The LLR method in Lattice Gauge Theories

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[Based on Phys.Rev.D 108 (2023) and Phys.Rev.D 111 (2025)]

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TELOS collaboration
Centre for Mathematical Sciences
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Bridging analytical and numerical methods in QFT - 24th–30th of August 2025

Outline

- The density of states in statistical mechanics and LGT
- The LLR algorithm
- Application to the deconfinement transition of the SU(3) and Sp(4) LGTs.
- Conclusions

The Density of States

The Density of states - Definition

The complete knowledge about the system is contained in the partition function Z, defined as

$$Z(\beta) = \int \mathcal{D}\phi e^{-\beta S[\phi]} = \int dE \rho(E) e^{-\beta E}$$

The density of states is defined as

$$\rho(E) = \int \mathcal{D}\phi \delta(E - S[\phi])$$

"the number of states with energy between E and $E+dE$ "

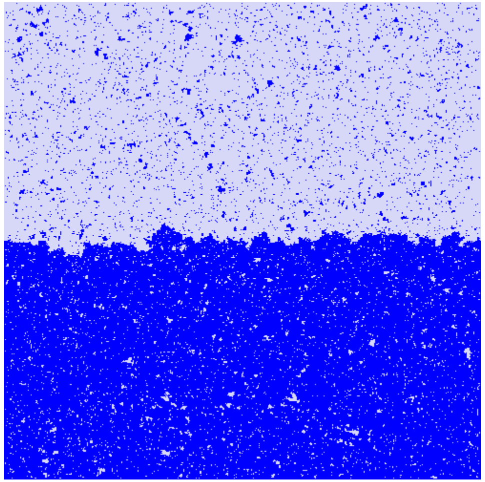
Vacuum expectation values (VEVs) can then be computed as

$$\langle O \rangle = \frac{1}{Z} \int dE O(E) \rho(E) e^{-\beta E}$$

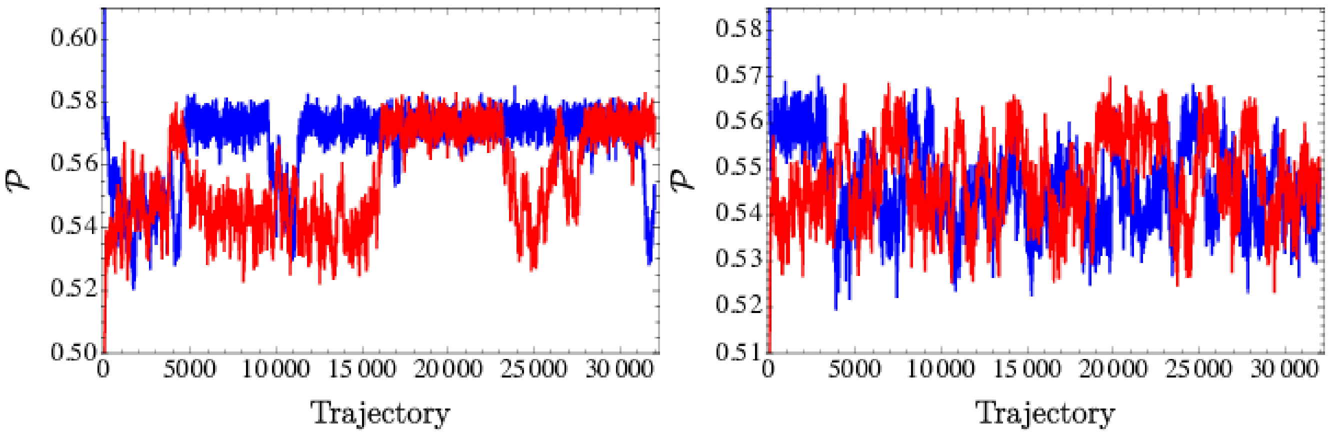
The Density of states

When is it useful to compute the DoS?

- When strong metastabilities are present: **first order phase transitions**,...
- When observables cannot be expressed as VEVs: **interface free energies**,...
- When path-integral measure is not positive semi-definite: **sign problem**,...

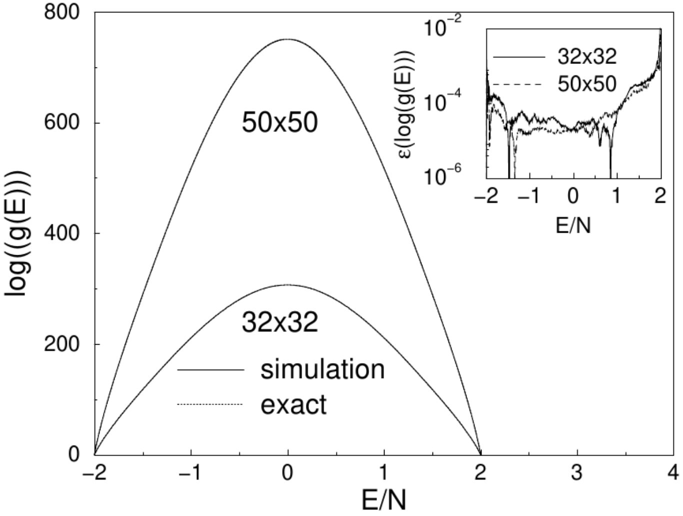


[Liquid-Gas interface. Taken from PhD Thesis of L. Coquille]



[Trace of a 1st order phase transition on the history of the elementary plaquette in a 3AS+2F Sp(4) LGT. Taken from D.V. et al PRD 106 (2022)]

The Density of states - How to compute it?



[The density of states for the 3d Ising model. Taken from Wang & Landau PRL (2001)]

- With discrete degrees of freedom, **the Wang-Landau algorithm** "*Random Walk in energy space with a flat histogram*".

$$P(1 \to 2) = \min\left(\frac{\rho(E_1)}{\rho(E_2)}, 1\right)$$

- With continuous degrees of freedom, **the LLR algorithm.**

The LLR idea:

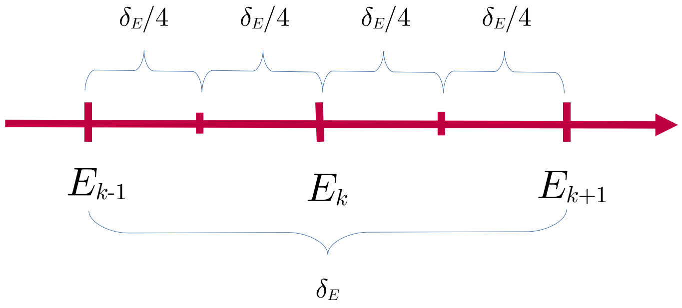
1) Approximate $\rho(E)$ in the interval $[E - \delta_E/2, E + \delta_E/2]$
2) Find a such that $\rho(E)e^{-aE}$ is flat

The LLR algorithm

The LLR algorithm - The approximate DoS

Consider the energy interval $[E_k - \delta_E/4, E_k + \delta_E/4]$, expand in a Taylor's series,

$$\log \rho(E) = \log \rho\left(E_k\right) + \left.\frac{\mathrm{d}\log\rho(E)}{\mathrm{d}E}\right|_{E_k}\left(E - E_k\right) + R_k(E)$$



where $$R_k(E) = \frac{1}{2}\left.\frac{\mathrm{d}^2\log\rho}{\mathrm{d}E^2}\right|_{E_k}\left(E - E_k\right)^2 + O(\delta_E^3)$$

And **define** $$\log\tilde{\rho}(E) = c_k + a_k(E - E_k)$$

for $E \in [E_k - \delta_E/4,\ E_k + \delta_E/4]$ where continuity imposes $$c_k = c_1 + (a_1 + a_k)\frac{\delta_E}{4} + \frac{\delta_E}{2}\sum_{l=1}^{k-1} a_l$$

Questions:

- How good an approximation is $\tilde{\rho}$ to ρ?
- How to compute a_k ?

The LLR algorithm - How good an approximation is it?

From

$$\ln \frac{\rho(E_{k+1})}{\rho(E_k)} = \int_{E_k}^{E_{k+1}} \mathrm{d}E \frac{\mathrm{d}\ln\rho}{\mathrm{d}E} = \frac{\delta_E}{4}(a_k + a_{k+1}) + O(\delta_E^3)$$

One obtains, by recursion

$$\rho(E) = \tilde{\rho}(E) e^{\left\{O(\delta_E^2)\right\}}$$

Hence:

- The density of states is approximated at *constant relative error*,

$$1 - \frac{\tilde{\rho}(E)}{\rho(E)} = O(\delta_E^2)$$

- For observables,

$$\langle O \rangle = \frac{1}{Z} \int dE O(E) \tilde{\rho}(E) e^{-\beta E} + O(\delta_E^2) = \langle O^{\mathrm{app}} \rangle + O(\delta_E^2)$$

The LLR algorithm - How to compute a_k ?

