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Reweighting Lefschetz Thimbles

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We present a novel reweighting technique to calculate the relative weights in the Lefschetz thimble decomposition of a path integral. Our method is put to work using a $U(1)$ one-link model providing for a suitable testing ground and sharing many features with realistic gauge theories with fermions at finite density. We discuss prospects and future challenges to our method.

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1. Introduction

The exploration of the phase diagram of Quantum Chromodynamics (QCD) provides a formidable challenge to lattice simulations due to the sign problem. The latter arises for finite chemical potential μ rendering the Euclidean action complex. Consequently, importance sampling based methods relying on a positive definite Boltzmann measure become inapplicable. In recent years, a plethora of contenders have been proposed towards mitigating the sign problem, see e.g. [1]. So far none of the method has been able to produce reliable results for $\mu/T \geq 1$. Amongst those, promising candidates operating on complex manifolds are the Complex Langevin evolution [2, 3] the Lefschetz thimble method [4] and flowed manifolds [5]. Recently, methods to find an optimal complex integration manifold where the sign problem is mild have been proposed in [6, 7, 8]. In this work we consider the Lefschetz thimbles which have been applied recently to one-dimensional QCD in [9, 10]. We propose algorithmic improvements addressing the determination of the relative weights of the contributing thimbles to the partition function. To this end we present a novel reweighting procedure which can be generalized to higher dimensional theories. Our method is demonstrated by using a $U(1)$ one-link model representing a suitable testing ground towards gauge theories with fermions at finite density.

2. Lefschetz thimbles

For simplicity we consider a complex action $S(x)$ of a real variable that we extend to the complex plane $x \to z = x + iy$. The Lefschetz thimbles [4, 11] are the paths of steepest descent $D_\sigma \in \mathbb{C}$ of the real part of the action and are obtained from the flow equation

$$\frac{\partial z}{\partial \tau} = -\overline{\frac{\partial S}{\partial z}}. \tag{2.1}$$

The thimbles end in the critical points $z_\sigma \in \mathbb{C}$ of the action which are the stationary solutions to the right-hand side of (2.1). Along the thimble the real part of the action decreases and has its minimum at the critical point z_σ. Importantly, the imaginary part of the action is constant along each thimble which can ameliorate the sign problem. The partition function can be rewritten as an integral over the union of the thimbles whose anti-thimbles (path of steepest ascent of $\mathrm{Re}[S]$) cross the real axis. If the critical points are non-degenerate this holds by continuously deforming the original real integration contour into the thimbles. Hence, for the partition function we have

$$Z = \int_I dx\, e^{-S(x)} = \sum_\sigma n_\sigma e^{-i\mathrm{Im}[S(z_\sigma)]} \underbrace{\int_{D_\sigma} dz\, e^{-\mathrm{Re}[S(z)]}}_{=:Z_\sigma}. \tag{2.2}$$

Here, $I \subset \mathbb{R}$ denotes the original real integration domain. n_σ counts the number of intersections of a given anti-thimble with I. The latter is also called the unstable thimble since the action is not bounded from below. Observables are obtained from the expression

$$\langle \mathscr{O} \rangle = \frac{1}{Z} \sum_\sigma n_\sigma e^{-i\mathrm{Im}[S(z_\sigma)]} \int_{D_\sigma} dz\, \mathscr{O} e^{-\mathrm{Re}[S(z)]} = \frac{\sum_\sigma n_\sigma e^{-i\mathrm{Im}S(z_\sigma)} Z_\sigma \langle \mathscr{O} \rangle_\sigma}{\sum_\sigma n_\sigma e^{-i\mathrm{Im}S(z_\sigma)} Z_\sigma}, \tag{2.3}$$

where we have defined

$$\langle \mathscr{O} \rangle_\sigma := \frac{1}{Z_\sigma} \int_{D_\sigma} dz e^{-\mathrm{Re}[S(z)]} \mathscr{O} \,. \tag{2.4}$$

This approach has two practical challenges:

1. Monte Carlo sampling on the (main) contributing thimbles based on finding a numerical parametrization implicitly or explicitly.

