

A density-of-states method for Lattice Gauge Theories

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(partially) based on :

[K. Langfeld, B. Lucini, AR, *Phys.Rev.Lett.* **109** (2012)]

[R. Pellegrini, K. Langfeld, B. Lucini, AR, *PoS LATTICE2014* (2015)]

[K. Langfeld, B. Lucini, AR, R. Pellegrini and L. Bongiovanni, *J. Phys. Conf. Ser.* **631** (2015)]

[K. Langfeld, B. Lucini, R. Pellegrini and AR, *Eur. Phys. J. C* **76** (2016)]

Motivations

- A large part of the success of Lattice Gauge Theory inherently tied with advances in Monte Carlo simulations
- Monte Carlo methods used in Lattice Gauge Theory are importance sampling methods
- Most quantities of interest can be expressed in the path integral formalism as ensemble averages over a positive-definite (and sharply peaked) measure.
- Importance sampling methods are inefficient for
 - ▶ Studying systems with strong metastabilities or more generically systems with a rough free action landscape.
 - ▶ Direct computations of free energies.
 - ▶ Every time exceptional configurations play a role.
 - ▶ Studying systems with a sign problem.

An alternative approach to numerical simulations could accelerate progress in those cases (or at least in some of those).

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

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

which leads to

$$Z[\beta] = \int d\mathcal{S} e^{-\beta \mathcal{S}} \rho(\mathcal{S})$$

But is the computation of $\rho(\mathcal{S})$ any easier?

Density of states

- The computation of $\rho(\mathcal{S})$ has been attempted many times in the past (e.g. reweighting), with limited success
- A breakthrough has been the Wang-Landau algorithm, which is a numerical technique to extract the density of states in statistical mechanics using a non-Markovian process (random walk in configuration space with Boltzmann weights depending on the history of the system) [Wang and Landau, *Phys. Rev. Lett.* 86 (2001)]
- Due to the fact that the algorithm relies on a frequency histogram, a direct generalisation to continuum systems does not seem very efficient
- For continuous systems, we need a method that iteratively compute a continuous density of state

The Logarithmic Linear Relaxation (LLR)

Consider the action interval $[\mathcal{S}_k - \delta_S/2, \mathcal{S}_k + \delta_S/2]$.

If the density of states is a smooth function in this interval, the logarithm of the latter quantity can be written as

$$\ln \rho(\mathcal{S}) \sim \ln \rho(\mathcal{S}_k) + \left. \frac{d \ln \rho}{d\mathcal{S}} \right|_{\mathcal{S}=\mathcal{S}_k} (\mathcal{S} - \mathcal{S}_k) + \frac{1}{2} \left. \frac{d^2 \ln \rho}{d\mathcal{S}^2} \right|_{\mathcal{S}=\mathcal{S}_k} (\mathcal{S} - \mathcal{S}_k)^2 + \mathcal{O}((\mathcal{S} - \mathcal{S}_k)^3).$$

Our goal will be to devise a numerical method to calculate the Taylor coefficients

$$a_k = \left. \frac{d \ln \rho}{d\mathcal{S}} \right|_{\mathcal{S}=\mathcal{S}_k}$$

Why should this be a good expansion?

$$\left. \frac{d \ln \rho}{d\mathcal{S}} \right|_{\mathcal{S}=\mathcal{S}_k} = a_k = \frac{1}{T_k} \qquad \left. \frac{d^2 \ln \rho}{d\mathcal{S}^2} \right|_{\mathcal{S}=\mathcal{S}_k} = -\frac{1}{T_k^2} \frac{1}{c_k}.$$

T_k and c_k are *intrinsic* quantities

The Logarithmic Linear Relaxation (LLR)

Our program:

- Divide the action interval in N sub-intervals of amplitude δ_S , each centered at $\mathcal{S}_i = \mathcal{S}_{\min} + (i - \frac{1}{2})\delta_S$
- In each sub-interval, compute $a_i = \left. \frac{d \ln \rho}{d\mathcal{S}} \right|_{\mathcal{S}=\mathcal{S}_i} + \mathcal{O}(\delta_S^2)$ (next slide)
- From the knowledge of the coefficients a_i reconstruct the density of states as

$$\rho_{\text{LLR}}(\mathcal{S}) = \rho_0 \prod_{i=1}^{k-1} e^{a_i \delta_S} \exp(a_k (\mathcal{S} - \mathcal{S}_k)), \quad \mathcal{S}_k \leq \mathcal{S} < \mathcal{S}_{k+1}$$

