DENSITY OF STATE METHOD FOR COMPLEX ACTION SYSTEMS*

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While importance sampling Monte Carlo algorithms have proved to be a crucial tool for numerical studies in modern physics, they fail when we consider complex action systems. The density of states approach provides a way to simulate such systems and reduce the sign problem that afflicts them to a 1-dimensional oscillatory integral. In this work, we shall review the density of states approach as well as the Linear Logarithmic Relaxation algorithm and present some recent development concerning the control of systematics in this algorithm. The results of a benchmark study on the relativistic Bose gas shall be presented as well.

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1. Introduction

For a wide range of models at finite density, the partition function of the system can be cast in the form of

$$Z(\mu) = \int \mathcal{D}\phi \; \mathrm{e}^{S_{\mathrm{R}}[\phi]} \; \mathrm{e}^{i\mu S_{\mathrm{I}}[\phi]} \, . \tag{1}$$

When $\mu = 0$, Eq. (1) can be interpreted as a Boltzmann weight and standard importance sampling techniques can be used in numerical studies. At finite values of μ, the probability interpretation of the Boltzmann weight

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cease to be valid, thus Markov Chain Monte Carlo methods fail to generate configurations in the correct ensemble. This is generally referred to as the *sign problem* (see [1] for a recent review), as the signal comes from cancellations over multiple orders of magnitude due to the integration over the phase in the partition function.

In our contribution (see also [2]), we further develop the density of states method (originally proposed in [3] and recently discussed in [4–7]) with the LLR algorithm [8, 9]. At the core of the (*generalized*) DoS method, there is the definition of the density of state function

$$\rho(s) = N \int \mathcal{D}\phi \; \delta(s - S_{\mathrm{I}}[\phi]) \; e^{-S_{\mathrm{R}}[\phi]} \,, \tag{2}$$

so that the partition function (1) simply becomes a one-dimensional Fourier transform of this DoS function

$$Z(\mu) = \int \rho(s) \; e^{-i\mu s} \; \mathrm{d}s \,. \tag{3}$$

The severity of the sign problem is then quantified by the vacuum expectation value of the phase factor, defined by

$$\left\langle e^{i\varphi} \right\rangle = Z/Z_{pq} = \frac{\int \rho(s) \;\; \cos(\mu s) \; \mathrm{d}s}{\int \rho(s) \; \mathrm{d}s} = e^{-V \, \Delta F} \,, \tag{4}$$

where ΔF is the free energy difference between the original system and the phase quenched counterpart.

In this work, we will study the self-interacting Bose gas in four Euclidean dimensions at finite density. Already studied within a sign problem free dual formulation [10] as well as by a complex Langevin approach and analytical mean field [11], this system provides a good test model for alternatives approaches to the sign problem. The model is described by the following action:

$$\begin{aligned} S_{\mathrm{R}} \;&=\; \sum_x \Bigg[\frac{1}{2} \left(2d + m^2\right) \phi_{a,x}^2 + \frac{\lambda}{4} \left(\phi_{a,x}^2\right)^2 \\ &\qquad - \sum_{i=1}^{3} \phi_{a,x} \phi_{a,x+\hat{i}} - \cosh(\mu) \;\; \phi_{a,x} \phi_{a,x+\hat{4}} \Bigg] \\ S_{\mathrm{I}} \;&=\; \sum_x \; \varepsilon_{ab} \phi_{a,x} \phi_{b,x+\hat{4}} \end{aligned}$$

with the full action defined as $S = S_{\mathrm{R}} + i \sinh(\mu) S_{\mathrm{I}}$.

