Ergodic sampling with the density of states

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Outline

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The density of states

Let us consider an Euclidean quantum field theory

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

The density of states is defined as

$$\rho(E) = \int [D\phi] \delta_E(S[\phi] - E)$$

which leads to

$$Z(\beta) = \int dE \rho(E) e^{-\beta E} = e^{-\beta F}$$

$\hookrightarrow$ if the density of states is known then free energies and expectation values are accessible via a simple integration, e.g. for an observable that depends only on E

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

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But is the computation of $\rho(E)$ any easier?

LLR express

- Divide the (continuum) energy interval in N sub-intervals of amplitude δ_E
- 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

$$\lim_{m \to \infty} a_n^{(m)} = a_n \;, \qquad a_n^{(m+1)} = a_n^{(m)} - \frac{\alpha}{m} \frac{\langle\langle \Delta E \rangle\rangle_{a_n^{(m)}}}{\langle\langle \Delta E^2 \rangle\rangle_{a_n^{(m)}}}$$

At fixed m, Gaussian fluctuations of $a_n^{(m)}$ around a_n

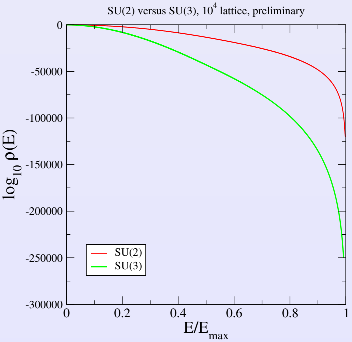
- Define

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

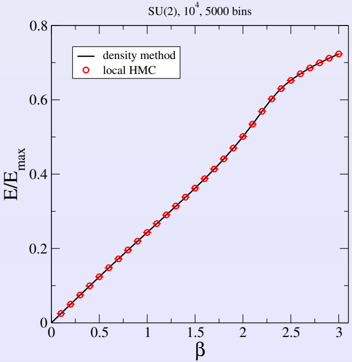
[Langfeld, Lucini and Rago, Phys. Rev. Lett. 109 (2012) 111601; Langfeld, Lucini, Pellegrini and Rago, Eur. Phys. J. C76 (2016) no.6, 306]

Exponential error suppression – YM

Density of states (LLR result)



Reconstructed plaquette for SU(2)



Exponential error reduction is at work!

(K. Langfeld, B. Lucini and A. Rago, Phys. Rev. Lett. 109 (2012) 111601)

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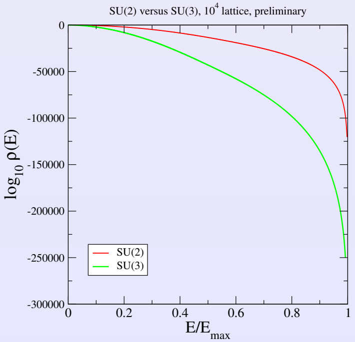
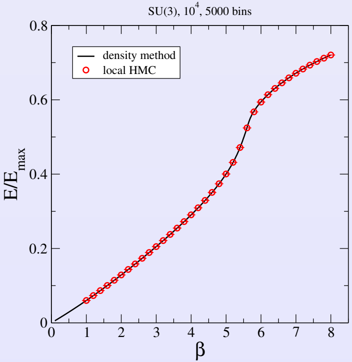


Reconstructed plaquette for SU(3)



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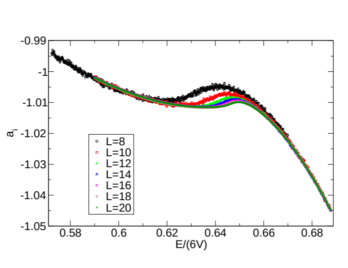
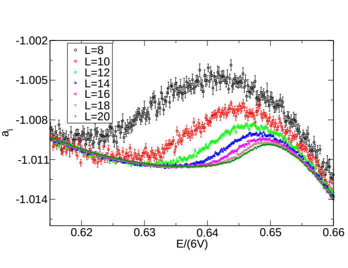
4D U(1) LGT: a vs E_0



