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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,

$$Z = \int_{\mathbb{R}^n} \mathrm{d}^n x\, \mathrm{e}^{-S(x)}, \tag{1.1}$$

where $S(x)$ is a complex action functional of the real field $x = (x_1, \dots, x_n) \in \mathbb{R}^n$. 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^σ in $\mathbb{C}^n$ ($\sigma \in \Sigma$). Consider Morse's flow equation for complexified variables z [2]:

$$\frac{\mathrm{d}z_i}{\mathrm{d}t} = \overline{\left(\frac{\partial S(z)}{\partial z_i}\right)}. \tag{1.2}$$

The Lefschetz thimble $\mathfrak{J}_\sigma$ is identified as the set of points reached by some flows emanating from z^σ. The partition function can now be computed as the sum of the nicely converging integrations;

$$Z = \sum_{\sigma\in\Sigma} n_\sigma \int_{\mathfrak{J}_\sigma} \mathrm{d}^n z\, \mathrm{e}^{-S(z)}. \tag{1.3}$$

The coefficient n_σ is given by the intersection number between $\mathbb{R}^n$ and $\mathfrak{K}_\sigma$; $n_\sigma = \langle \mathfrak{K}_\sigma, \mathbb{R}^n \rangle$. The dual thimble $\mathfrak{K}_\sigma$ is defined as the set of the points reached by flows getting sucked into z^σ. 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

$$Z = \int \mathscr{D}\phi \exp -S[\phi]. \tag{2.1}$$

Let us consider a background field method. The constrained effective action is given by

$$\exp -S_{\mathrm{eff}}[\phi_{\mathrm{MF}}] = \int \mathscr{D}\phi\ \delta(\langle\phi\rangle - \phi_{\mathrm{MF}})\ \exp -S[\phi], \tag{2.2}$$

where $\langle\phi\rangle = \int \mathrm{d}x \phi(x)/V$. In order to reproduce the original partition function, we need an integration over the background field ϕ_{MF}, i.e.,

$$Z = \int \mathrm{d}\phi_{\mathrm{MF}} \exp -S_{\mathrm{eff}}(\phi_{\mathrm{MF}}). \tag{2.3}$$

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Since $S_{\rm eff}$ is typically proportional to the volume V, the saddle-point approximation is useful. If the original action S is real, so is $S_{\rm eff}$ and the saddle-point approximation can be done without any difficulty. If S takes complex values, however, $S_{\rm eff}$ 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 $\ell_{\bf 3}$ is an order parameter of confinement;

$$\ell_{\bf 3}=\frac{1}{3}\mathrm{tr}\left[\boldsymbol{L}\right],\quad \boldsymbol{L}=\mathscr{P}\exp\left(\mathrm{i}g\int_0^\beta A_4\mathrm{d}x^4\right), \tag{3.1}$$

where $\mathscr{P}$ 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:

$$Z=\int_{SU(3)}\mathrm{d}\boldsymbol{L}\,\exp\left[-S_{\rm eff}(\boldsymbol{L})\right], \tag{3.2}$$

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

$$S_{\rm eff}(L)=-h\frac{(3^2-1)}{2}\left(e^{\mu}\ell_{\bf 3}+e^{-\mu}\ell_{\bar{\bf 3}}\right) \tag{3.3}$$

Here, $\ell_{\bar{\bf 3}}=\mathrm{tr}\boldsymbol{L}^{-1}/3$. When $h\neq 0$ and $\mu=\beta\mu_{\rm qk}\neq 0$, the integration (3.5) is oscillatory because $S_{\rm eff}$ takes complex values. When the quark chemical potential $\mu_{\rm qk}$ is turned on under the nontrivial Polyakov-loop background, the effective action $S_{\rm eff}(\theta)$ 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:

$$\boldsymbol{L}=\mathrm{diag}\left[\mathrm{e}^{\mathrm{i}(\theta_1+\theta_2)},\mathrm{e}^{\mathrm{i}(-\theta_1+\theta_2)},\mathrm{e}^{-2\mathrm{i}\theta_2}\right], \tag{3.4}$$

where $\theta_{1,2}$ are real parameters if $\boldsymbol{L}\in SU(3)$. The Weyl group acts on these parameters (θ_1,θ_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 $\mathfrak{C}=\{(\theta_1,\theta_2)\mid 3|\theta_2|\leq\theta_1\leq\pi\}$, and the partition function becomes

$$Z=\int_{\mathfrak{C}}\mathrm{d}\theta_1\mathrm{d}\theta_2 H(\theta_1,\theta_2)\exp\left[-S_{\rm eff}(\theta_1,\theta_2)\right]. \tag{3.5}$$

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

$$\begin{aligned}S_{\rm eff}-\ln H &= -\frac{8h}{3}(2\cos\theta_1\cos(\theta_2-\mathrm{i}\mu)+\cos(2\theta_2+\mathrm{i}\mu))\\ &\quad -\ln\left[\sin^2\theta_1\sin^2\left(\frac{\theta_1+3\theta_2}{2}\right)\sin^2\left(\frac{\theta_1-3\theta_2}{2}\right)\right].\end{aligned} \tag{3.6}$$

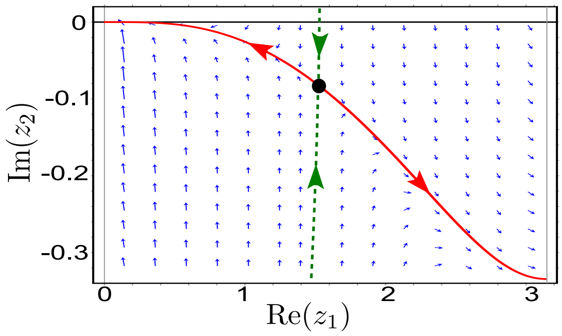

Figure 1: Morse's flow (1.2) around the saddle point (the black blob) z^* in the $\mathrm{Re}(z_1)$-$\mathrm{Im}(z_2)$ plane ($h = 0.1$, $\mu = 2$) [1]. The red solid and green dashed lines are the Lefschetz thimble $\mathfrak{J}_*$ and its dual $\mathfrak{K}_*$, respectively.

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 $\boldsymbol{L} \in SL(3,\mathbb{C})$, 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

$$z_1^* \simeq \frac{3e^{-\mu/2}}{2\sqrt{h}}, \quad z_2^* \simeq -\mathrm{i}\frac{e^{-\mu}}{8h}, \tag{3.7}$$

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

Using the saddle-point approximation, we can find that the effective action S_{eff} and Polyakov loops $\ell_{\mathbf{3}}$, $\ell_{\bar{\mathbf{3}}}$ 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,

$$\langle \ell_{\bar{\mathbf{3}}} \rangle - \langle \ell_{\mathbf{3}} \rangle \simeq \frac{2}{3}(\sinh 2\mathrm{i}z_2^* - 2\cos z_1^* \sinh \mathrm{i}z_2^*) > 0, \tag{3.8}$$

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

$$\overline{S(x)} = S(C \cdot x). \tag{4.1}$$

The linear map C on $\mathbb{R}^n$ can be extended to an antilinear map on $\mathbb{C}^n$ by

$$CK : (z_i) \mapsto (C_{ij}\overline{z_j}). \tag{4.2}$$

Using Eq.(4.1), the Morse's flow equation shows covariance under the conjugation,

$$\frac{\mathrm{d}\overline{z_i}}{\mathrm{d}t} = \overline{\left(\frac{\partial S(C\cdot\overline{z})}{\partial \overline{z_i}}\right)}. \tag{4.3}$$

