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The $\mathbb{Z}_3$ model with the density of states method

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In this contribution we apply a new variant of the density of states method to the $\mathbb{Z}_3$ spin model at finite density. We use restricted expectation values evaluated with Monte Carlo simulations and study their dependence on a control parameter λ. We show that a sequence of one-parameter fits to the Monte-Carlo data as a function of λ is sufficient to completely determine the density of states. We expect that this method has smaller statistical errors than other approaches since all generated Monte Carlo data are used in the determination of the density. We compare results for magnetization and susceptibility to a reference simulation in the dual representation of the $\mathbb{Z}_3$ spin model and find good agreement for a wide range of parameters.

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1. Introduction

Lattice QCD at finite chemical potential μ is notoriously difficult for Monte Carlo simulations since for $\mu > 0$ the fermion determinant and thus the effective fermion action are complex. The corresponding Boltzmann factor can no longer be interpreted as a probability and thus is not suitable for importance sampling. Various methods to overcome this so-called complex action problem have been explored, such as reweighting, complex Langevin, various expansions around $\mu = 0$ and rewriting partition sums to different degrees of freedom (dual variables).

Another possible approach is the density of states (DoS) method. Here the complex action problem manifests itself in the fact that for the evaluation of observables the density of states is multiplied with a rapidly oscillating factor, such that for reliable results the density of states has to be determined with very high accuracy. Recently an interesting variant of the DoS method has been proposed [1, 2] for lattice field theories where a restricted Monte Carlo update is used to obtain exponential error reduction in the determination of the density of states.

In this contribution we apply the density of states method to the $\mathbb{Z}_3$ spin model, where a lattice simulation with dual variables is available [3] and provides reference data to test the reliability and accuracy of the DoS approach. The model has been studied also using fugacity and Taylor expansion [4] and also a previous study with DoS techniques has been published in [2].

The variant of the DoS approach we present here is slightly different from the one in [2]: We use a similar ansatz to parameterize the density of states ρ, but determine the coefficients of this parameterization in a different way, which we refer to as the functional fit approach (FFA): In the restricted Monte Carlo simulation we study the dependence on a free control parameter λ and fit the known functional form as a function of λ to the Monte Carlo data. We show that a sequence of one parameter fits is sufficient to obtain all parameters of the density. We expect that this approach has smaller statistical errors and is numerically more stable than root finding or iterative techniques, since all Monte Carlo data generated for different values of λ are used to determine ρ.

2. Definition of the model and the density of states

The $\mathbb{Z}_3$ spin model in an external field with strength κ, a chemical potential μ and a temperature parameter τ is described by the action

$$S[P] = \sum_x \left[\tau \sum_{\nu=1}^{3} \left(P_x^\star P_{x+\hat{\nu}} + c.c. - 2 \right) + \kappa e^{\mu} (P_x - 1) + \kappa e^{-\mu} (P_x^\star - 1) \right], \tag{2.1}$$

where the dynamical degrees of freedom (spins) are $P_x \in \mathbb{Z}_3 = \{1, e^{i2\pi/3}, e^{-i2\pi/3}\}$, living on the sites x of a 3-dimensional lattice with periodic boundary conditions. The action is normalized such that $S[P] = 0$ if $P_x = 1 \, \forall x$. The partition function is obtained by summing the Boltzmann factor over all configurations $\{P\}$, i.e., $Z = \sum_{\{P\}} e^{S[P]}$. It is obvious that for finite chemical potential, $\mu \neq 0$, the action (2.1) has a non-zero imaginary part and the model has a complex action problem.

For a more convenient notation we introduce abbreviations for the total numbers of spins pointing in each of the three directions as $N_0[P] = \sum_x \delta(P_x, 1)$ and $N_\pm[P] = \sum_x \delta\left(P_x, e^{\pm i2\pi/3}\right)$, and note that obviously $N_0 + N_+ + N_- = V$, where V denotes the lattice volume, i.e., the total number

of sites of the lattice. Using these we can rewrite the action to the form

$$\begin{aligned} S[P] &= S_R[P] + iS_I[P] \,, \\ S_R[P] &= \tau \sum_x \sum_{\nu=1}^{3} \left(P_x^\star P_{x+\hat{\nu}} + c.c. - 2 \right) \; + \; \kappa 3 (N_0[P] - V) \cosh \mu \,, \\ S_I[P] &= \kappa \sqrt{3} \sinh \mu \, \Delta N[P] \,, \end{aligned} \tag{2.2}$$

where we have defined $\Delta N[P] = N_+[P] - N_-[P] \in \{-V, -V+1, \ldots, V\}$.

