Overcoming strong metastabilities with the LLR method

Biagio Lucini

(Work in collaboration with W. Fall and K. Langfeld)

Swansea University
Prifysgol Abertawe

Lattice 2016, University of Southampton, 26th July 2016

Outline

1. The LLR method
2. Replica exchange method
3. Numerical results for Potts models in D=2,3
4. Conclusions and outlook

Outline

1. The LLR method
2. Replica exchange method
3. Numerical results for Potts models in D=2,3
4. Conclusions and outlook

LLR cheat sheet

- Divide the (continuum) energy interval in N sub-intervals of amplitude $\delta_E/2$
- For each interval, given its centre E_n, define

$$\log \tilde{\rho}(E) = a_n \left(E - E_n - \delta_E/2\right) + c_n \qquad \text{for } E_n - \delta_E/2 \leq E \leq E_n + \delta_E/2$$

- Obtain a_n as the root of the stochastic equation

$$\langle\langle \Delta E \rangle\rangle_{a_n} = 0 \Rightarrow \int_{E_n - \frac{\delta_E}{2}}^{E_n + \frac{\delta_E}{2}} \left(E - E_n - \delta_E/2\right) \rho(E) e^{-a_n E} dE = 0$$

using the Robbins-Monro iterative method

$$\lim_{m \to \infty} a_n^{(m)} = a_n \; , \qquad a_n^{(m+1)} = a_n^{(m)} - \frac{1}{m} \langle\langle \Delta E \rangle\rangle_{a_n^{(m)}}$$

- Define

$$c_n = \frac{\delta}{2} a_1 + \delta \sum_{k=2}^{n-1} a_k + \frac{\delta}{2} a_n \qquad \text{(piecewise continuity of } \log \tilde{\rho}(E))$$

[Langfeld, Lucini and Rago, Phys. Rev. Lett. 109 (2012) 111601; Langfeld, Lucini, Pellegrini and Rago, Eur. Phys. J. C76 (2016) no.6, 306]

LLR method – rigorous results

One can prove that:

1. For small δ_E, $\tilde{\rho}(E)$ converges to the density of states $\rho(E)$, i.e.

$$\lim_{\delta_E \to 0} \tilde{\rho}(E) = \rho(E)$$

   "almost everywhere"

2. With $\beta_\mu(E)$ the microcanonical temperature at fixed E

$$\lim_{\delta_E \to 0} a_n = \left. \frac{\mathrm{d} \log \rho(E)}{\mathrm{d}E} \right|_{E=E_n} = \beta_\mu(E_n)$$

3. For ensemble averages of observables of the form O(E)

$$\langle \tilde{O} \rangle_\beta = \frac{\int O(E) \tilde{\rho}(E) e^{-\beta E} \mathrm{d}E}{\int \tilde{\rho}(E) e^{-\beta E} \mathrm{d}E} = \langle O \rangle_\beta + \mathcal{O}\left(\delta_E^2\right)$$

4. $\tilde{\rho}(E)$ is measured with constant relative error (exponential error reduction)

$$\frac{\Delta \tilde{\rho}(E)}{\tilde{\rho}(E)} \simeq \text{constant}$$

[Langfeld, Lucini, Pellegrini and Rago, Eur. Phys. J. C76 (2016) no.6, 306]

LLR method – hints and directions

Available numerical results [see Kurt Langfeld's plenary] suggest that

1. The convergence is precocious in δ_E
2. Potential ergodicity issues can be resolved with the replica exchange method
3. The cost of the algorithm is quadratic in V even at first order phase transitions (where importance sampling has an exponentially long tunnelling time between the degenerate equilibrium states)
4. The method allows to compute partition functions (and hence interfaces)
5. A simple modification of the method can be used to simulate efficiently systems afflicted by a sign problem
6. The method can be extended to generic observables, for which one still get quadratic convergence in δ_E to the correct result
7. At finite δ_E, δ_E^2 errors can be corrected with a multicanonical algorithm

LLR method – hints and directions

Available numerical results [see Kurt Langfeld's plenary] suggest that

1. The convergence is precocious in δ_E
2. Potential ergodicity issues can be resolved with the replica exchange method
3. The cost of the algorithm is quadratic in V even at first order phase transitions (where importance sampling has an exponentially long tunnelling time between the degenerate equilibrium states)
4. The method allows to compute partition functions (and hence interfaces)
5. A simple modification of the method can be used to simulate efficiently systems afflicted by a sign problem
6. The method can be extended to generic observables, for which one still get quadratic convergence in δ_E to the correct result
7. At finite δ_E, δ_E^2 errors can be corrected with a multicanonical algorithm