Define the double-bracket e.v.

$$\langle\langle O \rangle\rangle_k(a) = \frac{1}{\mathcal{N}(a)} \int_{E_k-\delta_E/2}^{E_k+\delta_E/2} dE O(E) \rho(E) e^{-aE}$$

where $\mathcal{N}(a) = \int_{E_k-\delta_E/2}^{E_k+\delta_E/2} \mathrm{d}E\, \rho(E) e^{-aE}$

For the appropriate value of a, $\rho(E)\, e^{-aE}$ is a constant, and

$$\boxed{\langle\langle E - E_k \rangle\rangle_k(a) = f(a) = 0}$$

Two ingredients are necessary to obtain a:

- A way to compute double bracket e.v. --→ Very similar to a simulation at inverse coupling a with energy constraints.
- A way to solve the framed equation --→ Highly non-linear and stochastic, has to be solved iteratively.

The LLR algorithm - How to compute a_k ?

To compute the double bracket e.v., several strategies are possible:

- Perform a constrained Heat Bath, this is a *hard* implementation of the constraint.
- Perform a Global HMC simulation with an additional force, this is a *soft* implementation of the constraint.

To solve the framed equation, one can use the *Newton-Raphson* method and relatives,

$$\cdots \to a_k^{(n-1)} \to a_k^{(n)} \to a_k^{(n+1)} \to \cdots$$

where

$$a_k^{(n+1)} = a_k^{(n)} - \frac{f(a_k^{(n)})}{f'(a_k^{(n)})}$$

Since $f'(a_k^{(n)}) = \langle\langle \Delta E^2 \rangle\rangle(a_k^{(n)})$ this becomes

$$a_k^{(n+1)} = a_k^{(n)} - \frac{12}{n+1} \frac{\langle\langle \Delta E \rangle\rangle_k}{\langle\langle \Delta E^2 \rangle\rangle_k}$$

However, the framed equation is **stochastic, so we use the related Robbins-Monro algorithm**!!

$$a_k^{(n+1)} = a_k^{(n)} - \frac{12}{n+1} \frac{\langle\langle \Delta E \rangle\rangle_k}{\delta_E^2}$$

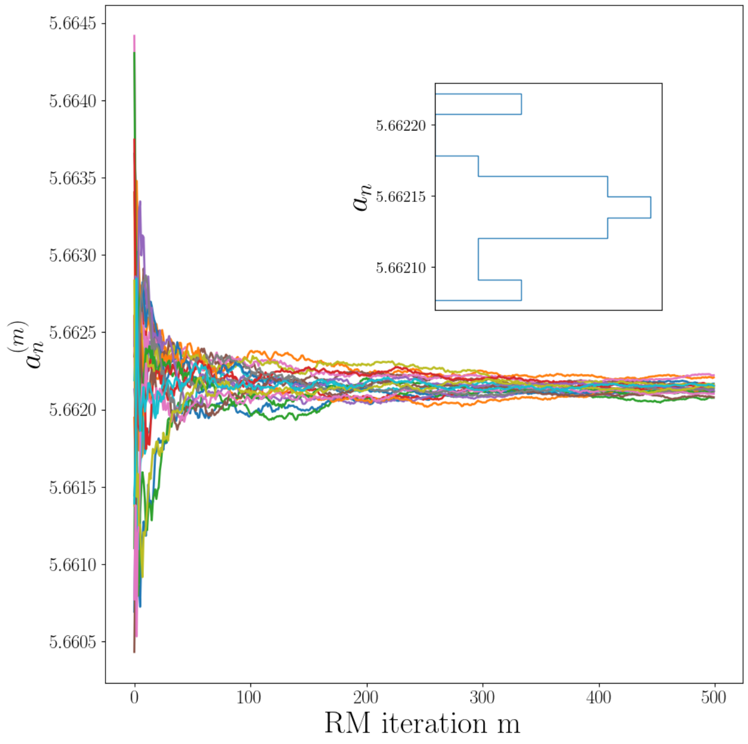
The Robbins-Monro algorithm

In practice:

- **How many updates to measure $<< \mathbf{E} >>_n$?** The more, the best: more lead to smaller oscillations around asymptotic value a*!! In any case, at least enough to sample the entire energy interval $[E-\delta_E/4, E+\delta_E/4]$.

- **How do we choose the initial value of a_k?** It is convenient to perform initial evolutions with the NR algorithm, and then switch to RM updates.

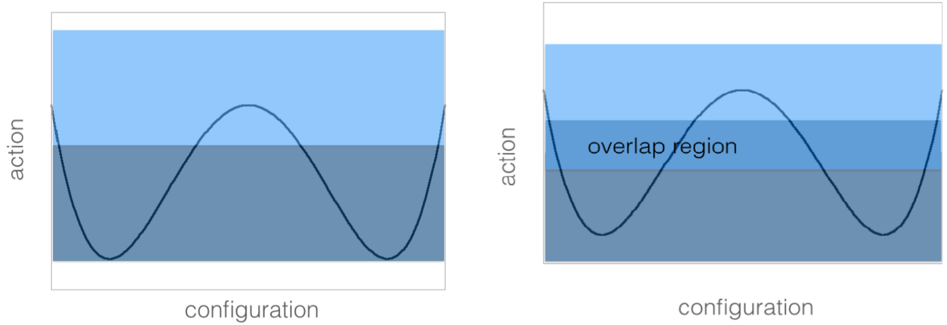
- **When do we stop the iterations of the RM algorithm?** Iterations can be stopped at any time once the distribution of repetitions of the algorithm are *normally* distributed.



[The case of SU(3) LGT. Taken from D.V. et al. PRD (2023)]

Ergodicity - Umbrella sampling

Each replica might remain trapped around a local action minimum.



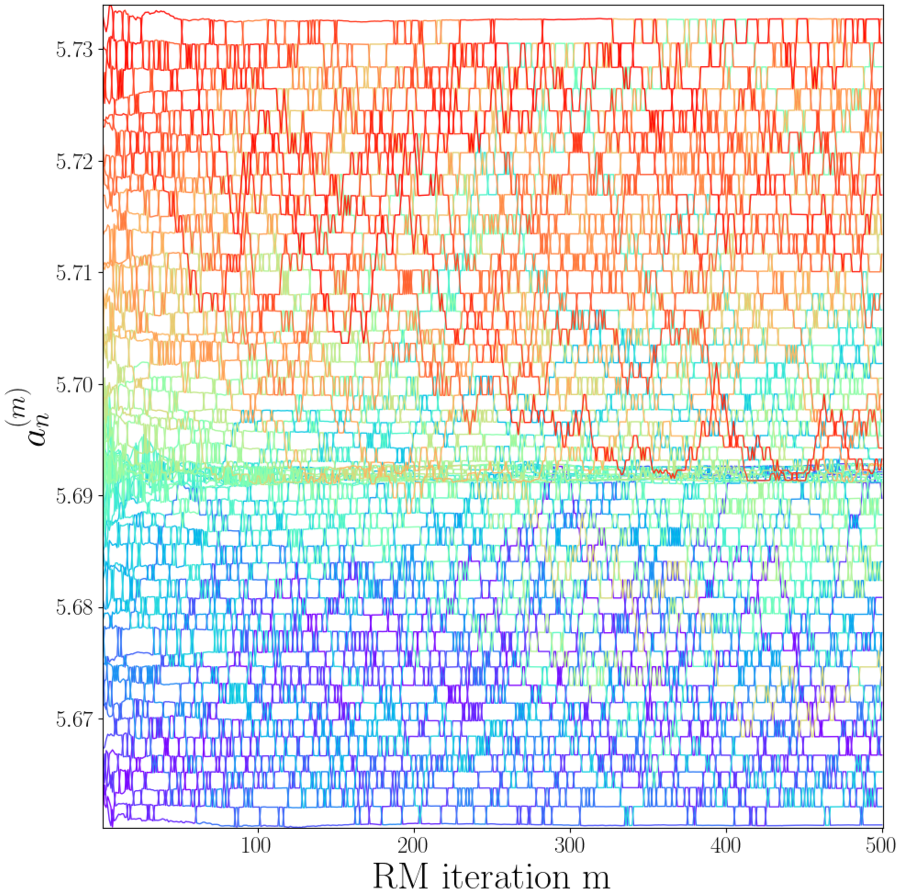
[Taken from Langfeld et al. EPJ C (2016)]

To avoid this:

- Overlapping energy intervals
- Replica exchange

For intervals k and l,

$$P_{\text{swap}} = \min\left(1,\, e^{(a_k - a_l)(E_k - E_l)}\right)$$



[The behaviour of a for replicas as a function of iterations of the RM algorithm. Taken from D.V. et al. PRD (2023)]

