

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

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E.N.S.E.A.

Organization of the thesis

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

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)

Organization of the talk

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

- 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. 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

I. Long-range Potts chain

Long-Range Q-state Potts Chain

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

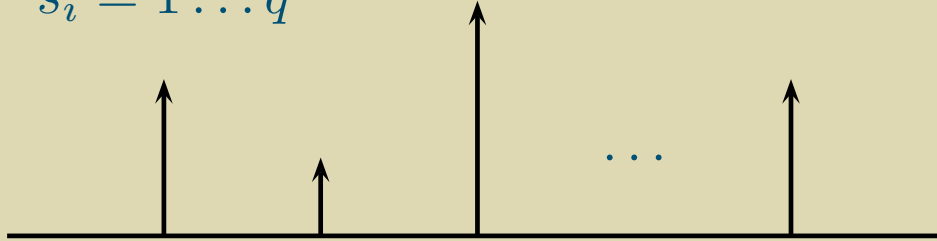
Accuracy

2D NN Potts

Surface tension

V. Conclusion

$$s_i = 1 \dots q$$



$$H = \sum_{i>j} J(|i-j|) \delta_{s_i, s_j}$$

- Algebraically decaying ferromagnetic potential:

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

- σ is an adjustable decay parameter of the interaction, akin to an *effective dimension*.
- Ordered phase: condensation in one of q phases.

LR spin models in microscopic modelling

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

In condensed matter physics:

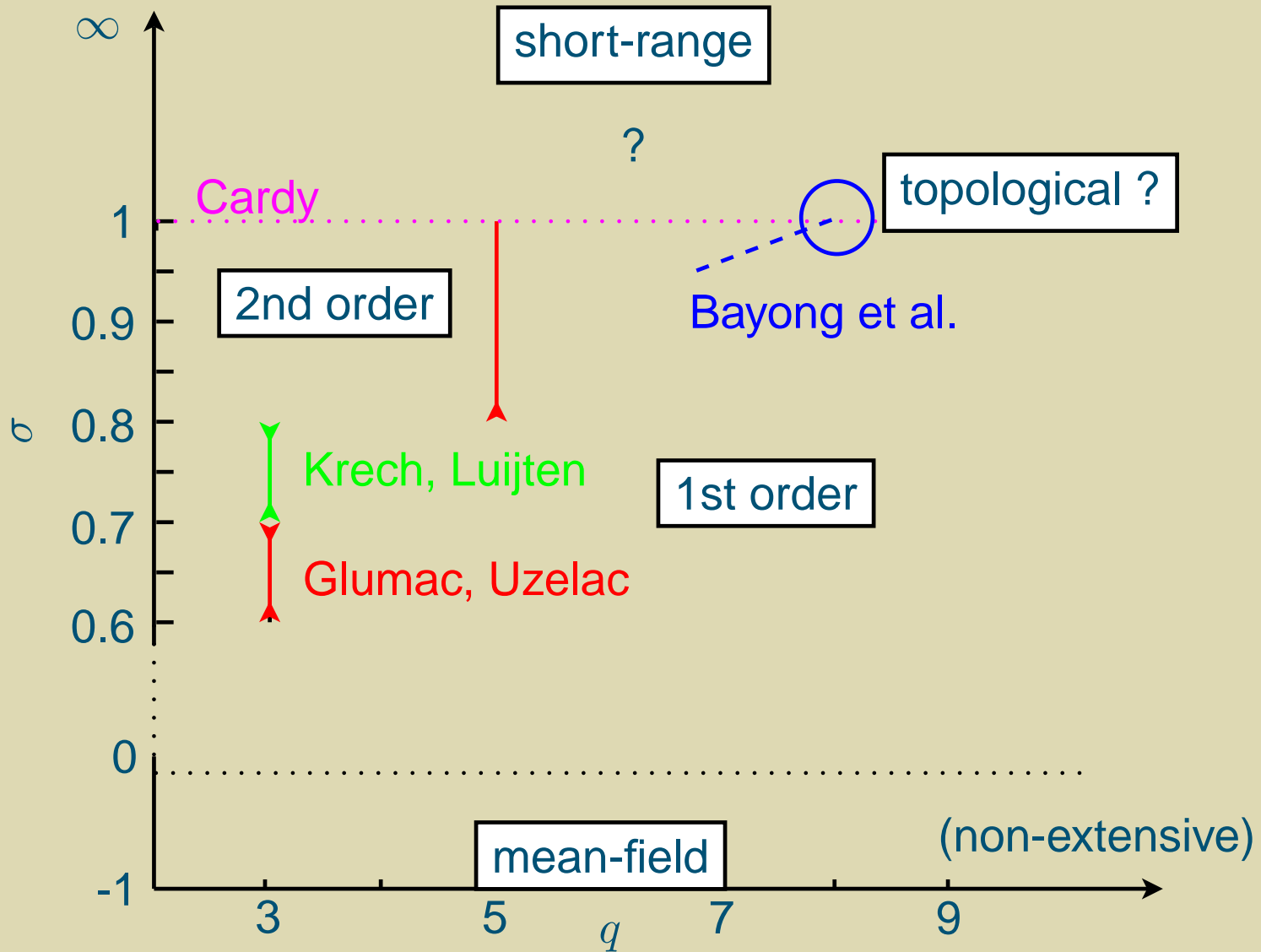
- Systems with Van der Waals forces, Casimir effect.
- Kondo effect: $1/r^2$ interactions
- Spin glasses: RKKY interaction $r^{-D} \cos(k_0 r + \phi)$
- Thin magnetic films

In connected fields:

- Neural networks, small-world networks.
- Spreading epidemics and Lévy flights
- Tsallis generalized thermodynamics

Phase diagram: open questions and controversies

- 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 diagram: addressed issues

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

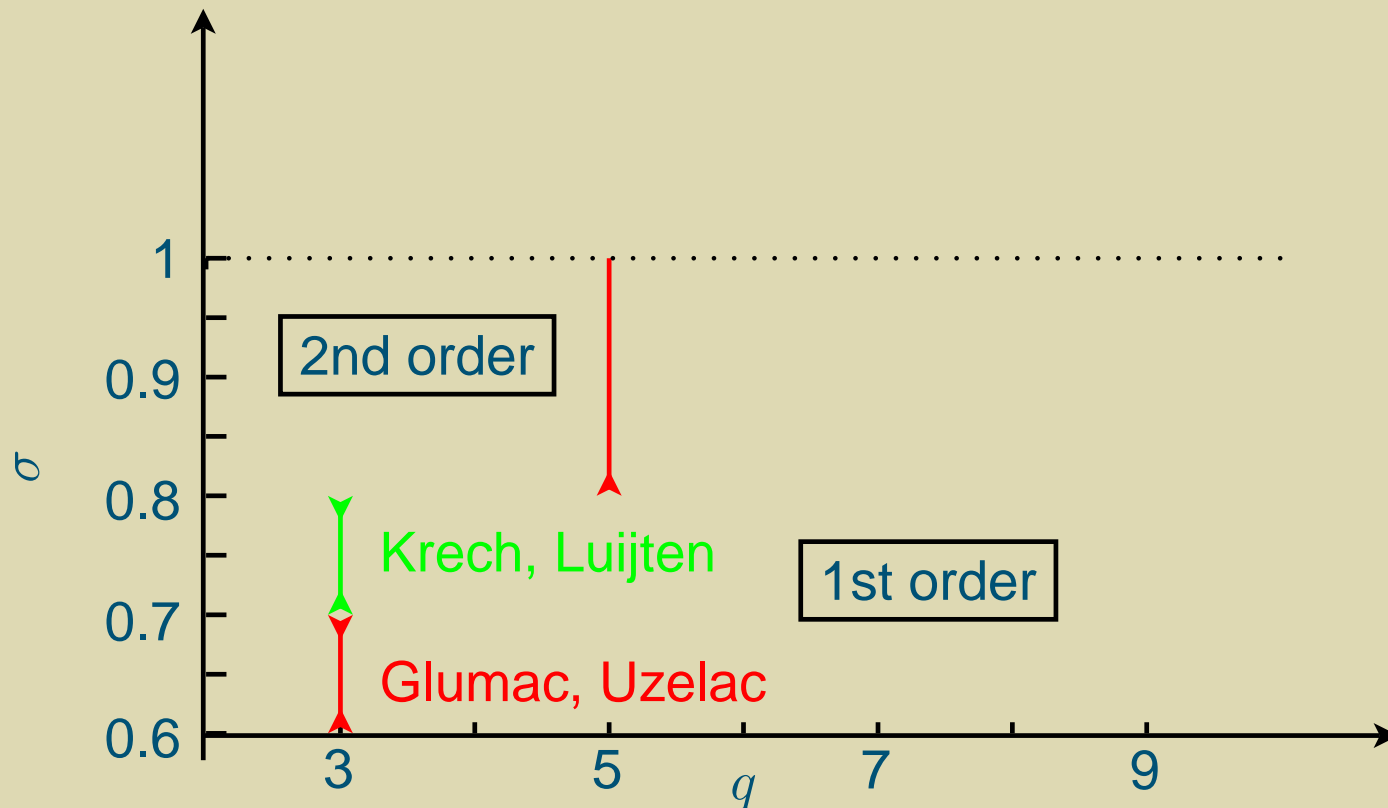
Accuracy

2D NN Potts

Surface tension

V. Conclusion

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



- Krech/Luijten, Glumac/Uzelac: standard Monte Carlo (cluster, histogramming)

Phase diagram: addressed issues

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

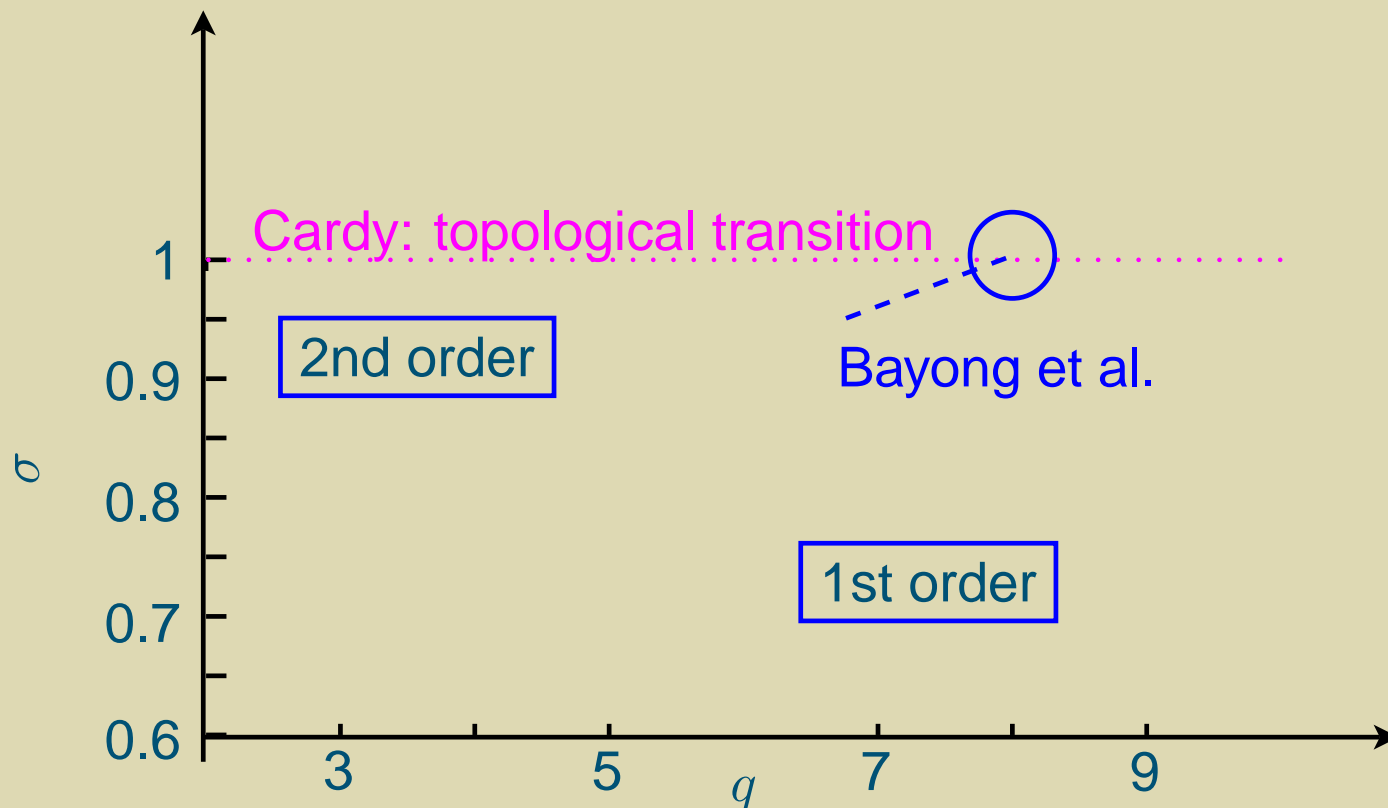
Accuracy

2D NN Potts

Surface tension

V. Conclusion

Nature of the transition at $\sigma = 1.0$: topological vs first-order?