2. In most realistic theories multiple thimbles contribute to the partition function. Hence, we need to determine the relative weights weights Z_ρ/Z_σ where $\rho \neq \sigma$ in (2.3).

Numerical cost and complexity of the above tasks increase with the dimensionality of the considered theory. So far there has not been a general solution capturing both problems. However, the first difficulty can be tackled by the holomorphic flow equations continuously deforming the original integration contour towards the thimbles [12]. Another approach addresses the second problem by means of a semi-classical approximation [13]. Methods tackling both problems have been proposed in [14]. In this presentation, we focus only on the second problem and present a technique to compute the relative weights.

3. Simulation method on Lefschetz thimbles

In this section we present an algorithm for a Monte Carlo simulation on Lefschetz thimbles, assumed that we know a parametrization of all contributing thimbles. For the discussion of finding a numerical parametrization in simple models we refer the reader to [14]. The method is divided up into two steps. First we discuss how to compute the expectation value of a given observable on a single thimble D_σ according to (2.4). In the second step we demonstrate how the ratios of partition functions determining the relative weights of the thimbles can be computed within the Monte Carlo simulation. For the first step let $[a,b] \subset \mathbb{R} \to D_\sigma : \tau \mapsto z(\tau)$ be a (numerical) parametrization of the thimble D_σ. Its associated partition function reads

$$Z_\sigma = \int_{D_\sigma} dz e^{-\mathrm{Re}[S(z)]} = \int_a^b d\tau\, e^{-\mathrm{Re}[S_\sigma(\tau)]} J_\sigma(z(\tau)) \,. \tag{3.1}$$

Here $S_\sigma(\tau) = S(z(\tau))$ denotes the action evaluated on D_σ. Moreover, the complex Jacobian $J_\sigma(\tau) := \partial z(\tau)/\partial \tau$ on D_σ has been introduced. We define

$$\langle \mathscr{O} \rangle_\sigma^r = \frac{1}{Z_\sigma^r} \int_a^b d\tau\, e^{-\mathrm{Re}[S_\sigma(\tau)]} \mathscr{O} \,, \tag{3.2}$$

as well as

$$Z_\sigma^r = \int_a^b d\tau\, e^{-\mathrm{Re}[S_\sigma(\tau)]} \,. \tag{3.3}$$

Thus, to calculate an observable on a single thimble we sample τ distributed according to $e^{-\mathrm{Re}[S_\sigma(\tau)]}/Z_\sigma^r$ and take into account the Jacobian via conventional reweighting

$$\langle \mathscr{O} \rangle_\sigma = \frac{\langle \mathscr{O} J_\sigma \rangle_\sigma^r}{\langle J_\sigma \rangle_\sigma^r} \,. \tag{3.4}$$

The phase of the Jacobian gives rise to the so-called residual sign problem. The expectation value of an observable reads

$$\langle \mathscr{O} \rangle = \frac{\sum_\sigma n_\sigma e^{-i\mathrm{Im}[S(z_\sigma)]} Z^r_\sigma \langle \mathscr{O} J_\sigma \rangle^r_\sigma}{\sum_\sigma n_\sigma e^{-i\mathrm{Im}[S(z_\sigma)]} Z^r_\sigma \langle J_\sigma \rangle^r_\sigma} \,. \tag{3.5}$$

It is obvious that in the case of a single contributing thimble (3.5) reduces to (3.4). In the second step we capture the weights from the partition functions Z^r_σ from within the Monte Carlo simulation. For simplicity we consider (3.5) with only two contributing thimbles, i.e. $\sigma = 1,2$. Without loss of generality we choose the second thimble and factor out Z^r_2 in (3.5). This thimble is refered to as the "master thimble". Hence, we are left with computing the ratio of the partition functions Z^r_1 and Z^r_2 which can be straightforwardly written in terms of the expectation value (3.2) of the ratio of the associated Boltzmann factors

$$\frac{Z^r_1}{Z^r_2} = \left\langle e^{\mathrm{Re}[S_2 - S_1]} \right\rangle^r_2 \,. \tag{3.6}$$