This talk will focus on the ergodicity properties and the efficiency of the LLR algorithm with replica exchange at first order phase transitions, by applying the method to Potts models in D=2 and D=3 [See also Guagnelli, arXiv:1209.4443]

Outline

1 The LLR method

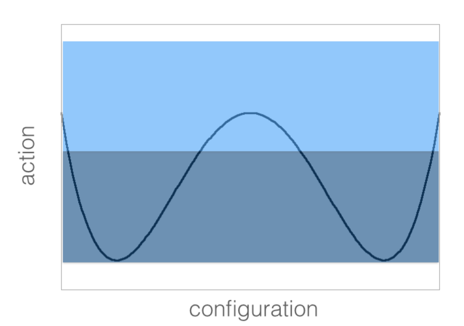
2 Replica exchange method

3 Numerical results for Potts models in D=2,3

4 Conclusions and outlook

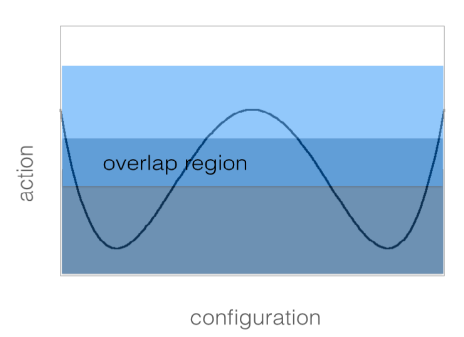
Trapping and ergodicity

Trapping occurs when, due to the small value of δ_E, a disconnection in configuration space is created between regions with the same energy



Trapping and ergodicity

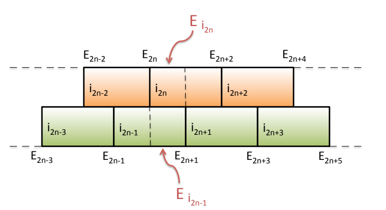
Trapping occurs when, due to the small value of δ_E, a disconnection in configuration space is created between regions with the same energy



Ergodicity can be recovered by having suitably overlapping energy intervals and allowing exchange of configurations if both energies are compatible with the restrictions of both intervals

Replica exchange

We use a second set of simulations, with centres of intervals shifted by $\delta_E/2$



After a certain number m of Robbins-Monro steps, we check if both energies in two overlapping intervals are in the common region and if this happens we swap configurations with probability

$$P_{\mathrm{swap}} = \min\left(1, e^{\left(a_{2n}^{(m)} - a_{2n-1}^{(m)}\right)\left(E_{i_{2n}} - E_{i_{2n-1}}\right)}\right)$$

Subsequent exchanges allow any of the configuration sequences to travel through all energies, hence overcoming trapping

Outline

1. The LLR method
2. Replica exchange method
3. Numerical results for Potts models in D=2,3
4. Conclusions and outlook

The q-state Potts model

On a D-dimensional lattice, the Hamiltonian of the q-state Potts model is given by

$$H = 2J \sum_{\langle ij \rangle} \left(\frac{1}{q} - \delta_{\sigma_i,\sigma_j} \right) \ , \qquad J > 0$$

with the spin variables $\sigma_i = 0, \ldots, q-1$

In D=2,3 the system undergoes an order-disorder phase transition driven by the $\mathbb{Z}_q$ symmetry

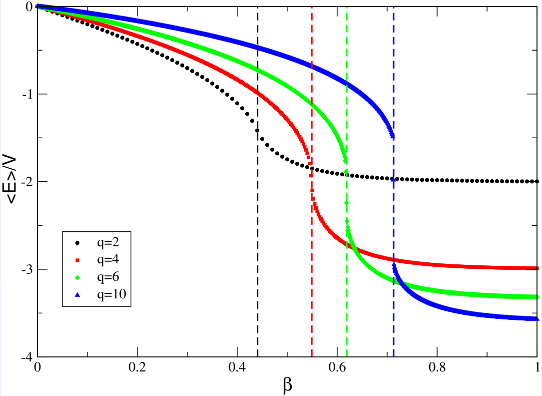
For D=2, the transition is first order for $q > 4$, second order for $q \leq 4$

