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Density of states approach to dense quantum systems

Kurt Langfeld[1] and Biagio Lucini[2]
[1]*School of Computing & Mathematics, Plymouth PL4 8AA, United Kingdom*
[2]*College of Science, Swansea University, Swansea SA2 8PP, United Kingdom*
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We develop a first-principle generalized density-of-states method for numerically studying quantum field theories with a complex action. As a proof of concept, we show that with our approach we can numerically solve the strong sign problem of the Z_3 spin model at finite density. Our results are confirmed by standard simulations of the theory dual to the considered model, which is free from a sign problem. Our method opens new perspectives on *ab initio* simulations of cold dense quantum systems, and in particular of Yang-Mills theories with matter at finite densities, for which Monte Carlo-based importance sampling is unable to produce sufficiently accurate results.

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I. INTRODUCTION

Monte Carlo simulations [1] of the theory regularized on a lattice [2] are key for obtaining first-principle results in QCD [3] and in other strongly interacting systems, like for instance correlated electrons in solid state physics [4]. Monte Carlo simulations rely on importance sampling, which exposes the configurations that dominate the partition function. Importance sampling requires a real positive Gibbs factor. Because of this restriction, many crucial problems in physics that could in principle have been addressed by numerical simulations have remained unexplored. In particular, quantum systems with matter at finite densities, including cold and dense baryon matter, are described by a complex action. The corresponding Monte Carlo simulations are hampered by the notorious sign problem, which severely limits the applicability of this method.

In recent years, there has been noticeable progress in numerical studies of complex-action systems, both with Monte Carlo methods and techniques that do not rely on importance sampling. Among the most promising methods are the complexification of the fields in a Langevin-based approach [5,6], worm or flux algorithms [7,8] to simulate the dual theory when the corresponding duality transformation is known and exposes a real action [9–12] and the use of techniques that explicitly exploit the cancellations of classes of fields [13].

Among alternative approaches to conventional Monte Carlo sampling, an efficient strategy relies on the numerical computation of the density of states [14]. Once this quantity has been determined, the partition function and derived expectation values of observables can be computed semianalytically, integrating numerically the density of states with the appropriate Boltzmann weight. The multicanonical algorithm [15] allows one to effectively compute the density of states in gauge and spin systems (see e.g. Ref. [16]). More recently, an alternative technique has been discussed in Refs. [17,18]. Originally introduced to obtain an efficient sampling of the density of states for continuous systems using a Wang-Landau-inspired procedure, this algorithm has been proven to work effectively for discrete systems as well [19].

It was observed long ago that density-of-states methods can be used to study complex-action problems in numerical simulations [20]. A natural question is whether an appropriate generalization of the method proposed in Refs. [17,18], referred to as the LLR algorithm, which does not rely on action-based importance samplings, could be effective at simulating systems with a sign problem. In this paper, we show that a density-of-states approach in the LLR formulation appropriately generalized to complex-action systems can provide a viable solution to the sign problem. As a test case to demonstrate the method, we study the Z_3 spin model for finite chemical potentials μ, which serves as a toy model for finite-density QCD [21]. This system, which has also been studied with complex Langevin techniques [5], provides an ideal benchmark test for our approach, since it possesses a "strong" sign problem but can be simulated with flux-type algorithms after dualization [22]. We will show that our method (which does not rely on the existence of a dual theory with a real action, but rather is formulated using the original degrees of freedom), can achieve reliable results for a wide range of μ.

The rest of the paper is organized as follows. In Sec. II, we introduce our proposal. Section III presents the system we have chosen to test our method with, which can also be simulated using the more conventional method described in Sec. IV. The numerical results obtained with our method (Sec. V) are then used to show that our proposal is effective at dealing with the sign problem in this model (Sec. VI). A critical discussion of our findings and an overview of further studies (Sec. VII) conclude this work.

II. GENERALIZED DENSITY OF STATES

Before discussing in detail the considered model and our solution technique, we shall outline how the relevant quantities (i.e. the generalized density of states and observables sensitive to strong cancellations) are identified in a more general setup. We consider a quantum field theory (QFT) with a complex action. In general terms, the partition function of such a system is given in terms of a functional integral over the degrees of freedom $\phi(x)$:

$$Z(\mu) = \int \mathcal{D}\phi \exp\{iS_I[\phi](\mu)\} e^{S_R[\Phi](\mu)}, \tag{1}$$

