The density of states approach to Lattice Gauge Theory

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Based on:
[K. Langfeld, B. Lucini, A. Rago *Phys.Rev.Lett.* **109** (2012)]
[RP, K. Langfeld, B. Lucini, A. Rago PoS **LATTICE2014** (2015)]
[K. Langfeld, B. Lucini, A. Rago, RP, L. Bongiovanni, J. Phys. Conf. Ser **631** (2015)]
[K. Langfeld, B. Lucini, RP, A. Rago, Eur. Phys. J. C **76** (2016)]

Motivations

Lattice gauge theory

- Advances in Monte Carlo simulations are largely responsible for the success of LGT
- Typical Monte Carlo methods used in LGT are importance sampling Markov Chain Monte Carlo
- State of the art Monte Carlo simulations are very efficient when the quantity of interest can be expressed as averages over a (sharply peaked) probability measure.

Methods based on importance sampling are inefficient for

- Computation of free energies
- Systems with meta-stabilities
- System with complex action

Alternative approaches could lead to significant improvement in these cases.

Density of states

Consider an Euclidean quantum field theory

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

The DoS is defined by

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

Which gives

$$Z\left[\beta\right]=\int dEe^{-\beta E}\rho(E)$$

Is the computation any easier?

Algorithms for the DoS

- The computation of the DoS has been attempted in the past with limited success
- The Wang-Landau algorithm was the major breakthrough, it is a numerical technique to extract the DoS using a non-Markovian process [Wang and Landau, Phys. Rev. Lett. 86 (2001)]
- The WL algorithm uses a frequency histogram, which does not seem ideal for continuum systems
- New proposal for continuum systems

Logarithmic Linear Relaxation (LLR)

Consider the energy interval

$$[E_k - \delta_E/2, E_k + \delta_E/2] \, .$$

If the logarithm of the DoS is a smooth function

$$\ln \rho(E) = \ln \rho(E_k) + a_k(E - E_k) + O({\delta_E}^2)$$

The program of the algorithm is to divide the energy in intervals and compute the coefficients a in every interval; the DoS can be reconstructed using the following

$$\rho(E) = \rho_0 \prod_{i=1}^{k-1} e^{a_i \delta_E + a_k (E - E_k)}, \quad E_k \leq E < E_{k+1}$$

Computing the a_k

We consider the expectation value

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

If the interval is small enough and the log linear approximation is valid we have

$$\rho(E) e^{-a_k E} = \text{constant} + \mathcal{O}({\delta_E}^2)$$

Which gives

$$\langle\langle E - E_k \rangle\rangle_k(a = a_k) = 0 + \mathcal{O}({\delta_E}^2)$$

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

Robbins-Monro algorithm

A root-finding procedure for stochastic equation is the Robbins-Monro iteration, which has the form[Robbins and Monro, Ann. Math. Statist. **22** (09, 1951)]

$$a^{(n+1)} = a^{(n)} - c_n \langle\langle E - E_k \rangle\rangle (a^{(n)})$$

With

$$\sum c_n = \infty, \quad \sum {c_n}^2 < \infty$$

Under mild assumption it can be proven to converge to the true root of the stochastic equation.