Exploring the properties of $S_R[P]$ and $S_I[P]$ under complex conjugation of the spin variables we find for the partition sum

$$Z = \sum_{\{P\}} e^{S[P]} = \sum_{\{P\}} e^{S_R[P]} \cos\left(S_I[P]\right) = \sum_{\{P\}} e^{S_R[P]} \cos\left(\kappa \sqrt{3} \sinh \mu \; \Delta N[P] \right) \,. \tag{2.3}$$

We now define a weighted density of states which is a function of $d \equiv \Delta N$,

$$\rho(d) = \sum_{\{P\}} e^{S_R[P]} \, \delta\left(d - \Delta N[P]\right) \,, \tag{2.4}$$

which can be shown to be an even function of d, i.e., $\rho(-d) = \rho(d)$. Using the density of states, the partition sum and expectation values of observables which are a function $O(\Delta N)$ of ΔN can be written as

$$Z = \sum_{d=-V}^{V} \rho(d) \cos\left(\kappa \sqrt{3} \sinh \mu \; d \right) \,, \tag{2.5}$$

$$\langle O \rangle = \frac{1}{Z} \sum_{d=-V}^{V} \rho(d) \left[\cos\left(\kappa \sqrt{3} \sinh \mu \, d \right) O_E(d) \; + \; i \sin\left(\kappa \sqrt{3} \sinh \mu \, d \right) O_O(d) \right] , \tag{2.6}$$

where O_E and O_O denote the even and odd parts of $O(\Delta N)$.

The partition sum and expectation values are obtained by reweighting the density $\rho(d)$ with the factors $\cos\left(\kappa\sqrt{3}\sinh(\mu)\, d\right)$ and $\sin\left(\kappa\sqrt{3}\sinh(\mu)\, d\right)$. While the density $\rho(d)$ is strictly positive, these factors are oscillating with d and the frequency of oscillation increases exponentially with μ. Thus for larger values of μ the density $\rho(d)$ has to be computed very accurately. This is how the complex action problem manifests itself in the density of states approach.

3. Computing the density of states

For the numerical computation we parameterize the density of states $\rho(d)$, with $d \in [-V, V]$, as

$$\rho(d) = \prod_{i=0}^{|d|} e^{-a_i} = \exp\left(- \sum_{i=0}^{|d|} a_i \right) \,, \tag{3.1}$$

with real parameters a_i. Note that this parameterization is exact in the sense that it contains $V+1$ parameters, precisely the number of independent degrees of freedom $\rho(d)$ has (remember that $\rho(d)$ is an even function). We also remark, that an overall normalization of $\rho(d)$ can be chosen freely, since it cancels in the expectation values (2.6). Here we choose the normalization $\rho(0) = 1$, which corresponds to setting $a_0 = 0$.

For the calculation of the coefficients a_i we define restricted expectation values $\langle\langle O\rangle\rangle_n(\lambda)$, $n = 0,1,\ldots V-1$, which depend on a free parameter λ,

$$Z_n(\lambda) = \sum_{\{P\}} \theta_n\big(\Delta N[P]\big)\, e^{S_R[P]}\, e^{\lambda\,\Delta N[P]}\;,\; \langle\langle O\rangle\rangle_n(\lambda) = \frac{1}{Z_n(\lambda)} \sum_{\{P\}} \theta_n\big(\Delta N[P]\big)\, e^{S_R[P]}\, e^{\lambda\,\Delta N[P]}\, O(\Delta N[P])\;. \tag{3.2}$$

Here we defined

$$\theta_0(d) \;=\; \begin{cases} 1\;, & \text{for } d = 0,1 \\ 0\;, & \text{otherwise} \end{cases}\;, \quad \text{and } \theta_n(d) \;=\; \begin{cases} 1\;, & \text{for } |d-n| \le 1 \\ 0\;, & \text{otherwise} \end{cases} \text{ for } n = 1,2,\ldots V-1\;. \tag{3.3}$$

In the restricted expectation values (3.2) only real and positive weight factors appear, such that they can be evaluated with a restricted Monte Carlo strategy which we will discuss below. In particular we are here interested in the observable $O = \Delta N$.