2. LLR algorithm

Inspired by the successful Wang–Landau approach to systems with a discrete energy spectrum [12], the LLR algorithm is an algorithm that allows us to reconstruct the DoS of continuous systems over several orders of magnitude. It is implemented through the following steps:

1. Divide the complex action domain in N intervals of width Δ;
2. For each interval, approximate the true density ρ as
$$\hat{\rho}_k(s) = C_k \exp\left(a_k(s - S_k)\right) \quad \text{with} \quad a_k = \partial \log \rho / \partial s|_{s=S_k}\,; \tag{5}$$
3. Obtain a_k as the root of the stochastic equation
$$\langle\langle \Delta S \rangle\rangle_k(a) = \int_{S_k - \Delta/2}^{S_k + \Delta/2} \rho(s)\ (s - S_k)\ \mathrm{e}^{-a(s-S_k)}\ \mathrm{d}s = 0 \tag{6}$$
using the Robbins–Monro iterative method [13]
$$a^{(n+1)} = a^{(n)} + \frac{12\ \langle\langle \Delta S \rangle\rangle_k \left(a^{(n)}\right)}{(n+1)\ \Delta^2}\,, \qquad \lim_{n\to\infty} a^n = a_k\,. \tag{7}$$

By linking the so-defined DoS, one obtains a piecewise estimation of ρ that becomes exact in the limit of vanishing Δ. Moreover, we can prove that $\hat{\rho}$ is measured with constant relative error over several orders of magnitude.

2.1. DoS rebuilding

However, once we consider the oscillatory integrals needed to measure the average phase (4), the piecewise approximation does not achieve the required accuracy. To overcome this difficulty, we have found a rebuilding technique based on global polynomial fitting best suited. In this approach, the LLR results are fitted to an odd polynomial (due to the symmetry property of the DoS) and a continuous DoS can be estimated as
$$\tilde{\rho}_n(s) = \mathcal{N}\ \exp\left\{\int_0^s p_n(x)\ \mathrm{d}x\right\} = \mathcal{N}\ \exp\left\{\sum_{i=1}^{n} \frac{c_{(2i-1)}}{2i}\ s^{2i}\right\}. \tag{8}$$
As shown in Fig. 1, where we show the result of the partially integrated phase factor defined as
$$\left\langle \mathrm{e}^{i\varphi} \right\rangle (s') = \int_0^{s'} \mathrm{d}s\ \rho(s)\ \cos(\sinh(\mu)s) \Big/ \int \mathrm{d}s\ \rho(s)\,, \tag{9}$$
the fitting approach has a huge advantage over the piecewise reconstruction.

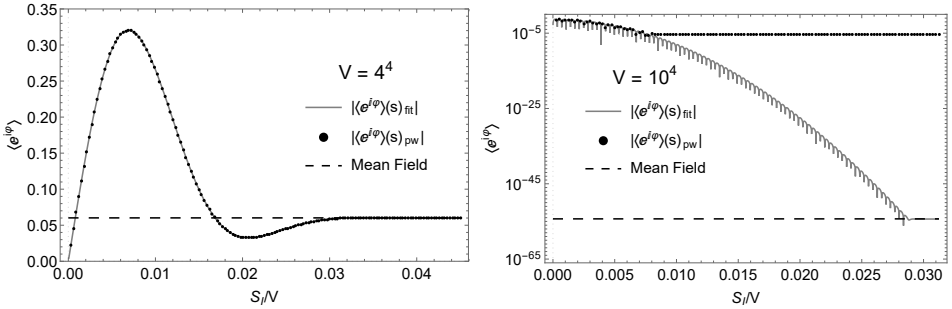

Fig. 1. Partially integrated phase factor, Eq. (9), as a function of the upper integration limit. Left: $V = 4^4$ corresponding to an easy sign problem scenario. Right: $V = 10^4$ corresponding to a hard sign problem scenario. Here, we plot the absolute value of the partially integrated phase factor on a logarithmic scale.

