Efficient calculations in Lattice Field Theories using the density of states

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RIKEN-CCS, (Virtual) Kobe, Japan, 5th Oct. 2021

Bibliography

Talk widely based on

- K. Langfeld, B. Lucini and A. Rago, Phys. Rev. Lett. 109 (2012) 111601
- k. Langfeld and B. Lucini, Phys. Rev. D90 (2014) no.9, 094502
- K. Langfeld, B. Lucini, R. Pellegrini and A. Rago, Eur. Phys. J. C76 (2016) no.6, 306
- B. Lucini, W. Fall and K. Langfeld, PoS LATTICE2016 (2016) 275
- R. Pellegrini, B. Lucini, A. Rago and D. Vadacchino, PoS LATTICE2016 (2017) 276
- O. Francesconi, M. Holzmann, B. Lucini and A. Rago, Phys. Rev. D 101 (2020)
- G. Cossu, D. Lancaster, B. Lucini, R. Pellegrini and A. Rago, Eur. Phys.J.C 81 (2021) 4

Outline

Outline

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

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

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

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

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

- Obtain a_n as the root of the stochastic equation

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

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

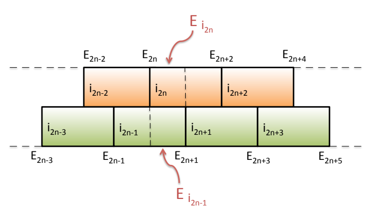
- Piecewise continuity of $\tilde{\rho}(E)$ plus setting $c_1 = 0$ leads to

$$c_n = \frac{\delta}{2} a_1 + \delta \sum_{k=2}^{n-1} a_k + \frac{\delta}{2} a_n \,, \qquad n \geq 2$$

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

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

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

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

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, hopes and prayers

Potential advantages over importance sampling:

1. More efficient at metastable points (exponential vs. polinomial cost)
2. May allow us to compute partition functions
3. Might allow to solve the sign problem by direct integration

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All supported by available numerical evidence

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In addition

1. The convergence is precocious in δ_E
2. At finite δ_E, δ_E^2 errors can be corrected with a multicanonical algorithm
3. The method can be extended to generic observables, for which one still gets quadratic convergence in δ_E to the correct result

Sharp vs. smooth cut-off

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

$$\theta(E_i + \delta/2 - E)\theta(E - E_i + \delta/2) \qquad \rightarrow \qquad e^{-\frac{(E-E_i)^2}{2\sigma^2}}$$

This introduces the effective density $\tilde{\rho}$ as

$$\tilde{\rho}(E) = e^{-a_i(E-E_i) - \frac{(E-E_i)^2}{2\sigma^2}}$$

which can be interpreted as an effective Hamiltonian giving rice to the force

$$f_i = -\frac{\delta E}{\delta \phi_i}\left(a_i + \frac{1}{\sigma^2}(E - E_i)\right)$$

Recursion relation

$$a_i^{(m+1)} = a_i^{(m)} - \frac{\alpha}{m}\frac{\langle\langle \Delta E \rangle\rangle_{a_i^{(m)}}}{\langle\langle \Delta E^2 \rangle\rangle_{a_i^{(m)}}}$$

amenable to simulations with an unconstrained global HMC and hence to parallelisation)

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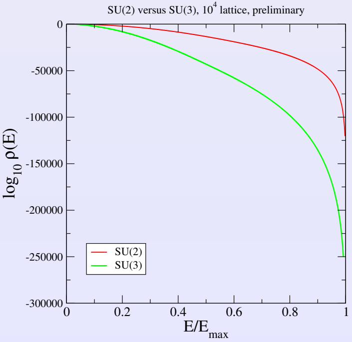
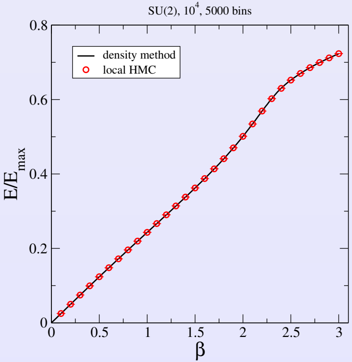
$\hookrightarrow$ First step towards inclusion of dynamical fermions