We can now also use the density of states $\rho(d)$ in the form of (3.1) to evaluate the restricted expectation values $\langle\langle \Delta N\rangle\rangle_n(\lambda)$. A straightforward calculation gives

$$\langle\langle \Delta N\rangle\rangle_0(\lambda) \;=\; \frac{e^{\lambda - a_1}}{e^{\lambda - a_1} + 1}\;,\; \langle\langle \Delta N\rangle\rangle_n(\lambda) - n \quad = \frac{e^{2\lambda - a_n - a_{n+1}} - 1}{e^{2\lambda - a_n - a_{n+1}} + e^{\lambda - a_n} + 1}\;,\; n = 1,\ldots V-1\;. \tag{3.4}$$

The right hand sides are simple functions of λ: They are monotonically increasing (their derivatives with respect to λ are easily shown to be positive) and for $n \ge 1$ they have a single zero ($\lim_{\lambda\to-\infty}$ is negative, $\lim_{\lambda\to+\infty}$ is positive). Examples for different n are shown in Fig. 1 below.

Using Monte Carlo simulations we can evaluate $\langle\langle \Delta N\rangle\rangle_n(\lambda) - n$ for different values λ_i, $i = 1,2,\ldots N_\lambda$ (typically $N_\lambda = \mathcal{O}(10)$) and fit the results according to the right hand sides of (3.4). The one-parameter fit for $\langle\langle \Delta N\rangle\rangle_0(\lambda)$ determines the first non-trivial coefficient a_1 (remember that we chose the normalization $a_0 = 0$). The fit value for a_1 can then be inserted in the right hand side of (3.4) for $n = 1$ such that with another one-parameter fit of $\langle\langle \Delta N\rangle\rangle_1(\lambda) - 1$ we can determine a_2, which in turn is then inserted in the fit function for $\langle\langle \Delta N\rangle\rangle_2(\lambda) - 2$, which gives a_3 from a one-parameter fit, et cetera. Using this sequence of fits we can determine all coefficients a_i from fits of the Monte Carlo data with simple functions depending on a single parameter (compare Fig. 1).

4. Restricted Monte Carlo

The variant of the density of states method described here is based on fitting the Monte Carlo data for the restricted expectation values $\langle\langle \Delta N\rangle\rangle_n(\lambda)$ as defined in (3.2). For this purpose we first need to generate initial configurations P of the spin variables, such that the constraint $\Delta N[P] \in \{n-1, n, n+1\}$ is obeyed (for $n > 0$). These configurations can easily constructed by hand, but of course need to be equilibrated before taking measurements (we use 10^6 equilibration sweeps for the data we show). Once the initial configurations that obey the constraints are generated, a slightly modified conventional Monte Carlo update can be used, with the additional restriction that proposed trial configurations which violate the constraint $\Delta N[P] \in \{n-1, n, n+1\}$ are rejected. The acceptance rate is very good throughout and only for n very close to the maximum value of $n = V$ (i.e., the cases $n = V, V-1, V-2$) we observe a strong drop in the acceptance rate. In principle it is easy to compute $\rho(d)$ for these largest values of d exactly with a low temperature

