The density of states approach to dense quantum systems

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We develop a first-principle generalised density of state method for studying numerically quantum field theories with a complex action. As a proof of concept, we show that with our approach we can solve numerically 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 are unable to produce sufficiently accurate results.

Monte Carlo simulations [1] of the theory regularised on a lattice [2] are key for obtaining first principle results in Quantum Chromo Dynamics (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, among which is cold and dense baryon matter, are described by a complex action. The corresponding Monte Carlo simulations are hampered by the notorious sign problem, which limits severely 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, 10] and the use of techniques that explicit exploit the cancellations of classes of fields [11].

Among alternative approaches to conventional Monte Carlo sampling, an efficient strategy relies on the numerical computation of the density of states [12]. Once this quantity has been determined, the partition function and derived expectation values of observables can be computed semi-analytically, integrating numerically the density of states with the appropriate Boltzmann weight. An effective technique for computing the density of states for systems with a continuous spectrum has been discussed in [13, 14]. A natural question is whether this method, referred to as the LLR algorithm, not relying on action-based importance samplings, could be effective at simulating systems with a sign problem. In this letter, we show that a density of state approach in the LLR

formulation appropriately generalised 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. This system, which has been studied also 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 dualisation [15]. We will show that our method (which does not rely on a the existence of a dual theory with real action, but is formulated using the original degrees of freedom), can achieve reliable results for a wide range of μ.

Before discussing in detail the considered model and our solution technique, we shall outline how the relevant quantities (i.e. the generalised 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 $\phi(x)$:

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

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

$$Z_{\mathrm{mod}}(\mu) \; = \; \int \mathcal{D}\phi \; \mathrm{e}^{S_R[\Phi](\mu)} \, . \qquad (2)$$

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

$$Q(\mu) \; = \; \frac{Z(\mu)}{Z_{\mathrm{mod}}(\mu)} \; = \; \Big\langle \exp\Big\{iS_I[\phi](\mu)\Big\} \Big\rangle_{\mathrm{mod}}, \qquad (3)$$
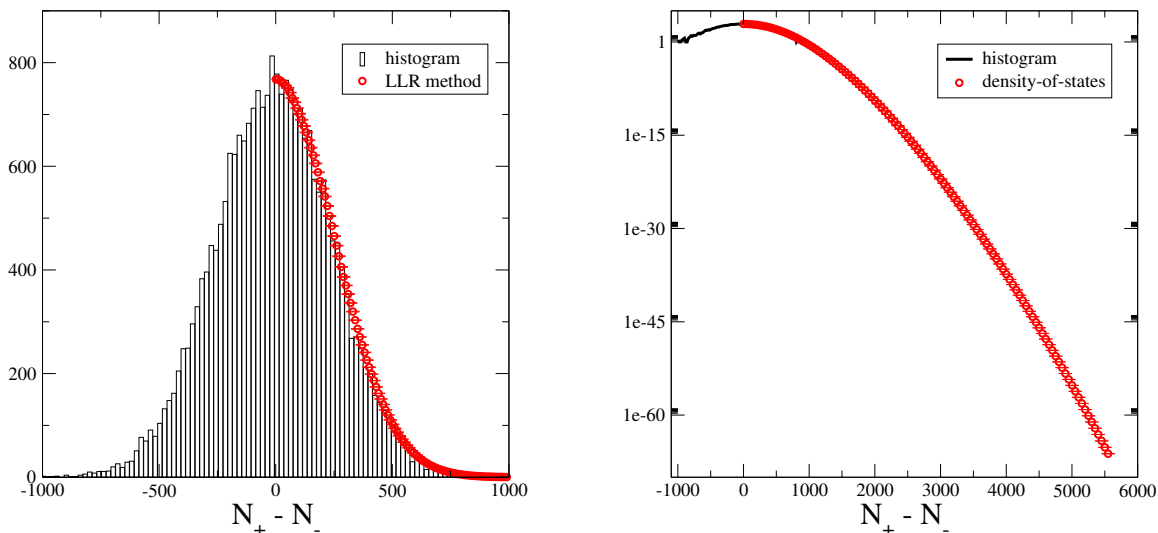
FIG. 1. The probability distribution ρ for $n = \Delta N = N_+ - N_-$ from a direct simulation using a histogram (black steps) and from our LLR method (left). Same probability distribution on a logarithmic scale (right), for a wider range of n. 24^3 lattice, $\tau = 0.17$, and $\kappa = 0.05$.