with $S_R, S_I \in \mathbb{R}$ and where μ is the chemical potential. In finite-density QFTs, the imaginary part vanishes with vanishing μ, i.e., $S_I(\mu) \to 0$ for $\mu \to 0$. The simplest way to deal with the sign problem is to adopt a "quenched" approximation and to ignore the phase factor. This is undoubtedly a good approximation at small μ, but most likely it will fail when density effects start to play a significant role. To quantify the importance of the phase factor, we introduce

$$Z_{\rm mod}(\mu) = \int \mathcal{D}\phi e^{S_R[\Phi](\mu)}. \tag{2}$$

We point out that observables of the modified theory can be easily estimated by standard importance sampling methods. If we succeed in calculating the phase-factor expectation value

$$Q(\mu) = \frac{Z(\mu)}{Z_{\rm mod}(\mu)} = \langle \exp\{iS_I[\phi](\mu)\}\rangle_{\rm mod}, \tag{3}$$

observables such as the density σ would be accessible as well:

$$\sigma(\mu) = \frac{d\ln Z}{d\mu} = \frac{d\ln Q(\mu)}{d\mu} + \frac{d\ln Z_{\rm mod}}{d\mu}. \tag{4}$$

Our strategy to calculate $Q(\mu)$ is based upon the density-of-states method originally proposed by Wang and Landau [14] in its LLR version [17]. At the heart of our approach is the generalized density of states $\rho(s)$:

$$\rho(s) = N \int \mathcal{D}\phi \delta(s - S_I[\phi](\mu)) e^{S_R[\Phi](\mu)}. \tag{5}$$

Later, we will choose the normalization N such that $\rho(0) = 1$. Such a generalized density of states was first introduced by Gocksch [20] to address the phase factor of the quark determinant of finite-density QCD. Using a binning method without the Wang-Landau-type refinements, it has been argued that a solution of the overlap problem might only come with polynomial costs in the volume. The generalized density of states (5) was also introduced in Refs. [23–27] to study the θ-angle dependence in spin systems using a saddle-point approximation, which becomes exact in the thermodynamic limit.

The phase factor $Q(\mu)$ [Eq. (3)] can be obtained by calculating two integrals:

$$Q(\mu) = \frac{\int ds \rho(s) \exp\{is\}}{\int ds \rho(s)}. \tag{6}$$

Note that the normalization N drops out. The challenge is that for sizable and phenomenologically interesting values of μ the phase factor can be very small ($Q \approx 10^{-16}$ in the example below) and exponentially depends on the system volume. The smallness of Q arises from cancellations in the numerator of Eq. (6). On the other hand, $\rho(s)$ is at times of order one and only known numerically. Thus, any algorithm which addresses $\rho(s)$ must feature an exponential error suppression in order to muster enough precision to obtain a sensible result upon the integration in Eq. (6). As we detail below, the LLR algorithm delivers just that.

III. THE Z_3 SPIN SYSTEM

As a showcase of our approach, we are going study the Z_3 spin model at finite chemical potential μ: the degrees of freedom $\phi(x) \in Z_3$ are associated with the sites of the N^3 three-dimensional lattice. The partition function and the action of the system are given by

$$Z(\mu) = \sum_{\{\phi\}} \exp\{S[\phi] + S_h[\phi]\}, \tag{7}$$

$$S[\phi] = \tau \sum_{x,\nu} \phi_x \phi^*_{x+\nu}, S_h[\phi] = \sum_x (\eta\phi_x + \bar{\eta}\phi^*_x), \tag{8}$$

with $\eta = \kappa e^{\mu}$ and $\bar{\eta} = \kappa e^{-\mu}$. The model can be derived from QCD in the heavy-quark and strong-coupling limit [28,29]. Therefore, κ is related to the quark hopping constant, and μ is the chemical potential. For $\mu = \mathcal{O}(1)$, this theory possesses a strong sign problem in the above formulation. However, the reformulation of this model with dual variables is real (even at finite μ) and can be effectively simulated using flux-type algorithms [22]. This makes this theory an ideal benchmark test for the LLR approach.

IV. THE FLUX ALGORITHM

Before showing our numerical findings, we briefly detail the calculation of the phase factor using the flux algorithm developed by Gattringer *et al.* [22]. The partition function can be expressed in terms of dual variables ϕ_D:

$$Z(\mu) = \sum_{\{\phi_D\}} M(\mu, \phi_D) P(\phi_D). \tag{9}$$

$Z(\mu)$ can be computed in terms of $Z(0)$. However, a simplistic approach to this calculation will be affected by the so-called overlap problem, whereby a partition function is sampled using configurations derived from a statistical sampling that are in principle related, but in practice have different dominant contributions. To resolve the overlap problem, we adopt a variant of the snake algorithm [30]. We firstly observe that

$$\frac{Z(\mu+\Delta\mu)}{Z(\mu)} = \frac{1}{Z(\mu)}\sum_{\{\phi_D\}}\frac{M(\mu+\Delta\mu,\phi_D)}{M(\mu,\phi_D)} \times M(\mu,\phi_D)P(\phi_D) = \left\langle\frac{M(\mu+\Delta\mu,\phi_D)}{M(\mu,\phi_D)}\right\rangle_\mu. \quad (10)$$