Quick recap

The algorithm in three steps

1. Divide the energy span of interest in small intervals centered at

$$E_i = E_{min} + i\delta_E$$

2. Compute the coefficients a using the RM algorithm in every interval

$$a_i = \left.\frac{d\log\rho}{dE}\right|_{E_i} + \mathcal{O}({\delta_E}^2)$$

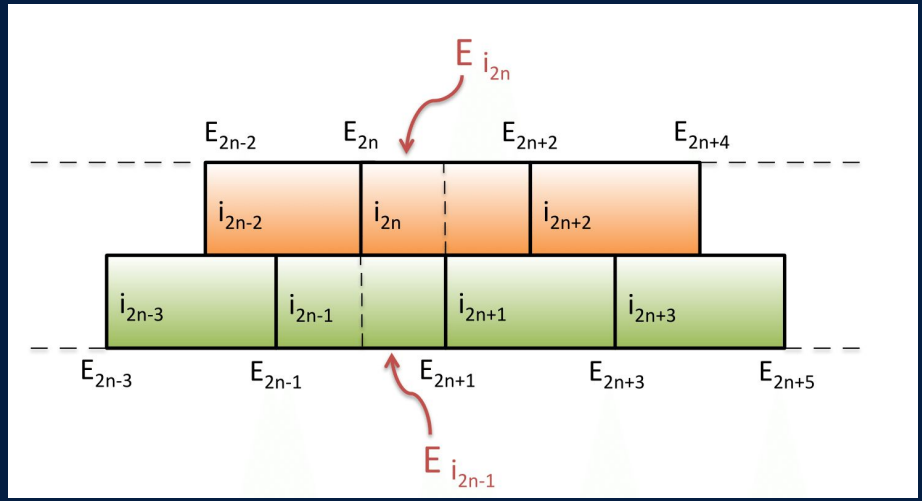
3. Reconstruct the DoS using

$$\rho(E) = \rho_0 \prod_{i=1}^{k-1} e^{a_i\delta_E + a_k(E-E_k)}, \quad E_k \leq E < E_{k+1}$$

Solving the ergodicity problem with replica exchange

We use a second set of simulations with center of energies shifted.

After a certain number of updates, if two system are in the same overlapping region we propose a swap with probability



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

Sharp vs smooth cut-off

It is possible to use a smooth localized function instead of the energy intervals.

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

$$\langle\langle E - E_k \rangle\rangle_k(a) = \frac{1}{\mathcal{Z}} \int_{-\infty}^{+\infty} dE (E - E_k) e^{-aE} \rho(E) e^{\frac{(E-E_k)^2}{\sigma^2}}$$

The weight is a smooth function and can be sampled using the Hybrid Monte Carlo sampler

$$W(\phi) \propto e^{-aE - \frac{(E-E_k)^2}{\sigma^2}}$$

Remarks

- The LLR algorithm is similar in spirit to the Wang-Landau; it computes the DoS iteratively using a non-Markovian process but the general principles are different
- The LLR is a first principle method with convergence theorem:

$$\log \rho\left(E\right) = \log \rho_{LLR}\left(E\right) + \mathcal{O}\left({\delta_E}^2\right)$$

almost everywhere.

- The relative error does not depend on the magnitude of the DoS and the method works for several (thousands) orders of magnitude.
- For observable the convergence to its continuum energy value is is again $\mathcal{O}\left({\delta_E}^2\right)$

Application: 4d U(1) LGT

The action is $$S = \beta \sum (1 - \cos(\Theta_{\mu\nu}(x)))$$

The system has a weak first order phase transition near $\beta_c = 1.01$

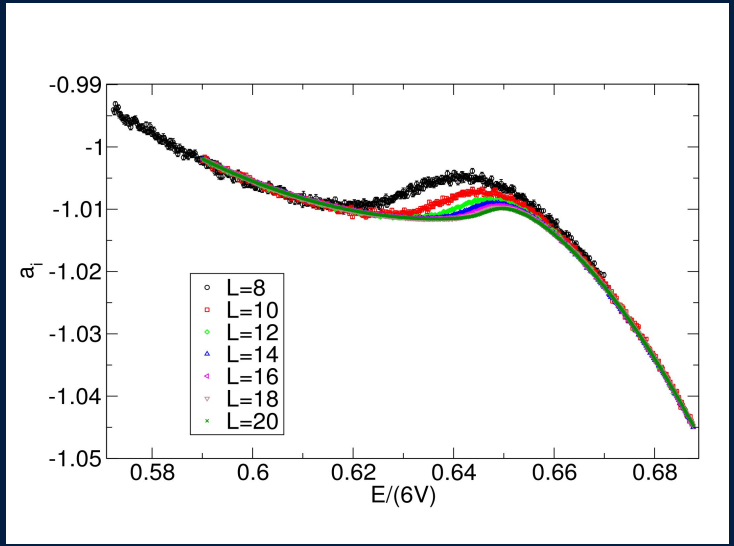
The meta-stabilities of the system make it very expensive to simulate.