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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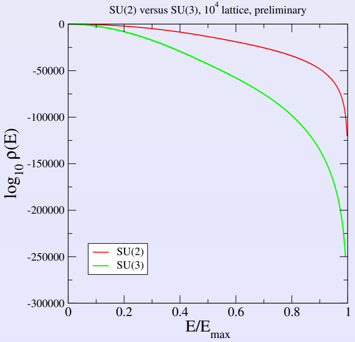

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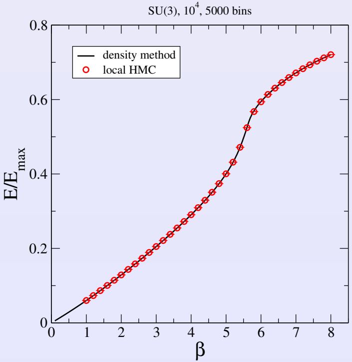

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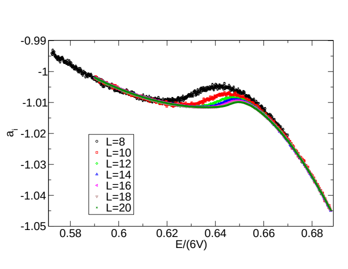
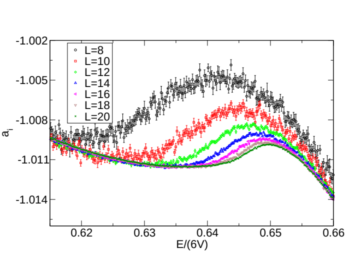
Outline

U(1) LGT: a vs E_0

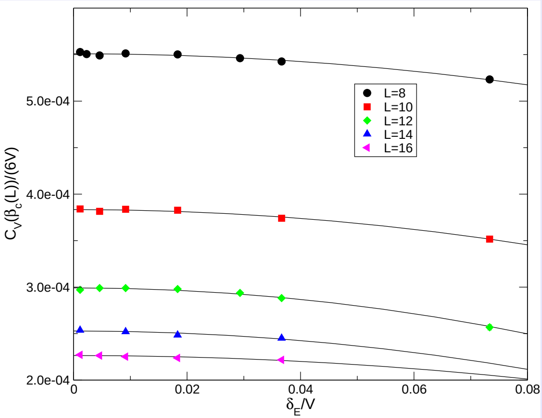




- The non-monotonicity is a signature of a first order phase transition
- The a seem to converge to their thermodynamic limit

U(1) LGT: δ_E dependence of observables

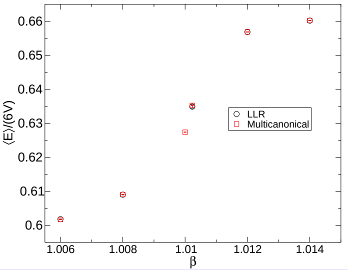
Example: peak of the specific heat at various volumes

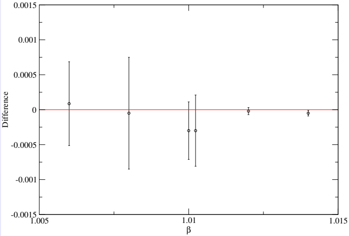


- A quadratic dependence in δ_E/V fits well the data
- The cost of the algorithm seems to be quadratic in V

U(1) LGT: LLR and multicanonical

Lattice 12^4

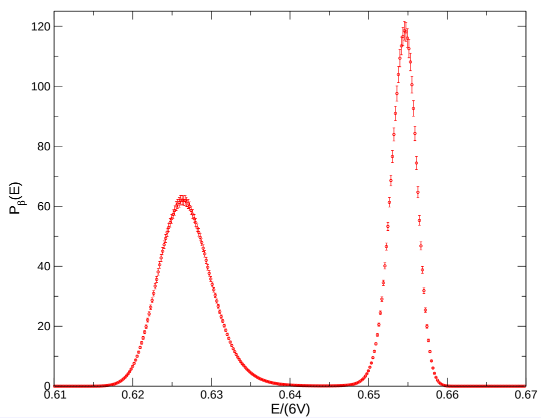




- The LLR method performs at least on pair with specialised methods such as the Multicanonical Algorithm
- The LLR algorithm reproduces the results of Arnold *et al.* at a more modest computational cost