For D=3, the transition is second order only for $q = 2$ (Ising case), first order for $q > 2$

The strength of the transition increases with $q \Rightarrow$ strong metastabilities pose a challenge for simulations at large q

The phase transition in D=2

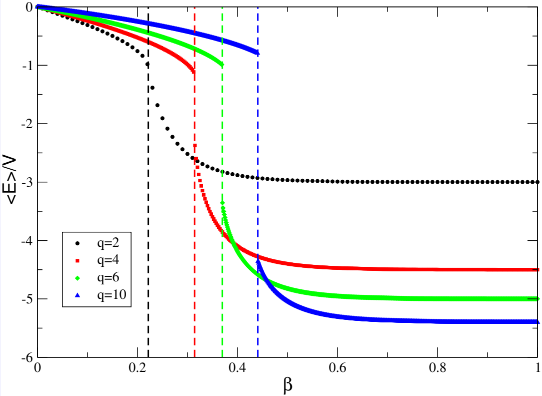
$\langle E \rangle$ vs β, lattice size $L = 64$



Exact $\beta_c = \frac{1}{2} \log \left(1 + \sqrt{q}\right)$

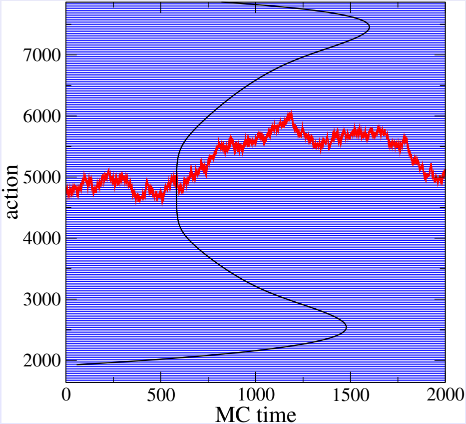
The phase transition in D=3

$\langle E \rangle$ vs β, lattice size $L = 16$



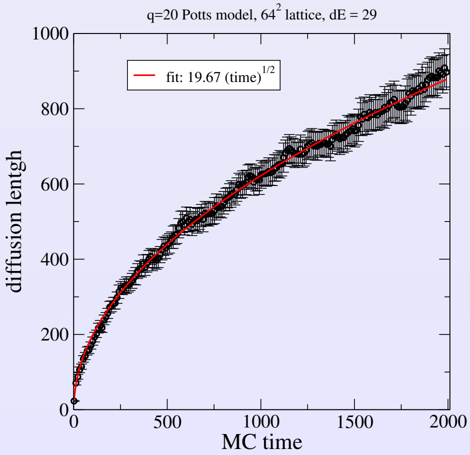
β_c from Bazavov, Berg and Dubey, Nucl. Phys. B802 (2008) 421-434

Efficiency of replica swapping (D=2 q=20)



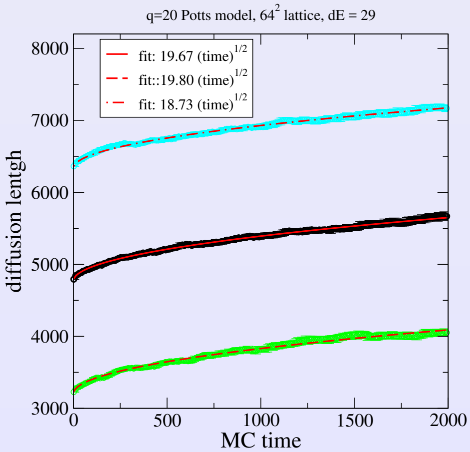
The hopping of configurations across intervals is reminiscent of a random walk

Replica swap and diffusive dynamics



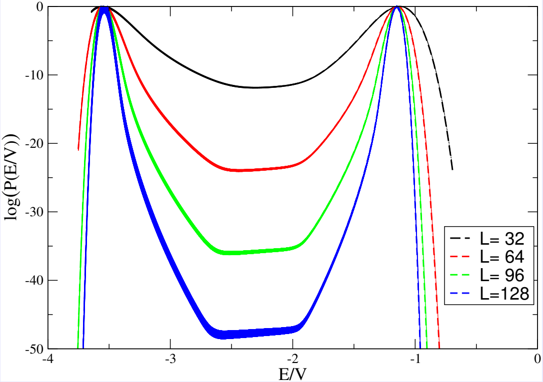
Mean path in energy space: $\langle (E_{\bar{f}} - E_{\bar{\imath}})^2 \rangle^{1/2} = D t^{1/2}$