The latter expectation value can be efficiently evaluated with the flux algorithm. The partition function is then obtained from

$$Z(k\Delta\mu) = Z(0)\prod_{i=1}^{k}\frac{Z(i\Delta\mu)}{Z((i-1)\Delta\mu)}, \quad (11)$$

with each factor $Z(i\Delta\mu)/Z((i-1)\Delta\mu)$ evaluated with the snake algorithm. The same approach is repeated for the "quenched" partition function Z_{mod}, and the phase factor is finally obtained from

$$Q(k\Delta\mu) = Z(k\Delta\mu)/Z_{\mathrm{mod}}(k\Delta\mu). \quad (12)$$

V. MEASURING THE GENERALIZED DENSITY OF STATES

To proceed with our method, we introduce the center elements

$$\phi \in \{1, z, z^\dagger\}, \qquad z \coloneqq \frac{1}{2}+\frac{\sqrt{3}}{2}i. \quad (13)$$

The linear term of the action can then be written as

$$S_h[\phi] = \kappa\sum_x[\mathrm{e}^{\mu}\phi(x)+\mathrm{e}^{-\mu}\phi^\dagger(x)] = \kappa[(2N_0-N_z-N_{z^*})\cosh(\mu) + i\sqrt{3}(N_z-N_{z^*})\sinh(\mu)], \quad (14)$$

where N_0, N_z and N_{z^*} are the numbers of time-like links equalling a particular center element, i.e.

$$N_0 = \sum_x\delta(\phi(x),1), \qquad N_z = \sum_x\delta(\phi(x),z), \qquad N_{z^*} = \sum_x\delta(\phi(x),z^*). \quad (15)$$

The probability distribution for the variable $\Delta N \coloneqq N_z - N_{z^*}$ is symmetric around zero. Thus, the partition function is real and given by

$$Z(\mu) = \sum_{\{\phi\}}\exp\{S[\phi]+\kappa(3N_0-V)\cosh(\mu)\} \times\cos\left(\sqrt{3}\kappa\Delta N\times\sinh(\mu)\right), \quad (16)$$

where we have used the constraint

$$N_0+N_z+N_{z^*} = N^3 \coloneqq V. \quad (17)$$

For a fixed lattice volume V, we now define the density of states ρ by

$$\rho(n) \coloneqq \sum_{\{\phi\}}\delta(n,\Delta N[\phi])\exp\{S[\phi] + \kappa(3N_0[\phi]-V)\cosh(\mu)\}. \quad (18)$$

With this definition, the partition function can be written as a simple sum:

$$Z(\mu) = \sum_n\rho(n)\cos(\sqrt{3}\kappa\times\sinh(\mu)n). \quad (19)$$

Using a standard Monte Carlo simulation and casting the observed values ΔN into a histogram would only provide enough precision to calculate the partition function for very small values of μ. Nevertheless, this histogram provides first insights into $\rho(n)$ and later will serve as an important cross-check for more elaborate methods. Our results for a 24^3 lattice using $\tau = 0.17$ and $\kappa = 0.05$ are shown in Fig. 1.

Our aim will be to calculate $\rho(n)$ with a precision of many of orders of magnitude such that a direct evaluation of Eq. (19) does yield a statistically significant result despite cancellations. For this purpose, we follow Ref. [17] and write

$$\rho(n) = \prod_{i=0}^{n}\exp\{-a_i\}. \quad (20)$$

We then define the "double-bracket" expectation values by

$$\langle\!\langle F\rangle\!\rangle(a_n) = \frac{1}{\mathcal{N}}\sum_{\{\phi\}}F(\Delta N[\phi])\theta(\Delta N,n)\exp\{a_n\Delta N\} \times\exp\{S[\phi]+\kappa(3N_0[\phi]-V)\cosh(\mu)\}, \quad (21)$$

$$\mathcal{N} = \sum_{\{\phi\}}\theta(\Delta N,n)\exp\{a_n\Delta N\} \times\exp\{S[\phi]+\kappa(3N_0[\phi]-V)\cosh(\mu)\}, \quad (22)$$

where $\theta(\Delta N,n) = 1$ for $|\Delta N[\phi]-n| \le 1$ and $\theta(\Delta N,n) = 0$ otherwise. Note that these expectation values can be