- Cardy: renormalization of kink-gas model
- Bayong: single-histogram Monte Carlo

Phase diagram: addressed issues

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

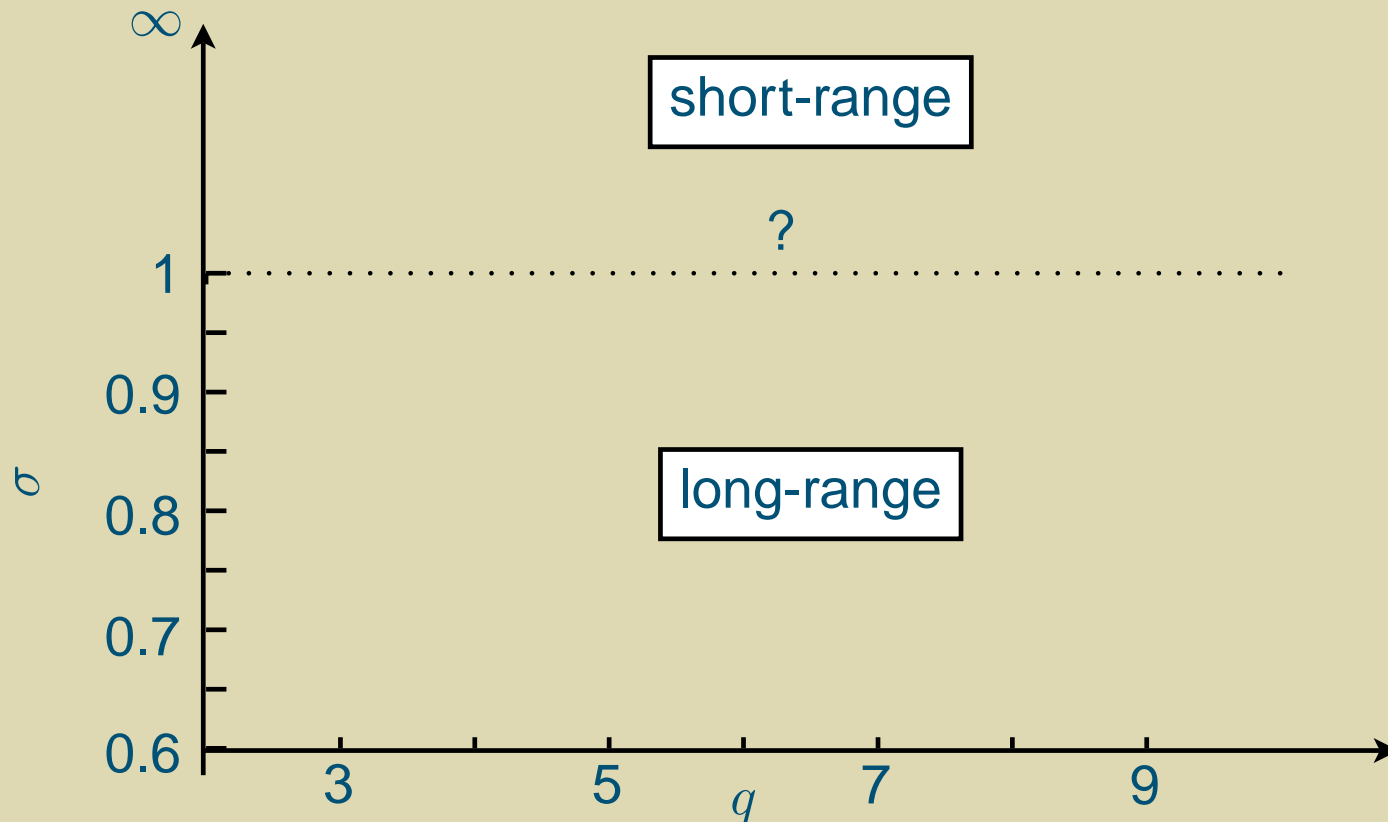
Accuracy

2D NN Potts

Surface tension

V. Conclusion

Cross-over from LR to SR behavior



- Sak, Theumann/Gusmao: renormalization group ($\sigma_{co} = 1$)

Results

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

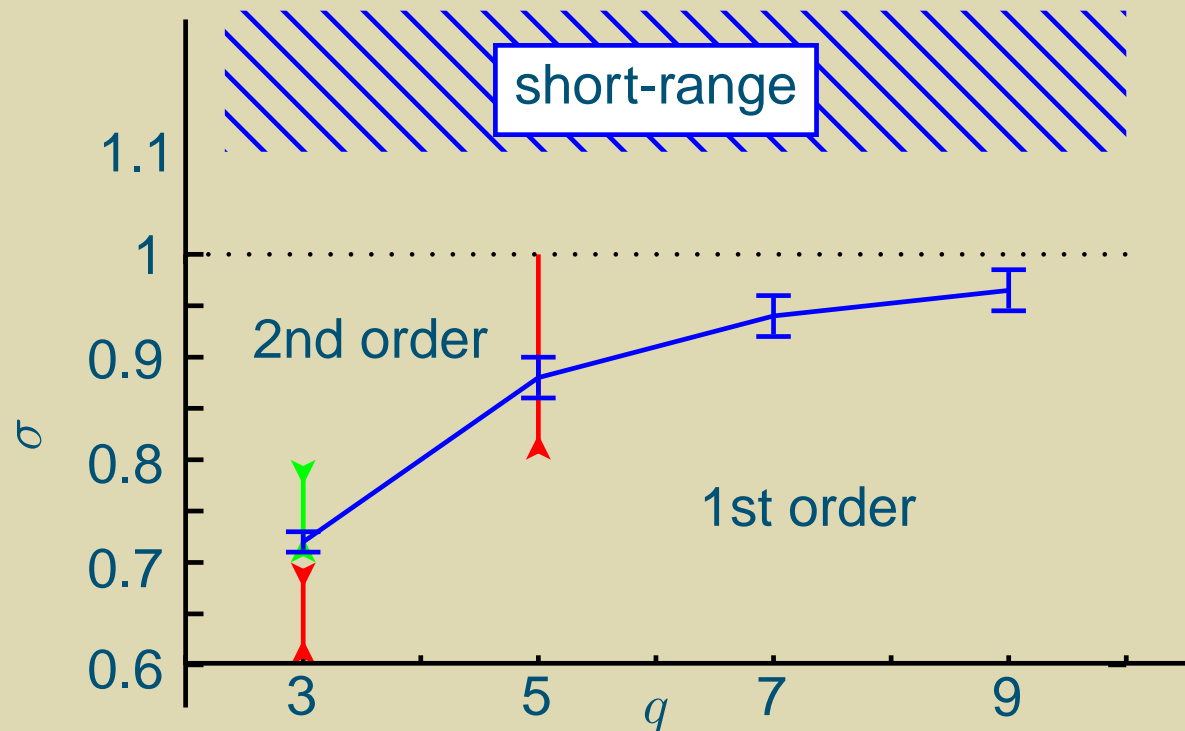
FFT

Accuracy

2D NN Potts

Surface tension

V. Conclusion



- Phase 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.

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

II. Multicanonical ensemble

Markov chains and detailed balance

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

- Generate a Markov chain of configurations $\{\sigma_1, \sigma_2, \dots\}$ using a transition probability $W(i \rightarrow f)$ from σ_i to σ_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

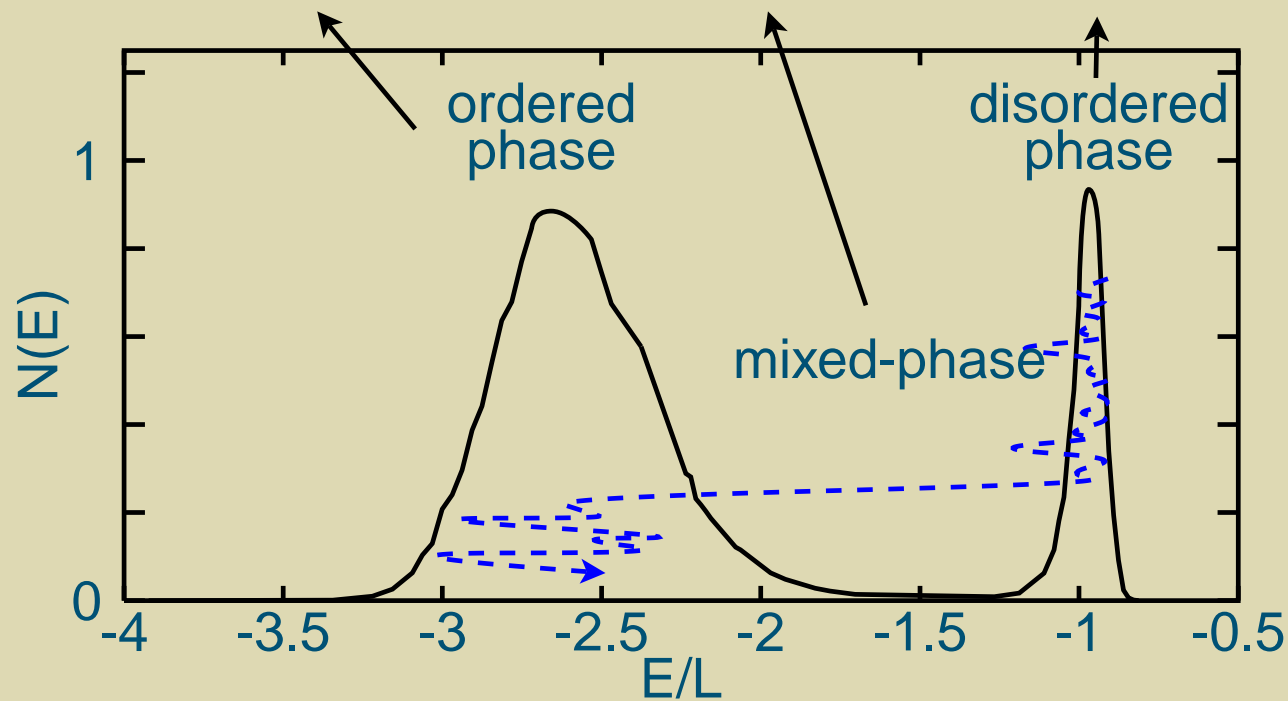
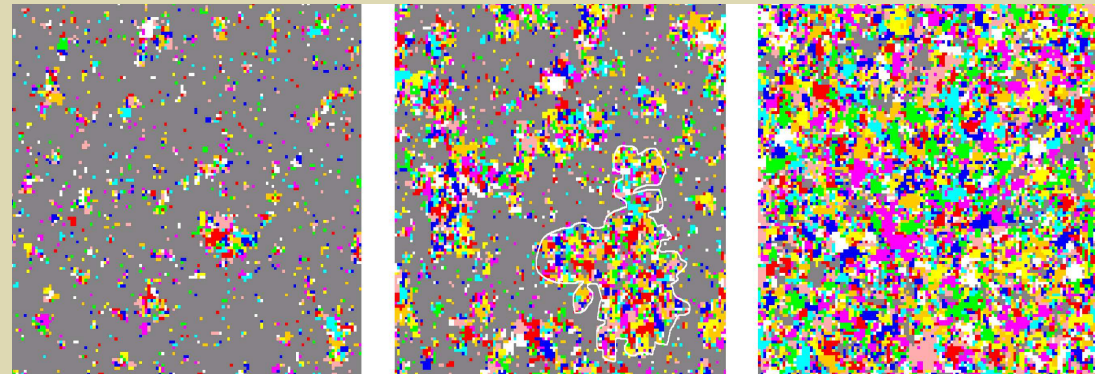
FFT