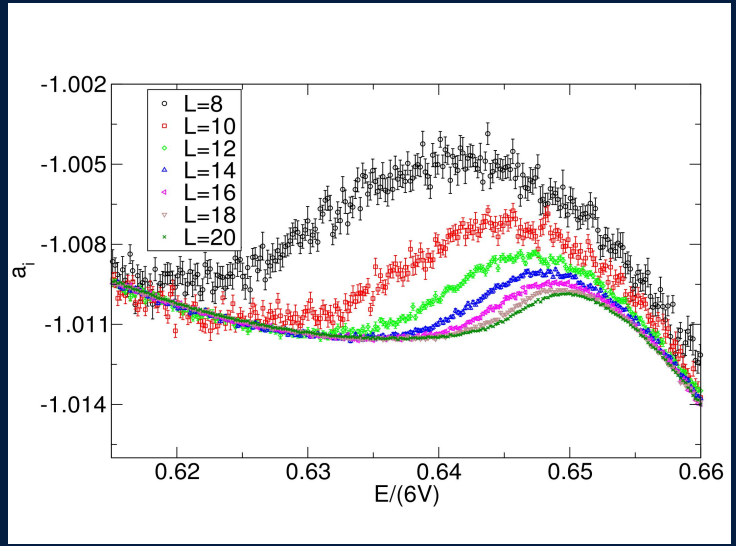
Supercomputer were needed for a relatively small lattice 18^4 [Arnold, Bunk, Lippert, Schilling Nucl. Phys. Proc. Suppl. **119** (2003)]

Scaling of a's with the volume

The coefficients a can be interpreted as the inverse microcanonical temperature, which has a well defined thermodynamical limit.

$$a_i = \left. \frac{d \log \rho(E)}{dE} \right|_{E_i} = \frac{1}{T_{mc}}$$





Comparison with the literature

The pseudo critical coupling is defined such as the coupling at which the peak of the specific heat occurs.

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

L	Present method	Reference
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)]*

Theories with sign problem

Consider a system with complex action

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

It is possible to define a generalized DoS

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

Such that the partition function is the Fourier transform of the DoS

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

Fourier transform

The DoS is not known exactly but just up to Noise coming from the numerical simulation.

$$P_{LLR}(s) = P_{TRUE}(s) + \epsilon(s)$$

The partition function is the fourier transform of the DoS (sign problem)

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

Z is a fast decaying function while the fourier transform of white noise does not depend on the frequency. A simple FFT will break down at relatively low chemical potential.

Filtering the noise

A simple alternative to FFT is to fit the computed log derivative of the DoS to a polynomial

$$\frac{d \log P(s)}{ds} = \sum_i c_i s^{2i+1}$$

The statistical error is reported to the coefficients and the Fourier transform can be performed using multiprecision numerical integration.

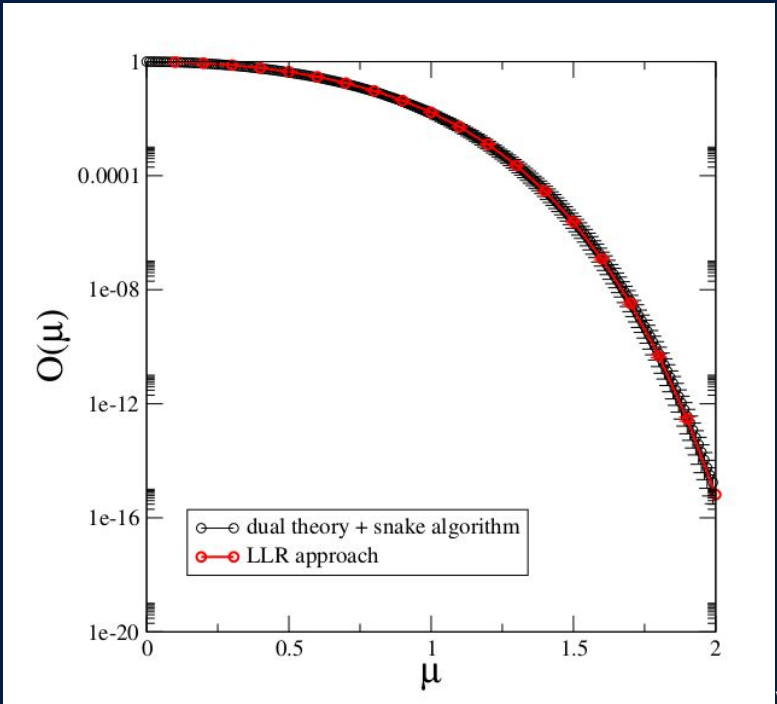
In order to quantify the sign problem we are interested in the expectation value of the phase