Probability distribution on large lattices

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

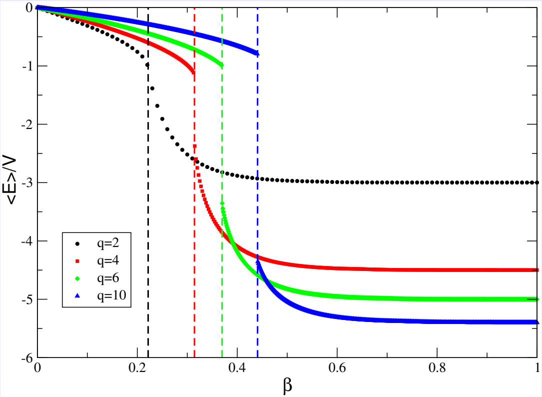


Obtained in 2 weeks on 512 Sandy Bridge cores

Outline

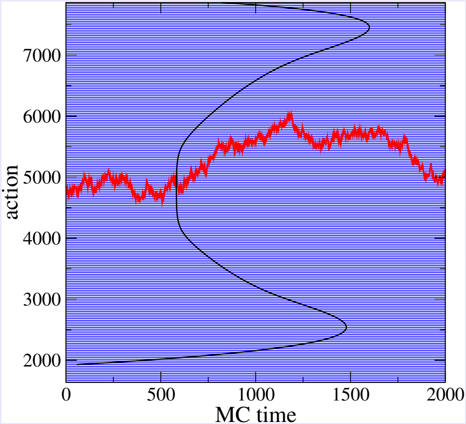
Potts models – phase transition in D=3

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



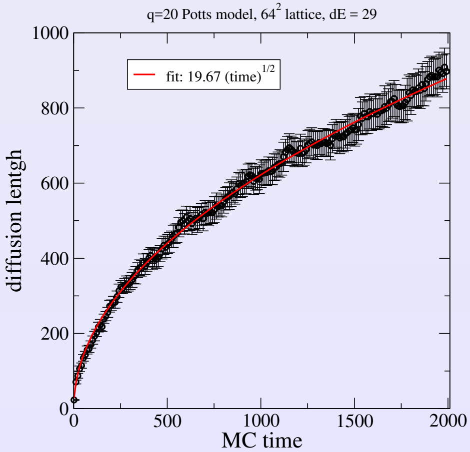
β_c from Bazavov, Berg and Dubey, Nucl. Phys. B802 (2008) 421-434
[B. Lucini, W. Fall and K. Langfeld, PoS LATTICE2016 (2016) 275]

Potts: replica swapping for D=2 q=20



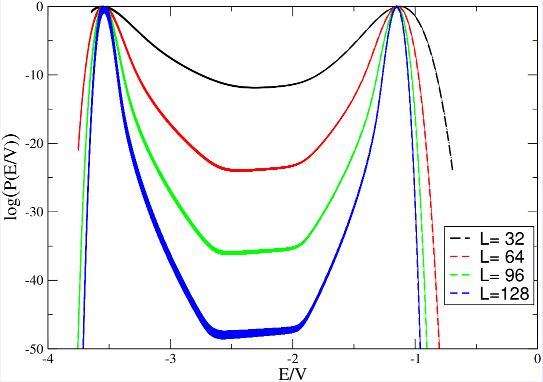
The hopping of configurations across intervals is reminiscent of a random walk (as expected)

Replica and diffusive dynamics



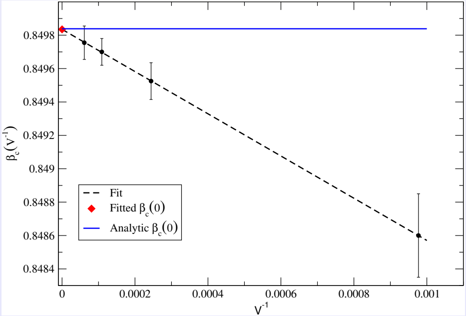
Mean path in energy space: $\langle (E_{\bar{f}} - E_{\bar{\imath}})^2 \rangle^{1/2} = D t^{1/2}$