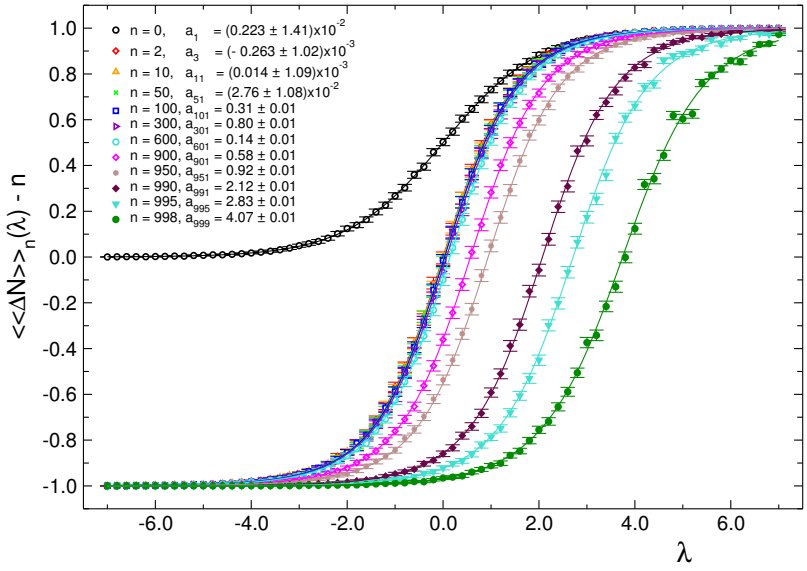

Figure 1: Monte Carlo results (symbols) for $\langle\langle\Delta N\rangle\rangle_n(\lambda)-n$ for $n = 0$, 2, 10, 50, 100, 300, 600, 900, 950, 990, 995 and 998 as a function of λ. The data are for the parameters $\tau = 0.16$, $\kappa = 0.01$ and $\mu = 1.0$. The full curves are the fits with the functions on the rhs. of (3.4). The resulting values for the corresponding coefficients a_n are given in the legend.

expansion. However, since for the values of d where the quality of the Monte Carlo data decreases $\rho(d)$ is already very small, we simply use the data as we obtain them from the simulation.

In Fig. 1 we show the Monte Carlo results (symbols) for $\langle\langle\Delta N\rangle\rangle_n(\lambda)-n$ with $n = 0$, 2, 10, 50, 100, 300, 600, 900, 950, 990, 995 and 998 for several values of λ in the interval $[-7,7]$. The data were generated on 10^3 lattices for the parameter values $\tau = 0.16$, $\kappa = 0.01$ and $\mu = 1.0$. After 10^6 equilibration sweeps we sample 10^5 configurations separated by 100 sweeps for each data point, and the errors we show are the statistical errors. The figure demonstrates that the Monte Carlo data show the expected simple behavior as a function of λ and can easily be fit (we use a standard χ^2 procedure) with the functions given in the right hand sides of (3.4). The results of the fits are shown in Fig. 1 as full curves and it is obvious that they perfectly describe the numerical data.

Once the coefficients a_i are determined from the fits, we can build up the density of states $\rho(d)$ as given in (3.1). Results for the density $\rho(d)$ at different values of μ are presented in Fig. 2. The data we show in the lhs. plot are for $\tau = 0.16$, $\kappa = 0.01$, while in the rhs. plot $\tau = 0.178$, $\kappa = 0.001$ were used. It is remarkable that the range of the values for $\rho(d)$ strongly depends on the parameters, including also μ. This is due to the fact that the density we use here also includes the μ-dependent Boltzmann factor e^{S_R}.

5. Results for physical observables

Having determined the density $\rho(d)$ we can finalize the calculation and evaluate expectation values of observables using (2.6). We consider $\langle M-M^*\rangle$ and $\chi_{M-M^*} = \langle(M-M^*)^2\rangle - \langle M-M^*\rangle^2$, where $M = \sum_x P_x$. In Fig. 3 we show the results from the FFA for $\langle M-M^*\rangle$ and χ_{M-M^*} as a function of μ (red circles). We display results for two sets of parameters, $\tau = 0.16$, $\kappa = 0.01$ on the lhs., and