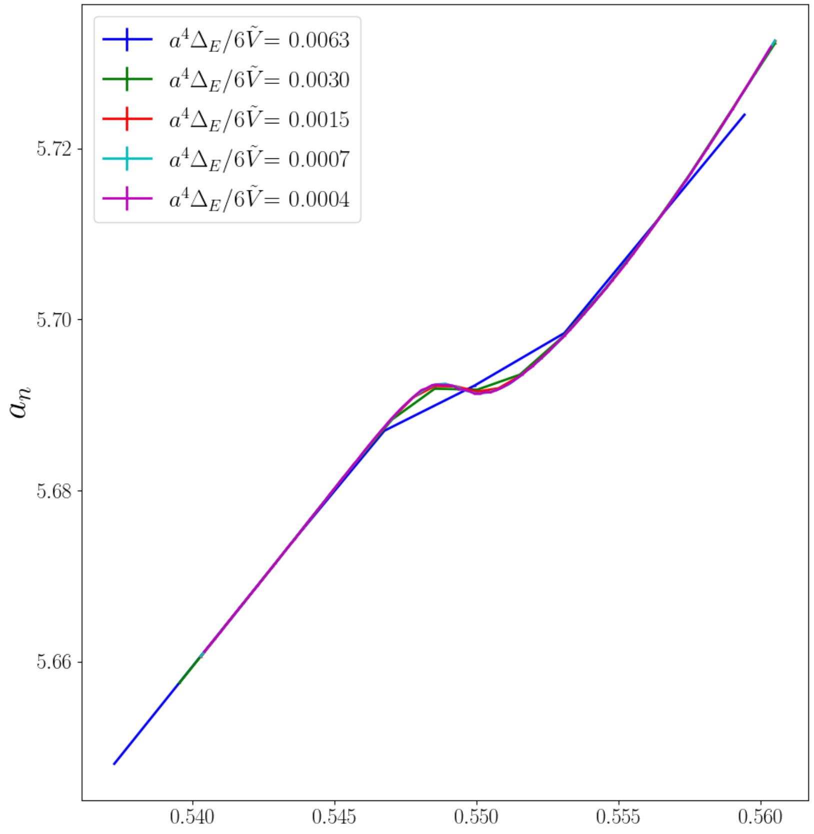
a_k as a function of E - at last!!

To summarize:

- Partition the energy axis in (overlapping) sub-intervals of amplitude δ_E centred at E_n
- For each interval, compute $\langle\langle E \rangle\rangle_n$ and update a
- Exchange replicas to prevent ergodicity problems.
- After an appropriate number of iterations, collect a for each energy interval.

One finally obtains

$$\tilde{\rho}(E) = \prod_{k=1}^{n} e^{c_i + a_i(E - E_k)} \quad = e^{c_n + a_n(E - E_n)}$$



[a_n as a function of u_p for different values of δ_E for the $SU(3)$ LGT. Taken from D.V. et al. PRD (2023)]

A bit of literature

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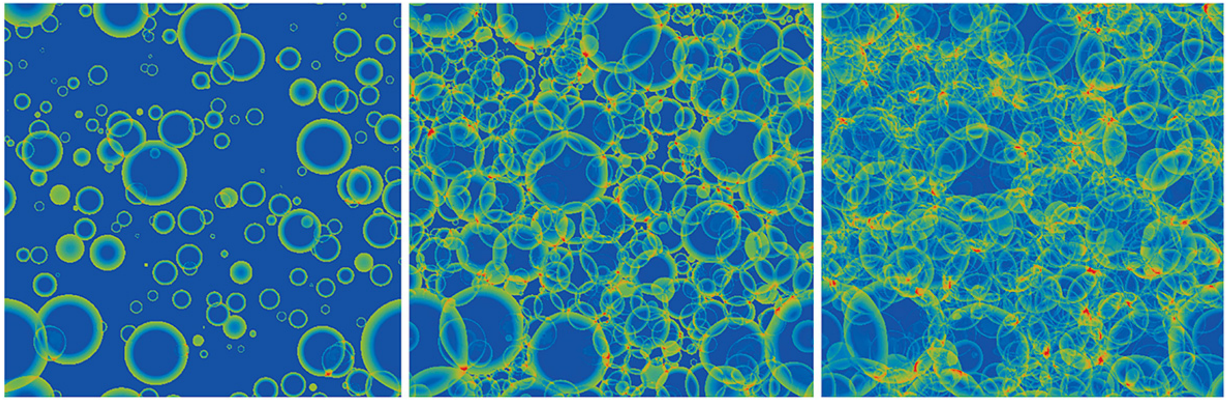
Application to the deconfinement transition of the SU(3) and Sp(4) LGTs

Phase transitions in YM theories - ElectroWeak BaryoGenesis

- EWBG in the SM requires a **strong** 1^{st} order phase transition, which in the SM requires a light enough Higgs (~$70\ GeV$).
- Bubbles are created during the transition: turbulence and their collisions source a background of GWs whose spectrum could be accessible today.
- BSM sectors are necessary to make the transtion stronger and to generate a strong enough CP asymmetry.



[Bubble nucleation, growth and collisions source GWs. Taken from Servant et al. JCAP04014]

The spectrum of the generated GW background depends on:

- The latent heat.
- The critical temperature.
- The bubble nucleation rate.
- The Sphaleron Rate.

Lattice Gauge Theories

- Deconfining phase transition provided the number of fermions is not too large.
- For $N_c > 3$, the phase transition is first order and its strength grows with N_c.
- Order parameter: the Polaykov loop, corresponding to broken centre symmetry.
- Pure gauge theories allow non-perturbative calculations at moderate computational cost.

We specialize to a system defined on a $N_s^3 \times N_t$ hypercubic lattice of spacing a, with an action

$$S = \sum_p \left(1 - \frac{1}{N_c} \Re \operatorname{Tr} U_p\right) \quad (= E)$$

N_c number of colors
U_p elementary plaquette

The partition function is then

$$Z(\beta) = \int \mathcal{D}U \; e^{-\beta S}$$

The temperature is set by $T = 1/N_t a$, where N_t is the number of lattice spacings in the time direction.

Lattice Gauge Theories

Our aims:

- Compute the density of states
- Compute the critical temperature
- Compute the Latent heat
- …?

Our approach:

- We define a workflow and benchmark our approach on the best understood SU(3) theory on one representative lattice of geometry 4 x 20^3.
- We explore more systematically the Sp(4) theory, i.e. we attempt an infinite (spatial) volume limit.

Observables with the LLR

For observables O that depend on E,

$$\langle O \rangle = \frac{1}{Z(\beta)} \int dE O(E) \rho(E) e^{-\beta E}$$

Hence, if we approximate $\varrho(E)$ with

$$\tilde{\rho}(E) = e^{c_n + a_n (E - E_n)}$$

we obtain

$$\langle O \rangle = \sum_{n=1}^{2N-1} \frac{e^{c_n - a_n E_n}}{Z(\beta)} \int_{E_n - \delta_E/4}^{E_n + \delta_E/4} \mathrm{d}E \, O(E) \, e^{(a_n - \beta) E}$$

with

$$Z(\beta) = \sum_{n=1}^{2N-1} e^{c_n - a_n E} \int_{E_n - \delta_E/4}^{E_n + \delta_E/4} \mathrm{d}E \, e^{(a_n - \beta) E}$$

Observables with the LLR - $<u_p>$

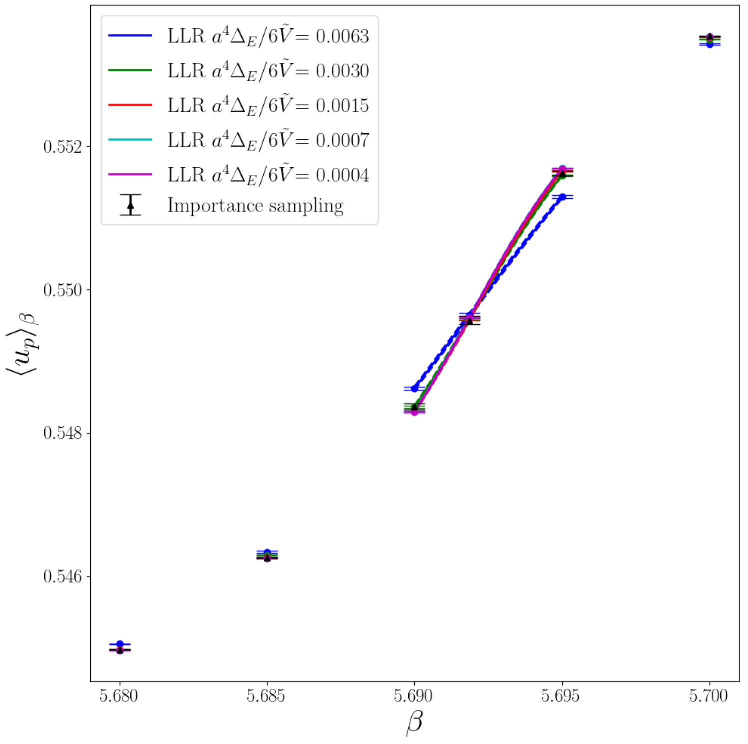
Simplest example and a useful check: $u_p = 1 - \frac{E}{6N_s^3 N_t}$

$$\langle u_p \rangle = \sum_{n=1}^{2N-1} \frac{e^{c_n - a_n E_n}}{Z(\beta)} \int_{E_n - \delta_E/4}^{E_n + \delta_E/4} \mathrm{d}E\, u_p\, e^{(a_n - \beta)E}$$