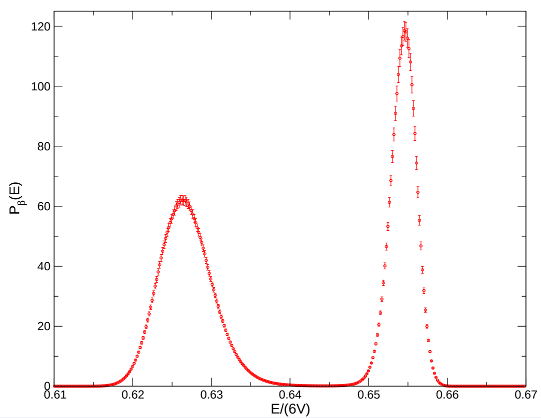


- The non-monotonicity is a signature of a first order phase transition
- The a seem to converge to their thermodynamic limit

(K. Langfeld, B. Lucini, R. Pellegrini and A. Rago, Eur. Phys. J. C76 (2016) no.6, 306, arXiv:1509.08391)

The phase transition in 4D U(1) LGT

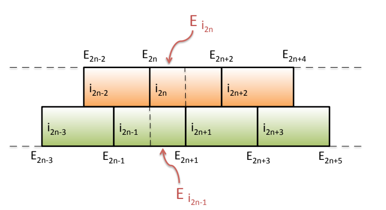
Probability distribution on a 20^4 lattice at pseudo-critical point (current "world record")



(K. Langfeld, B. Lucini, R. Pellegrini and A. Rago, Eur. Phys. J. C76 (2016) no.6, 306, arXiv:1509.08391)

Replica exchange

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

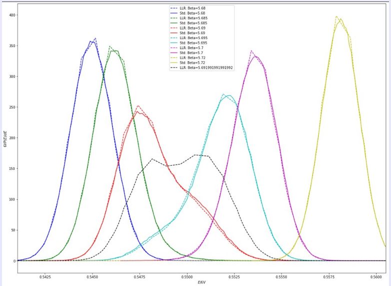


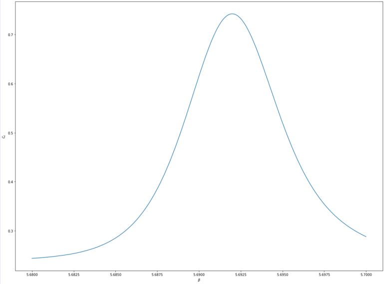
After a certain number m of Robbins-Monro steps, we check if both energies in two overlapping intervals are in the common region and if this happens we swap configurations with probability

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

Subsequent exchanges allow any of the configuration sequences to travel through all energies, hence overcoming trapping
(B. Lucini, W. Fall and K. Langfeld, PoS LATTICE **2016** (2016) 275)

The deconfinement phase transition in SU(3)





Lattice size $20^3 \times 4$

(B. Lucini, D. Mason, M. Piai, E. Rinaldi, D. Vadacchino, in progress)

Sharp vs. smooth cut-off

Algorithmic modification: for double-angle expectation values $\langle\langle O(E)\rangle\rangle$, we have replaced

$$\theta(E_i + \delta_E/2 - E)\theta(E - E_i + \delta_E/2) \qquad \to \qquad e^{-\frac{(E-E_i)^2}{2\delta_E^2}}$$

Minimal modification of the recursion relation, but amenable to simulations with an unconstrained global HMC (and hence to parallelisation)

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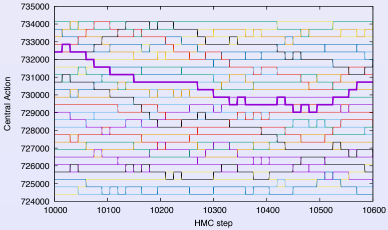
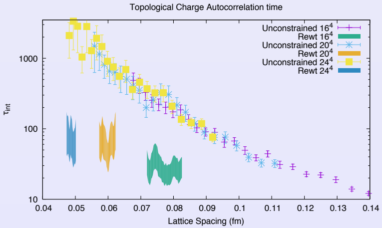
$\hookrightarrow$ First step towards inclusion of dynamical fermions?