- The above equation shows exponential error suppression.
The relative approximation error does not depend on the magnitude of $\rho(\mathcal{S})$.

$$1 - \frac{\rho_{\text{LLR}}(\mathcal{S})}{\rho(\mathcal{S})} = \mathcal{O}(\delta_S^2)$$

Evaluating the a_k

- If we restrict the system to a small action interval of amplitude δ_S , we can consider

$$\begin{aligned}\langle\langle O \rangle\rangle_k(a) &= \frac{1}{\mathcal{N}} \int d\mathcal{S} \Gamma(\mathcal{S}_k, \delta_S) \rho(\mathcal{S}) O(\mathcal{S}) e^{-a\mathcal{S}}, \\ \mathcal{N} &= \int d\mathcal{S} \Gamma(\mathcal{S}_k, \delta_S) \rho(\mathcal{S}) e^{-a\mathcal{S}},\end{aligned}$$

Where $\Gamma(\mathcal{S}_k, \delta_S)$ is a support function localised around \mathcal{S}_k and a is a parameter.

- If the interval is small enough our linear approximation will be valid hence there must exist a value of a such that

$$\rho(\mathcal{S}) \exp(-a\mathcal{S}) = \text{constant} + \mathcal{O}(\delta_S^2)$$

- The value of a that fulfils the above equation will be

$$a_k = \left. \frac{d \ln \rho}{d\mathcal{S}} \right|_{\mathcal{S}=\mathcal{S}_k}$$

How to use this observation to evaluate the a_k ?

Evaluating the a_k

- We choose to evaluate $O(\mathcal{S}) = \Delta\mathcal{S} = \mathcal{S} - \mathcal{S}_k$

$$\langle\langle \Delta\mathcal{S} \rangle\rangle_{k, \delta_S}(a) = \frac{1}{\mathcal{N}} \int d\mathcal{S} \Gamma(\mathcal{S}_k, \delta_S) \rho(\mathcal{S}) (\mathcal{S} - \mathcal{S}_k) e^{-a\mathcal{S}},$$

- If the interval is small enough and a log linear approximation is valid

$$\rho(\mathcal{S}) \exp(-a\mathcal{S}) = \text{constant} + \mathcal{O}(\delta_S^2)$$

under rather mild assumptions on the support function, it can be shown

$$\langle\langle \Delta\mathcal{S} \rangle\rangle_{k, \delta_S}(a) = \delta_S^2 \frac{\frac{d\rho}{d\mathcal{S}}(\mathcal{S}_k) - a\rho(\mathcal{S}_k)}{\rho(\mathcal{S}_k)e^{-a\mathcal{S}_k}} + \mathcal{O}(\delta_S^4).$$

$$\langle\langle \Delta\mathcal{S} \rangle\rangle_k(a = a_k) = 0 + \mathcal{O}(\delta_S^4)$$

- Determining a can hence be rephrased as a root-finding problem involving a stochastic average.

A root-finding problem

- The standard Newton-Raphson method, starting from an initial guess $a^{(0)}$ which converges to the true solution a_k . [Langfeld, Lucini, AR, *Phys.Rev.Lett.* **109** (2012)]
With

$$a^{(n+1)} = a^{(n)} + \frac{\langle\langle \Delta \mathcal{S} \rangle\rangle_k(a^{(n)})}{\sigma^2(\Delta \mathcal{S}; a^{(n)})} = a^{(n)} + \frac{12}{\delta_S^2} \langle\langle \Delta \mathcal{S} \rangle\rangle(a^{(n)})$$

- For stochastic equations, a root-finding procedure suitable for our purpose is the Robbins-Monro iteration
The iterative Robbins-Monro algorithm has the form

$$a^{(n+1)} = a^{(n)} - c_n \langle\langle \Delta \mathcal{S} \rangle\rangle_k(a^{(n)}), \quad \text{with } \sum c_n = \infty \text{ and } \sum c_n^2 < \infty$$

It can be proved that

$$\lim_{n \rightarrow \infty} a^{(n)} = a_k$$

in L_2 with an asymptotically normal distribution.