Analogously one can obtain the specific heat and the Binder cumulant,

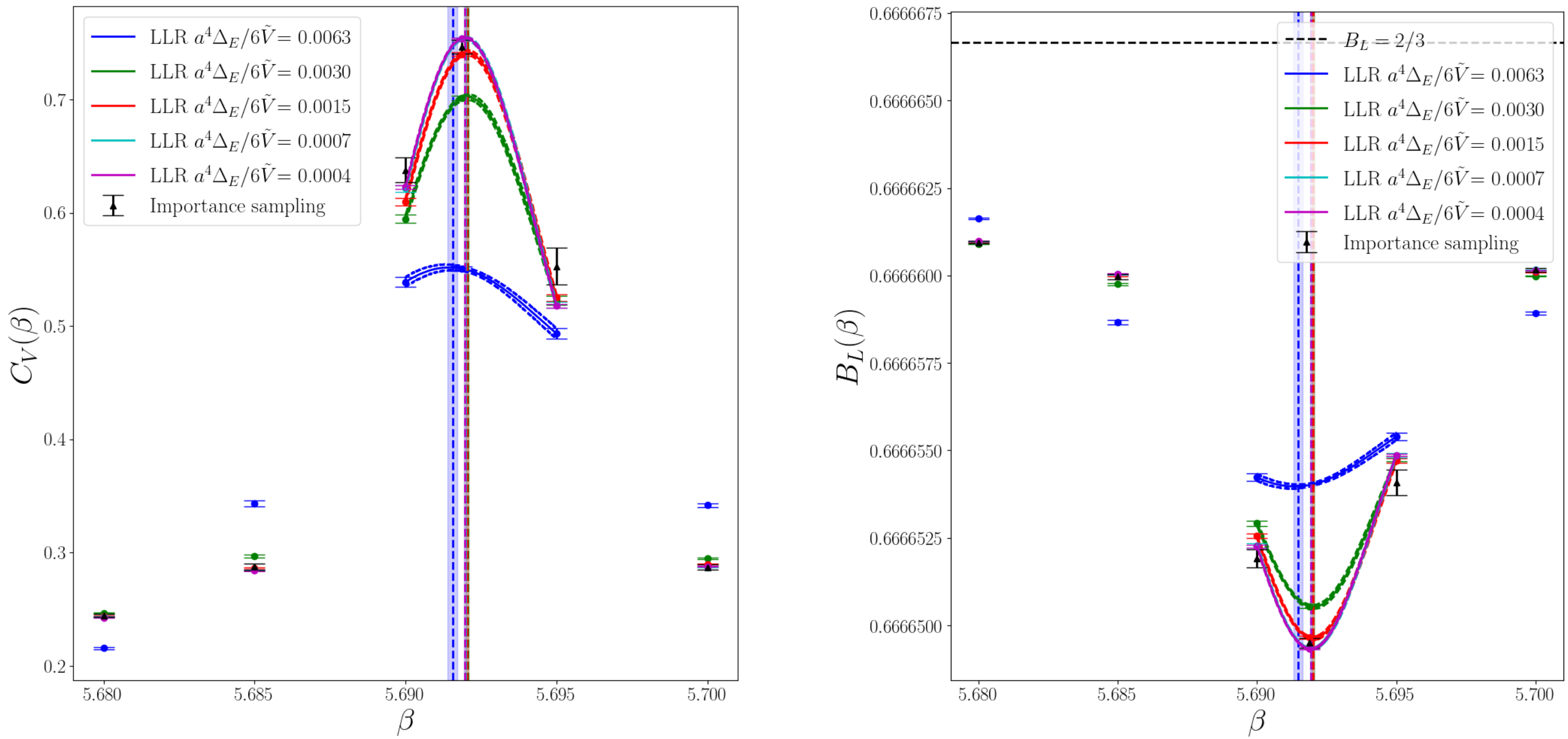
$$C_V(\beta) = 6N_t N_s^3 \left(\langle u_p^2 \rangle_\beta - \langle u_p \rangle_\beta^2\right)$$

$$B_V(\beta) = 1 - \frac{\langle u_p^4 \rangle_\beta}{3\langle u_p^2 \rangle_\beta^2}$$



[Average plaquette in SU(3) gauge theory on a 4×20^4 lattice. Taken from D.V. et al. PRD 108(2023)]

Observables with the LLR - C_V and B_L



[The specific heat and the Binder cumulant as functions of the inverse coupling in SU(3) gauge theory on a 4×20^4 lattice. Taken from D.V. et al. PRD 108(2023)]

Observables with the LLR - u_p distribution

One can easily compute the probability of E

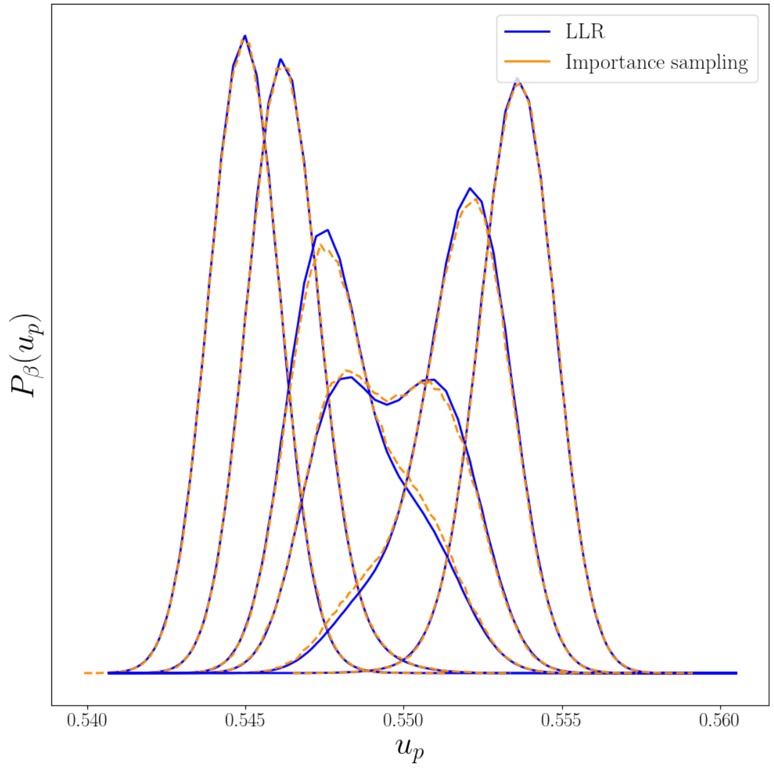
$$P_\beta(E) = \rho(E)\frac{e^{-\beta E}}{Z(\beta)}$$

where

$$E = \frac{6\tilde{V}}{a^4}(1 - u_p)$$

Note:

- Two peaks are present, as expected from a 1st order phase transition
- Small discrepancies can be observed around the peaks and near the bottom of the distributions



[The distribution of E in the SU(3) LGT for several different values of β on a 4×20^3 lattice. Taken from D.V. et al. PRD (2023)]

Critical β

We define the critical inverse coupling in several different ways:

- As the β at which

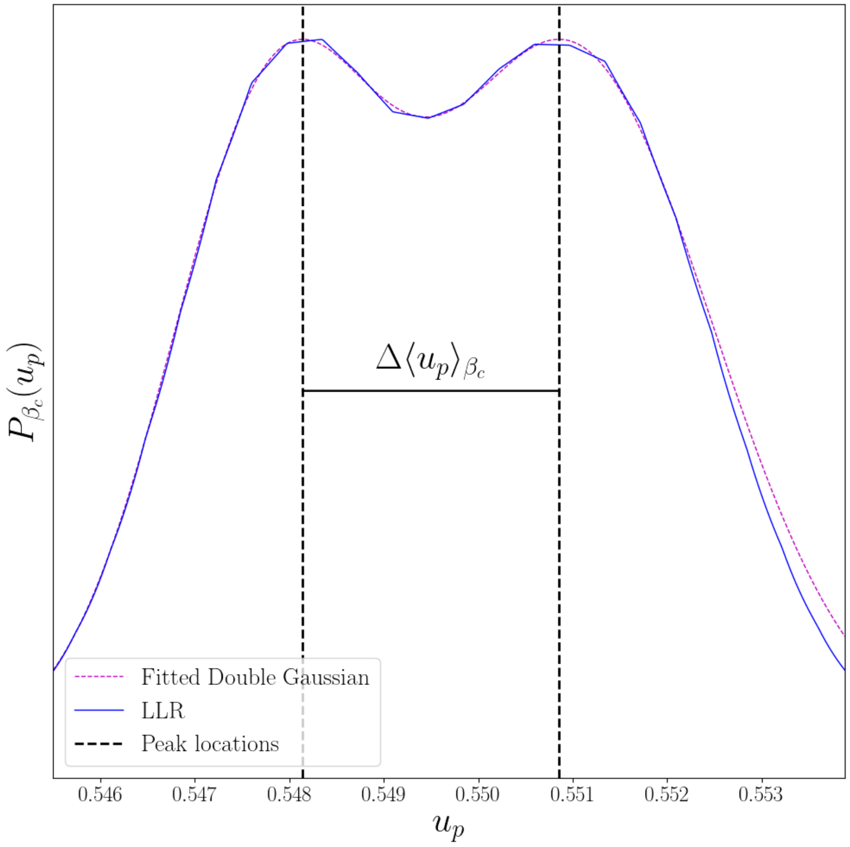
$$P_{\beta_c}(E_+) = P_{\beta_c}(E_-)$$

- As the β at which

$$C_V(\beta) = \frac{6\tilde{V}}{a^4}\left(\langle u_p^2\rangle_\beta - \langle u_p\rangle_\beta^2\right)$$

$$B_V(\beta) = 1 - \frac{\langle u_p^4\rangle_\beta}{3\langle u_p^2\rangle_\beta^2}$$