Decorrelation of topology in SU(3)





Correlation time reduced by one order of magnitude at fine lattice spacing

(G. Cossu, D. Lancaster, B. Lucini, R. Pellegrini and A. Rago, Eur. Phys. J. C81 (2021) 4, 375)

Outline

The sign problem

The sign problem is a **numerical** difficulty that arises from the obstruction in implementing importance sampling methods if the action is complex

Prototype example

$$Z(\beta) = \int [D\phi] e^{-\beta S_R[\phi] + i\mu S_I[\phi]}$$

- $\mu = 0 \Rightarrow [D\phi] e^{-\beta S_R[\phi]}$ can be interpreted as a Boltzmann weight and standard Markov Chain Monte Carlo methods can be used in numerical studies
- $\mu \neq 0 \Rightarrow$ the path integral mesure does not have an interpretation as a Boltzmann weight and standard Markov Chain Monte Carlo methods fail spectacularly

Examples: QCD at non-zero baryon density, dense quantum matter, strongly correlated electron systems, . . .

Note that

- There is no algorithm that solves all systems affected by the sign problem, unless $P = NP$ (Troyer-Wiese)
- The problem might be just due to an unfortunate choice of variables (some systems solved by duality!)

The generalised density of states

Let us consider an Euclidean quantum field theory with complex action

$$Z(\beta) = \int [D\phi] e^{-\beta S[\phi] + i\mu Q[\phi]}$$

The generalised density of states is defined as

$$\rho(q) = \int [D\phi] e^{-\beta S[\phi]} \delta(Q[\phi] - q)$$

which leads to

$$Z(\mu) = \int dq \rho(q) e^{i\mu q}$$

The integral is strongly oscillating and hence $\rho(q)$ needs to be known with an extraordinary accuracy

Sign problem as an overlap problem

The severity of the sign problem is indicated by the *vev* of the phase factor in the phase quenched ensemble:

$$\langle e^{i\mu q} \rangle = \frac{Z(\mu)}{Z(0)} = e^{-V\Delta F} \to 0 \qquad \text{exponentially in } V$$

In this language, the sign problem is an *overlap problem*

The LLR algorithm can solve severe overlap problems

However, one still needs to perform the integral with the required accuracy, and for this the most direct approach does not work

Proposed solutions:

- *compression* of the generalised density of states, e.g.

$$\log \rho(q) = \sum_{i=1}^{k} \alpha_i q^{2i}$$

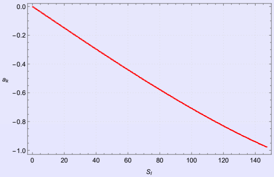
  with the polynomium to be fitted (Langfeld and Lucini)
- cumulant expansion through polynomial fit (Garron and Langfeld)

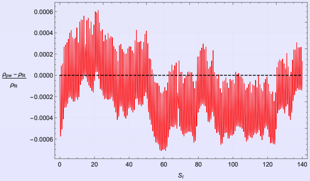
The Bose Gas

The model

$$\begin{aligned} S &= \sum_i \left[\frac{1}{2} \left(2d + m^2 \right) \phi_{a,i}^2 + \frac{\lambda}{4} \left(\phi_{a,i}^2 \right)^2 - \sum_i \sum_{\nu=1}^{3} \phi_{a,i} \phi_{a,i+\hat{\nu}} \right] \\ & \sum_i \left[-\cosh(\mu)\, \phi_{a,i} \phi_{a,i+\hat{4}} + i \sinh(\mu)\, \varepsilon_{ab} \phi_{a,i} \phi_{b,i+\hat{4}} \right] \\ &= S_R + i \sinh(\mu) S_I \end{aligned}$$