[Robbins and Monro, *Ann. Math. Statist.* **22** (09, 1951)]

- To minimise the variance of the result one choses

$$c_n = \frac{12}{\delta_S^2(n+1)}$$

A quick recap

- Divide the action interval in N sub-intervals of amplitude δ_S , each centered at $\mathcal{S}_i = \mathcal{S}_{\min} + (i - \frac{1}{2})\delta_S$
- In each sub-interval, compute $a_i = \left. \frac{d \ln \rho}{dS} \right|_{\mathcal{S}=\mathcal{S}_i} + \mathcal{O}(\delta_S^2)$ with Robbins-Monro
- From the knowledge of the coefficients a_i reconstruct the density of states as

$$\rho_{\text{LLR}}(\mathcal{S}) = \rho_0 \prod_{i=1}^{k-1} e^{a_i \delta_S} \exp(a_k (\mathcal{S} - \mathcal{S}_k)), \quad \mathcal{S}_k \leq \mathcal{S} < \mathcal{S}_{k+1}$$

- Evaluate the action dependant observable by mean of a numerical one dimensional integration

$$\langle O \rangle = \frac{1}{Z} \int d\mathcal{S} O(\mathcal{S}) \rho_{\text{LLR}}(\mathcal{S}) e^{-\beta \mathcal{S}}$$

Few remarks

- As for the Wang-Landau method, the density of states is computed iteratively, using non-Markovian processes, but the recursion and the general principles (continuous density of states, piecewise approximation, no frequency histogram used) are different from those of Wang-Landau
- The LLR algorithm is a first principle method:

$$\rho(\mathcal{S}) = \rho_{\text{LLR}}(\mathcal{S})e^{c\delta_{\mathcal{S}}^2}$$

almost everywhere (the $\rho(\mathcal{S})$ is supposed to be almost everywhere C_2).

- The above equation shows exponential error suppression: the relative approximation error does not depend on the magnitude of ρ the method works over several orders of magnitude!
- For observables, the convergence to its continuum action value is $\mathcal{O}(\delta_{\mathcal{S}}^2)$
- The method allows us to compute generic observables, and not only observables that can be expressed as a function of the action
- The choice of support function can affect the efficiency of the update algorithm and its ergodicity properties.

A first application: Compact U(1)

The action

$$S = \beta \sum (1 - \cos \Theta_{\mu\nu}(x))$$
$$\Theta_{\mu\nu}(x) = \theta_\mu(x) + \theta_\nu(x + \hat{\mu}) - \theta_\mu(x + \hat{\nu}) - \theta_\nu(x)$$

The system has a bulk first order phase transition around $\beta_c \sim 1.01$

The system shows strong metastabilities close to the phase transition that make its simulation very expensive.

State of the art supercomputer are needed to evaluate a 18^4 volume. [[Arnold,Bunk, Lippert, Schilling, Nucl.Phys.Proc.Suppl. 119 \(2003\)](#)]

Simulation details

L	$\mathcal{S}_{\min}/(6V)$	$\mathcal{S}_{\max}/(6V)$	N_{SW}	N_{RM}	$(\mathcal{S}_{\max} - \mathcal{S}_{\min})/\delta_S$
8	0.5722222	0.67	250	600	512
10,12,14, 16,18,20	0.59	0.687777	200	400	512

We have used a simple step function as support function

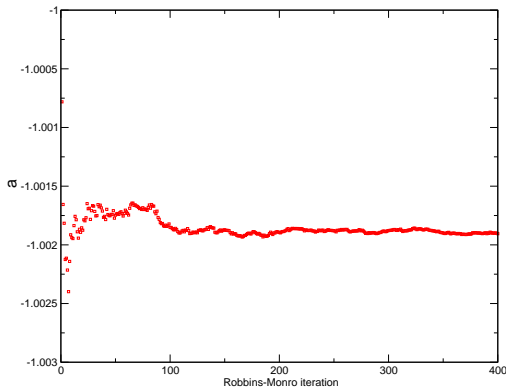
$$\Gamma(\mathcal{S}_k, \delta_S) = H(\mathcal{S} - \mathcal{S}_k + \delta_S/2) + H(\mathcal{S} - \mathcal{S}_k - \delta_S/2)$$

and a local Metropolis update.