Have peaks



[The distribution of E in the SU(3) LGT at β_c on a 4×20^3 lattice. Taken from D.V. et al. PRD (2023)]

The Latent Heat

The latent heat can defined from the internal energy density,

$$\varepsilon(T) = \frac{T^4}{V}\frac{\partial \ln Z(T)}{\partial T}$$

as

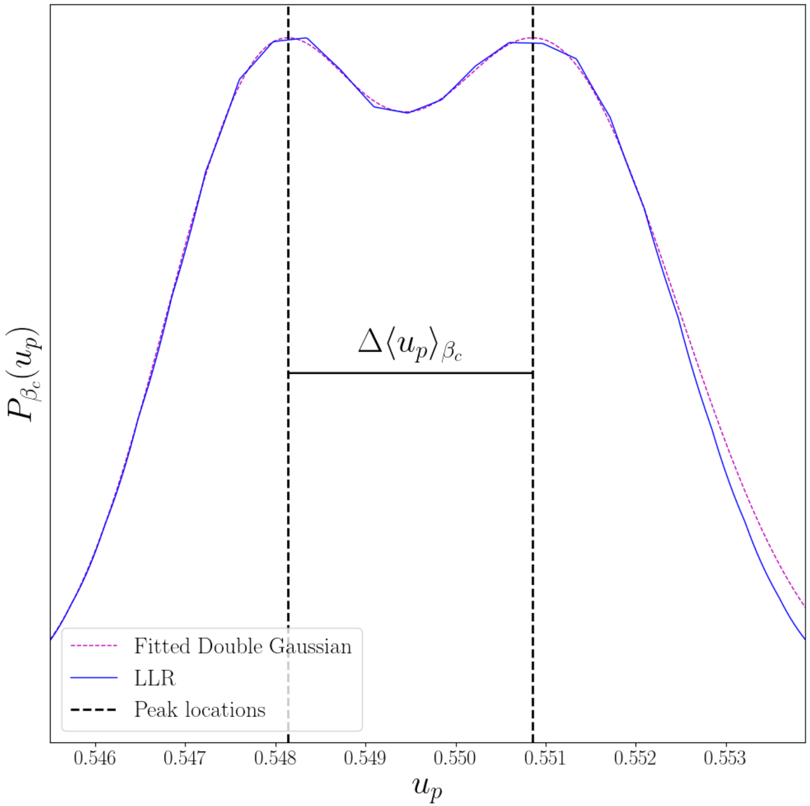
$$L_h = |\varepsilon_+ - \varepsilon_-|$$

Where $\varepsilon_\mp$ are the internal energies of each of the coexisting phases at the critical temperature.

Then
$$\frac{L_h}{T^4} = -\left(6N_t^4 a\frac{\partial\beta}{\partial a}\Delta\langle u_p\rangle_\beta\right)_{\beta=\beta_c}$$

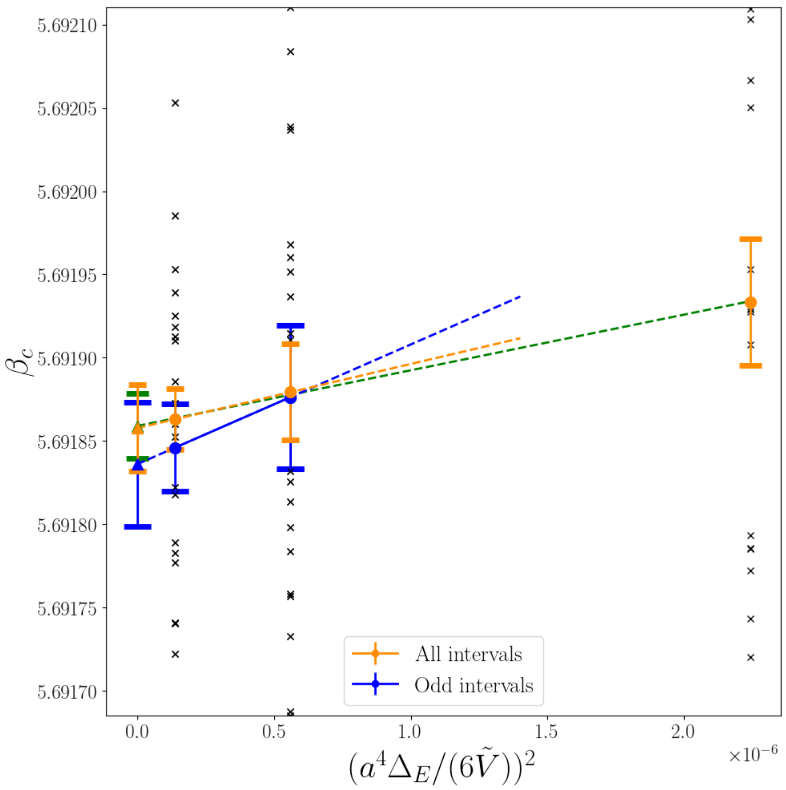
where

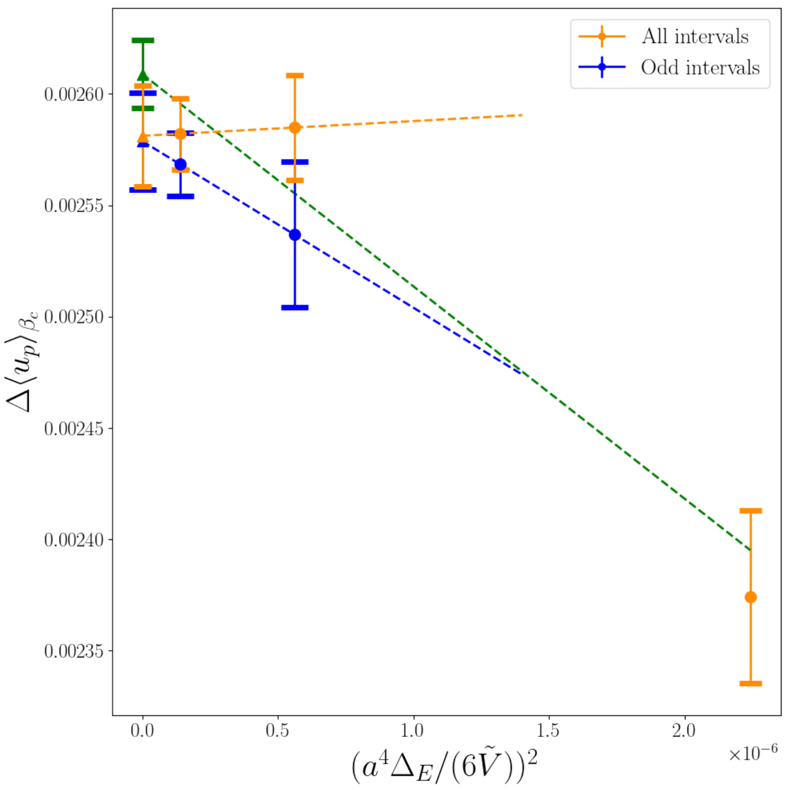
$$\Delta\langle u_p\rangle_\beta = |u_{p+} - u_{p-}|$$



[The distribution of E in the SU(3) LGT at β_c on a 4×20^3 lattice. Taken from D.V. et al. PRD (2023)]

The $\delta_E \to 0$ limit for β_c and Δu_p





Note: for SU(3) <u>in infinite volume</u> at N_t=4, β_c=5.69236(15)

From [Lucini, Teper, Wegner JHEP 01 061(2005)]

[The results for the calculation of β_c and Δ<u_p> on a 4×20^3 lattice for several values of δ_E^2. Taken from D.V. et al. PRD (2023)]