The antilinearly transformed function $\widetilde{z}(t) := CK(z(t))$ satisfies

$$\frac{\mathrm{d}\widetilde{z}_i}{\mathrm{d}t} = C_{ij}\cdot\overline{\left(\frac{\partial S(\widetilde{z})}{\partial \overline{z_j}}\right)} = \overline{\left(\frac{\partial S(\widetilde{z})}{\partial \widetilde{z}_i}\right)}, \tag{4.4}$$

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 Σ into three disjoint parts. For simplicity, we assume that $S(z^\sigma)\in\mathbb{R}$ only if the saddle point satisfies $z^\sigma = K(z^\sigma)$; then, $\Sigma = \Sigma_0\cup\Sigma_+\cup\Sigma_-$, where

$$\Sigma_0 = \{\sigma \mid z^\sigma = L\cdot\overline{z^\sigma}\},\quad \Sigma_\pm = \{\sigma \mid \mathrm{Im}S(z^\sigma)\gtrless 0\}. \tag{4.5}$$

The transformation CK induces a bijection $\Sigma_+\to\Sigma_-$. Equation (1.3) becomes

$$Z = \sum_{\sigma\in\Sigma_0} n_\sigma \int_{\mathfrak{J}_\sigma} \mathrm{d}^n z\, \mathrm{e}^{-S(z)} + \sum_{\tau\in\Sigma_+} n_\tau \int_{\mathfrak{J}_\tau+\mathfrak{J}_\tau^K} \mathrm{d}^n z\, \mathrm{e}^{-S(z)}. \tag{4.6}$$

Each integral on the r.h.s. of the formula (4.6) is real or purely imaginary depending on whether CK changes orientation of $\mathfrak{J}_\sigma$ and of $\mathfrak{J}_\sigma\cup\mathfrak{J}_\sigma^K$. Since the l.h.s. is real, n_τ must be zero unless the integral on $\mathfrak{J}_\tau$ or on $\mathfrak{J}_\tau+\mathfrak{J}_\tau^K$ 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

$$CK : (z_1, z_2) \mapsto (\overline{z_1}, -\overline{z_2}), \tag{4.7}$$

and the saddle point z^* satisfies the invariance under CK. This is the reason why the Lefschetz-thimble integration on $\mathfrak{J}_*$ 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 μ_{qk} is

$$Z_{\mathrm{QCD}} = \int \mathscr{D}A\, \det\mathscr{M}(\mu_{\mathrm{qk}}, A)\, \mathrm{e}^{-S_{\mathrm{YM}}[A]}, \tag{4.8}$$

where $S_{\mathrm{YM}} = \frac{1}{2}\mathrm{tr}\int_0^\beta \mathrm{d}x^4 \int \mathrm{d}^3\boldsymbol{x} |F_{\mu\nu}|^2\ (>0)$ is the Yang-Mills action, and

$$\det\mathscr{M}(\mu_{\mathrm{qk}}, A) = \det\left[\gamma^\nu(\partial_\nu + \mathrm{i}gA_\nu) + \gamma^4\mu_{\mathrm{qk}} + m_{\mathrm{qk}}\right] \tag{4.9}$$

is the quark determinant. When $\mu_{\mathrm{qk}}\neq 0$, the quark determinant becomes an oscillatory functional of the gauge field A, and the sign problem emerges. Even when $\mu_{\mathrm{qk}}\neq 0$, the charge conjugation $A\mapsto -A^t$ with the γ_5 hermiticity implies that the fermion determinant still satisfies the identity [6],

$$\overline{\det\mathscr{M}(\mu_{\mathrm{qk}}, A)} = \det\mathscr{M}(-\mu_{\mathrm{qk}}, A^\dagger) = \det\mathscr{M}(\mu_{\mathrm{qk}}, -\overline{A}). \tag{4.10}$$

The charge $\mathscr{C}$ and complex $\mathscr{K}$ conjugation, or the $\mathscr{C}\mathscr{K}$ 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 $\mathscr{C}\mathscr{K}$ symmetry so that $Z_{\mathrm{QCD}} \in \mathbb{R}$.

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