As the fitting approach compresses the set of a_k values to a handful of polynomial coefficient, the choice of the polynomial order n becomes of fundamental importance. The minimum order is easy to obtain with a χ^2 analysis, instead, to ensure that we are not *overfitting*, we independently evaluate in each interval the second derivative of $\log \rho$

$$f''(S_k) = \left(360/\Delta^4\right) \left(\left\langle\left\langle \Delta S^2 \right\rangle\right\rangle_k - \Delta^2/12\right) + \mathcal{O}\left(\Delta^2\right) . \tag{10}$$

Rather than using the second derivative directly in the fitting procedure, we look at how well the polynomial fit of the a_k describes this quantity. This gives us a quantitative indication of whether the chosen functional form is overfitting the data.

2.2. LLR intrinsic bias

As previously stated, the LLR algorithm becomes exact in the limit of $\Delta \to 0$, however, as in numerical simulations the interval width will always be a finite quantity, we study how a finite Δ will affect the final result.

To do so, we evaluate what are the corrections to Eq. (6) that do not vanish when $a = a_k = \partial \log(\rho)/\partial s|_{s=S_k}$. In particular, the first correction generated by this bias is

$$a_{\text{biased}} = a_k + \left(\Delta^2/40\right) \; f^{(3)}(S_k) + \mathcal{O}\left(\Delta^4\right) . \tag{11}$$

Based on this estimation, we are able to control this intrinsic bias reducing Δ to achieve unbiased results.

3. Results

Following the steps described in the previous sections, we run simulations at different lattice volumes ($V = 6^4, 8^4, 10^4, 16^4$) and different values of the

chemical potential ($\mu = 0.6, 0.8, 0.9$). For each combination of volume and chemical potential, we performed a bootstrap analysis consisting in the resampling of the a_k values to obtain a family of fitted functions used to integrate the phase factor. Performing this analysis at different polynomial orders, we have been able to obtain consistent results in the sweet spot region indicated by the χ^2 and second derivative analysis.

As shown in Fig. 2, the results obtained in this way are precise enough to enable us to extrapolate to the infinite volume limit.

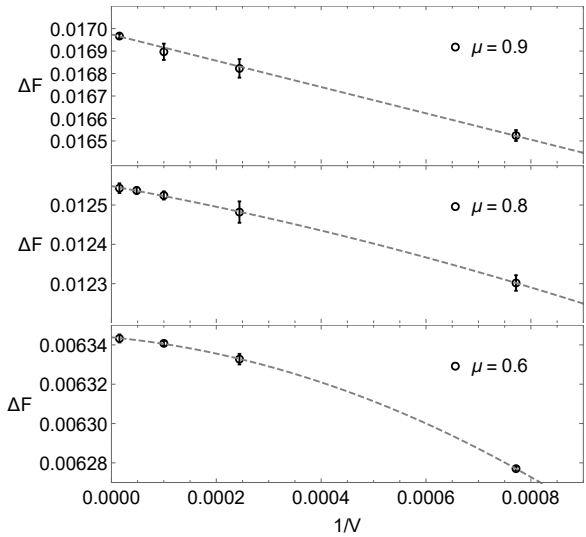

Fig. 2. Plot of the extrapolation at infinite volume of the free energy difference at chemical potential $\mu = 0.6, 0.8, 0.9$, the data points are relative to volumes $V = 6^4, 8^4, 10^4, 12^4$(only $\mu = 0.8$) and 16^4.

4. Conclusion

We have performed a numerical study of the self-interacting Bose gas using the density of states method. We have applied the LLR algorithm to study the DoS corresponding to the imaginary part of the action and studied the systematic bias due to the piecewise linear approximation and the influence of any non-vanishing interval width on the final result. We have shown that a polynomial fitting approach is able to provide numerically stable and reliable results integrating highly oscillatory integrals with phase factors down to $\mathcal{O}\left(10^{-480}\right)$ occurring in situations with a "hard sign problem". We have provided a methodology to determine an optimal range of polynomial order. For the relativistic Bose gas, we have shown that precise extrapolations to the infinite volume of the overlap free energies are possible within a broad range of chemical potentials.

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