A novel density of state method for complex action systems

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(Based on *K. Langfeld and B. Lucini, arXiv:1404.7187*)

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Lattice 2014, Columbia University, 27th June 2014

Outline

1. Motivations
2. The method
3. The system
4. The algorithm
5. Results
6. Conclusions and outlook

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1 Motivations

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Motivations

- Numerical simulations of dense QCD still problematic
- The Monte Carlo approach is hindered by the sign problem
- In recent years, much progress has been achieved using an array of new methods
- A different perspective on the approach can give further insights on the problem and on the best solution
- Here we propose an approach based on the density of states and we test it on the $\mathbb{Z}(3)$ spin model

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The approach

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- Is it a good idea?
  - the density of states is hard to determine with numerical techniques
  - There is an overlap problem that goes exponentially with the volume

The approach

- Using the density of states (or a generalisation thereof) we reduce the partition function to an oscillating one-dimensional integral
- Is it a good idea?
  - the density of states is hard to determine with numerical techniques OR IS IT?
  - There is an overlap problem that goes exponentially with the volume OR IS THERE?

The approach

- Using the density of states (or a generalisation thereof) we reduce the partition function to an oscillating one-dimensional integral
- The density of states can be computed efficiently with the LLR method, which is a first principle approach providing exponential error suppression

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Highly-oscillatory integrals are allegedly difficult to calculate. The main assertion of this paper is that impression is incorrect. As long as appropriate quadrature methods are used, their accuracy increases when oscillation becomes faster. . .
[Arieh Iserles, 2003]

The approach

- Using the density of states (or a generalisation thereof) we reduce the partition function to an oscillating one-dimensional integral
- The density of states can be computed efficiently with the LLR method, which is a first principle approach providing exponential error suppression
- The remaining oscillating integral can be performed with well-established numerical techniques

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

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

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

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

The action is complex, but the partition function is real

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

Alternative representation for Z

With
$$N_0 = \sum_x \delta\Big(\phi(x), 1\Big), \qquad N_z = \sum_x \delta\Big(\phi(x), z\Big),$$
$$N_{z^*} = \sum_x \delta\Big(\phi(x), z^*\Big), \qquad N_0 + N_z + N_{z^*} = V = L^3$$

S_h can be written as

$$S_h = \kappa \left[(2\,N_0 - N_z - N_{z^*})\,\cosh(\mu) + i\sqrt{3}\,(N_z - N_{z^*})\,\sinh(\mu) \right]$$

and $Z(\mu)$ as

$$Z(\mu) = \sum_{\{\phi\}} \exp\Big\{ S[\phi] + \kappa\,(3N_0 - V)\,\cosh(\mu) \Big\} \cos\Big(\sqrt{3}\,\kappa\,\Delta N\,\sinh(\mu)\Big)\,, \qquad \Delta N = N_z - N_{z^*}$$

In this form $Z(\mu)$ can be determined using the LLR algorithm

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- We define the generalised density of state as

$$\rho(n) = \sum_{\{\phi\}} \delta\Big(n, \Delta N[\phi]\Big) \exp\Big\{S[\phi] + \kappa\Big(3N_0[\phi] - V\Big)\cosh(\mu)\Big\}$$

so that

$$Z(\mu) = \sum_{n} \rho(n) \cos\Big(\sqrt{3}\,\kappa \sinh(\mu) n\Big)$$

Note that $\rho(-n) = \rho(n)$

The algorithm

- $\rho(n) = \sum \delta\left(n, \Delta N\right) \exp\left\{S + \kappa\left(3N_0 - V\right) \cosh(\mu)\right\}$
  $Z(\mu) = \sum_n \rho(n) \cos\left(\sqrt{3}\,\kappa \sinh(\mu) n\right)$

The algorithm

- $\rho(n) = \sum \delta\left(n, \Delta N\right) \exp\left\{S + \kappa\left(3N_0 - V\right) \mathsf{cosh}(\mu)\right\}$
  $Z(\mu) = \sum_n \ \rho(n) \cos\left(\sqrt{3}\,\kappa\, \mathsf{sinh}(\mu) n\right)$
- We use the ansatz

$$\rho(n) \ = \ \prod_{i=0}^{n} \exp\{-a_i\}$$

The algorithm

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  $Z(\mu) = \sum_n \; \rho(n) \cos\Big(\sqrt{3}\,\kappa \sinh(\mu) n\Big)$
- Ansatz $\rho(n) \; = \; \prod_{i=0}^{n} \exp\{-a_i\}$
- Define n-restricted expectation values