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



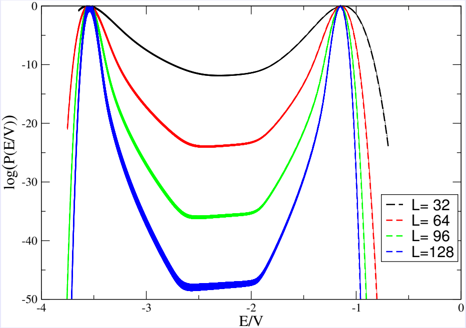
For first order phase transitions

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

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



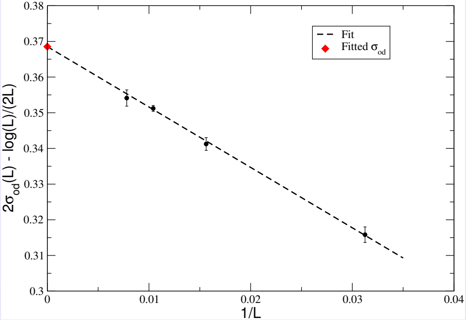
At finite L

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

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



Ansatz

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

Strong coupling calculation (Borgs-Janke):

$$2\sigma_{od}(L) = 0.3709881649\ldots \qquad \Delta\sigma/\sigma = 0.0066(23)$$

Outline

Energy-momentum tensor in SU(N) YM

On the lattice

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

with Z_T, z_t, z_s renormalisation constants to be determined non-perturbatively

Using shifted boundary condition

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

It is possible to write Ward Identities that fix the normalisation constant Z_T [L. Giusti and M. Pepe Phys. Rev. D 91, 114504]

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

where

$$f(\beta, L_0, \boldsymbol{\xi}) = \frac{\log \int dE e^{-\beta E} \rho(E)}{V} + c$$

The DoS in SU(2)

Computation time 48 hours per point, but covers a range of β.

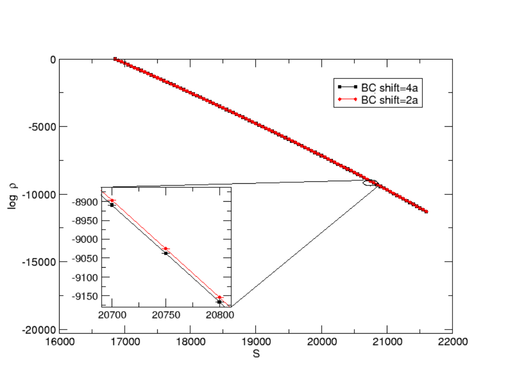


Figure: Vol $= 12^3 x3$ and shift $= \left(\frac{4}{3}, 0, 0\right)$, $\left(\frac{2}{3}, 0, 0\right)$

[R. Pellegrini, B. Lucini, A. Rago and D. Vadacchino, PoS LATTICE2016 (2017) 276]

The probability density in SU(2)

$$\Delta f = \frac{1}{V}\left[\log\left(\int dS e^{-\beta S}\rho_{\xi}(S)\right) - \log\left(\int dS e^{-\beta S}\rho_{\xi'}(S)\right)\right] = 0.002319(21)$$

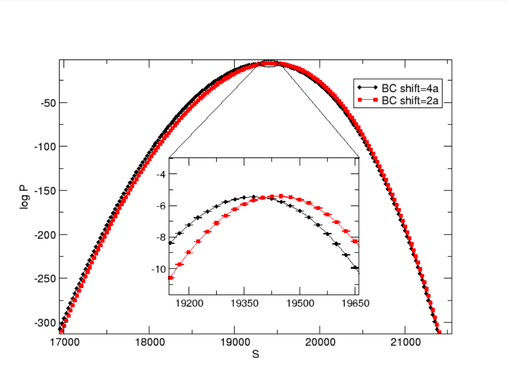
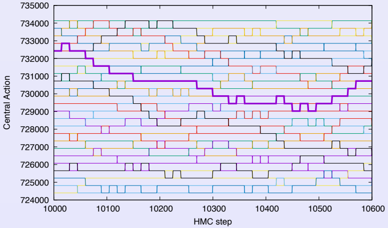


