Lefschetz-thimble path integral for solving the mean-field sign problem

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The sign problem is a serious obstacle not only for the Monte Carlo method in lattice field theories, but also for the mean-field approximation in the effective models. The Lefschetz-thimble approach can be a key clue to understand these problems, and we show that the mean-field sign problem can be solved.

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1. Lefschetz-thimble method

The Lefschetz-thimble path integral is a new approach to the sign problem of quantum Monte Carlo simulation. The Boltzmann weight need not be semi-positive definite, and the quark (fermion) determinant causes its oscillatory behavior in finite-density lattice QCD (and many other condensed matter systems). In those systems, importance sampling breaks down for practical purpose, and moreover the mean-field approximation requires a great care to give a consistent result with physical requirements. We review our result on the Lefschetz-thimble approach to the sign problem appearing in the mean-field approximation [1].

Let us consider a multiple integration that gives the partition function,
\[
Z = \int_{\mathbb{R}^n} d^n x \, e^{-S(x)}, \tag{1.1}
\]
where \(S(x)\) is a complex action functional of the real field \(x = (x_1, \ldots, x_n) \in \mathbb{R}^n\). In order to circumvent the oscillatory integral, we perform integrations on steepest descent paths, called Lefschetz thimbles, instead of (1.1). Each Lefschetz thimble is an \(n\)-dimensional space spanned around a saddle point \(z_\sigma\) in \(\mathbb{C}^n\) (\(\sigma \in \Sigma\)). Consider Morse’s flow equation for complexified variables \(z\) [2]:
\[
\frac{dz_i}{dt} = \left(\frac{\partial S(z)}{\partial z_i}\right). \tag{1.2}
\]
The Lefschetz thimble \(\mathcal{J}_\sigma\) is identified as the set of points reached by some flows emanating from \(z_\sigma\). The partition function can now be computed as the sum of the nicely converging integrations:
\[
Z = \sum_{\sigma \in \Sigma} n_\sigma \int_{\mathcal{J}_\sigma} d^n z \, e^{-S(z)}. \tag{1.3}
\]
The coefficient \(n_\sigma\) is given by the intersection number between \(\mathbb{R}^n\) and \(\mathcal{K}_\sigma = \langle \mathcal{J}_\sigma, \mathbb{R}^n \rangle\). The dual thimble \(\mathcal{K}_\sigma\) is defined as the set of the points reached by flows getting sucked into \(z_\sigma\). This method turns out to be useful for evading the sign problem in some lattice field theories [3]. For recent developments of this technique in various other contexts, see [4, 5].

2. Sign problem in the mean-field approximation

In order to understand how the sign problem appears in the mean-field approximation, let us consider a field theory \(S[\phi]\) with finite volume \(V\). The partition function is given by
\[
Z = \int D\phi \exp -S[\phi]. \tag{2.1}
\]
Let us consider a background field method. The constrained effective action is given by
\[
\exp -S_{\text{eff}}[\phi_{\text{MF}}] = \int D\phi \, \delta(\langle \phi \rangle - \phi_{\text{MF}}) \exp -S[\phi], \tag{2.2}
\]
where \(\langle \phi \rangle = \int dx \phi(x)/V\). In order to reproduce the original partition function, we need an integration over the background field \(\phi_{\text{MF}}\), i.e.,
\[
Z = \int d\phi_{\text{MF}} \exp -S_{\text{eff}}(\phi_{\text{MF}}). \tag{2.3}
\]
Since $S_{\text{eff}}$ is typically proportional to the volume $V$, the saddle-point approximation is useful. If the original action $S$ is real, so is $S_{\text{eff}}$ and the saddle-point approximation can be done without any difficulty. If $S$ takes complex values, however, $S_{\text{eff}}$ is also complex. One cannot find saddle points in the original integration cycle, and cannot conclude physically sensible results. This is the sign problem appearing in the mean-field approximation [6], and we will tackle this problem for a Polyakov-loop effective model of the dense-heavy quark system [1].

3. Application to the sign problem of Dense QCD

The fundamental Polyakov loop $\ell_3$ is an order parameter of confinement;

$$\ell_3 = \frac{1}{3} \text{tr}[L], \quad L = \mathcal{P} \exp \left( ig \int_0^\beta A_4 dx^4 \right),$$  \hspace{1cm} (3.1)

where $\mathcal{P}$ refers to the path ordering. Using the background field method, or the mean-field approximation, we consider an effective action for the Polyakov loop. It gives an $SU(3)$ matrix integral:

$$Z = \int_{SU(3)} dL \exp[-S_{\text{eff}}(L)],$$  \hspace{1cm} (3.2)

For our demonstration, we take a simplified heavy-quark model [6, 9]:

$$S_{\text{eff}}(L) = -h \left( \frac{3^2 - 1}{2} \right) \left( e^\mu \ell_3 + e^{-\mu} \ell_3^{-1} \right)$$  \hspace{1cm} (3.3)

Here, $\ell_3 = \text{tr}L^{-1}/3$. When $h \neq 0$ and $\mu = \beta \mu_q \neq 0$, the integration (3.5) is oscillatory because $S_{\text{eff}}$ takes complex values. When the quark chemical potential $\mu_q$ is turned on under the nontrivial Polyakov-loop background, the effective action $S_{\text{eff}}(\theta)$ takes complex values in general due to the quark determinant. This makes the integration (3.5) oscillatory, and the sign problem remains in the mean-field approximation [6].