$$\langle\langle F \rangle\rangle(a_n) \;=\; \frac{1}{\mathcal{N}} \sum_{\{\phi\}} F\left(\Delta N\left[\phi\right]\right) \; \theta(\Delta N, n) \; \exp\{a_n\}$$
$$\exp\Big\{S[\phi] \; + \; \kappa\Big(3N_0[\phi] - V\Big) \cosh(\mu)\Big\} \; ,$$

where $\theta(\Delta N, n) = 1$ for $|\Delta N[\phi] - n| \leq 1$ and
$\theta(\Delta N, n) = 0$ otherwise
$\mathcal{N}$ normalisation factor such that $\langle\langle 1 \rangle\rangle = 1$

The algorithm

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  $Z(\mu) = \sum_n \; \rho(n) \cos\Big(\sqrt{3}\, \kappa \sinh(\mu) n\Big)$
- Ansatz $\rho(n) \;=\; \prod_{i=0}^{n} \exp\{-a_i\}$
- Define n-restricted expectation values $\langle\!\langle F \rangle\!\rangle(a_n)$, which can be evaluated by standard Monte Carlo techniques

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- Define n-restricted expectation values $\langle\langle F \rangle\rangle(a_n)$, which can be evaluated by standard Monte Carlo techniques
- In each interval $[n-1; n+1]$, starting from a trial a_n^0, determine a_n from the recursion

$$a_n^{k+1} \ = \ a_n^k \ - \ \frac{\langle\langle \Delta N \rangle\rangle(a_n^k)}{\langle\langle \Delta N^2 \rangle\rangle(a_n^k)}$$

The algorithm

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- Statistical errors evaluated through a bootstrap procedure

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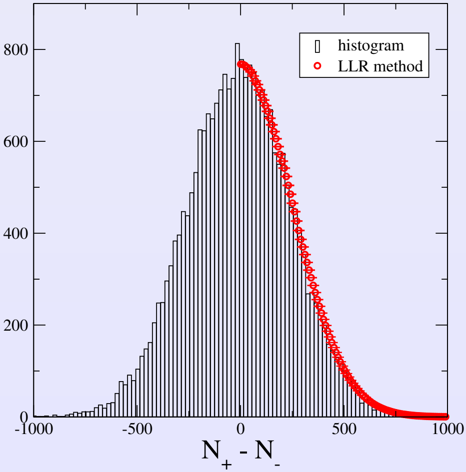
The density of states near the peak

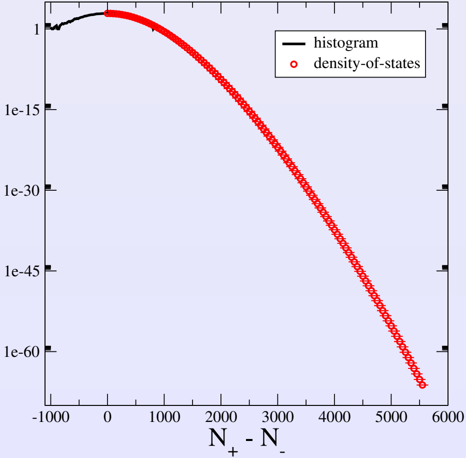
$L = 24, \tau = 0.17, \kappa = 0.05$



The two determinations are compatible

The density of states far from the peak

$L = 24$, $\tau = 0.17$, $\kappa = 0.05$



ρ determined well over 60 orders of magnitude!

The phase factor

- The phase factor $O(\mu)$ is given by

$$O(\mu) = \frac{\sum_n \rho(n) \cos\left(\sqrt{3}\, \kappa \sinh(\mu)\, n\right)}{\sum_n \rho(n)} = \frac{Z(\mu)}{Z(0)}$$

- Values of $O(\mu)$ close to one mean that the sign problem is mild; conversely, $O(\mu) \ll 1$ means that the system is afflicted by a severe sign problem
- Within the LLR method, $O(\mu)$ can be computed directly using the numerical determination of ρ, and more accurately using a polynomial interpolation $\ln \rho(n) = \sum_{k=0}^{p} c_k\, n^{2k}$
- $O(\mu)$ can be computed using a snake algorithm with worm updates, and results obtained with the two methods can be compared