The LLR algorithm - Thermodynamics

From

$$s(E) = \log \rho(E) \simeq \log \prod_{k=1}^{n} e^{c_k + a_k (E - E_k)}$$

One obtains

$$F(t) = E - t\,s = f(t)\tilde{V}$$

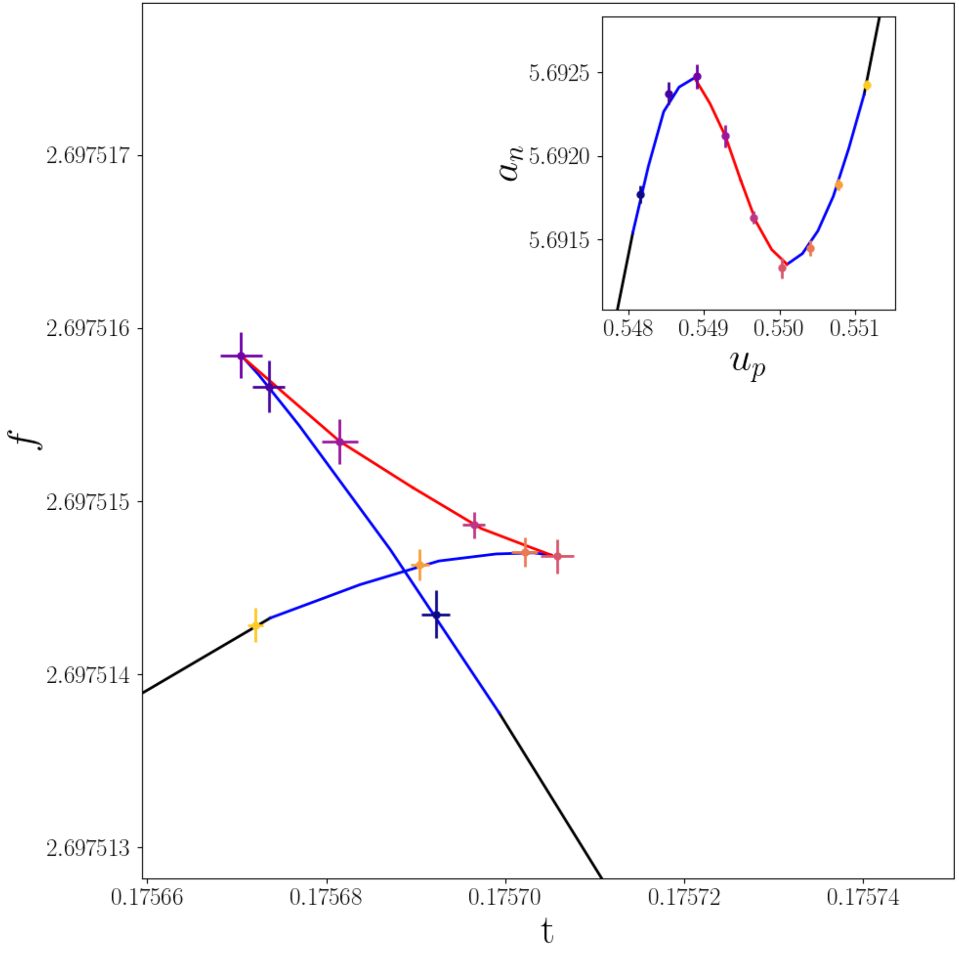
with

$$\frac{1}{t} = \frac{\partial s(E)}{\partial E} = a_i$$

(inverse) microcanonical temperature.

Note the color coding:

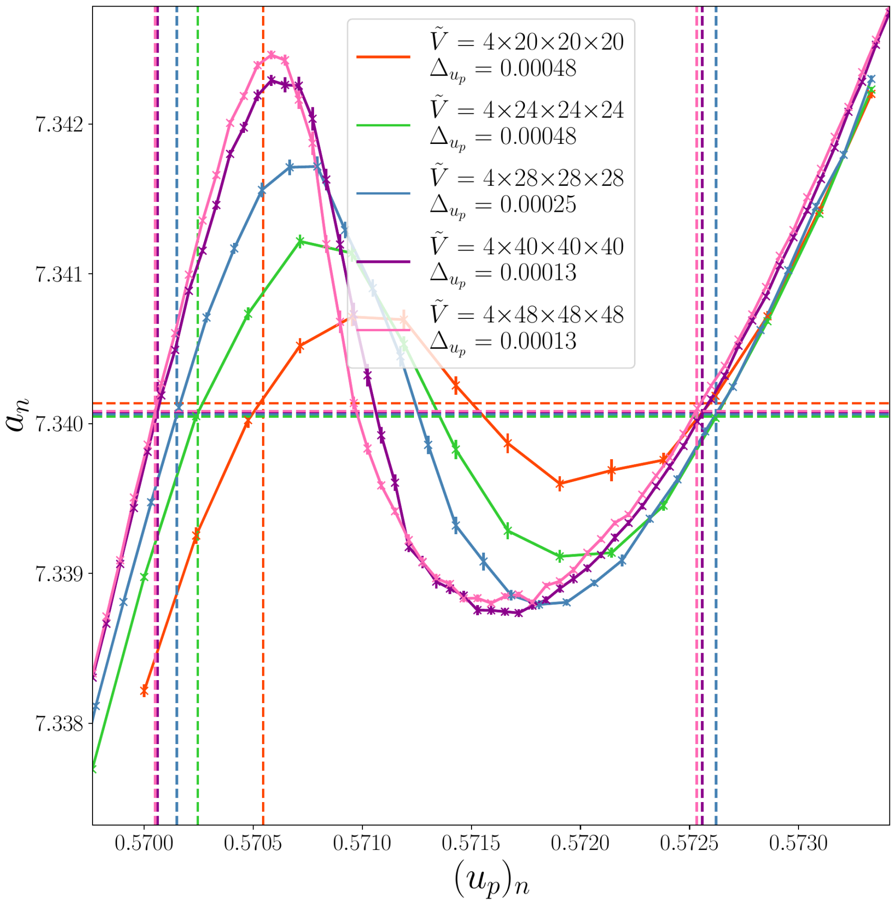
- In **black**, f is single valued
- In **blue**, f is multivalued, we have metastable states
- In **red**, unstable states

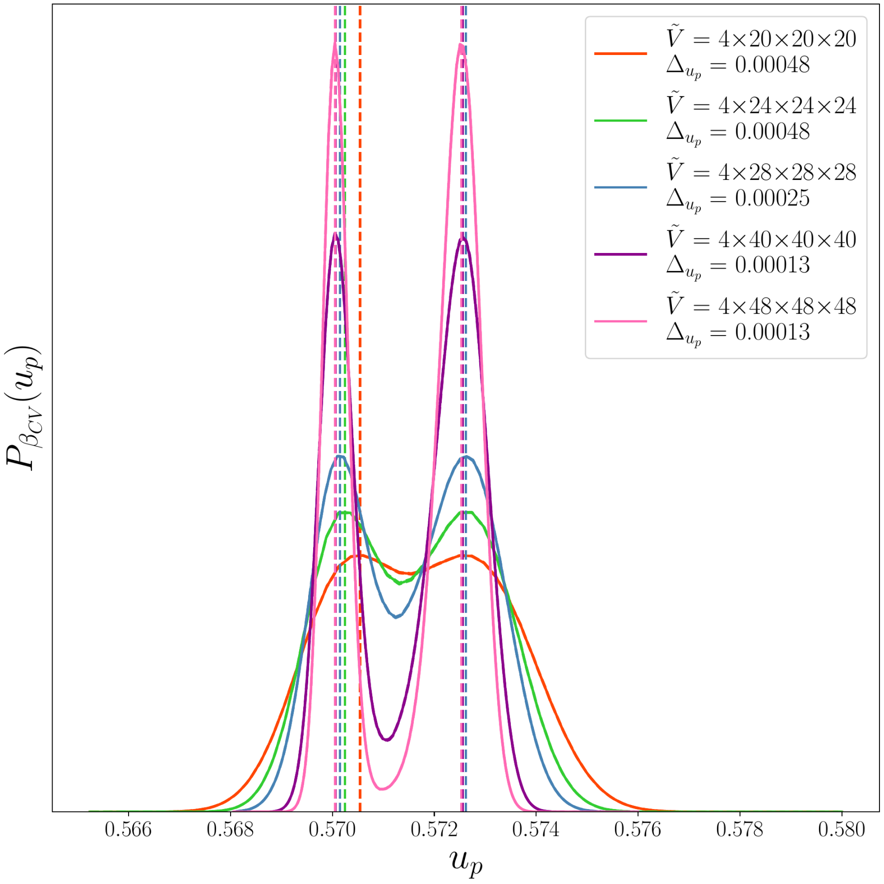


[Taken from D.V. et al. PRD (2023)]