Accuracy

2D NN Potts

Surface tension

V. Conclusion



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

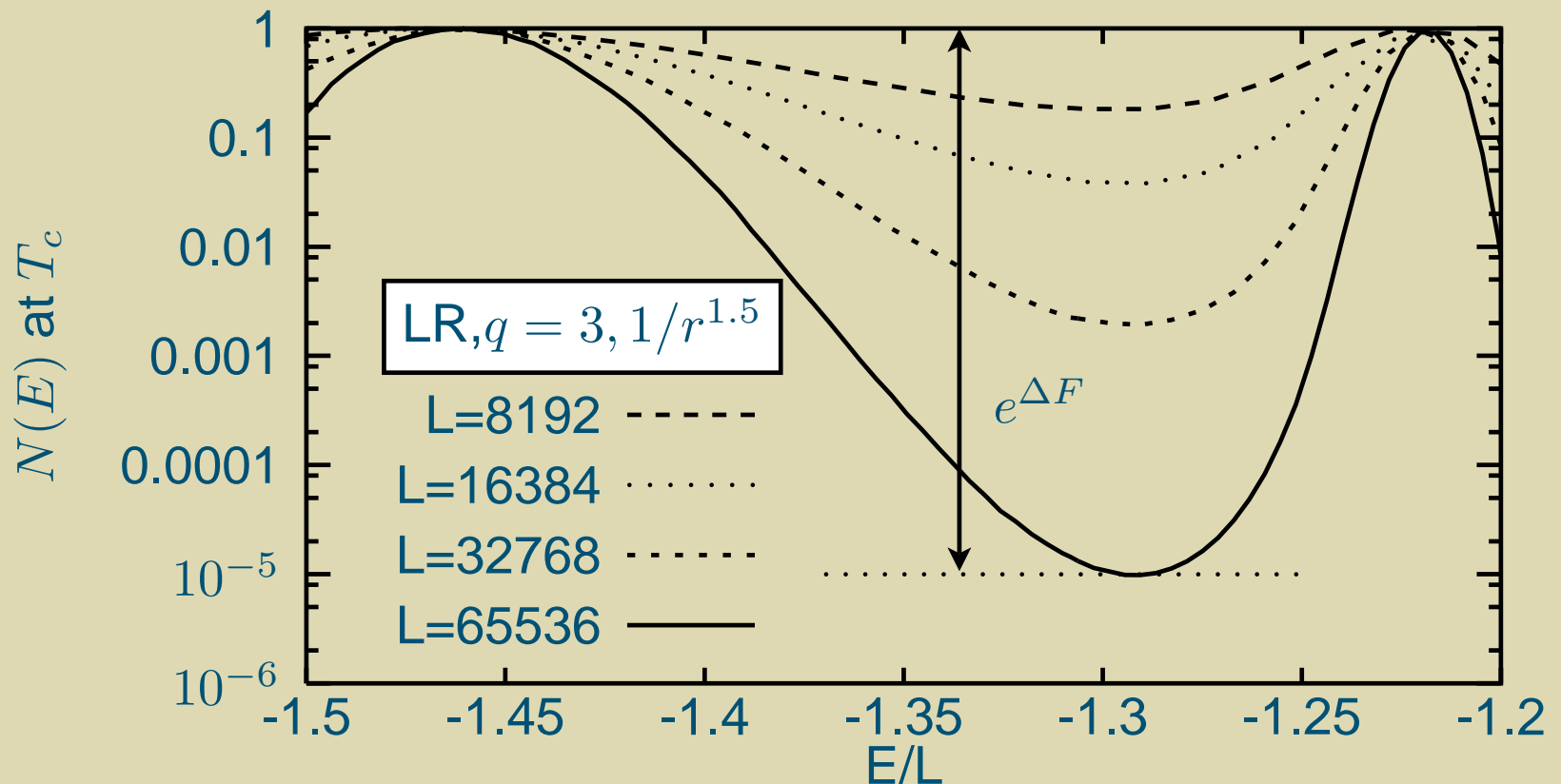
Accuracy

2D NN Potts

Surface tension

V. Conclusion

The surface tension ΔF increases with the lattice size
→ exponential suppression of mixed-phase configurations.