Let us simplify the matrix integral by taking the Polyakov gauge, in which the Polyakov loop becomes diagonal:

$$L = \text{diag} \left[ e^{i(\theta_1+\theta_2)}, e^{i(-\theta_1+\theta_2)}, e^{-2i\theta_2} \right],$$  \hspace{1cm} (3.4)

where $\theta_{1,2}$ are real parameters if $L \in SU(3)$. The Weyl group acts on these parameters $(\theta_1, \theta_2)$ as $(\theta_1, \theta_2) \mapsto (-\theta_1, \theta_2)$, $(\theta_1, \theta_2) \mapsto ((\theta_1 + 3\theta_2)/2, (\theta_1 - \theta_2)/2)$ and it only permutes eigenvalues of the Polyakov loop (3.4). Thus, the parameter region can be restricted to $\mathcal{C} = \{(\theta_1, \theta_2) \mid |3\theta_2| \leq \theta_1 \leq \pi \}$, and the partition function becomes

$$Z = \int_{\mathcal{C}} d\theta_1 d\theta_2 H(\theta_1, \theta_2) \exp[-S_{\text{eff}}(\theta_1, \theta_2)].$$  \hspace{1cm} (3.5)

$H(\theta) = \sin^2 \theta_1 \sin^2((\theta_1 + 3\theta_2)/2) \sin^2((\theta_1 - 3\theta_2)/2)$ is the Vandermonde determinant, which comes from the Haar measure. In this parametrization,

$$S_{\text{eff}} - \ln H = \frac{8h}{3} \left( 2 \cos \theta_1 \cos(\theta_2 - i\mu) + \cos(2\theta_2 + i\mu) \right)$$  \hspace{1cm} (3.6)

$$- \ln \left[ \sin^2 \theta_1 \sin^2 \left( \frac{\theta_1 + 3\theta_2}{2} \right) \sin^2 \left( \frac{\theta_1 - 3\theta_2}{2} \right) \right].$$
In order to apply the saddle-point approximation to this model, we rewrite the original integral (3.5) using the Lefschetz-thimble method. After complexification, the Polyakov line $\mathcal{L} \in \text{SL}(3, \mathbb{C})$, and let us denote the complexified variables of $\theta_{1,2}$ by $z_{1,2}$. In the limit $\mu \to +\infty$, the saddle-point equation can be approximately solved analytically, and we find

$$z^*_1 \simeq \frac{3e^{-\mu/2}}{2\sqrt{h}}, \quad z^*_2 \simeq -\frac{e^{-\mu}}{8h},$$

(3.7)

In general, the saddle point $z$ satisfies that $\text{Im}z_1^* = \text{Re}z_2^* = 0$. Figure 1 explicitly shows the behavior of Morse’s downward flow (1.2) around the saddle point in the two-dimensional subspace $\text{Im}z_1 = \text{Re}z_2 = 0$ of $\mathbb{C}^2$. The dual thimble $\mathfrak{J}_*$ of $z^*$ is shown with the green dashed curve, and it indeed intersects with the original integration cycle $\mathcal{C}$. Therefore, the complex saddle point contributes, and the integration on the Lefschetz thimble $\mathfrak{J}_*$ is identical to that on $\mathcal{C}$.

Using the saddle-point approximation, we can find that the effective action $S_{\text{eff}}$ and Polyakov loops $\ell_3, \bar{\ell}_3$ take real values. Therefore, even after performing the saddle-point approximation using the Lefschetz thimble method, the physical quantities turn out to be real. Furthermore,

$$\langle \ell_3 \rangle - \langle \bar{\ell}_3 \rangle \simeq \frac{2}{3} (\sinh 2iz_2^* - 2\cos z_1^* \sinh iz_2^*) > 0,$$

(3.8)

and the difference between two Polyakov loops at finite chemical potential can be captured correctly [6].

There exists a deep reason why the physical quantities remain real using the complexified saddle-point approximation, and the charge conjugation plays an important role there [7]. We will generalize this statement as a common property of the Lefschetz decomposition formula (1.3).