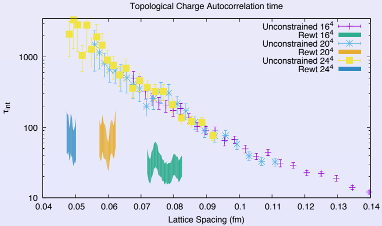
Figure: β=2.36869, vol $= 12^3 x3$ and shift $= \left(\frac{4}{3}, 0, 0\right)$, $\left(\frac{2}{3}, 0, 0\right)$

[R. Pellegrini, B. Lucini, A. Rago and D. Vadacchino, PoS LATTICE2016 (2017) 276]

Outline

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!)

Proposed remedies

1. Minimal modifications of standard methods treating the real part of the action in a standard way and dealing separately with the imaginary part, e.g.
   - reweighting
   - imaginary chemical potential
   - cumulant expansion
   - Taylor expansion
   - ...
2. Radically new approaches
   - Complex Langevin
   - Thimble methods
   - ...

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    - Thimble methods
    - ...
    - Density of the states

Outline

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 (Garron and Langfeld)

Outline

The $\mathbb{Z}(3)$ spin model

At strong coupling and for large fermion mass, for finite temperature and non-zero chemical potential QCD described by the three-dimensional spin model

$$
\begin{aligned}
Z(\mu) &= \sum_{\{\phi\}} \exp\left\{\tau \sum_{x,\nu} \left(\phi_x \phi^*_{x+\nu} + c.c.\right) + \sum_x \left(\eta\phi_x + \bar{\eta}\phi^*_x\right)\right\} \\
&= \sum_{\{\phi\}} \exp\left\{S_\tau[\phi] + S_\eta[\phi]\right\}
\end{aligned}
$$

with $\quad \phi \in \mathbb{Z}(3)\,, \qquad \eta = \kappa e^{\mu} \quad$ and $\quad \bar{\eta} = \kappa e^{-\mu}$

The action is complex, but the partition function is real

The model has been simulated using complex Langevin techniques and the worm algorithm

$\mathbb{Z}(3)$: Phase twist

Defined as

$$p(\mu) \; = \; i \, \frac{\sqrt{3}}{V} \, \langle N_z - N_{z^*} \rangle$$

Can be computed from the generalised density of states

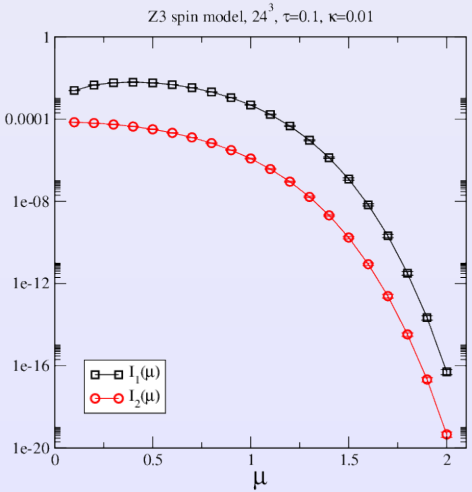
$$p(\mu) = \frac{\sum_n \rho(n) \; n \; \sin\left(\kappa\sqrt{3}\,\sinh(\mu)\; n\right)}{\sum_n \rho(n) \; \cos\left(\kappa\sqrt{3}\,\sinh(\mu)\; n\right)}$$

Can be expressed as the ratio of the oscillating sums

$$I_1(\mu) \quad = \quad \frac{\sum_n \rho(n) \; n \; \sin\left(\kappa\sqrt{3}\,\sinh(\mu)\; n\right)}{\sum_n \rho(n)}$$