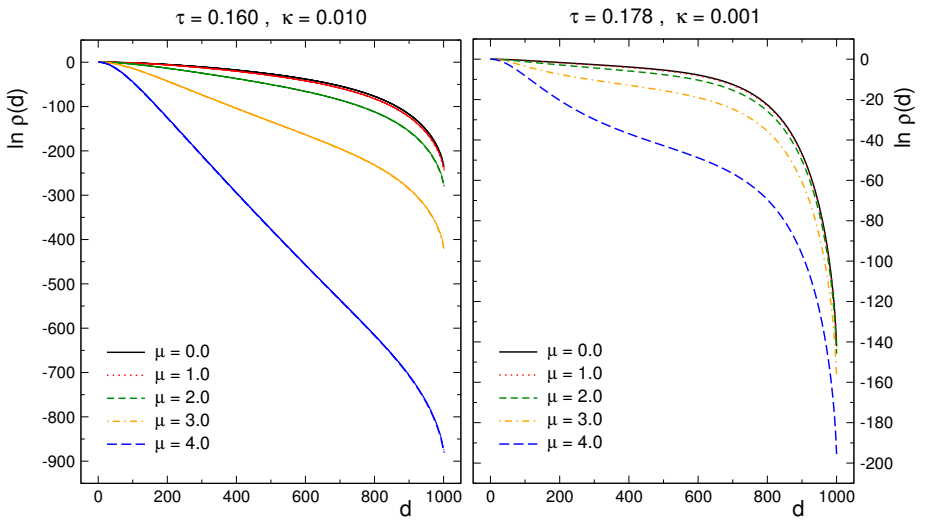

Figure 2: Results for the logarithm of $\rho(d)$ as a function of d from a 10^3 lattice for different values of μ. The data we show in the lhs. plot are for $\tau = 0.16$, $\kappa = 0.01$. On the rhs. we use $\tau = 0.178$ and $\kappa = 0.001$. The error bars are smaller than the line-width. Note the different vertical scales for the two plots.

$\tau = 0.178$, $\kappa = 0.001$ (rhs.). The data are for 10^3 lattices and the statistics is as described in the previous section. The results are compared to the observables evaluated with the LLR approach for the determination of the density (density parameterized with $\Delta d = 4$, same statistics as the FFA, black diamonds). It is obvious, that the results from the FFA and the LLR approach agree well, but that the FFA data have smaller statistical errors as expected.

As reference data in Fig. 3 we also show the results from a dual simulation [3] (10^6 measurements, crosses). For the $\tau = 0.178, \kappa = 0.001$ data (rhs.) the FFA and LLR results agree well with the dual results for all values of μ we show. However, for $\tau = 0.16$, $\kappa = 0.01$ (lhs.) the dual and the DoS data disagree for μ larger than 2. This discrepancy can be attributed to the fact, that for this parameter set the sign problem is much harder than for $\tau = 0.178, \kappa = 0.001$ (compare [4]). In addition we also show the results when the density $\rho(d)$ is replaced by a fit of $\rho(d)$ with a finite polynomial in d^2 [2]. This reduces the impact of local fluctuations and increases the range of μ where the DoS results agree with the dual simulation.

To summarize: Our assessment shows that the density of states method based on restricted Monte Carlo simulations [1, 2] is certainly a competitive and rather generally applicable method. To obtain a maximal range of values for the chemical potential μ, the density has to be computed as precisely as possible. In the variant we discuss here this is done by fitting the restricted Monte Carlo data to the dependence on the control parameter λ and in this way making optimal use of all computed Monte Carlo data. Technical improvements such as these will contribute to the further refinement of the density of states method.