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

$$\sigma(\mu) \;=\; \frac{d \ln Z}{d\mu} \;=\; \frac{d \ln Q(\mu)}{d\mu} \;+\; \frac{d \ln Z_{\mathrm{mod}}}{d\mu} \;. \qquad (4)$$

Our strategy to calculate $Q(\mu)$ is the based upon the density of state method originally proposed by Wang and Landau [12] in its LLR version [13]. At the heart of our approach is the generalised density of states $\rho(s)$:

$$\rho(s) \;=\; N \int \mathcal{D}\phi \; \delta\!\left(s - S_I[\phi](\mu)\right) \mathrm{e}^{S_R[\Phi](\mu)} \;. \qquad (5)$$

Later, we will choose the normalisation N such that $\rho(0) = 1$. The phase factor can be then obtained by calculating two integrals:

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

Note that the normalisation N drops out. The challenge is that for sizeable and phenomenological 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 (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 (6). As we detail below, the LLR algorithm is just delivering that.

For 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 3-dimensional lattice. The partition function and the action of the system are given by

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

$$S[\phi] = \tau \sum_{x,\nu} \phi_x \, \phi_{x+\nu}^* \;, \quad S_h[\phi] = \sum_x \Big(\eta\phi_x + \bar{\eta}\phi_x^* \Big) \;, (8)$$

with $\eta = \kappa\,\mathrm{e}^{\mu}$ and $\bar{\eta} = \kappa\,\mathrm{e}^{-\mu}$. The model can be derived from QCD in the heavy quark and strong coupling limit [16, 17]. Thereby, 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 [15]. This makes this theory an ideal benchmark test for the LLR approach.

Before showing our numerical findings, we briefly detail the calculation of the phase factor using the flux algorithm developed by Gattringer at al. [15]. The partition function can be expressed in terms of dual variables ϕ_D:

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

$Z(\mu)$ can be computed in terms of $Z(0)$. However, a simplistic approach to this calculation will be affected by a so-called overlap problem, whereby a partition function is sampled using configurations derived from a statistical sampling in principle related, but in practice with different dominant contributions. To resolve the overlap problem, we adopt a variant of the snake algorithm [18].

We firstly observe that

$$\frac{Z(\mu + \Delta\mu)}{Z(\mu)} = \frac{1}{Z(\mu)} \sum_{\{\phi_D\}} \frac{M(\mu + \Delta\mu, \phi_D)}{M(\mu, \phi_D)} \times \qquad (10)$$

$$M(\mu, \phi_D)\, P(\phi_D) = \left\langle \frac{M(\mu + \Delta\mu, \phi_D)}{M(\mu, \phi_D)} \right\rangle_\mu .$$

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

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

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

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

To proceed with our method, we introduce the centre elements

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

The linear term of the action can then be written

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

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

$$N_0 = \sum_x \delta\Big(\phi(x), 1\Big), \quad N_z = \sum_x \delta\Big(\phi(x), z\Big),$$

$$N_{z^*} = \sum_x \delta\Big(\phi(x), z^*\Big). \qquad (15)$$

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

$$\begin{aligned}
Z(\mu) = \sum_{\{\phi\}} \exp\Big\{ S[\phi] &+ \kappa\,(3N_0 - V)\, \cosh(\mu) \Big\} \\
&\cos\Big(\sqrt{3}\,\kappa\,\Delta N \sinh(\mu)\Big) ,
\end{aligned} \qquad (16)$$