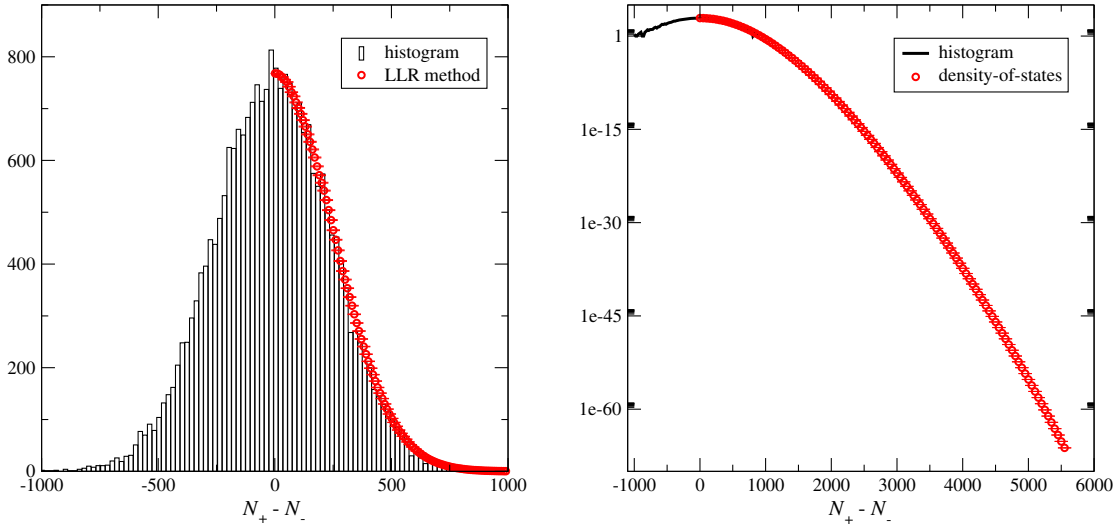

FIG. 1 (color online). Left: The probability distribution ρ for $n = \Delta N = N_+ - N_-$ from a direct simulation using a histogram (black steps) and from our LLR method. Right: Same probability distribution on a logarithmic scale, for a wider range of n. 24^3 lattice, $\tau = 0.17$, and $\kappa = 0.05$.

calculated using standard Monte Carlo methods. If a_n is chosen correctly, configurations with $\Delta N = n-1$, $\Delta N = n$ and $\Delta N = n+1$ possess the same probability. This yields a nonlinear equation to determine a_n:

$$\langle\langle \Delta N \rangle\rangle(a_n) = 0. \tag{23}$$

We solve the latter equations using a Newton-Raphson iteration:

$$a_n^{k+1} = a_n^k - \frac{\langle\langle \Delta N \rangle\rangle(a_n^k)}{\langle\langle \Delta N^2 \rangle\rangle(a_n^k)}. \tag{24}$$

Details of the algorithm will be presented elsewhere. Once we have obtained the coefficients a_n, we can reconstruct the density of states ρ with the help of Eq. (20). In practice, we have obtained 200 independent values for each of the a_n with n up to 5000. Our result for ρ_n is also shown in Fig. 1. Error bars are obtained using the bootstrap method. We find an excellent agreement with the histogram method, but can extend the observed range of ρ to over 60 orders of magnitude.

VI. TAMING THE SIGN PROBLEM WITH THE GENERALIZED DENSITY OF STATES

The phase factor $Q(\mu)$ can now obtained from Eq. (6) or, in the case of the Z_3 spin model, from

$$Q(\mu) = \frac{\sum_n \rho(n) \cos\left(\sqrt{3}\kappa \sinh(\mu) n\right)}{\sum_n \rho(n)}. \tag{25}$$

Error margins could once again be computed using the bootstrap method. However, we found it advantageous to exploit the smoothness of $\ln \rho(n)$ and fit this function to an even polynomial of degree $2p$:

$$\ln \rho(n) = \sum_{k=0}^{p} c_k n^{2k}. \tag{26}$$

In practice, we fitted polynomials of degree $2p = 2, 4, 6, 8$ and found very stable results with only the coefficients c_0 and c_2 significantly (within bootstrap error bars) different from zero. After the extraction of the Taylor coefficients, the phase factor (25) can be obtained "semianalytically" to a high precision.