- $N_{TH} \sim 100$, the number of Monte-Carlo updates in the restricted action interval before starting to measure expectation values;
- N_{SW} , the number of iterations used for computing expectation values;
- N_{RM} , the number of Robbins-Monro iterations for determining a_i ;
- $N_B = 20$, number of final values from the Robbins-Monro iteration subjected to a subsequent bootstrap analysis.

The Robbins-Monro convergence

Estimator of the a_i as function of the Robbins-Monro iteration.

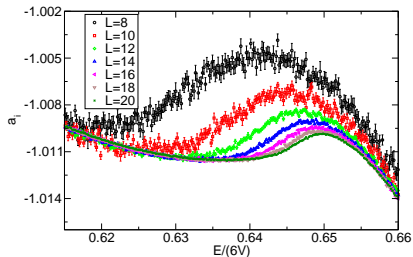
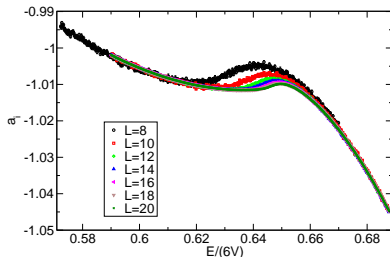


$$\begin{aligned}V &= 20^4 \\ \mathcal{S}/(6V) &= 0.59009548 \\ \delta_S/V &= 1.91 \times 10^{-4}\end{aligned}$$

$$\text{A reminder } a_k^{(n+1)} = a_k^{(n)} + \frac{12}{\delta_S^2(n+1)} \langle\langle \Delta \mathcal{S} \rangle\rangle_k(a_k^{(n)}).$$

Scaling of the a_i with the volume

The a_i have a well defined thermodynamic limit.



The non-monotonicity is a signature of a first order phase transition.

Results comparison

As usual we define the pseudo-critical coupling $\beta_c(L)$ such as the coupling at which the peak of the specific heat occurs for a fixed volume.

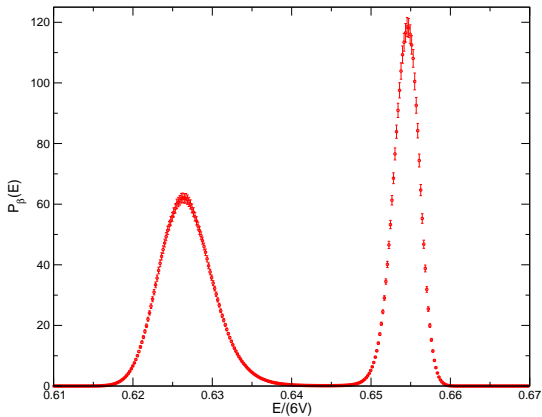
$$C_V(\beta) = \langle S^2(\beta) \rangle - \langle S(\beta) \rangle^2$$

L	$\beta_c(L)$ present method	$\beta_c(L)$ reference values
8	1.00744(2)	1.00741(1)
10	1.00939(2)	1.00938(2)
12	1.010245(1)	1.01023(1)
14	1.010635(5)	1.01063(1)
16	1.010833(4)	1.01084(1)
18	1.010948(2)	1.010943(8)
20	1.011006(2)	

Reference data from [\[Arnold,Bunk, Lippert, Schilling, Nucl.Phys.Proc.Suppl. 119 \(2003\)\]](#)

...as a byproduct

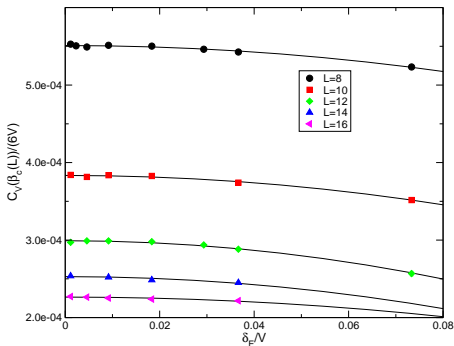
Probability distribution on a 20^4 lattice at pseudo-critical point (Discovered today that this is not the world record)



The entire set of simulations was obtained in 2 weeks on 512 Sandy Bridge cores.

