi) = 1.68765(2)$
Numerical results for the LR Potts chain

FSS behavior of the surface tension: fractal?

\[ \Delta F \propto L^\alpha \text{, with } \alpha(\sigma). \]

(reminder: \( \Delta F \propto L^{D-1} \) for SR models)
V. Conclusion
Conclusion

Method:

- Data analysis: spinodal method → follow the position of spinodal points + select the appropriate quantity ($T_2/T_c$) which yields the highest accuracy.

- Breathing cluster:
  1. Dramatically extends the range of attainable lattice sizes
  2. Better statistical quality
  3. Versatile (short-range models, transition matrix)
Model
- Long-range Random-field Ising model: first numerical study; controversy SR model (tricritical line).
- Fractal geometry of interface between phases

Method
- Combination with Optimized Ensemble (disordered models)