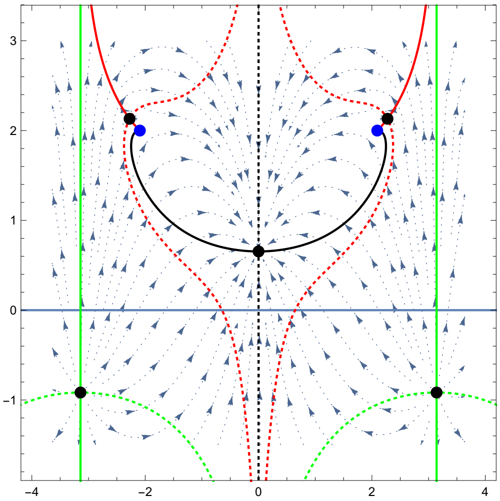
This means that we determine the relative weights in (3.5) by reweighting with respect to the master thimble. We remark that for (3.6) to hold (a) the integrals over the thimbles have the same parameter interval $[a,b]$ and (b) the parameters τ on both thimbles must be identified. In case the latter does not hold we need to take into account an additional Jacobian. For the example integrals considered in this work (a) can be realized by suitable variable transformations and (b) can be achieved by normalizing the steepest descent equation when determining the numerical parametrizations. For further details, see [14] and appendices A and B therein. Thus, we can compute the relative weights of the contributing thimbles (3.6) within the Monte Carlo simulation by reweighting with respect to the master thimble which completes the list of ingredients for (3.5). The reweighting method might also be useful in addressing higher dimensional integrals for field theories since it does not rely on an explicit (numerical) parametrization of the thimble.

4. Numerical results

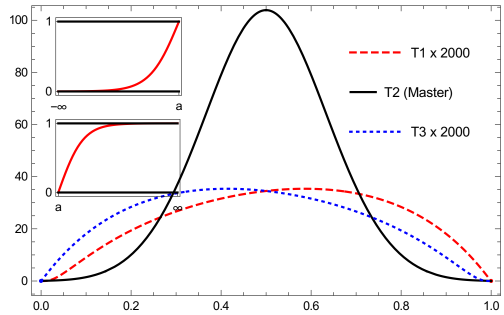
In this section we put to work our reweighting algorithm by using a $U(1)$ one-link model with a finite chemical potential μ

$$\begin{aligned} Z &= \int_{-\pi}^{\pi} dx \, e^{-S(x)} \,, \\ S(x) &= -\beta \cos(x) - \log(1 + \kappa \cos(x - i\mu)) \,. \end{aligned} \tag{4.1}$$

Despite its simplicity the model shares general features with more complicated theories such as QCD at finite chemical potential. In the following we consider the case $\beta = 1, \kappa = 2$ and $\mu = 2$. The model has been studied using the Complex Langevin evolution in [2]. Its thimble structure has been investigated in [15, 16]. There are three contributing thimbles, see the red and black full lines in Fig. 1 (a). The two red ones are related by symmetry and their partition functions are complex conjugates [16]. The second term in the effective action in (4.1) modeling a fermion determinant generates poles in the holomorphic flow (and equivalently in the Complex Langevin drift) in which the contributing thimbles end for finite flow time τ. Due to the presence of these poles the Complex Langevin evolution yields incorrect results for the given parameters above [16]. For the partition



(a) Contributing thimbles (full lines) and anti-thimbles (dashed lines) for the $U(1)$ one-link model. The critical points of the action are represented by the black dots and poles of the holomorphic flow are indicated by blue dots. The contributing thimbles all end in poles at finite flow times τ. The blue arrows in the background represent the drift force in the Complex Langevin evolution. Due to the periodicity of the model the non-contributing thimbles (green) at the edges of the original integration domain $[-\pi,\pi]$ coincide.