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

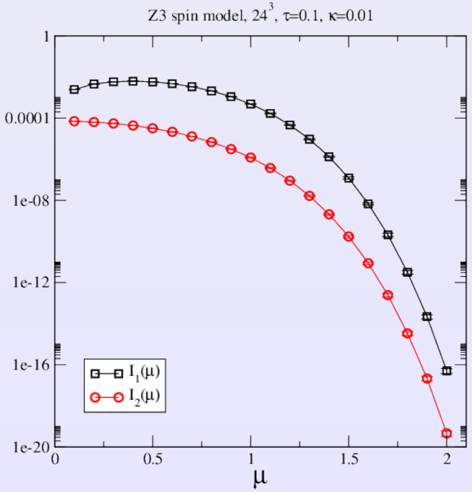
$$p(\mu) = \frac{\sum_n \rho(n)\; n\;\; \sin\Big(\kappa\sqrt{3}\;\sinh(\mu)\; n\Big)}{\sum_n \rho(n)\;\; \cos\Big(\kappa\sqrt{3}\;\sinh(\mu)\; n\Big)}$$

Can be expressed as the ratio of the oscillating sums

$$I_1(\mu) \;=\; \frac{\sum_n \rho(n)\; n\;\; \sin\Big(\kappa\sqrt{3}\;\sinh(\mu)\; n\Big)}{\sum_n \rho(n)}$$

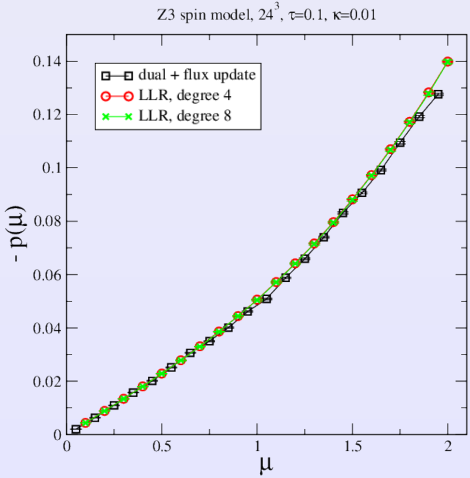
$$I_2(\mu) \;=\; \frac{\sum_n \rho(n)\;\; \cos\Big(\kappa\sqrt{3}\;\sinh(\mu)\; n\Big)}{\sum_n \rho(n)}$$

I_1 and I_2 *vs.* μ – Preliminary



Strong cancellations at high μ

$P(\mu)$ *vs.* μ – Preliminary



Good agreement with the worm algorithm

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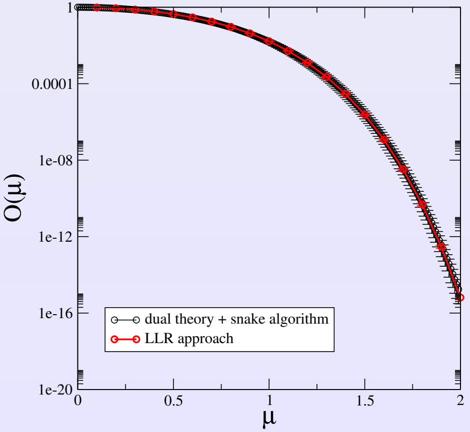
Conclusions

- We have proposed a new method for studying numerically systems afflicted by a sign problem
- The method rely on
  1. an efficient determination of the density of states with exponential error suppression (provided by the LLR sampling)
  2. a numerical interpolation of the measured density of states
  3. a high-precision semi-analytical determination of a unidimensional highly oscillating integral
- The method has been successfully tested on the $\mathbb{Z}(3)$ spin model
- In order to evaluate its effectiveness for more realistic systems, further studies are needed

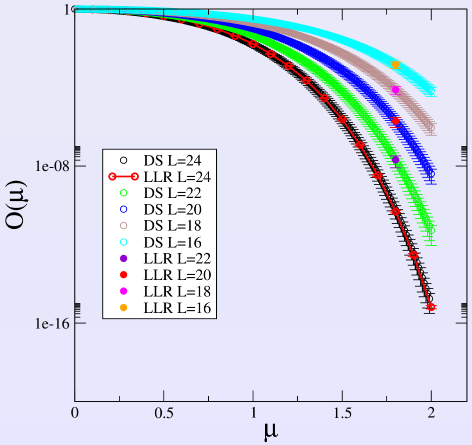
Numerical determinations

$L = 24, \tau = 0.1, \kappa = 0.01$



Excellent agreement even when cancellations are $\mathcal{O}(10^{-16})$

Volume scaling



Better precision of the LLR determination at any volume and no breaking of the agreement as the volume is increased