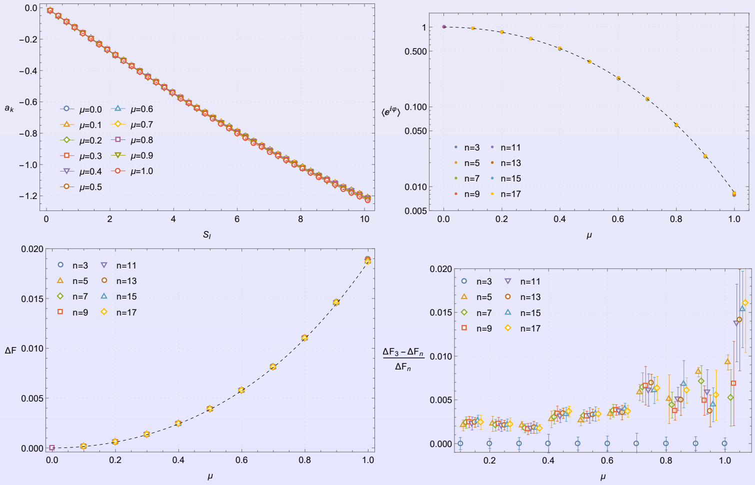
Oscillations of the piecewise approximation need to be treated through smoothing





(Example for $V = 8^4$, $m = \lambda = 1$, $\mu = 0.8$)

Results for $V = 4^4$



Region of fit stability not obvious when μ increases

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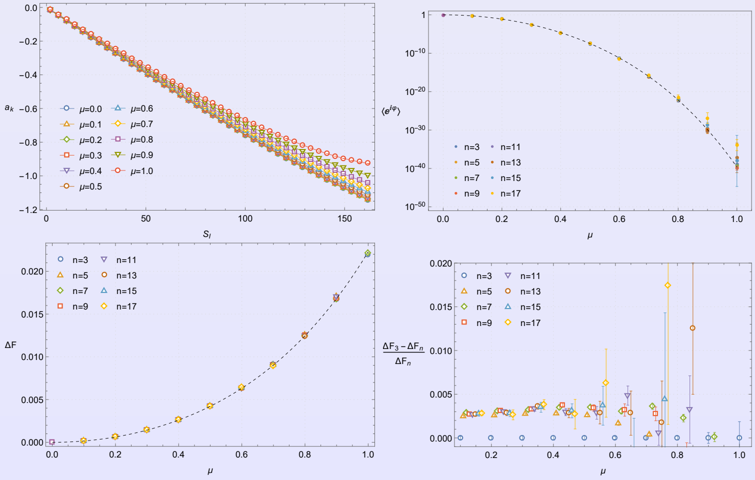
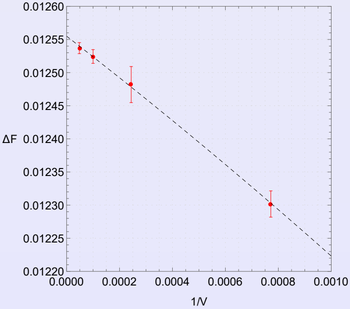


Fit stability seems to get worse as V increases

ΔF in the thermodynamic limit

For the Bose Gas at $\mu = 0.8$



$$\Delta F = (0.012557 \pm 0.000004) - \frac{(0.329 \pm 0.008)}{V} \, , \qquad \Delta F_{MF} \simeq 0.012522$$

Expected asymptotics seem to describe the data accurately
Small deviation from mean-field visible

(O. Francesconi, M. Holzmann, B. Lucini and A. Rago, Phys. Rev. D101 (2020) 1, 014504)

Outline

Conclusions and outlook

- For systems with a real action, the LLR algorithm has advantages over traditional importance sampling in cases in which exponentially suppressed signals need to be measured
- Supplemented with some smoothing technique or cumulant expansion, the LLR algorithm can solve the sign problem (tested in the $\mathbb{Z}(3)$ model, $\lambda\phi^4$ and Heavy-Dense QCD)
- Possible future applications:
  - Gravitational wave signatures from early-universe phase transitions
  - Systems with fermions
  - Proof of concept of the solution of the sign problem in QCD (e.g. small lattices)