δ_S dependences of the observables

Peak of the specific heat for various volumes and δ_S choices



L	$(S_{\max} - S_{\min})/\delta_S$
10	8, 16, 32, 64, 128, 512
12	8, 16, 20, 32, 64, 128, 512
14	16, 32, 64, 512
16	16, 32, 64, 128, 512

- A quadratic dependence in δ_S fits well the data at fixed volume
- The cost of the algorithm seems to be quadratic in V

- We have introduced a density of state method with a general domain of applicability
The key features of the algorithm are
 - ▶ It does not rely on importances sampling
 - ▶ It is first-principle
 - ▶ It implements exponential error reduction
 - ▶ It converges quadratically in δ_S to the exact result
- The efficiency of the algorithm has been proved in the case of a first order phase transition, for which it has been observed a scaling time that is polynomial in the volume (cfr. exponential time for importance sampling methods)
- Other applications are currently under study:
 - ▶ Extension of the method to global HMC and fermionic degrees of freedom
 - ▶ Ergodicity of the algorithm
 - ▶ Thermodynamical properties of gauge theories
 - ▶ Theories with a sign problem

Global HMC

- The basic idea is to use as support function a strongly localised and analytic function.
- The natural choice being a gaussian

$$\langle\langle \mathcal{O} \rangle\rangle_{k, \delta_S}(a) = \frac{1}{\mathcal{N}} \int d\mathcal{S} e^{-\frac{(\mathcal{S}-\mathcal{S}_k)^2}{2\delta_S^2}} \rho(\mathcal{S}) \mathcal{O} e^{-a\mathcal{S}},$$

with

$$\mathcal{N} = \int d\mathcal{S} e^{-\frac{(\mathcal{S}-\mathcal{S}_k)^2}{2\delta_S^2}} \rho(\mathcal{S}) e^{-a\mathcal{S}},$$

- In order to compute $\langle\langle \mathcal{O} \rangle\rangle_{k, \delta_S}(a)$ the weight that needs to be sampled is

$$W(\mathcal{S}[\phi], \mathcal{S}, \delta_S, a) \propto e^{-U[a, \phi, \mathcal{S}]}$$

where

$$U[a, \phi, \mathcal{S}] = a\mathcal{S}[\phi] + \frac{(\mathcal{S}[\phi] - \mathcal{S})^2}{2\delta_S^2}$$

Global HMC

- For the new action

$$U[a, \phi, \mathcal{S}] = aS[\phi] + \frac{(S[\phi] - \mathcal{S})^2}{2\delta_S^2}$$

- We can then define an Hamiltonian for the HMC evolution as:

$$H[p_i, \phi] = \sum_i \frac{p_i p_i}{2} + U[a, \phi, \mathcal{S}],$$

- The associated force is then:

$$f_i = -\frac{\partial U}{\partial \phi_i} = -\frac{\partial S}{\partial \phi_i} \left(a + \frac{1}{\delta_S^2} (S[\phi] - \mathcal{S})^2 \right)$$

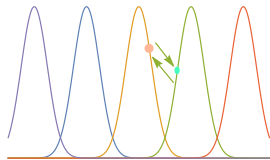
where $S[\phi]$ is the original action.

- The Hamiltonian evolution can be performed with the standard integration techniques.

Ergodicity and efficiency

- In principle, this algorithm is ergodic: given enough time, it will explore the entire phase space.
- However the probability of visiting states with action far from the peak of the Gaussian will be very small and this will lead to a slow dynamic of the Markov Chain.
- The idea is to simulate multiple overlapping intervals of energy in parallel and periodically propose a swap of two of them with probability given by

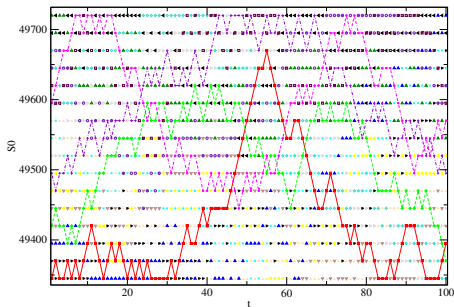
$$P_{sw} = \min(1, \exp(U[a_1, \phi^{(1)}, \mathcal{S}_1] + U[a_2, \phi^{(1)}, \mathcal{S}_2] - U[a_2, \phi^{(1)}, \mathcal{S}_2] - U[a_1, \phi^{(2)}, \mathcal{S}_1]))$$



Preserving the detailed balance of energy of the entire system.