$$\left\langle e^{iS_I[\phi]} \right\rangle = \frac{\mathcal{Z}(\mu)}{\mathcal{Z}_{pq}(\mu)}$$

Z_3 model [Langfeld, Lucini (2014)]

The Z_3 model action can be derived from QCD in the strong coupling and heavy quark limit

$$S[\phi] = \tau \sum_{x,\nu} \phi_x \phi^*_{x+\nu} + \kappa \sum_x \left(e^{\mu} \phi_x + e^{-\mu} \phi^*_x \right), \ \phi \in Z_3$$



Heavy dense QCD[N. Garron K.Langfeld]

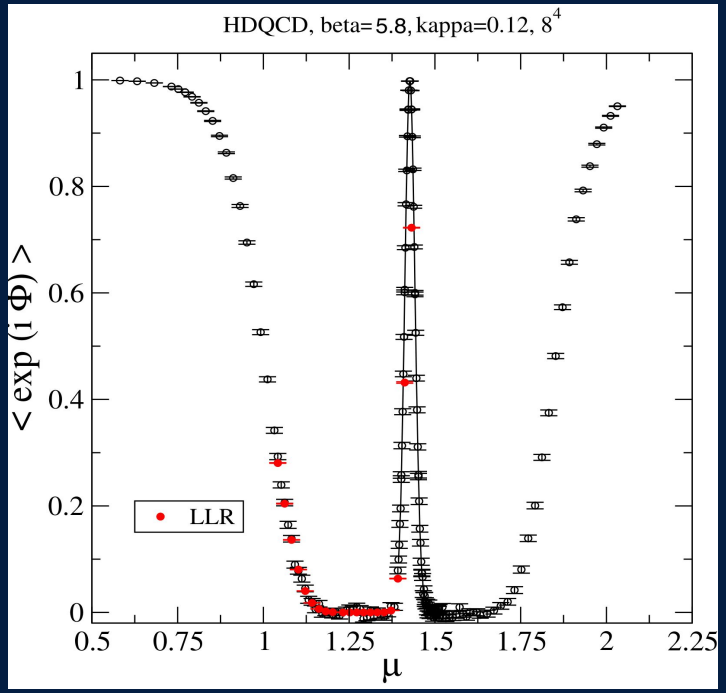
The action of QCD after integrating out the fermionic degrees of freedom is

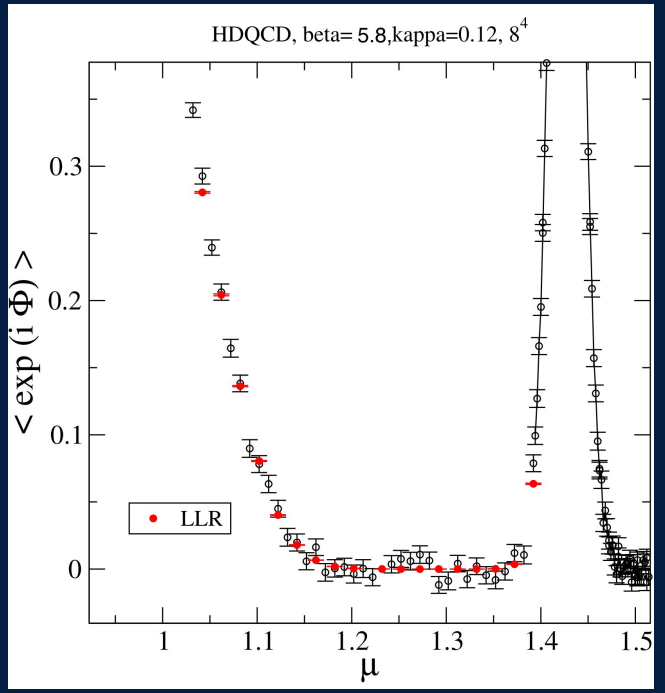
$$\mathcal{Z}(\mu) = \int \mathcal{D}U_\mu e^{-S_{ym}} \det M(\mu)$$