Multicanonical weights: algorithm

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

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

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

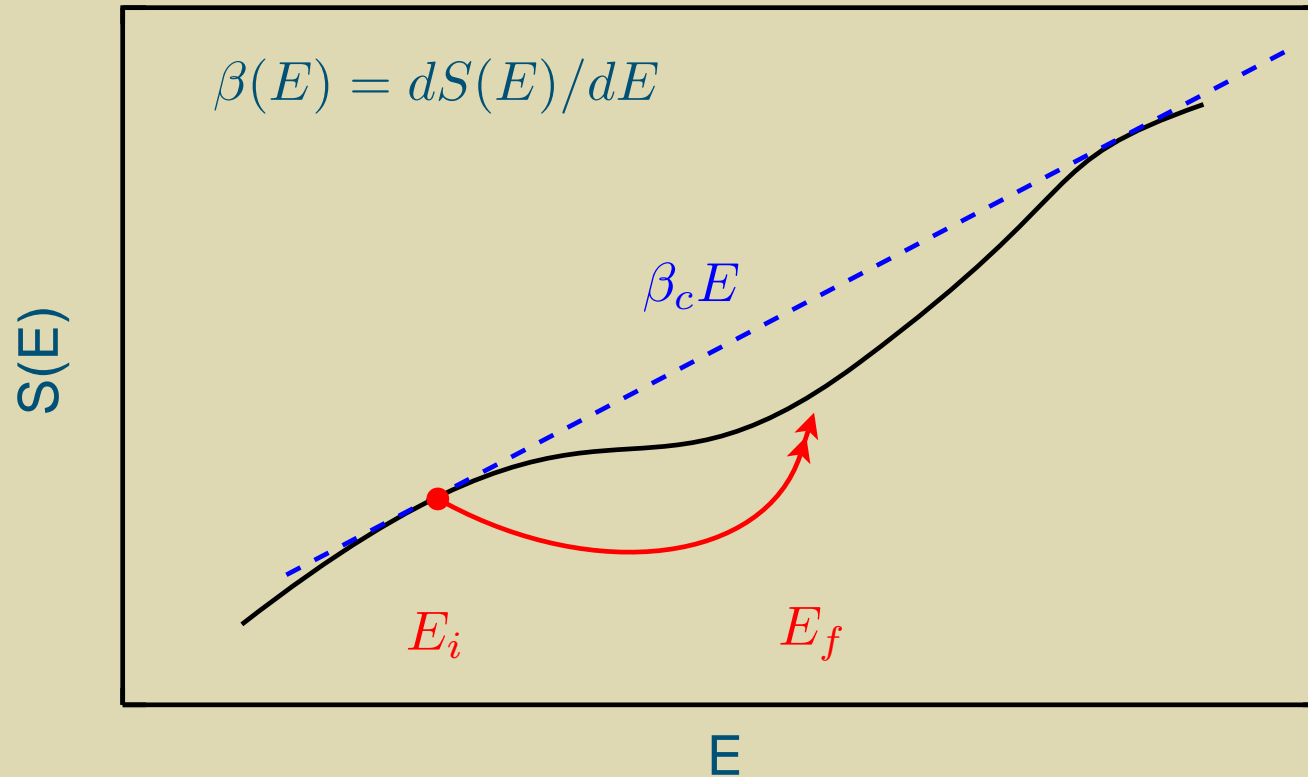
FFT

Accuracy

2D NN Potts

Surface tension

V. Conclusion



Multicanonical weights: random-walker

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

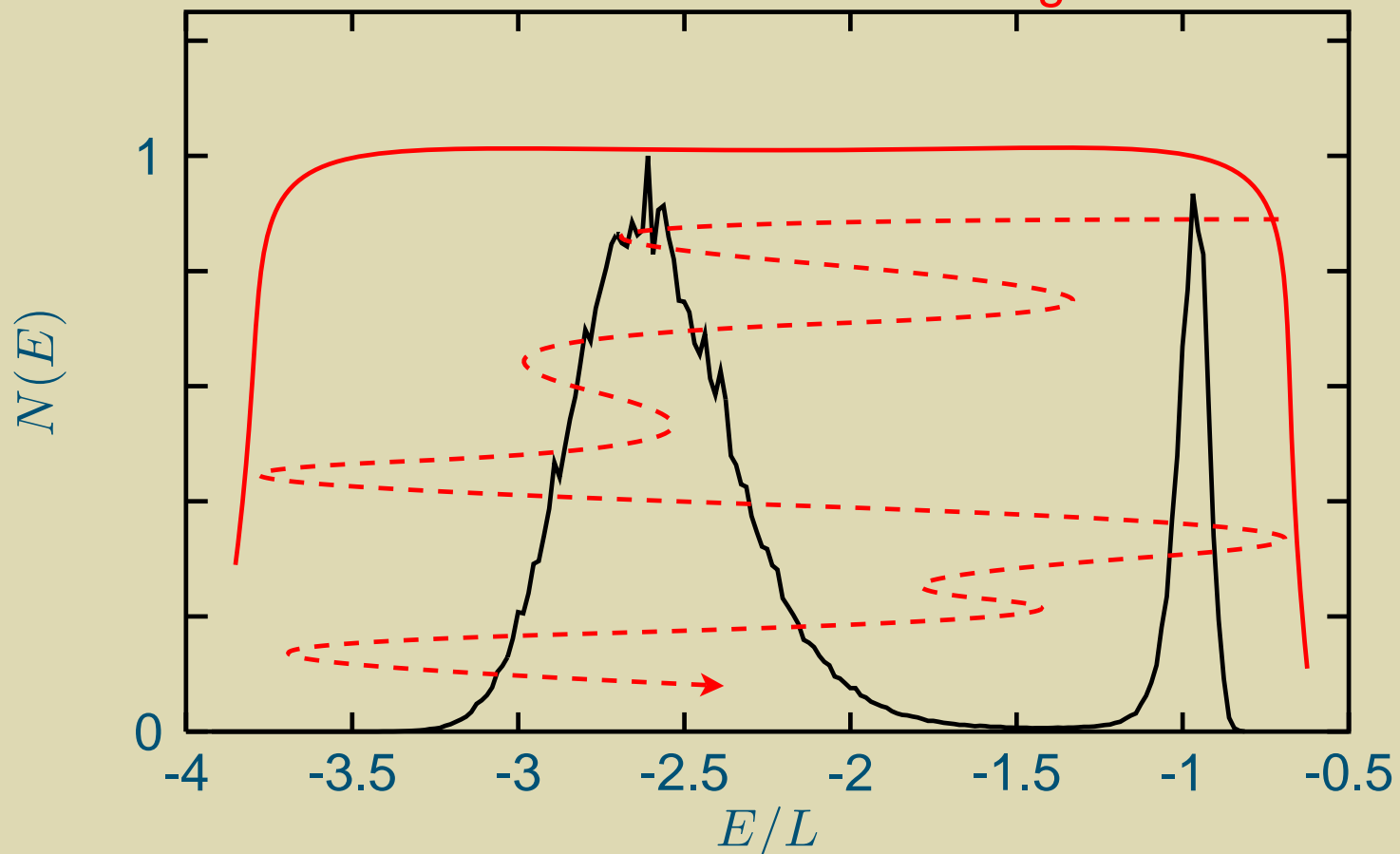
Surface tension

V. Conclusion

Random walk in energy space

Canonical histogram @ $T = T_c$ —

Multicanonical histogram



Reweighting of thermodynamic averages

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

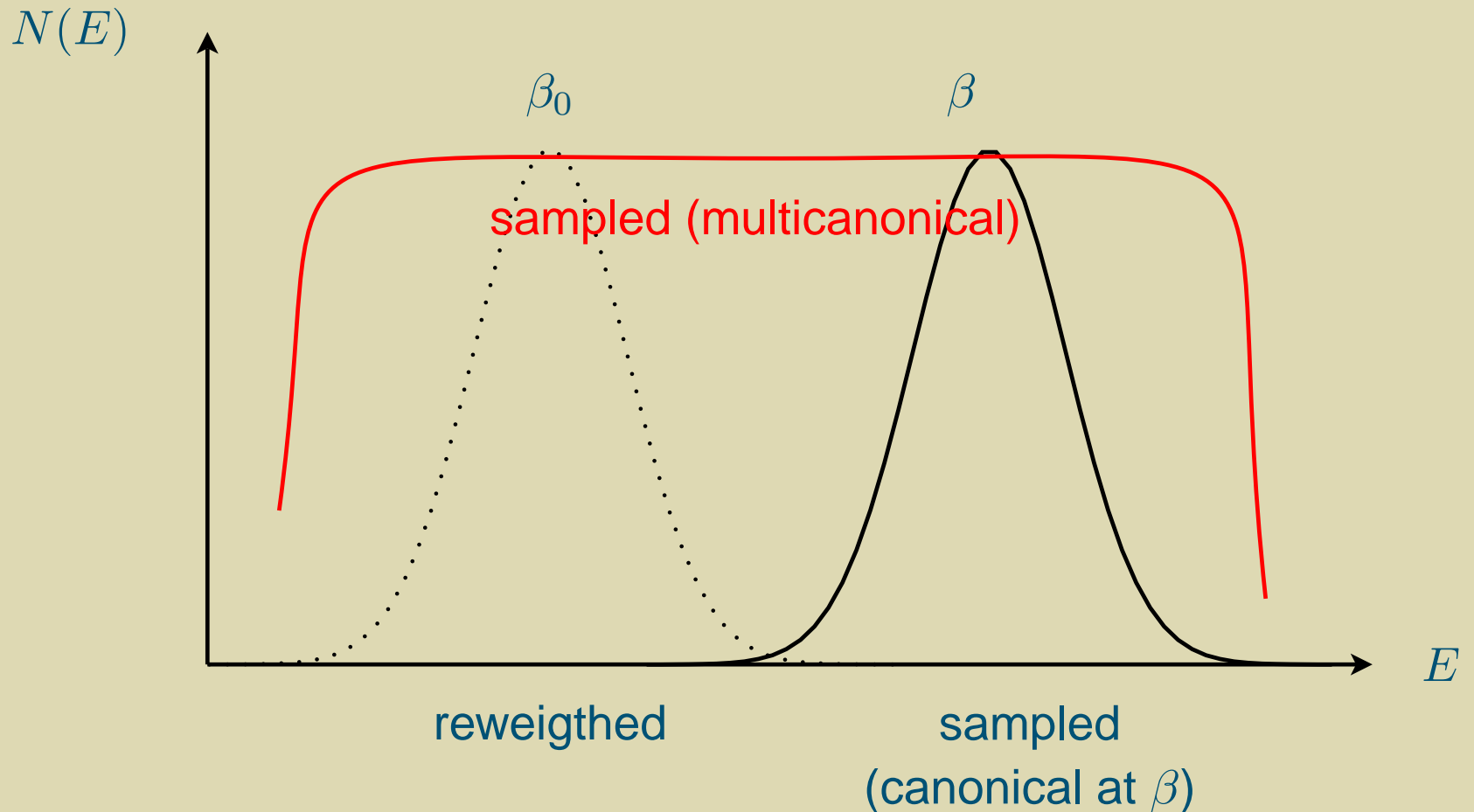
2D NN Potts

Surface tension

V. Conclusion

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

Energy distribution:



Multicanonical reweighting: metastable states

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

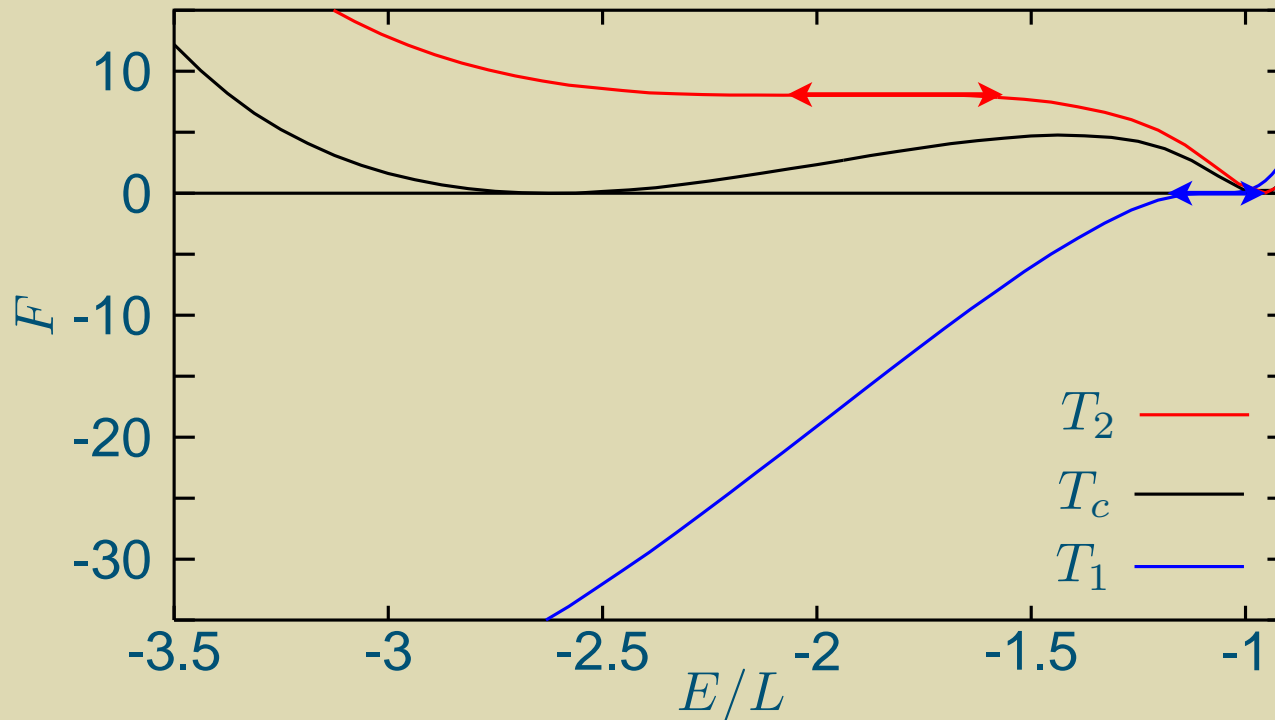
Accuracy

2D NN Potts

Surface tension

V. Conclusion

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.

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

III. Detecting the order of phase transitions: the spinodal method

Issue: weakening of the transition

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

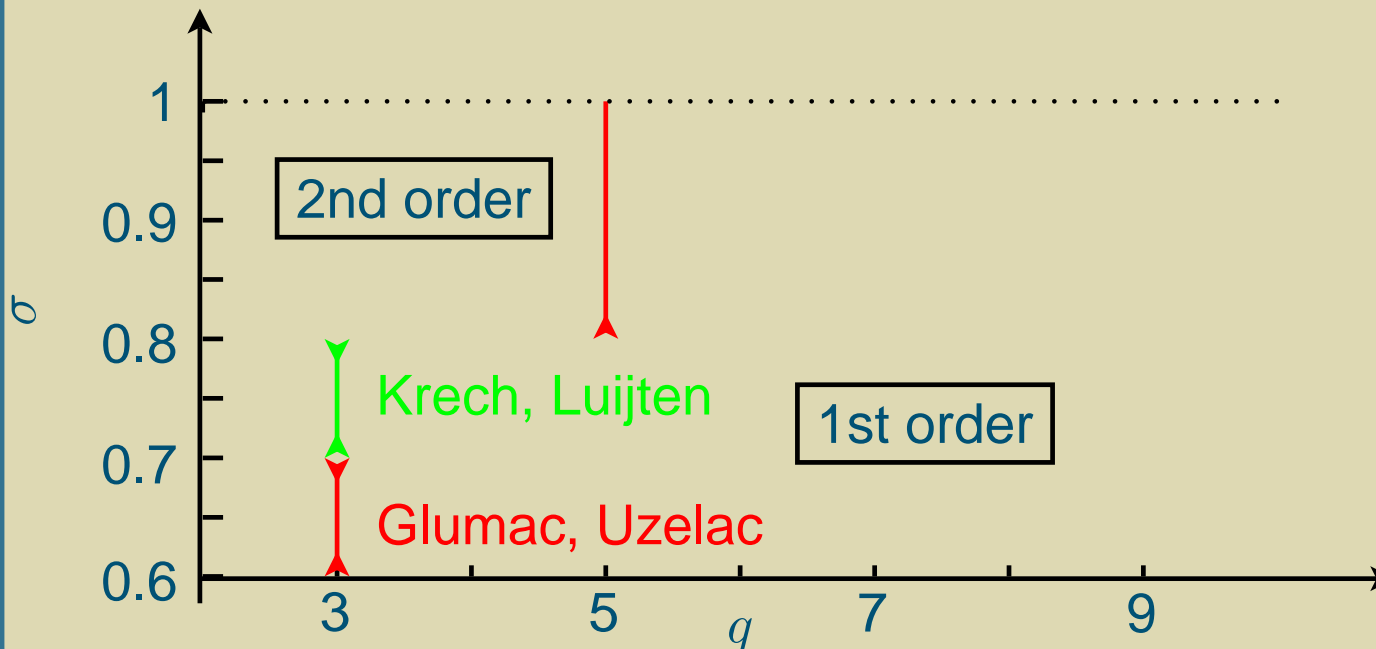
FFT

Accuracy

2D NN Potts

Surface tension

V. Conclusion



- As boundary is approached ($\sigma \rightarrow \sigma_c^-(q)$), cluster sizes diverge: transition weakens.
- Traditional estimators (ΔF , Binder cumulants) fail: tend to *smoothly* to their limit value
- Need distinct indicator: ratio of spinodals points

Weakening of the first-order transition

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

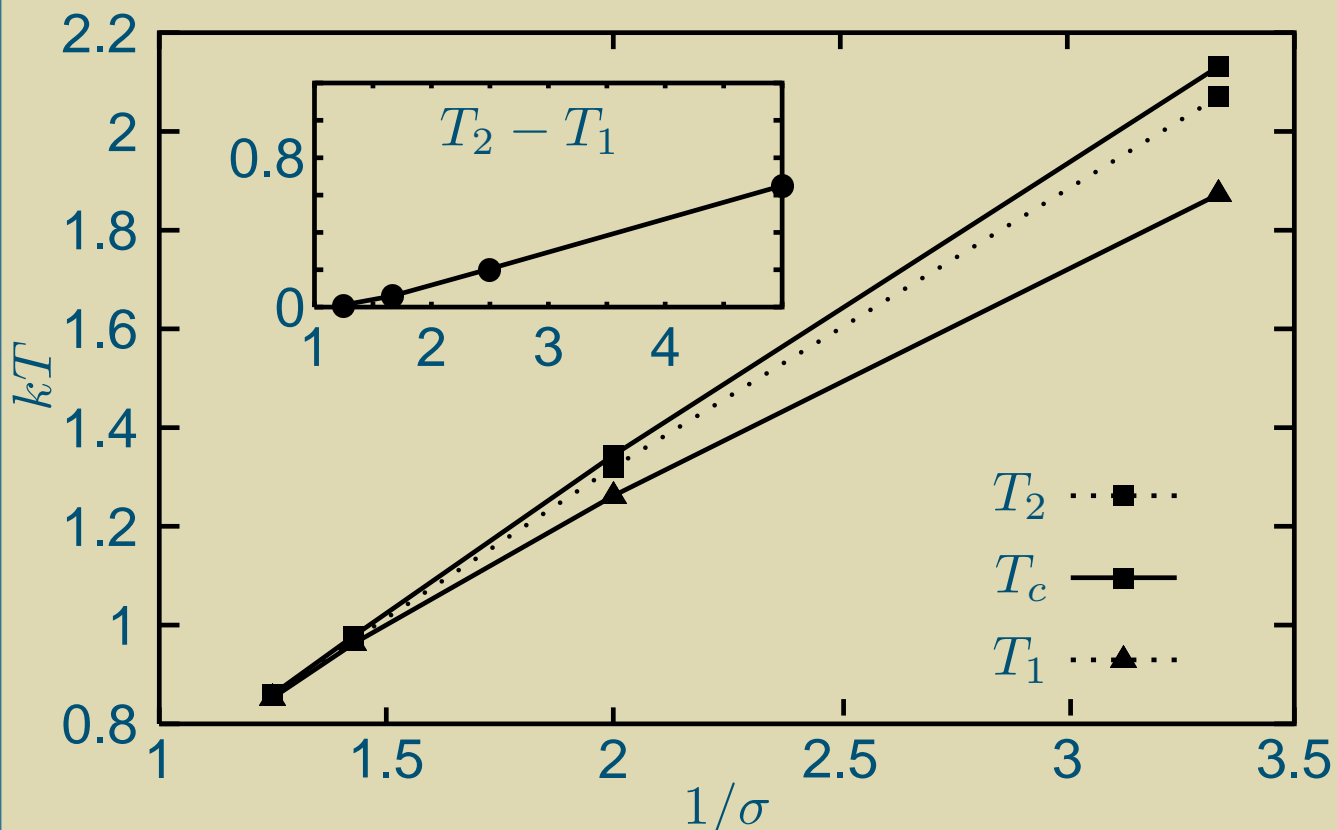
FFT

Accuracy

2D NN Potts

Surface tension

V. Conclusion



- 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 $\sigma \rightarrow \sigma_c$
- Yet $T_2 - T_1$ is **not** a good estimator.