Ergodicity and efficiency

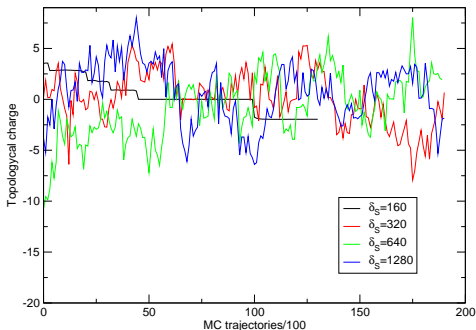
- Subsequent exchanges allow any of the configuration sequences to travel through all the action intervals, hence overcoming trapping.
The example below reports the case of a $16^3 \times 3$ SU(2) Yang-Mills.



Different symbols correspond to different replicas and we connected the symbols of four selected replicas to guide the eyes.

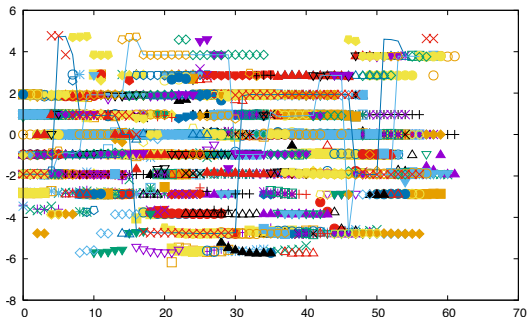
Topological charge (work in progress)

- The dynamics of the topological charge can be very different from the one of the action.
- For a single replica it strongly depends of the width of the gaussian support function.
- $SU(3)$ Yang-Mills Volume 16^4 , Central $S_0 = 227847.7$



Topological charge (work in progress)

- However when the replica swap is enabled



- Autocorrelation has to be defined on the final observable.
- Running...

EMT from shifted BC (work in progress)

- In Yang-Mills theory, if translations are preserved, the energy momentum tensor is

$$T_{\mu\nu} = \frac{1}{g^2} \left\{ F_{\mu\alpha} F_{\nu\alpha} - \frac{1}{4} \delta_{\mu\nu} F_{\alpha\beta} F_{\alpha\beta} \right\} .$$

- When using lattice regularisation the energy momentum tensor needs to be renormalised [S. Caracciolo et al., Nuclear Phys. B Vol 9 (1989)].

The renormalised energy momentum tensor can be written as the sum of three operators,

$$T_{R\mu\nu} = Z_T \left\{ T_{\mu\nu}^{[1]} + z_t T_{\mu\nu}^{[3]} + z_s \left(T_{\mu\nu}^{[2]} - \langle T_{\mu\nu}^{[2]} \rangle \right) \right\} ,$$

- Using shifted boundary conditions for the fields in the time direction [L. Giusti, H. B. Meyer Phys. Rev. Lett. 106 (2011).] .

$$A(L_0, \mathbf{x}) = A(0, \mathbf{x} - L_0 \boldsymbol{\xi}) ,$$

it is possible to find the renormalisation constants Z_T, z_t, z_s .

- Here we focus on the renormalisation constant Z_T which can be obtained from the formula

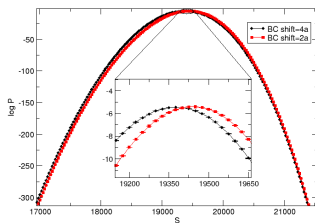
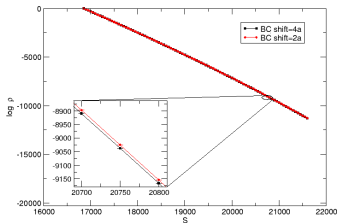
$$Z_T(\beta) = \frac{f(\beta, L_0, \boldsymbol{\xi} - a\hat{k}L_0) - f(\beta, L_0, \boldsymbol{\xi} + a\hat{k}L_0)}{2a} \frac{1}{\langle T_{0k}^{[1]}(\beta) \rangle_{\boldsymbol{\xi}}} ,$$

EMT from shifted BC (work in progress)

- $f(\beta, L_0, \xi)$ the free energy with shift ξ , coupling β and inverse temperature L_0 .
- The free energy can be computed from the density of states:

$$f(\beta, L_0, \xi) = \frac{\log \int dS e^{(-\beta S)} \rho(S)}{V} + c .$$

- In the left panel we plot the $SU(2)$ density of states as a function of the action for two $12^3 \times 3$ lattices with shifts $(\frac{4}{3}, 0, 0)$ and $(\frac{2}{3}, 0, 0)$ respectively.