A snapshot of the results for the Sp(4) LGT

The Sp(4) LGT - critical β_c and Latent Heat





The Sp(4) LGT - critical β

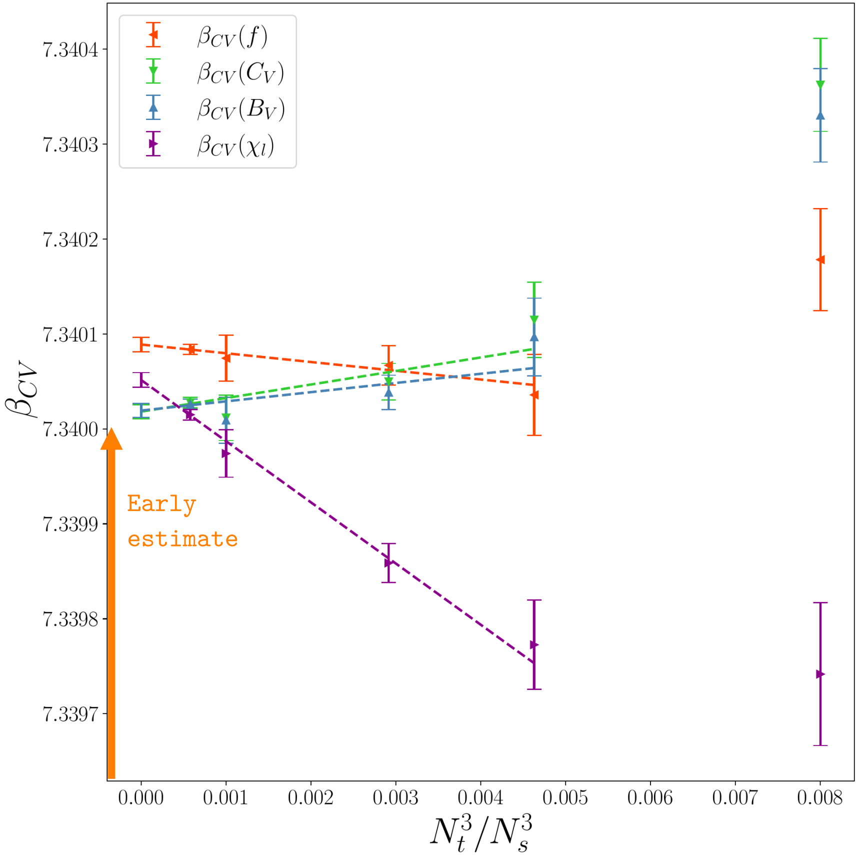
Early estimate:

$$\beta_c = 7.339(1)$$

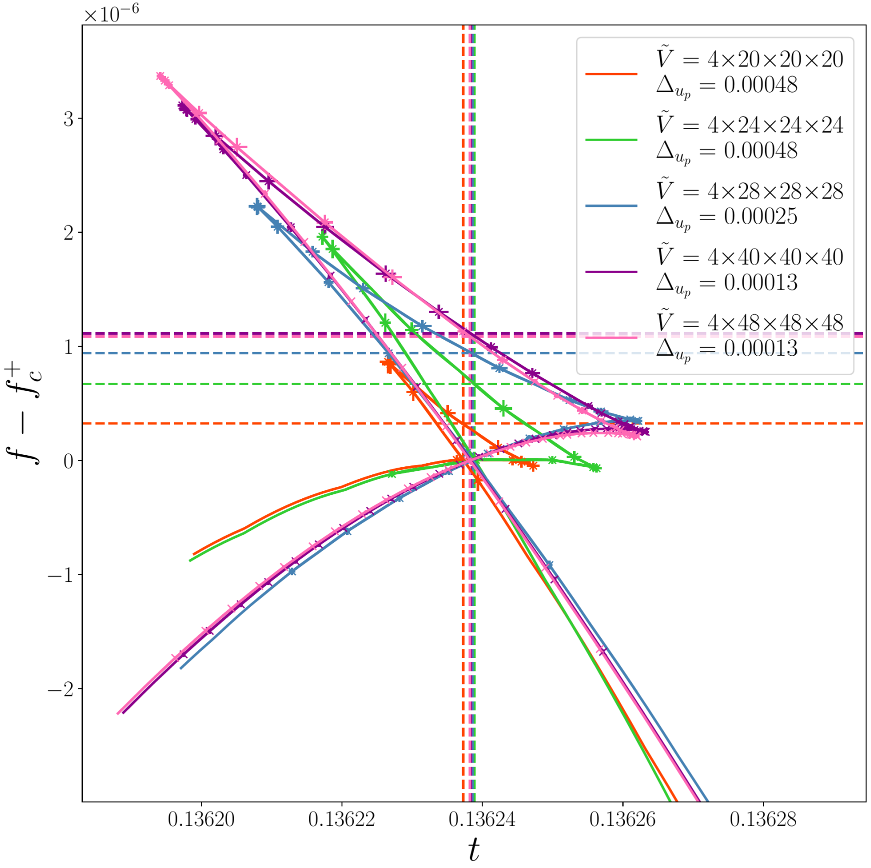
In *[Pepe, Wiese, Holland, Nucl. Phys. B 694 (2008)]*.

Note thatm in the $N_t/N_s \to 0$ limit:

- Our results are compatible with the early estimate
- Our errors are two orders of magnitude smaller
- Our errors are perhaps a bit too small!! (systematics…?)



The Sp(4) LGT - Thermodynamics



Conclusions

- An LLR workflow for the SU(3) LGT was probed for one representative lattice.
- The Sp(4) LGT were explored more systematically. Preliminary results seem to be compatible with expectations, but some more work is needed to reach the continuum limit.
- In general, the LLR seems to offer interesting possibilities, namely access information that is otherwise difficult to obtain.

Thank you for your attention!

Appendices

The effect of the Interface

If we ignore mixed phases, then

$$P_\beta(E) = P_\beta^+(E) + P_\beta^-(E)$$

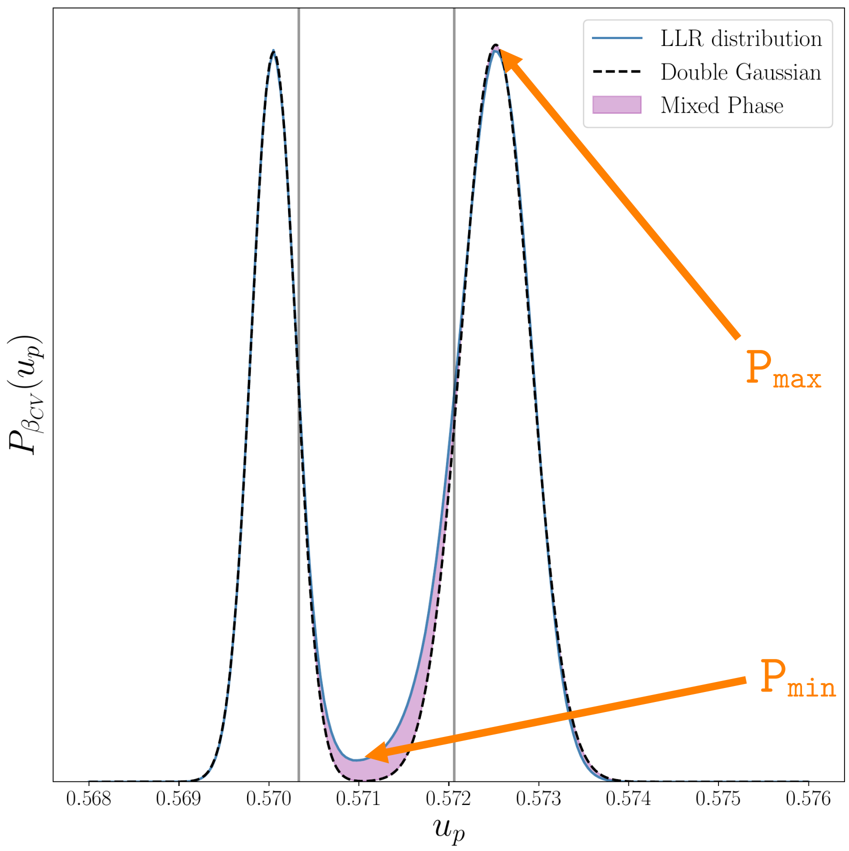
Where $P_\beta^\pm(E)$ are Gaussians

- A discrepancy with a sum of two Gaussians is apparent in the internal region
- We expect this to be caused by an **interface** with tension

$$\tilde{I} = -\frac{N_t^2}{2N_s^2}\log\frac{P_{\min}}{P_{\max}} - \frac{N_t^2}{4N_s^2}\log(N_s)$$