Spinodal points and the transition order

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

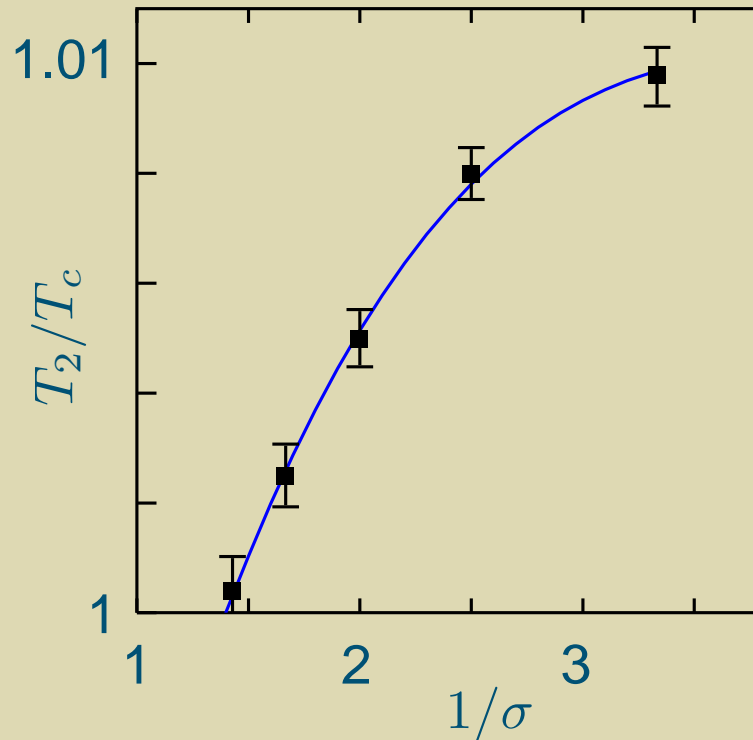
FFT

Accuracy

2D NN Potts

Surface tension

V. Conclusion



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 σ_c yields higher precision

$\sigma = 1.0$: controversy over the nature of the transition

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

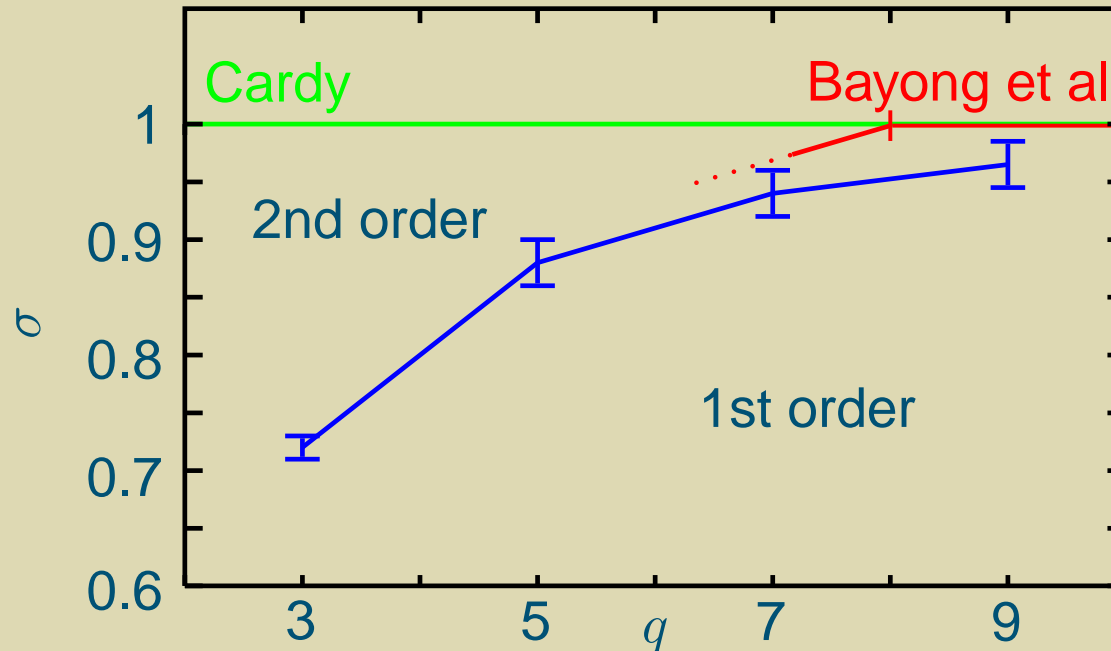
FFT

Accuracy

2D NN Potts

Surface tension

V. Conclusion



- 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

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

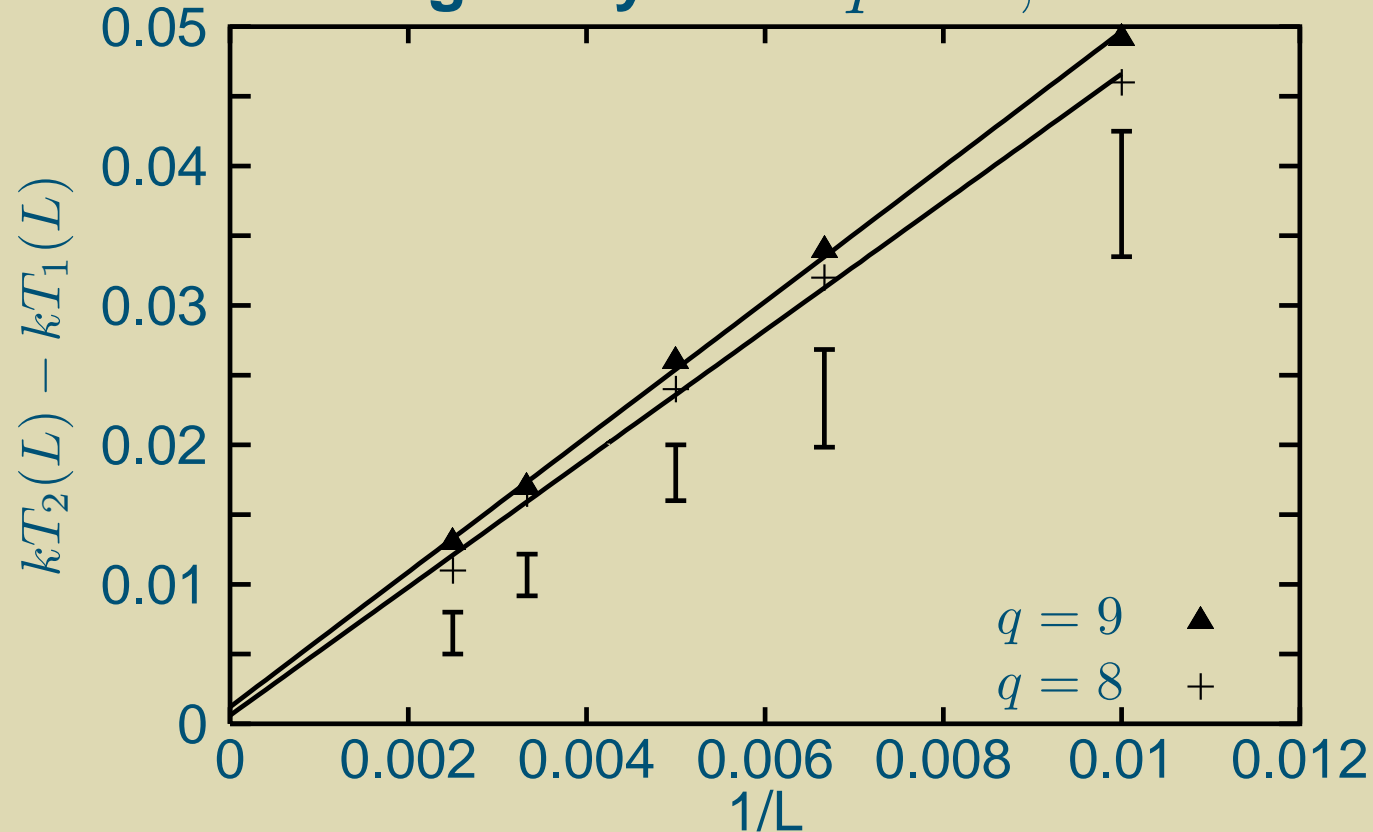
Accuracy

2D NN Potts

Surface tension

V. Conclusion

Finite-size scaling analysis at $q = 8, 9$:



- Transition appears discontinuous already for $L < 400$.
- FSS shows that it is continuous in the thermodynamic limit.

$\sigma = 1.0$: unusual finite-size effect

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

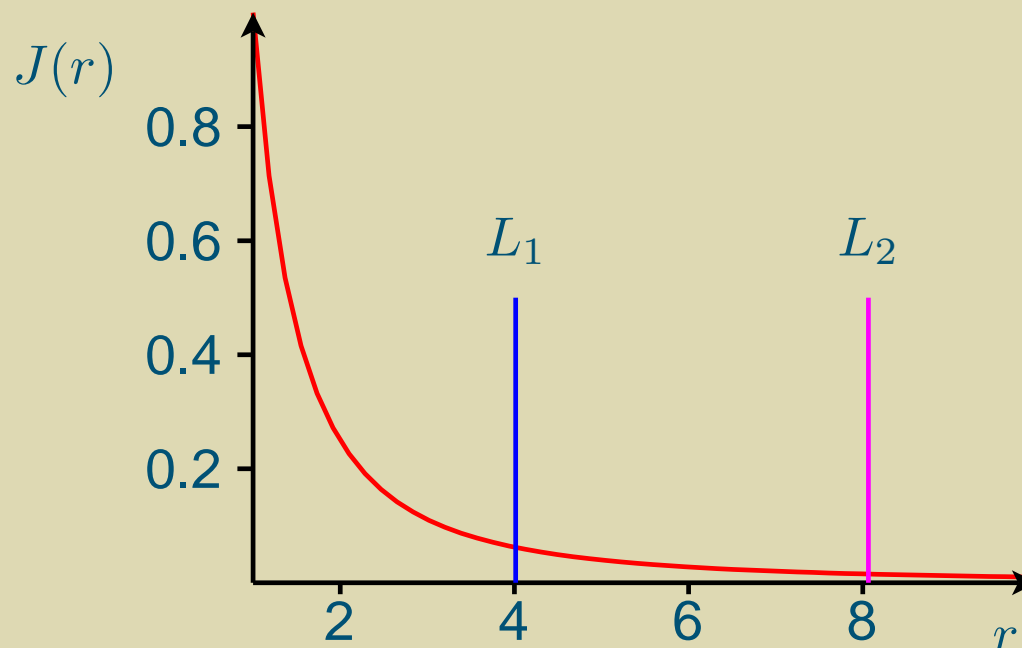
2D NN Potts

Surface tension

V. Conclusion

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 $\sigma_c(q)$



Conclusion (part I)