where we have used the constraint

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

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

$$\begin{aligned}
\rho(n) := \sum_{\{\phi\}} \delta\Big(n, \Delta N[\phi]\Big)\, \exp\Big\{ S[\phi] \\
+ \kappa\Big(3N_0[\phi] - V\Big) \cosh(\mu) \Big\} .
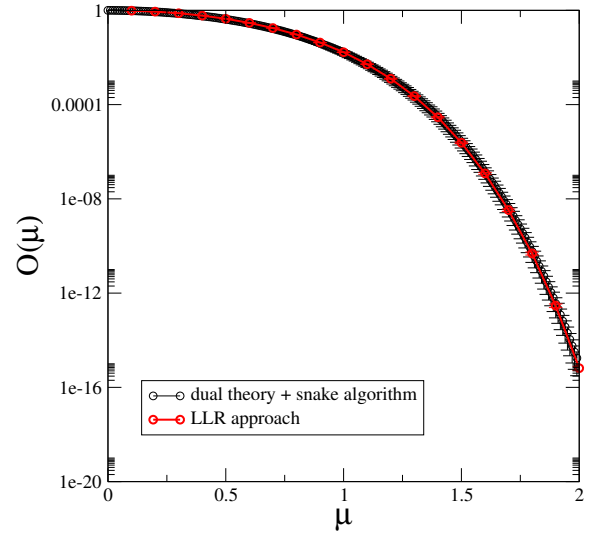\end{aligned} \qquad (18)$$

FIG. 2. The phase factor calculated using the flux algorithm and the dual formulation (black symbols) and the LLR algorithm applied to the original theory with a strong sign problem (red symbols). 24^3 lattice, $\tau = 0.1$ and $\kappa = 0.01$.

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

$$Z(\mu) = \sum_n \rho(n)\, \cos\Big(\sqrt{3}\,\kappa \sinh(\mu)\, n\Big) . \qquad (19)$$

Using a standard Monte Carlo simulation and casting the observed values ΔN into an 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 crosscheck for any more elaborate method. Our results for a 24^3 lattice using $\tau = 0.17$ and $\kappa = 0.05$ are shown in figure 1.

Our aim will be to calculate $\rho(n)$ with a precision of many of orders of magnitude such that a direct evaluation of (19) does yield a statistically significant result despite cancellations. For this purpose, we follow [13] and write

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

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

$$\langle\!\langle F \rangle\!\rangle(a_n) = \frac{1}{\mathcal{N}} \sum_{\{\phi\}} F\left(\Delta N[\phi]\right)\, \theta(\Delta N, n)\, \exp\{a_n\} \quad (21)$$

$$\exp\Big\{ S[\phi] + \kappa\Big(3N_0[\phi] - V\Big) \cosh(\mu) \Big\} ,$$

$$\mathcal{N} = \sum_{\{\phi\}} \theta(\Delta N, n)\, \exp\{a_n\} \qquad (22)$$

$$\exp\Big\{ S[\phi] + \kappa\Big(3N_0[\phi] - V\Big) \cosh(\mu) \Big\} ,$$

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

calculated using standard Monte Carlo methods. The LLR key ingredient is the observation that if the re-weighting factor $\exp\{a\}$ is chosen correctly, configurations with $\Delta N = n - 1$, $\Delta N = n$ and $\Delta N = n + 1$ possess the same probability. This yields a non-linear equation to determine a_n:

$$\langle\langle \Delta N \rangle\rangle (a_n) \; = \; 0 \; . \qquad (23)$$

It is the later equation which we solve using a Newton-Raphson iteration:

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

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 (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 figure 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.

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

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

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

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

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 "semi-analytical" to a high precision.

Our numerical findings for ρ are shown in figure 1, while our results for $Q(\mu)$ are summarised in figure 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 figure 1, left panel, for an example). The right panel of figure 1 demonstrates the ability of our method to determine the density of states over more than sixty 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 over a wide range of μ, which determines a variation of $Q(\mu)$ over sixteen orders of magnitude. A more detailed inspection shows that numerical results (obtained using quadruple precision) found with the two methods are always within errors.

In conclusion, we have proposed an efficient *ab initio* approach that allows us to compute numerically observables affected by strong cancellations in systems afflicted by a sign problem. The methods consists of: a) a generalisation of the density of states; b) a numerical determination of the generalised density of states using the LLR algorithm; c) a polynomial interpolation of the density of states; d) a semi-analytical determination of observables. This strategy has been successfully probed for the Z_3 spin system, for which numerical results are available since its dual formualtion 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. The final goal of our programme 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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