- By numerical integration

$$\Delta f(\beta = 2.36869) = 0.002319(21) .$$

Generalised density of states

At finite chemical potential we have

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

It is possible to define a generalised density of states as

$$P_\beta(s) = \int [D\phi] \delta(s - S_I[\phi]) e^{-\beta S_R[\phi]}$$

which leads to find the partition function as the Fourier transform of P

$$Z[\beta, \mu] = \int ds e^{i\mu s} P_\beta(s)$$

Bose gas at finite density (work in progress)

- LLR was already tested on a Z_3 spin model with complex action, where it seems to give reasonable results [[K. Langfeld and B. Lucini, Phys. Rev. D 90 \(2014\)](#)].
- The relativistic Bose gas is a different test since it is known to undergo a second-order phase transition at μ_c .
- Observables are independent from μ below a threshold μ_c (aka Silver Blaze phenomenon).
- It has been studied (solved) by means of an exact dual flux representation in [[Gattringer, Kloiber, Nucl. Phys. B 869 \(2013\)](#)]

Bose gas at finite density

(work in progress)

- We consider a self-interacting complex scalar field in the presence of a chemical potential μ , with the continuum action

$$S[\phi] = |\partial_\mu \phi|^2 + (m^2 - \mu^2)|\phi|^2 + \mu(\phi^* \partial_4 \phi - \partial_4 \phi^* \phi) + \lambda|\phi|^4$$

- On the lattice the chemical potential is introduced as a vector potential

$$S[\phi] = (8 + m^2)\phi_x^* \phi_x + \lambda(\phi_x^* \phi_x)^2 - \sum_{\nu=1}^4 \left(\phi_x^* e^{-\mu \delta_{\nu,4}} \phi_{x+\hat{\nu}} + \phi_{x+\hat{\nu}}^* e^{\mu \delta_{\nu,4}} \phi_x \right)$$

- The density of particles is given by (with $\phi_x = \frac{1}{\sqrt{2}}(\phi_{1,x} + i\phi_{2,x})$)

$$\langle n \rangle = \left. \frac{d \log(Z)}{d\mu} \right|_{\mu=0} = (\delta_{ab} \sinh \mu - i\epsilon_{ab} \cosh \mu) \phi_{a,x} \phi_{b,x+\hat{4}},$$

Bose gas at finite density (work in progress)

- The action can be divided in its real and complex part

$$S[\phi] = S_R[\phi, \mu] + i\kappa(\mu)S_I[\phi],$$

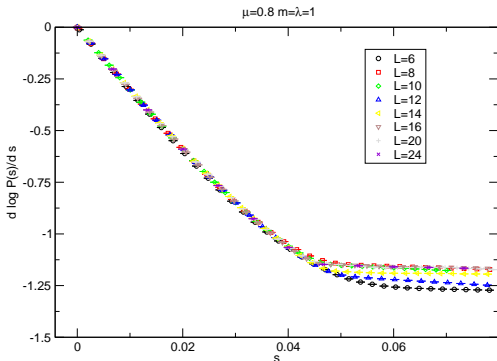
with

$$S_I[\phi] = \phi_{1,x}\phi_{2,x+\hat{4}}\phi_{2,x}\phi_{1,x+\hat{4}} \quad \kappa(\mu) = \sinh(\mu)$$

- To quantify the severity of sign problem we are interested in the expectation value of the quantity

$$\langle e^{-i\kappa(\mu)S_I} \rangle_{PQ} = \frac{Z[\mu]}{Z_{PQ}[\mu]} = e^{-V\Delta f}$$

Generalised DOS



The partition function is given by a Fourier transform of the DOS

$$Z[\mu] = \int ds e^{i\kappa(\mu)s} P(s)$$

- $P(s)$ is not known exactly but up to noise coming from the Montecarlo simulation.
- The Fourier transform of white noise does not depend on the frequency while $Z[\mu]$ is a fast decaying function.