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

- **Spinodal points method** offers a drastic refinement of the position of the boundary line an unprecedented range of q and σ 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 $[1.0, 1.1]$

Outlook:

- Single-spin update efficient to solve some controversies
- New questions arise regarding FSS
- Need for a large range of linear lattice sizes
- Hence the need to design a specific method (next part)

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

IV. Breathing clusters

Single-spin updates vs. cluster updates

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

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

Breathing clusters: algorithm complexity

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

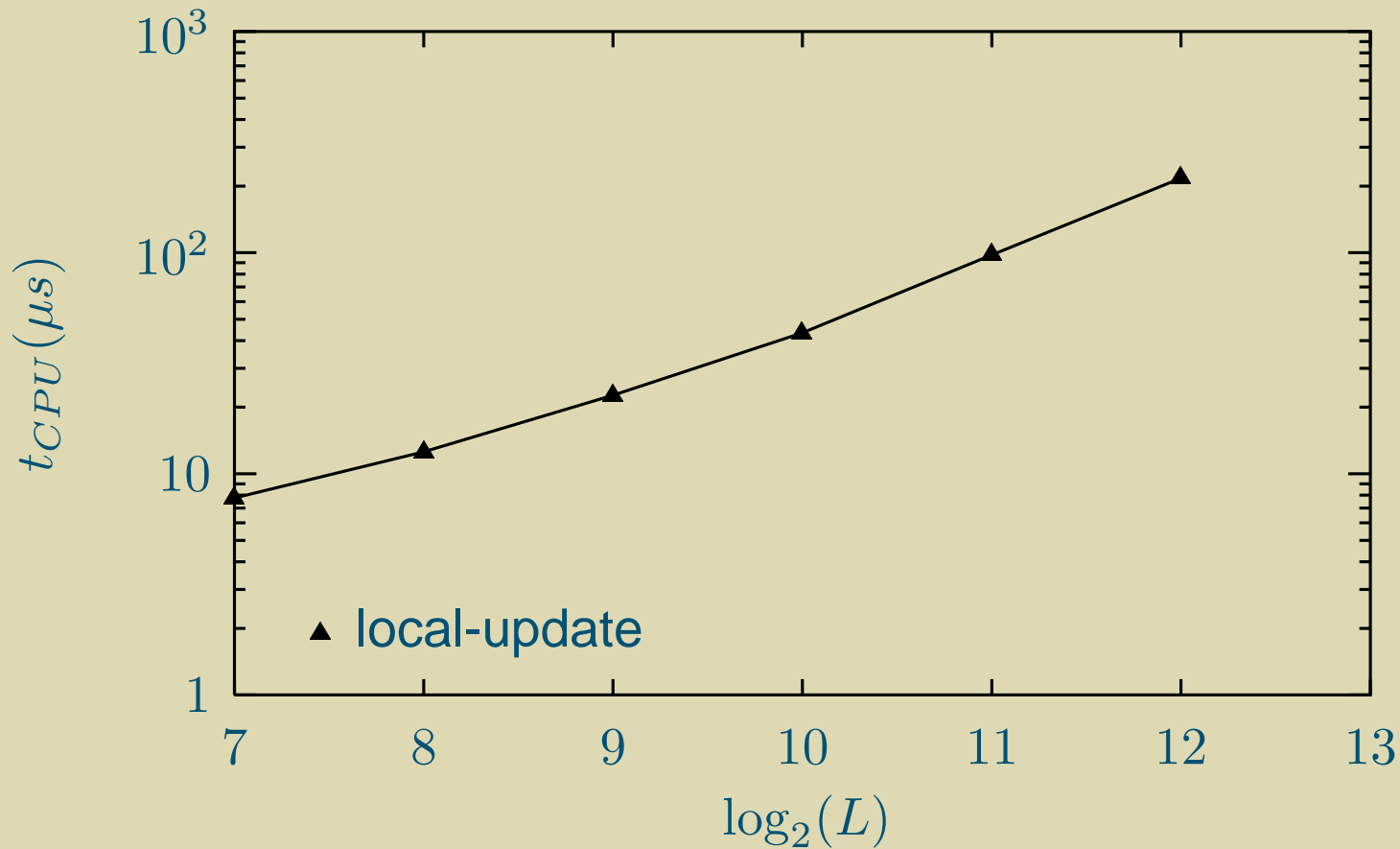
Accuracy

2D NN Potts

Surface tension

V. Conclusion

Goals: Cut down algorithm complexity from $O(N^2)$ to $O(N \log N)$ for Long-Ranged (LR) spin models.



Breathing clusters: algorithm complexity

I. LR Potts model
Modelling
Open questions
Addressed issues
Results

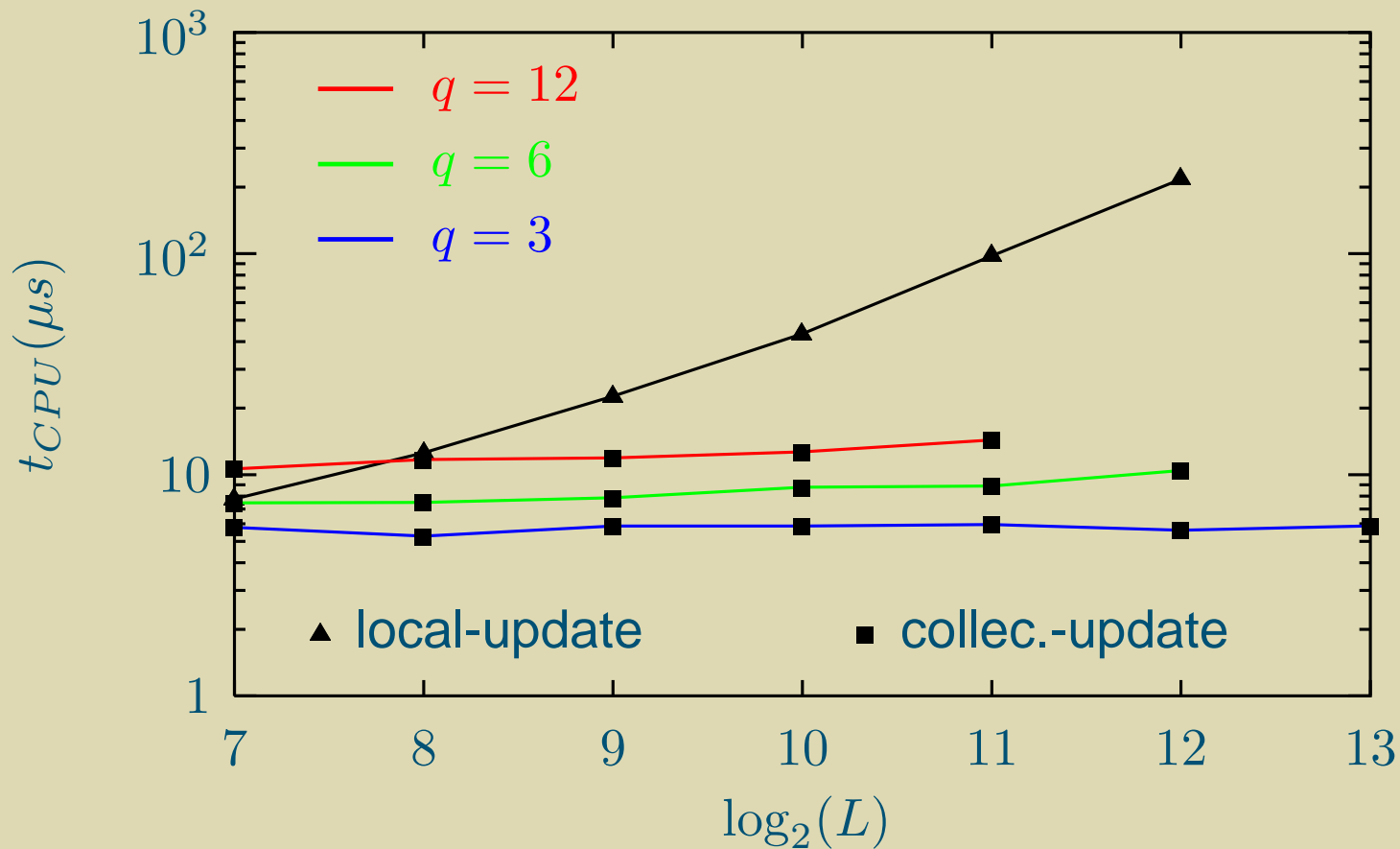
II. Multicanonical ensemble
Markov chains
Supercritical SD
Multicanonical weights

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

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Breathing clusters: dynamic characteristics

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

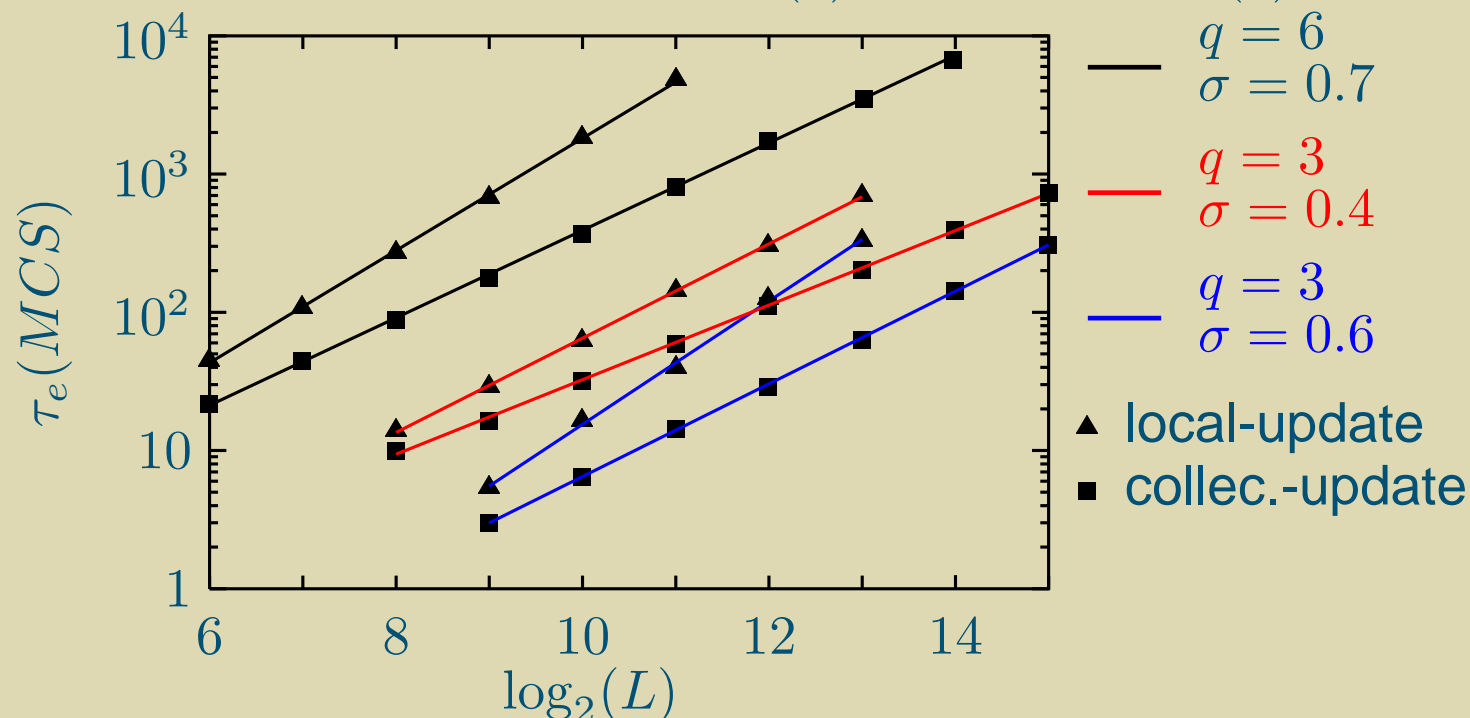
Surface tension

V. Conclusion

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

Tunneling times and dynamic exponents

$q =$	6	$\sigma =$	0.7	$z_{loc} =$	1.35(3)	$z_{col} =$	1.05(1)
	3		0.4		1.13(2)		0.89(1)
	3		0.6		1.48(2)		1.11(1)



Collective updates in multicanonical ensemble: issues

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

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!