4. General theorem on the mean-field approximation and charge conjugation

By definition, the partition function (1.1) for physical systems must be a real quantity, however the Boltzmann weight $S(x)$ may be complex. The condition $Z \in \mathbb{R}$ is manifestly ensured if there exists charge conjugation $C : (x_i) \mapsto (C_{ij} x_j)$, which satisfies $C_{ij} = C_{ji} \in \mathbb{R}, C^2 = 1$ and

$$S(x) = S(C \cdot x).$$

(4.1)
The linear map $C$ on $\mathbb{R}^n$ can be extended to an antilinear map on $\mathbb{C}^n$ by
\[
CK : (z_i) \mapsto (C_i \bar{z}_j).
\] (4.2)
Using Eq.(4.1), the Morse’s flow equation shows covariance under the conjugation,
\[
\frac{d\Sigma}{dt} = \left( \frac{\partial S(C: \bar{z})}{\partial \bar{z}_i} \right).
\] (4.3)
The antilinearly transformed function $\tilde{\Sigma}(t) := CK(\bar{z}(t))$ satisfies
\[
\frac{d\tilde{\Sigma}}{dt} = C_{ij} \cdot \left( \frac{\partial S(\bar{z})}{\partial \bar{z}_j} \right) = \left( \frac{\partial S(\bar{z})}{\partial z_i} \right),
\] (4.4)
which is nothing but the original flow equation (1.2). This shows that the downward flow itself has an invariance under the transformation $CK$.

Let us decompose the set of saddle points $\Sigma$ into three disjoint parts. For simplicity, we assume that $S(\varepsilon^\sigma) \in \mathbb{R}$ only if the saddle point satisfies $\varepsilon^\sigma = K(\varepsilon^\sigma)$; then, $\Sigma = \Sigma_0 \cup \Sigma_+ \cup \Sigma_-$, where
\[
\Sigma_0 = \{ \sigma \mid \varepsilon^\sigma = L \cdot L^\sigma \}, \quad \Sigma_\pm = \{ \sigma \mid \text{Im}(\varepsilon^\sigma) \gtrless 0 \}.
\] (4.5)
The transformation $CK$ induces a bijection $\Sigma_+ \to \Sigma_-$. Equation (1.3) becomes
\[
Z = \sum_{\sigma \in \Sigma_0} n_\sigma \int_{\Theta_0} d^2 z \, e^{-S(z)} + \sum_{\tau \in \Sigma_+} n_\tau \int_{\Theta_+} d^2 \bar{z} \, e^{-S(\bar{z})}.
\] (4.6)
Each integral on the r.h.s. of the formula (4.6) is real or purely imaginary depending on whether $CK$ changes orientation of $\Theta_\sigma$ and of $\Theta_\sigma \cup \Theta^K_\sigma$. Since the l.h.s. is real, $n_\tau$ must be zero unless the integral on $\Theta_\tau$ or on $\Theta_\tau + \Theta^K_\tau$ is real [1]. This conclusion can also be applied to expectation values of any physical observables that satisfy the symmetry (4.1). The decomposition formula (4.6) takes a suitable form for the saddle-point analysis.

We can easily check that the previous example (3.5) shows an invariance under the conjugation $CK : (z_1, z_2) \mapsto (\bar{z}_1, -\bar{z}_2)$, (4.7)
and the saddle point $\varepsilon^s$ satisfies the invariance under $CK$. This is the reason why the Lefschetz-thimble integration on $\Theta_\sigma$ gives real expectation values of physical quantities, and its saddle-point approximation also satisfies that property. Let us check our theorem also applies to the finite-density QCD. The QCD partition function at temperature $T = \beta^{-1}$ and quark chemical potential $\mu_{qk}$ is
\[
Z_{\text{QCD}} = \int \mathcal{D}A \, \text{det} \mathcal{M}(\mu_{qk}, A) \, e^{-S_{\text{YM}}[A]},
\] (4.8)
\[
S_{\text{YM}} = \frac{1}{2} \text{tr} \int_0^\beta d\tau \int d^4x \sum_{\mu, \nu} |F_{\mu\nu}|^2 \quad (> 0)
\]
is the Yang-Mills action, and
\[
\text{det} \mathcal{M}(\mu_{qk}, A) = \text{det} \left[ \gamma^\mu (\partial_\nu + igA_\nu) + \gamma^\lambda \mu_{qk} + m_{qk} \right]
\] (4.9)
is the quark determinant. When $\mu_{qk} \neq 0$, the quark determinant becomes an oscillatory functional of the gauge field $A$, and the sign problem emerges. Even when $\mu_{qk} \neq 0$, the charge conjugation $A \mapsto -A^\dagger$ with the $\gamma_5$ hermiticity implies that the fermion determinant still satisfies the identity [6],
\[
\text{det} \mathcal{M}(\mu_{qk}, A) = \text{det} \mathcal{M}(-\mu_{qk}, A^\dagger) = \text{det} \mathcal{M}(\mu_{qk}, -\bar{A}).
\] (4.10)
The charge $C$ and complex $\mathcal{K}$ conjugation, or the $C\mathcal{K}$ transformation, serves as the antilinear map (4.2) for finite-density QCD [7], and our theorem applies to it. The Lefschetz-thimble decomposition (4.6) manifestly respects the $C\mathcal{K}$ symmetry so that $Z_{\text{QCD}} \in \mathbb{R}$.

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