FFT breaks at relatively small chemical potential.

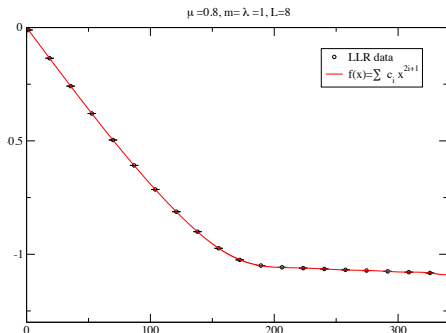
Filtering the noise

- A first alternative is a fit of the log-derivative of the density of states.

$$P(s) = \exp\left(\sum_i c_i s^{2i+1}\right)$$

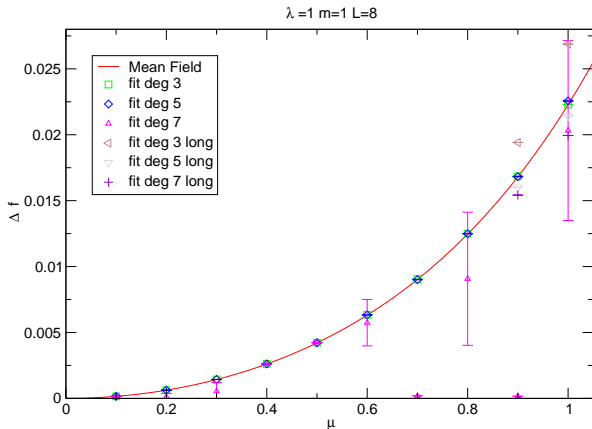
- The error is now reported the coefficients and the Fourier transform of every power is a fast decaying function.

However this introduces a systematic error.



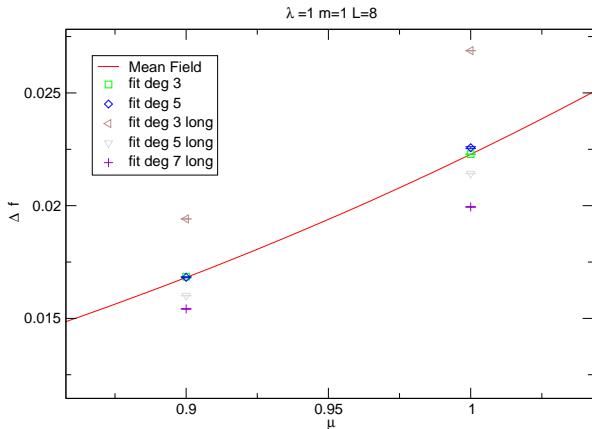
Filtering the noise

- All our fits have a $\chi^2 \leq 1$
- The Fourier transform with multi-precision numerical integration.
- The integration domain is kept always within the interpolation region and large enough not to influence the result.



Filtering the noise

- All our fits have a $\chi^2 \leq 1$
- The Fourier transform with multi-precision numerical integration.
- The integration domain is kept always within the interpolation region and large enough not to influence the result.



- We have introduced a density of state method with a general domain of applicability
The key features of the algorithm are
 - ▶ It does not rely on importances sampling
 - ▶ It is first-principle
 - ▶ It implements exponential error reduction
 - ▶ It converges quadratically in δ_S to the exact result
- The efficiency of the algorithm has been proved in the case of a first order phase transition, for which it has been observed a scaling time that is polynomial in the volume (cfr. exponential time for importance sampling methods)
- Other applications are currently under study:
 - ▶ Extension of the method to global HMC and fermionic degrees of freedom
 - ▶ Ergodicity of the algorithm
 - ▶ Thermodynamical properties of gauge theories
 - ▶ Theories with a sign problem

...an open question

- We presented an application of the LLR algorithm to a system with a severe sign problem.
- For the specific case under investigation the fitting procedure seems to introduce a systematic error.
- Although we capture the bulk part of the signal, further investigations and a better procedure to account for the systematic error are needed.