(b) Boltzmann factors $e^{-\mathrm{Re}[S_\sigma(\tau)]}$ vs. the flow parameter τ for the three contributing thimbles in the $U(1)$ one-link model. The black line represents the thimble with the largest weight – the master thimble used to determine the relative weights. To maximize overlap of the Boltzmann distributions, the different integration ranges of the three thimbles are mapped to the same interval $[0,1]$. With $a,b \in \mathbb{R}^+, a \neq b$ for the two symmetric thimbles on the sides T1 and T3 (red) the parameter ranges are of the form $(-\infty, a]$ and $[-a,\infty)$. Suitable mappings are hyperbolic tangent functions, see the inlays. A linear transformation is used for the central thimble T2 (black) with parameter range of the form $[-b,b]$. Futher remarks on the transformations can be found in [14] and the appendix B therein. For better visuability the distributions have been rescaled.

Figure 1: Thimble structure (a) and distribution of the Boltzmann weights for every contributing thimble (b) mapped to the interval $[0,1]$.

functions (3.3) associated with the contributing thimbles all integration ranges for the parameter τ differ. This demands to transform these to the same interval yielding overlap of the distributions $e^{-\mathrm{Re}[S_\sigma(\tau)]}$ which facilitates the reweighting procedure for the relative weights (3.6). The remapped distributions are shown in Fig. 1 (b) where details on the transformation mappings are provided in the caption. The central thimble (black) carries the largest weight. We choose it to be the master thimble. For a quantitative test of our method we compute the analogue of the Polyakov loop, its inverse, the plaquette and the density which are given in analytical form in [2]

$$\begin{aligned}\langle U\rangle &= \langle e^{ix}\rangle ,\\ \langle U^{-1}\rangle &= \langle e^{-ix}\rangle ,\\ \langle P\rangle &= \langle \cos(x)\rangle ,\\ \langle n\rangle &= \left\langle \frac{i\kappa\sin(x-i\mu)}{1+\kappa\cos(x-i\mu)}\right\rangle .\end{aligned} \tag{4.2}$$

The results of our Monte Carlo simulations are displayed in Table 1 in comparison with the exact results. This includes the relative weights for the contributing thimbles with respect to the master thimble of choice. The results for the observables agree with the exact ones from [2] within the

$\langle \mathscr{O} \rangle$	numerical	exact
$\mathrm{Re}\langle U \rangle$	0.315217(3)	0.315219
$\mathrm{Re}\langle U^{-1} \rangle$	1.800941(3)	1.800939
$\mathrm{Re}\langle P \rangle$	1.058079(3)	1.058079
$\mathrm{Re}\langle n \rangle$	0.742861(1)	0.742860
$Z_2/Z_1\|_{T_1} \times 10^{-3}$	2.99378(3)	2.99382
$Z_1/Z_2\|_{T_2} \times 10^{4}$	3.34032(4)	3.34022
$Z_2/Z_3\|_{T_3} \times 10^{-3}$	2.99377(3)	2.99382
$Z_3/Z_2\|_{T_2} \times 10^{4}$	3.34026(9)	3.34022

Table 1: Numerical results and exact values of observables for the U(1) one-link model together with the statistical errors. We have found the imaginary parts for the observables to be all consistent with zero within the statistical error. Possible deviations are caused by systematic errors from the numerical parametrization, see the main text for details.

statistical error as shown in Table 1. Systematic errors arise from the numerical parametrization of the thimble obtained by solving the holomorphic flow. For the simple integrals considered here this error is estimated by comparing with the exact solution to be of the order of 10^{-6} which compares to the statistical error. The ratio of partition functions appears to be influenced by these systematics, see Table 1. Combining the statistical and the systematic error we find that all quantities agree with the exact results. We remark that we obtained the same results within the combined errorbars for either choosing the central or the left (right) thimble as the master thimble.

5. Conclusions and outlook

In this work we have developed a novel reweighting procedure to determine the relative weights in the thimble decomposition. The approach is successfully put to work by considering a $U(1)$ one-link model representing a toy model for a gauge theory with fermions at finite density. Although its thimble structure is trivial to parametrize numerically it provides a valuable testbed. Numerical results for the expectation values of observables obtained with the novel method agree well with exact results within the combined statistical and systematic errors. The extension to higher dimesional theories is challenging since Monte Carlo sampling on the thimble is required with or without having an explicit parametrization. Nevertheless, the reweighting procedure straightforwardly generalizes to field theories and may be combined with existing simulation methods for thimbles. Applications in progress are higher dimensional gauge theories [17].

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