Diffusion coefficient vs. $E_{\bar{\imath}}$



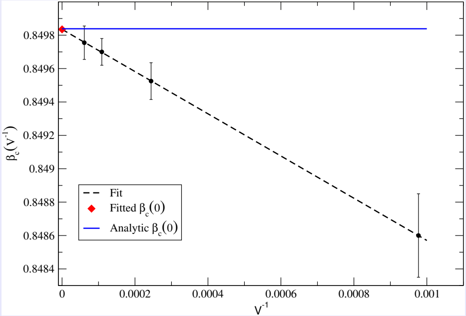
D seems independent from $E_{\bar{\imath}}$

Probability density at criticality



- The value of β for which $P(E/V)$ has two equal-height maxima is a possible definition of $\beta_c(V^{-1})$
- The minimal depth of the valley between the peaks is related to the order-disorder interface

Finite Size Scaling – β_c



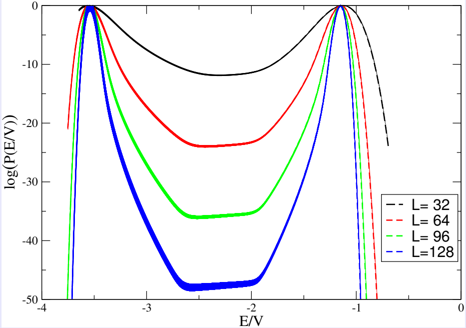
For first order phase transitions

$$\beta_c(V^{-1}) = \beta_c^{fit} + \frac{a_\beta}{V} + \dots$$

With a linear fit, we find

$$\beta_c^{fit} = 0.8498350(21) \, , \qquad \frac{\beta_c^{fit} - \beta_c^{exact}}{\beta_c^{exact}} = 1.7(2.5) \times 10^{-6}$$

Finite Size Scaling – order-disorder interface



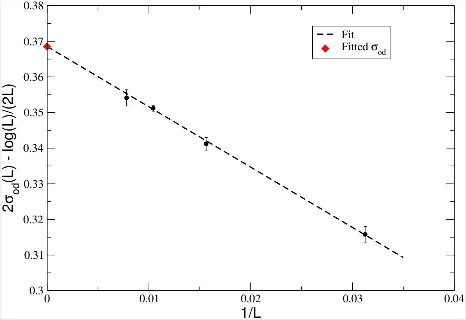
At finite L

$$2\sigma_{od}(L) = -\frac{1}{L}\log P_{min,valley}$$

Ansatz

$$2\sigma_{od}(L) - \frac{\log L}{2L} = 2\sigma_{od} + \frac{c_\sigma}{L} \qquad \Rightarrow \qquad 2\sigma_{od} = 0.36853(88)$$

Finite Size Scaling – order-disorder interface



At finite L

$$2\sigma_{od}(L) = -\frac{1}{L}\log P_{min,valley}$$

Ansatz

$$2\sigma_{od}(L) - \frac{\log L}{2L} = 2\sigma_{od} + \frac{c_\sigma}{L} \qquad \Rightarrow \qquad 2\sigma_{od} = 0.36853(88)$$

Outline

1. The LLR method
2. Replica exchange method
3. Numerical results for Potts models in D=2,3
4. Conclusions and outlook

Conclusions and outlook

- LLR algorithm (supplemented with replica exchange) works for Potts models in D=2 and D=3 $\Rightarrow$ perhaps because E/V $\rightarrow$ continuous when $V \rightarrow \infty$?
- The replica exchange method behaves as expected, providing a random walk in energy space even when the system is metastable $\Rightarrow$ cost of the algorithm scaling as V^2?
- To my knowledge, first determination of critical properties for $q = 20$, D=2 (including σ_{od})
- Future directions:
  - study the dependence V of the diffusion coefficient D
  - determine σ_{oo} and check if the perfect wetting condition is satisfied
  - perform a similar precision study in D=3