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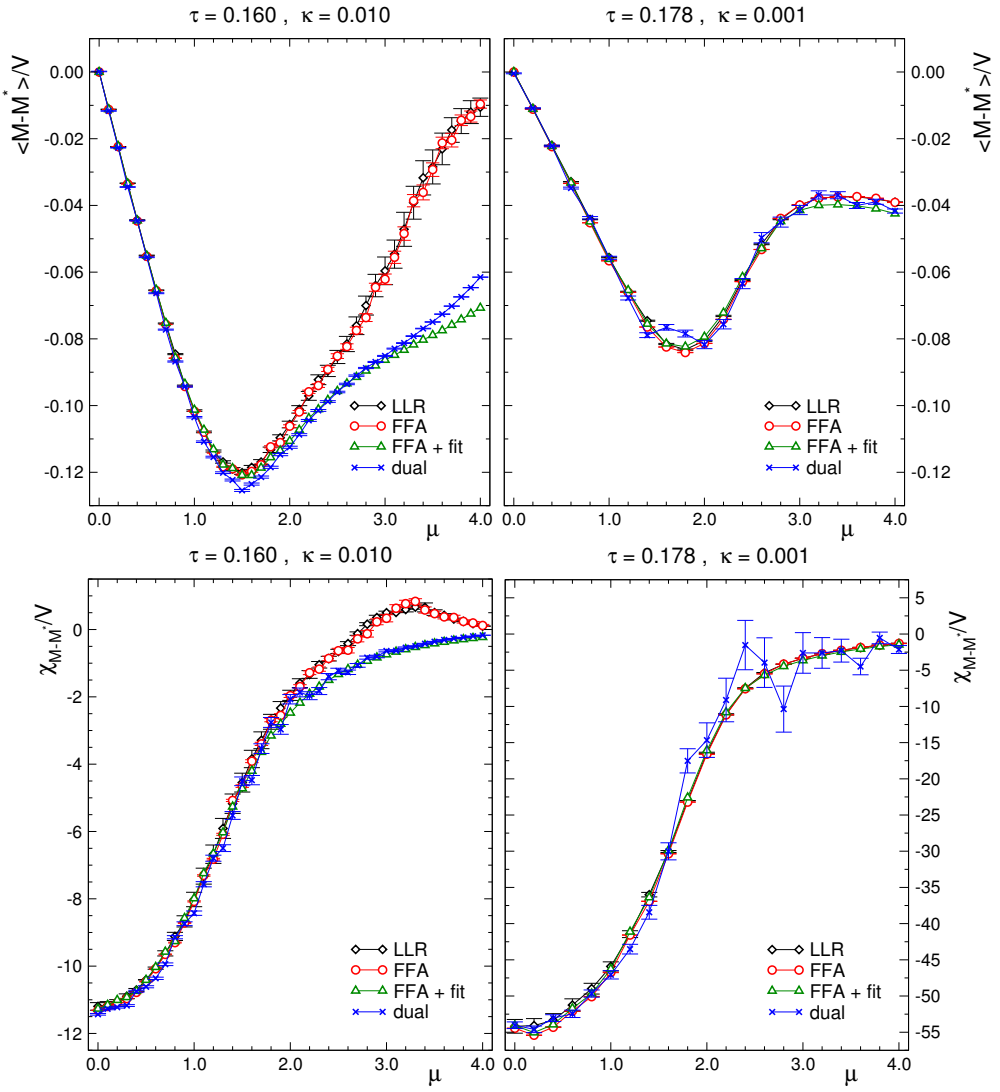

Figure 3: Results for the physical observables $M - M^*$ (top row of plots) and χ_{M-M^*} (bottom) on 10^3 lattices as a function of μ. We use two sets of parameters, $\tau = 0.16$, $\kappa = 0.01$ on the lhs., and $\tau = 0.178$ and $\kappa = 0.001$ on the rhs. We show results from the LLR algorithm, the FFA algorithm, the FFA algorithm combined with a fit of $\rho(d)$ and for comparison also the results from a simulation in the dual representation.

References

[1] K. Langfeld, B. Lucini and A. Rago, Phys. Rev. Lett. **109** (2012) 111601 [arXiv:1204.3243 [hep-lat]]. K. Langfeld, J. Pawlowski, B. Lucini, A. Rago and R. Pellegrini, arXiv:1310.8231 [hep-lat].

[2] K. Langfeld and B. Lucini, arXiv:1404.7187 [hep-lat].

[3] Y. D. Mercado, H. G. Evertz and C. Gattringer, Phys. Rev. Lett. **106** (2011) 222001 [arXiv:1102.3096 [hep-lat]]; Comput. Phys. Commun. **183** (2012) 1920 [arXiv:1202.4293 [hep-lat]].

[4] E. Grünwald, Y. D. Mercado and C. Gattringer, arXiv:1403.2086 [hep-lat]; PoS LATTICE **2013** (2013) 448 [arXiv:1310.6520 [hep-lat]].