where

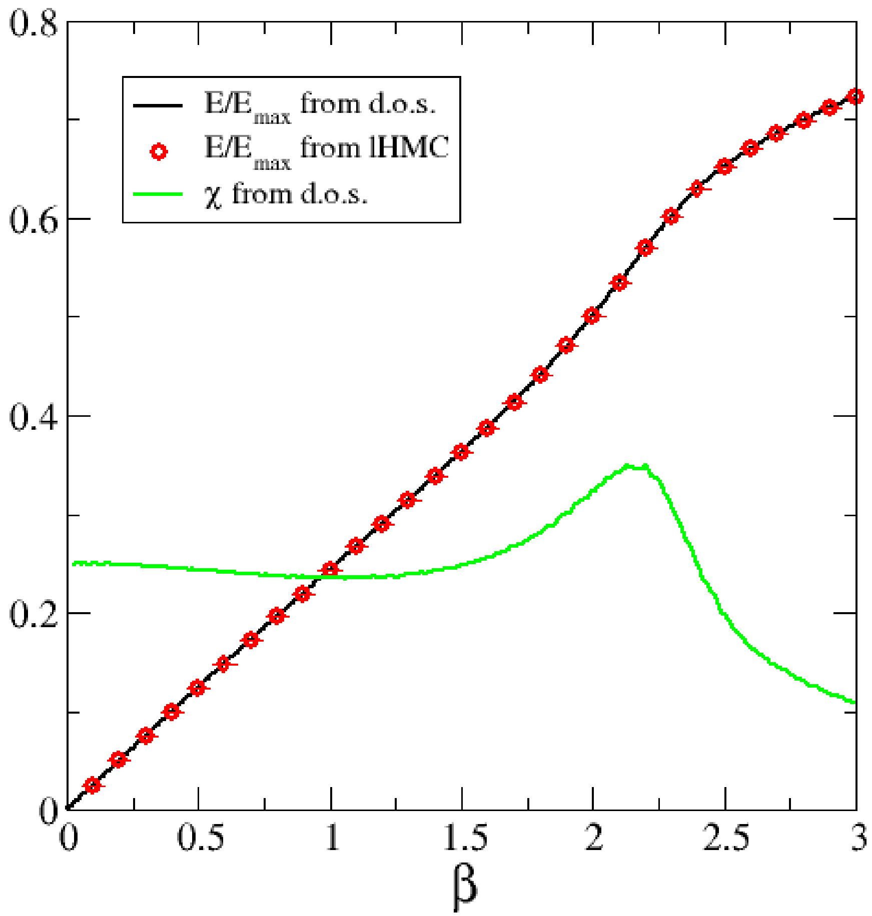
$$\lim_{N_t/N_s\to 0}\tilde{I} = \frac{\sigma_{cd}}{T_C^3}$$



[Taken from D.V. et al. PRD 108 (2023)]

σ_{cd} Confined-deconfined interface tension

The average plaquette - SU(2) LGT



The Robbins-Monro algorithm

$$a_{n+1} = a_n - c_n \left(N(a_n) - \alpha \right)$$

If c_n satisfies

$$\sum c_n = \infty \qquad \sum c_n^2 < \infty$$

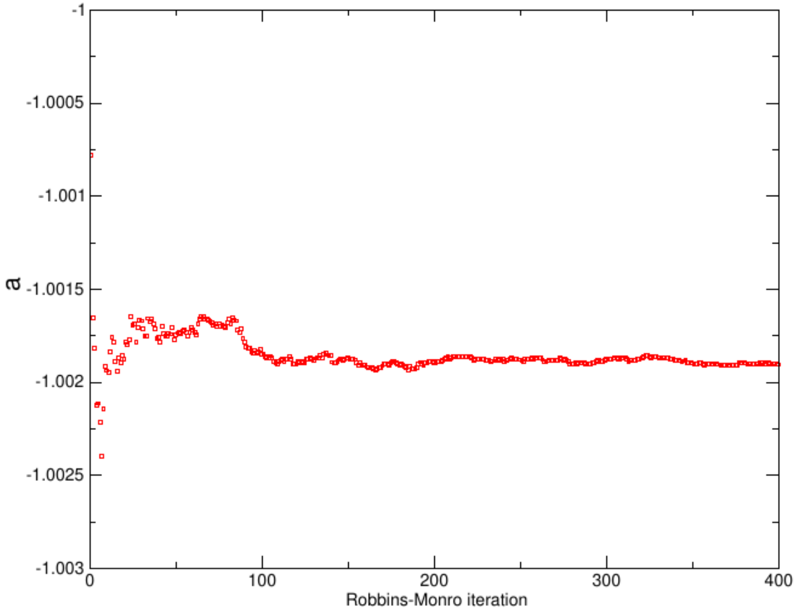
And other very general assumptions, then

$$\sqrt{n} \left(a_n - a^\star \right)$$

Is normally distributed around 0.

We can choose $c_n{=}c/(n{+}1)$ and

$$a_{n+1} = a_n - \frac{12}{n+1} \frac{\langle\langle \Delta E \rangle\rangle_n}{\delta_E^2}$$

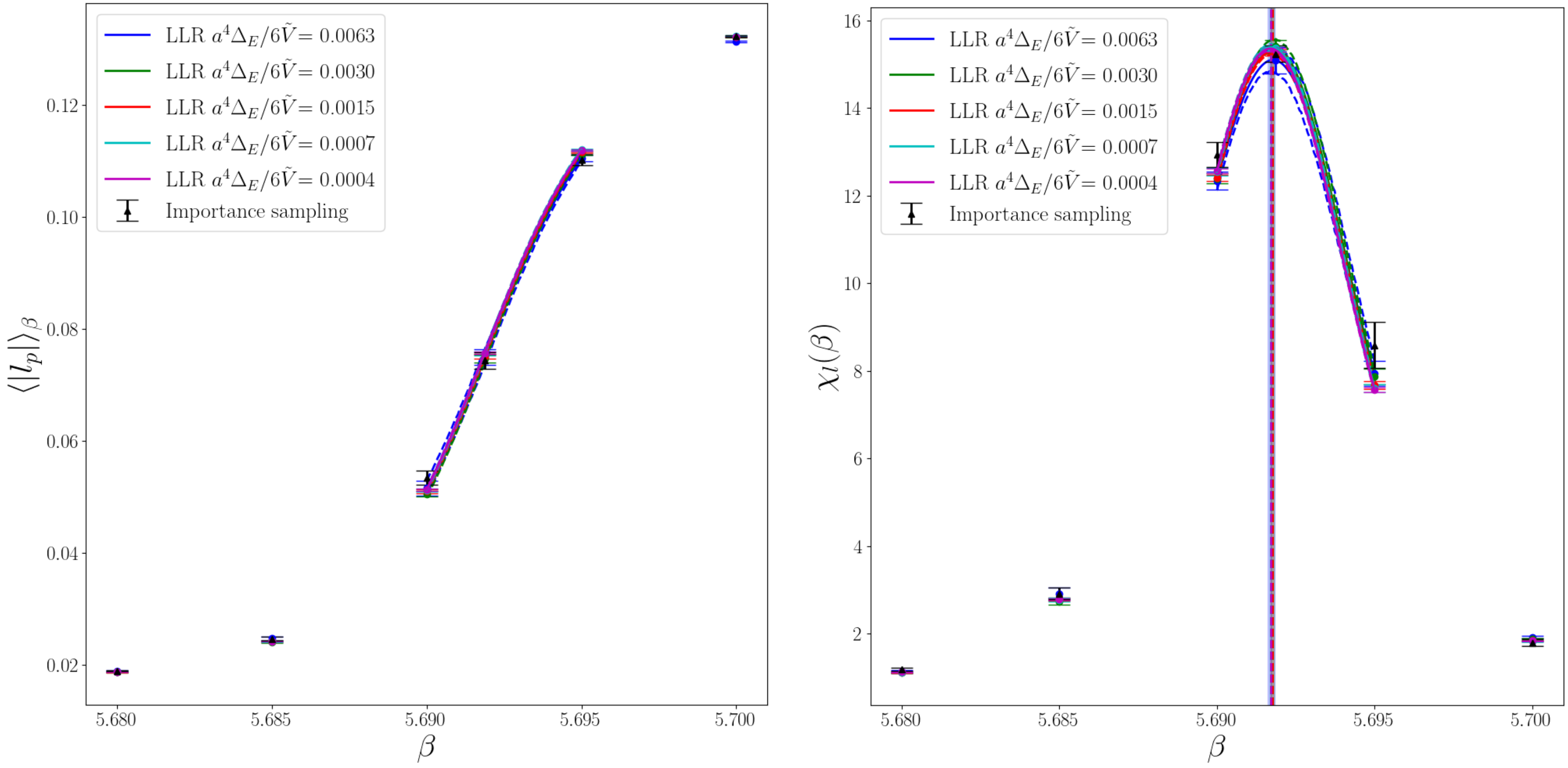


[The case of the U(1) theory. Taken from Langfeld et al. EPJ C (2016)]

It was shown by Robbins and Monro that:

- The values of a are normally distributed around asymptotic value
- The variance decreases as $1/n^2$

SU(3) Polyakov loop and its susceptibility



[The Polyakov loop e.v. and its susceptibility as functions of the inverse coupling in SU(3) gauge theory on a 4×20^4 lattice. Taken from D.V. et al. PRD 108(2023)]