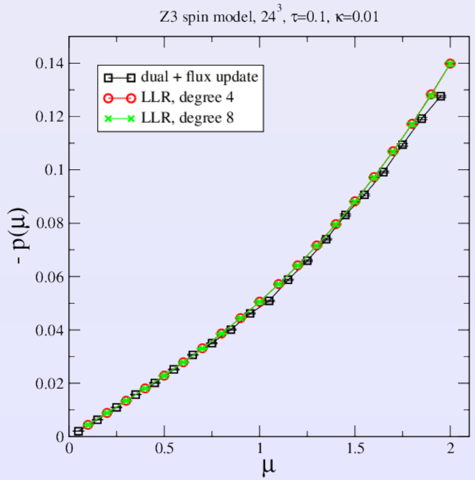
$$I_2(\mu) \quad = \quad \frac{\sum_n \rho(n) \; \cos\left(\kappa\sqrt{3}\,\sinh(\mu)\; n\right)}{\sum_n \rho(n)}$$

$\mathbb{Z}(3)$: I_1 and I_2 *vs.* μ



Strong cancellations at high μ

$\mathbb{Z}(3)$: $P(\mu)$ vs. μ



Good agreement with the worm algorithm

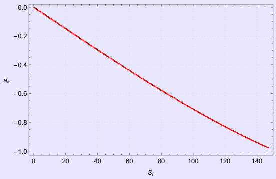
Outline

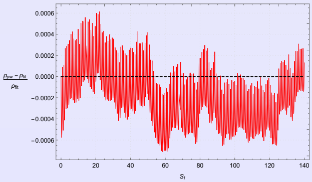
The Bose Gas

The model

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

Oscillations of the piecewise approximation need to be treated through smoothing





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

Controlling the fit

The order of the fit is arbitrary $\Rightarrow$ we need to make sure we are not under- or over-fitting

For under-fitting, the χ^2 gives a good criterion

For over-fitting, we extract from the data the second derivative and we use it to check how well our analytic derivative of the data describe those points

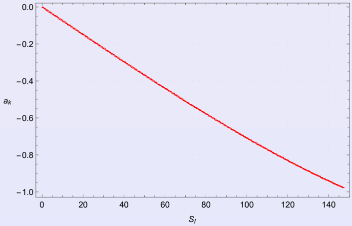
The second derivative can be extracted from an independent measurement

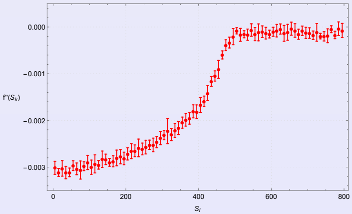
$$\frac{\mathrm{d}^2}{\mathrm{d}S_I^2} \log \rho \Big|_{S_I,k} = \frac{360}{\Delta^4} \left(s_2 - \frac{\Delta^2}{12} \right) + \mathcal{O}(\Delta^2) \; ,$$

with s_2 order two cumulant evaluated with an average restricted to the k-th interval