For large quark mass m and large chemical potential the determinant factorises into

$$\det M(\mu) = \prod_x \det{}^2 \left(1 + e^{\mu - m} P(x)\right) \det{}^2 \left(1 + e^{-(m+\mu)} P^\dagger(x)\right)$$

Comparison with reweighting





Bose gas at finite density

- We have seen that LLR gives good results in both Z_3 spin model and HDQCD [K. Langfeld B. Lucini, Phys. Rev. D **90** (2014)], [Garron, Langfeld (2016)]
- The relativistic Bose gas is a different test since it displays the Silver Blaze phenomenon
- Below the critical chemical potential the observables are independent from the chemical potential itself (Silver Blaze phenomenon)
- The Bose gas can be efficiently simulated using a dual flux representation which is not affected by the sign problem [Gattringer, Kloiber, Nucl. Phys. B **869** (2013)]

Bose gas at finite density

We consider a complex scalar field theory at finite density, the lattice action is

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

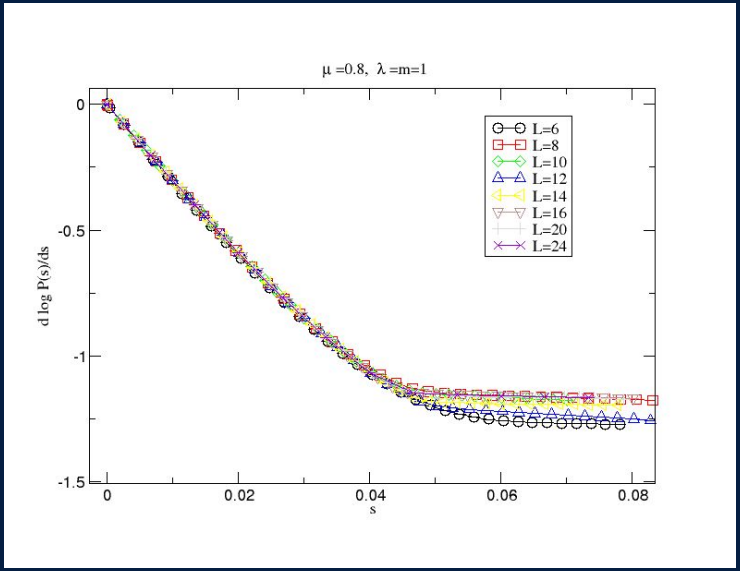
The action can be divided in complex and real part

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

In order to quantify the severity of the sign problem we are interested in the quantity