Fortuin-Kasteleyn mapping for LR models

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

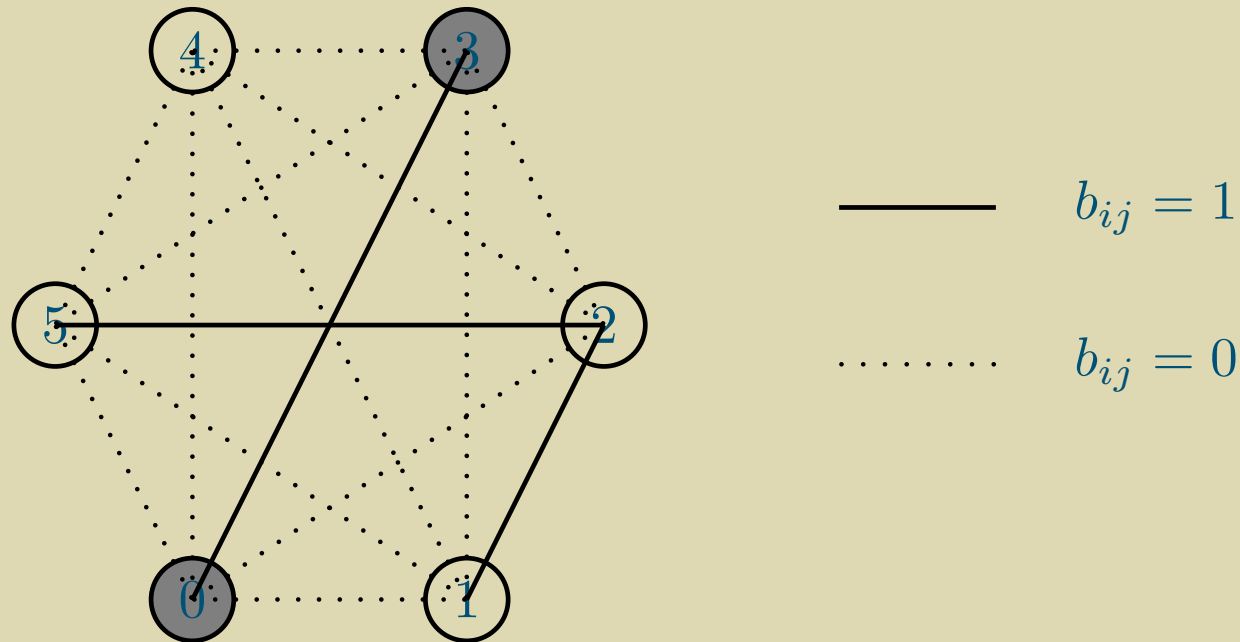
FFT

Accuracy

2D NN Potts

Surface tension

V. Conclusion



- Invoke the Fortuin-Kasteleyn representation and rewrite $w(E)$ as

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

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

Cluster construction

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

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 $B(l)$ = 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 !

Acceptance rate

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

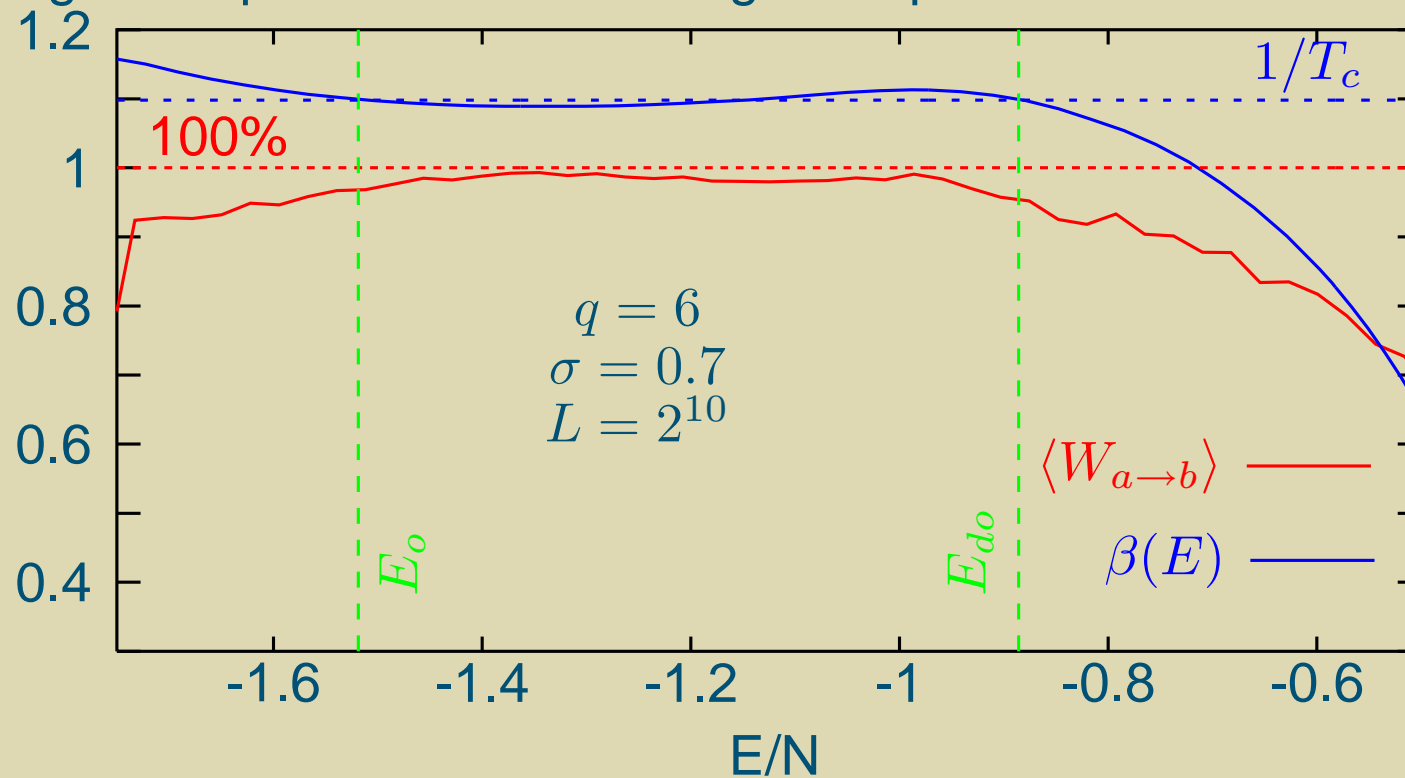
Surface tension

V. Conclusion

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

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

- 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

$$H = -\frac{1}{2N} \sum_{k=0}^{N-1} \tilde{J}(k) \tilde{\vec{S}}(k) \cdot \tilde{\vec{S}}(-k)$$

- 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

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

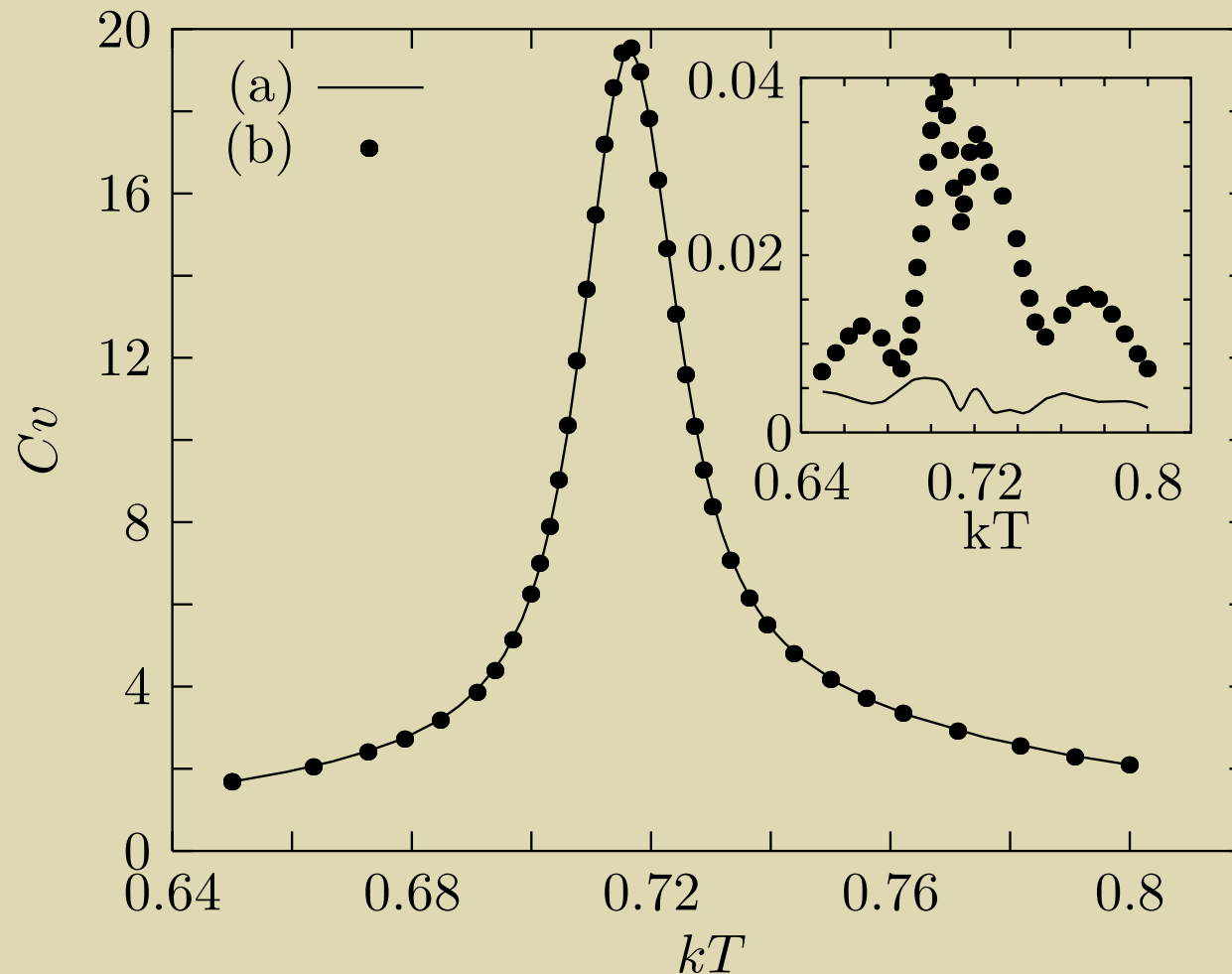
Accuracy

2D NN Potts

Surface tension

V. Conclusion

Lower statistical error on the computation of the density of states



Numerical results for the 2D NN Potts model

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

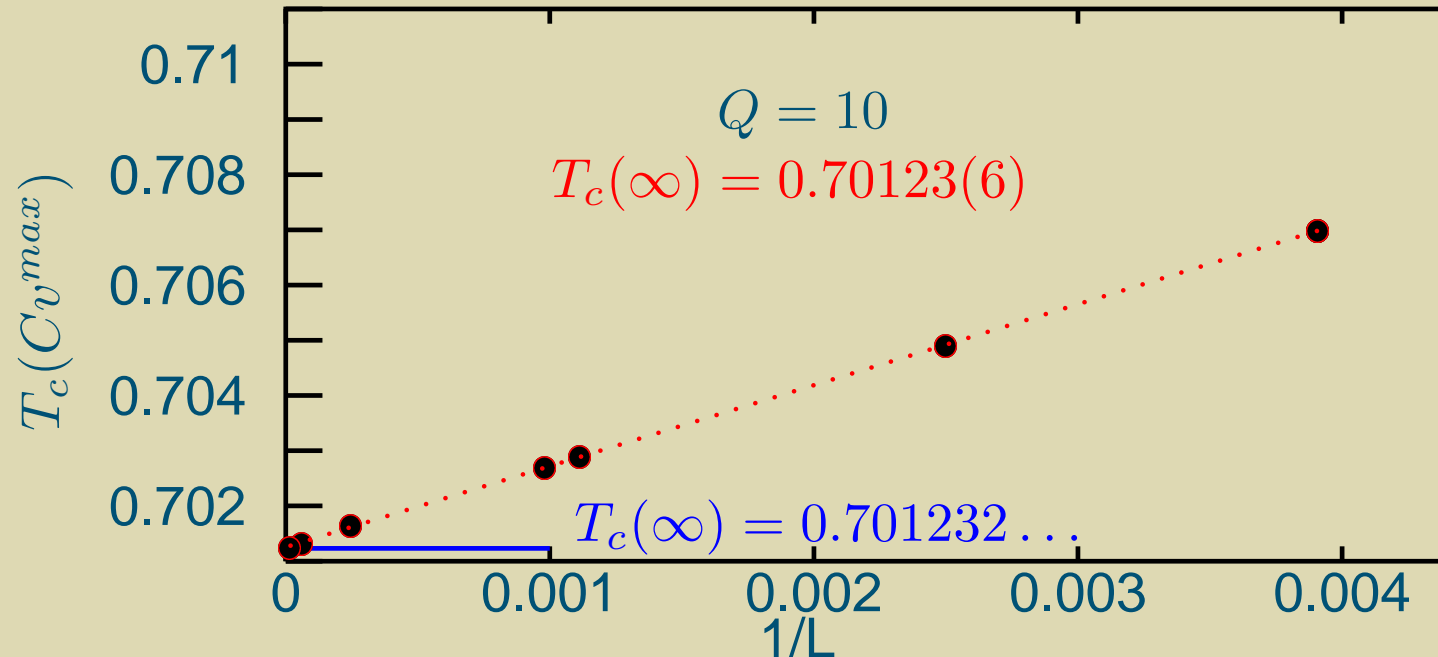
Surface tension

V. Conclusion

Tunneling times and dynamic exponents

q	z_{loc}	z_{col}	z_{mubo}
7	2.60(4)	1.82(2)	1.84
10	2.87(4)	2.23(1)	2.1

Finite-size temperatures:



Numerical results for the LR Potts chain

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

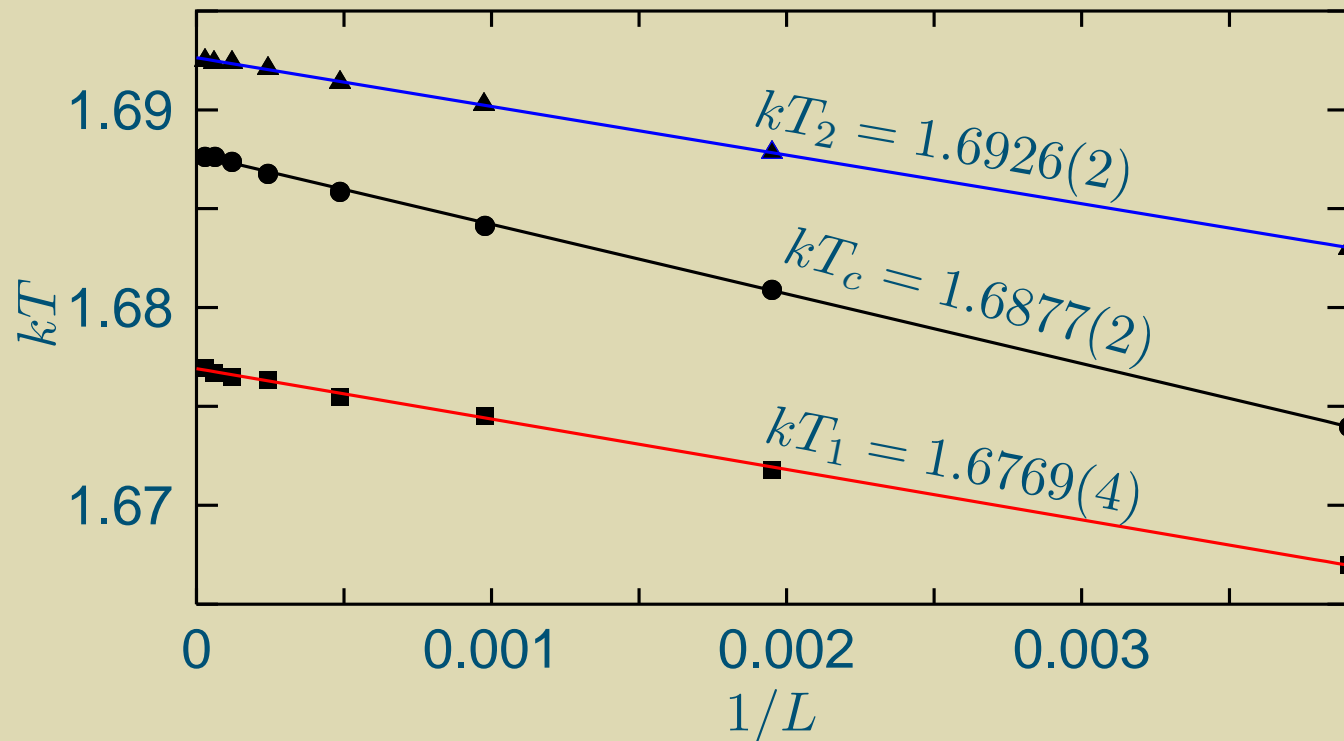
Accuracy

2D NN Potts

Surface tension

V. Conclusion

Finite-size temperatures



■ $T_c(C_v) = 1.68764(1)$

■ $T_c(\chi) = 1.68765(2)$

Numerical results for the LR Potts chain

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

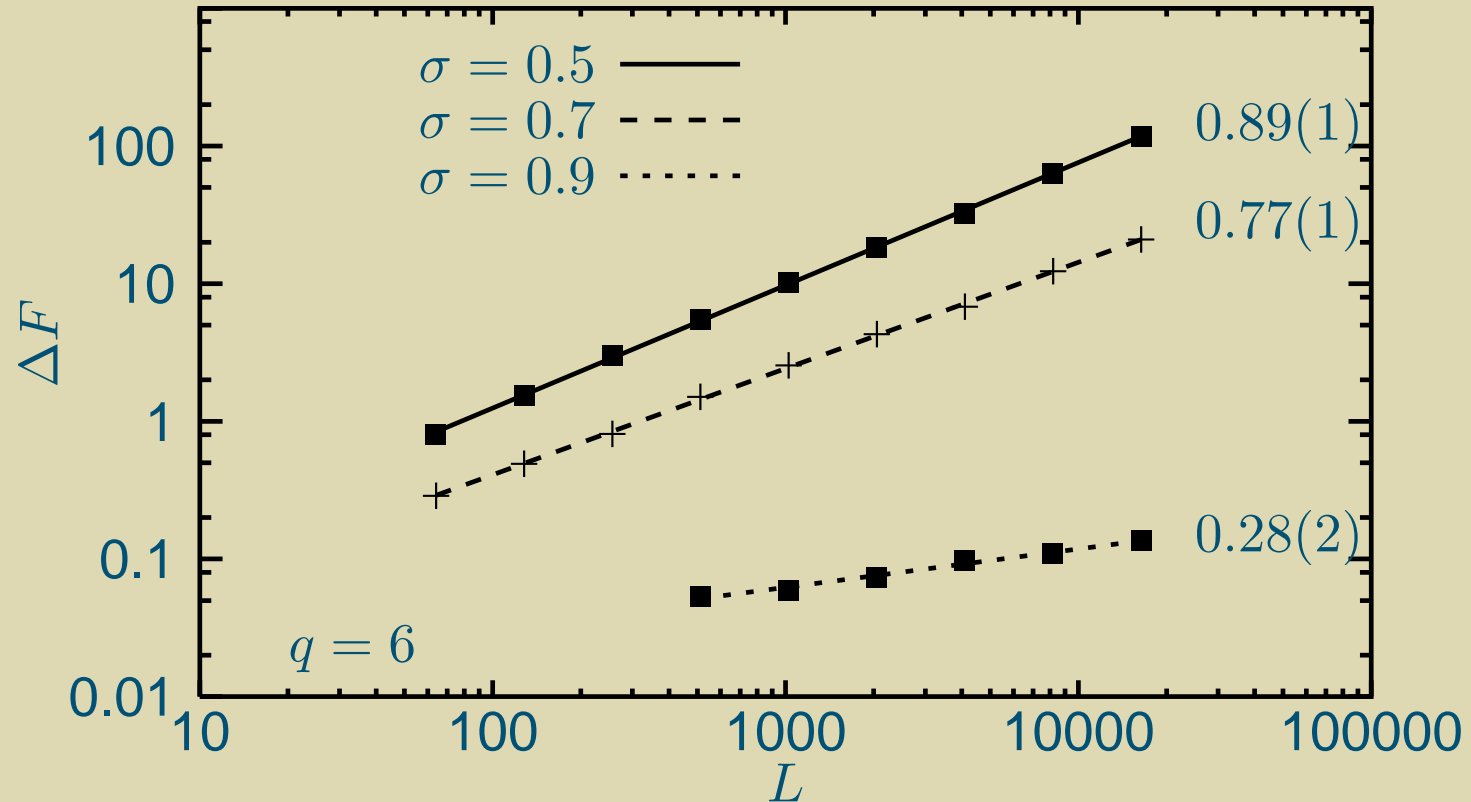
Accuracy

2D NN Potts

Surface tension

V. Conclusion

FSS behavior of the surface tension: fractal?



→ we find $\Delta F \propto L^\alpha$, with $\alpha(\sigma)$.

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

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

V. Conclusion

Conclusion

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

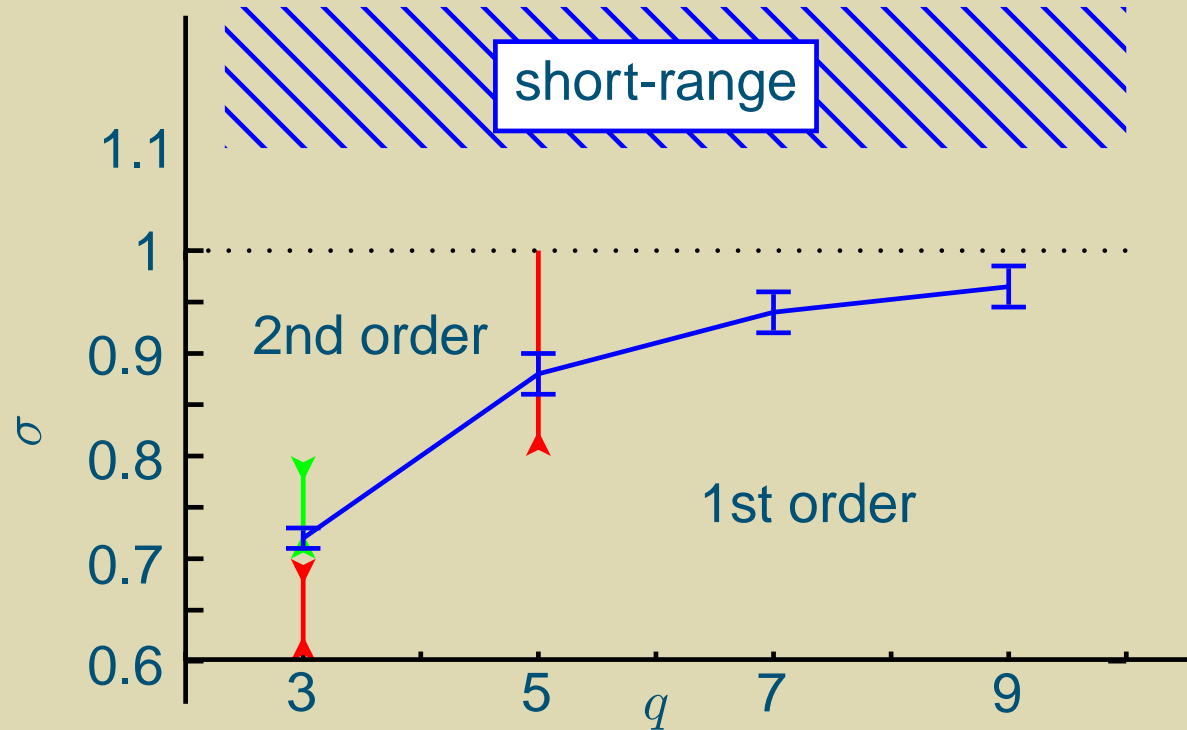
Accuracy

2D NN Potts

Surface tension

V. Conclusion

Model:



Conclusion

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

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)

Outlook and work underway

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

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)