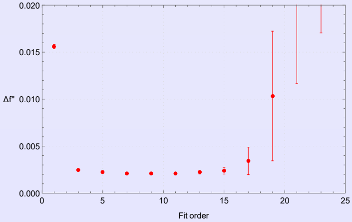
Constraints on the second derivative

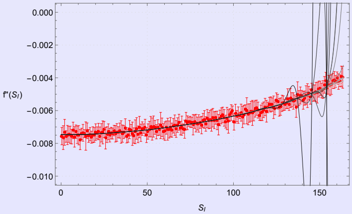
Quality of the first two derivatives





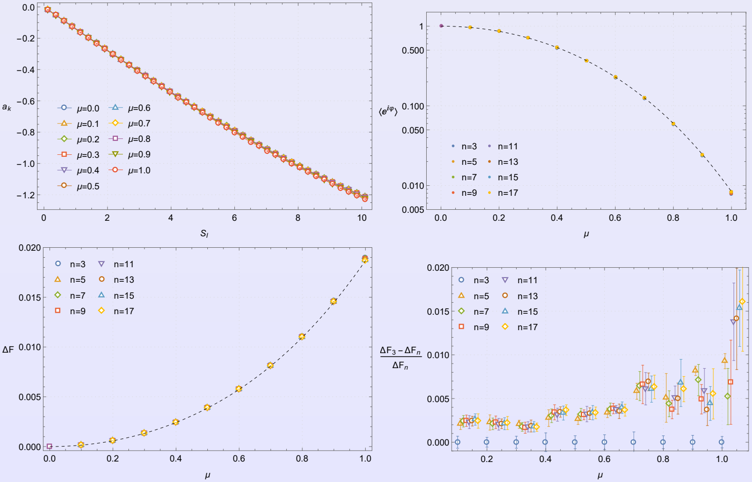
Various order polynomial interpolations





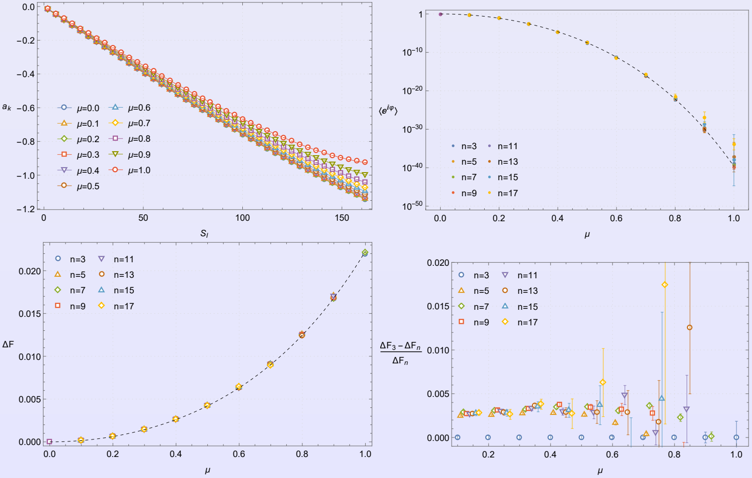
Region with good control over fit seems to exist

Results for $V = 4^4$



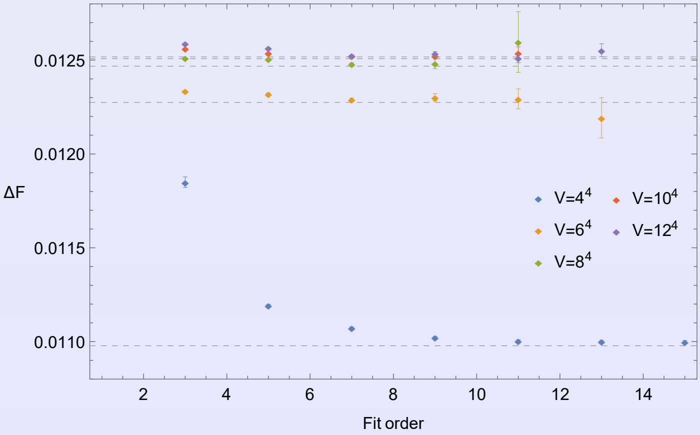
Region of fit stability not obvious when μ increases

Results for $V = 8^4$



Fit stability seems to get worse as V increases

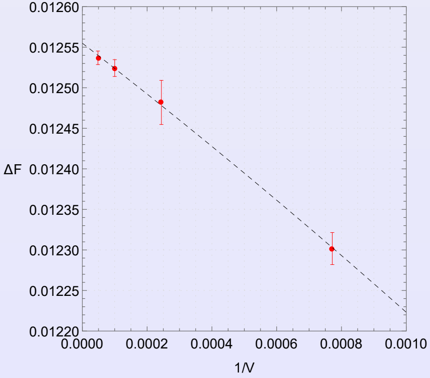
Higher statistics results for $\mu = 0.8$



Good control also for $V = 12^4$

Good agreement with mean field [see also Aarts, JHEP 0905 (2009) 052]

Overlap free energy in the thermodynamic limit



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

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)

Conclusions and outlook

- For systems with a real action, the LLR algorithm
  - Provides a controlled procedure for computing the density of states in models with a continuum spectrum (see U(1) study)
  - Can be used for efficient studies of metastable systems (see U(1) and Potts applications)
  - Allows to determine partition functions and free energies (see the E-M tensor application)
  - Decorrelates topological modes (see SU(3) study)
- 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:
  - Systematic investigation of the scaling of the algorithm with the volume
  - Determination of an optimal procedure for the smoothing of the density of the states
  - Application to systems with fermions
  - Proof of concept of the solution of the sign problem in QCD (e.g. small lattices)