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

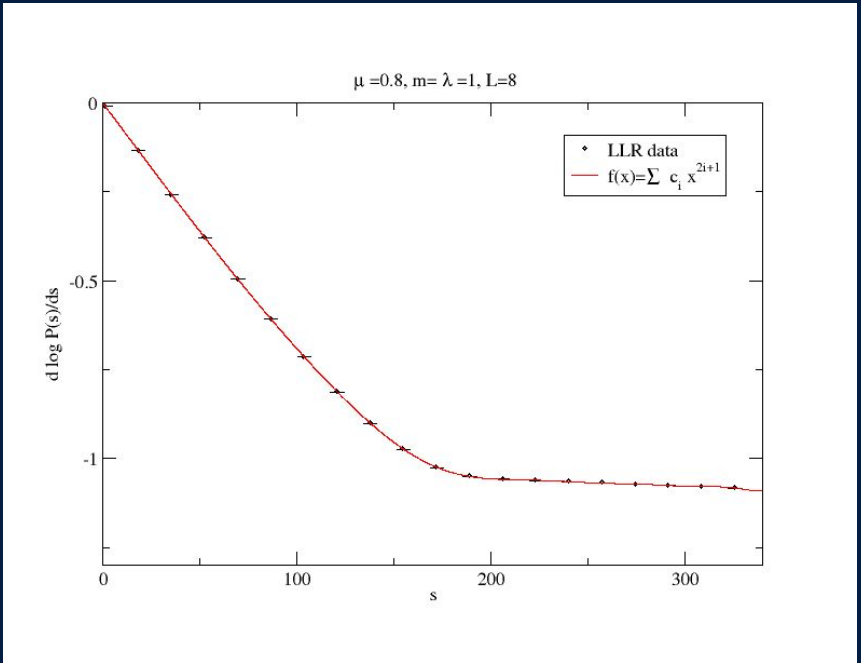
Generalized DoS



The partition function is given by the fourier transform of the DoS

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

Fit of the DoS

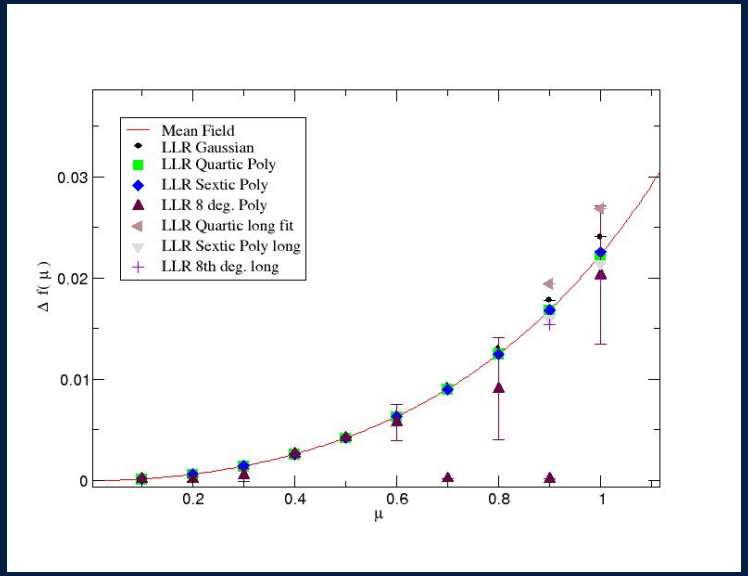


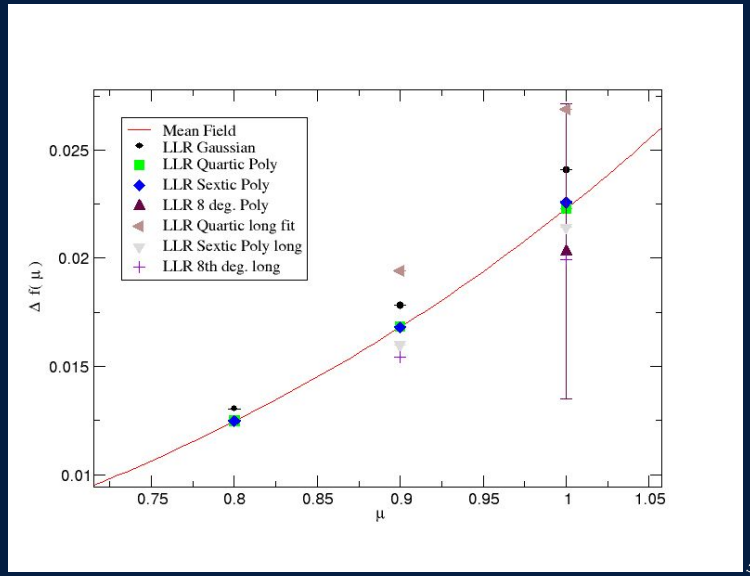
$$\frac{d\log P(s)}{ds} = \sum_i c_i s^{2i+1}$$

Systematic error

The fitting procedure seems to introduce a systematic error

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





An open question

- We presented an application of the LLR algorithm to a system affected by a severe sign problem
- A simple FFT breaks down at very small chemical potential
- Using a fitting procedure the range where it is possible to grasp the signal is greatly extended
- However, for the specific case of the Bose gas, the fitting procedure seems to introduce a systematic error
- Further investigation and a better procedure to account for the systematic error are needed