Our numerical findings for ρ are shown in Fig. 1, while our results for $Q(\mu)$ are summarized in Fig. 2. Our density of states agrees with the density of states extracted from the flux algorithm for all values for which the latter method is effective (see Fig. 1, left panel, for an example). The right panel of Fig. 1 demonstrates the ability of our method to determine the density of states over more than 60 orders of magnitude. The correctness of this determination can be checked by comparing our results for $Q(\mu)$ with results obtained with the flux algorithm. Figure 2 shows agreement for various lattice sizes at $\mu = 1.8$, where the sign problem is severe. Note that there is no sign of the method breaking at large volume, up to volumes that are known from other methods to be large enough for the asymptotic behavior to be manifest in the relevant observables. For the largest size, the same figure shows an agreement over a wide range of μ, which determines a variation of $Q(\mu)$ over 16 orders of magnitude. A more detailed inspection shows that numerical results (obtained using quadruple precision) found with the two methods are always within errors.

We finally present a rough estimate of the computational costs. The density ρ_n rapidly decreases with n such that the

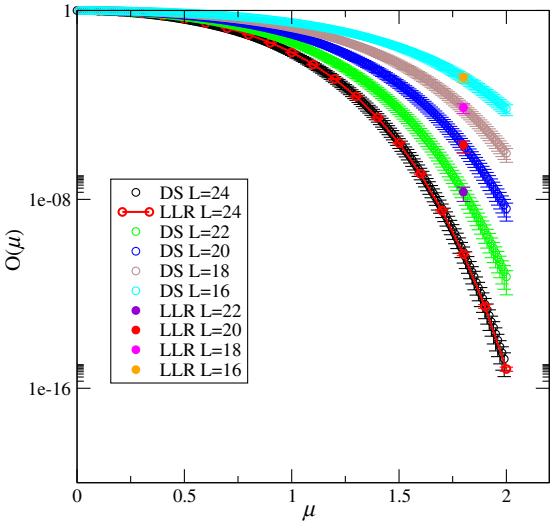

FIG. 2 (color online). The phase factor calculated using the flux algorithm in the dual formulation and the LLR algorithm applied to the original theory with a strong sign problem for various sizes and μ values, at $\tau = 0.1$ and $\kappa = 0.01$.

sum in Eq. (25) can be truncated at some value $n_{\max}$. Empirically, we find that this upper limit needs to scale with volume,

$$n_{\max} \approx 0.3V.$$

When calculating the coefficients a_n^k, the number of steps needed for the Newton-Raphson iteration (24) to achieve an acceptable precision is independent of the system size. However, the numerical costs to evaluate the estimators for the double-expectation values $\langle\langle \ldots \rangle\rangle$ are scaling with the volume. This leaves us with the observation that estimating the phase factor $Q(\mu)$ requires computational costs that increase polynomiall increase with the volume, V^p, $p \approx 2$. A detailed analysis of the volume dependence of the cost will be presented elsewhere. We here emphasize that costs follow a power law of the volume rather than increasing exponentially as it would be with standard Monte Carlo methods.

VII. DISCUSSION AND CONCLUSIONS

In conclusion, we have proposed an efficient *ab initio* approach that allows us to numerically compute observables affected by strong cancellations in systems afflicted by a sign problem. The methods consists of (a) a generalization of the density of states, (b) a numerical determination of the generalized density of states using the LLR algorithm, (c) a polynomial interpolation of the density of states, and (d) a semianalytical determination of observables. This strategy has been successfully probed for the Z_3 spin system, for which numerical results are available since its dual formulation is real and accessible by Monte Carlo methods. We have found that our method reproduces results of the dual formulation over a wide range of chemical potentials. In this first exploratory study, we explored a region of space that is deep in the symmetric phase. We found that a Gaussian approximation does work very well, which might be due to the fact that for our parameter choice the system is far from the phase transition. The validity of the Gaussian approximation in this regime has been argued in Ref. [31]. We are currently extending our studies to the phase diagram near the phase transition. We expect to find significant corrections to the Gaussian behavior [32].

Note that the method we have used in this work could in principle suffer from ergodicity problems if topological sectors with large energy barriers are present that would implicate long energy detours for tunnelings. While the agreement with the exact algorithm shows that this does not happen for the system studied here, for the general case an ergodic algorithm can be easily obtained following the technique exposed in Ref. [33].

The final goal of our program would be tackling the sign problem in QCD and in other real-world systems. In order to verify the effectiveness of our method, studies of more complicated toy models such as the O(2) system and the Bose gas at final temperature are currently in progress.

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Note added.—After submitting our work to this journal, Ref. [34] appeared in which the same system is studied with a similar technique in a wider range of parameters. That investigation shows that the density-of-states method agrees with the worm algorithm even in regions where the Gaussian approximation to the generalized density of states breaks down.

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