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

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Jul 15, 2015 @ LATTICE 2015

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Motivation

Path integral with complex weights appear in many important physics:

- Finite-density lattice QCD, spin-imbalanced nonrelativistic fermions
- Gauge theories with topological $\theta$ terms
- Real-time quantum mechanics

Oscillatory nature hides many important properties of partition functions.
Example: Airy integral

Let’s consider a one-dimensional oscillatory integration:

\[ \text{Ai}(a) = \int_{\mathbb{R}} \frac{dx}{2\pi} \exp i \left( \frac{x^3}{3} + ax \right). \]

RHS is well defined \textbf{only if} \( \text{Im}a = 0 \), though \( \text{Ai}(z) \) is holomorphic.

\[10^* \cos(x^3/3+x) \exp(-0.5x) \cos(x^3/3)\]

**Figure**: Real parts of integrands for \( a = 1 \) \((\times 10)\) & \( a = 0.5i \)
First thing first

Lefschetz decomposition formula

Oscillatory integrals with **many variables** can be evaluated using the “steepest descent” cycles $\mathcal{J}_\sigma$:

$$
\int_{\mathbb{R}^n} d^n x \ e^{-S(x)} = \sum_\sigma n_\sigma \int_{\mathcal{J}_\sigma} d^n z \ e^{-S(z)}.
$$

$\mathcal{J}_\sigma$ are called Lefschetz thimbles, and $\text{Im}[iS]$ is constant on it:

$$
\frac{dz_i}{dt} = \left( \frac{\partial S(z)}{\partial z_i} \right).
$$

$n_\sigma$: intersection numbers of duals $\mathcal{K}_\sigma$ and $\mathbb{R}^n$.

[Witten, arXiv:1001.2933, 1009.6032]

(⇒ Ünsal, Friday 9:00-; Scorzato, Sat. 14:15-)
Rewrite the Airy integral

There exists two Lefschetz thimbles $\mathcal{J}_\sigma$ ($\sigma = 1, 2$) for the Airy integral:

$$Ai(a) = \sum_\sigma n_\sigma \int_{\mathcal{J}_\sigma} \frac{dz}{2\pi} \exp i \left( \frac{z^3}{3} + a z \right).$$

$n_\sigma$: intersection number of the steepest ascent contour $\mathcal{K}_\sigma$ and $\mathbb{R}$.

Figure: Lefschetz thimbles $\mathcal{J}$ and duals $\mathcal{K}$ ($a = \exp(0.1i), \exp(\pi i)$)
Sign problem in MFA: Motivation

At finite-density QCD (in the heavy-dense limit), the Polyakov-loop effective action looks like

\[ S_{\text{eff}}(\ell) \simeq \int d^3 \mathbf{x} \left[ e^{\mu \ell(\mathbf{x})} + e^{-\mu \ell(\mathbf{x})} \right] \notin \mathbb{R}. \]

Even after the MFA, the effective potential becomes complex!

The integration over the order parameter plays a pivotal role for reality. (Fukushima, Hidaka, PRD75, 036002)

Question

*Can we make a tied connection bet. the saddle-point approximation and the mean-field approximation with complex \( S \)?*
Polyakov-loop effective model

The Polyakov line $\mathbf{L}$:

$$\mathbf{L} = \frac{1}{3} \text{diag} \left[ e^{i(\theta_1 + \theta_2)}, e^{i(-\theta_1 + \theta_2)}, e^{-2i\theta_2} \right].$$

Let us consider the $SU(3)$ matrix model:

$$Z_{\text{QCD}} = \int d\theta_1 d\theta_2 H(\theta_1, \theta_2) \exp \left[ -V_{\text{eff}}(\theta_1, \theta_2) \right],$$

where $H = \sin^2 \theta_1 \sin^2 \left( (\theta_1 + 3\theta_2)/2 \right) \sin^2 \left( (\theta_1 - 3\theta_2)/2 \right).$
Charge conjugation in the Polyakov loop model

Charge conjugation acts as $L(\theta_1, \theta_2) \leftrightarrow L^\dagger(\theta_1, \theta_2) \simeq L(\theta_1, -\theta_2)$:

$$V_{\text{eff}}(z_1, z_2) = V_{\text{eff}}(\overline{z}_1, -\overline{z}_2).$$

Simple model for dense quarks ($\ell := \text{tr} L$):

$$V_{\text{eff}} = -h \frac{(3^2 - 1)}{2} \left( e^\mu \ell_3(\theta_1, \theta_2) + e^{-\mu} \ell_3(\theta_1, \theta_2) \right)$$
Behaviors of the flow

Figure: Flow at $h = 0.1$ and $\mu = 2$ in the $\text{Re}(z_1)$-$\text{Im}(z_2)$ plane.

The black blob: a saddle point.
The red solid line: Lefschetz thimble $\mathcal{J}$.
The green dashed line: its dual $\mathcal{K}$.

(YT, Nishimura, Kashiwa, PRD91, 101701)
Saddle point approximation at finite density

The saddle point approximation can now be performed.

Polyakov-loop phases \((z_1, z_2)\) takes complex values, so that

\[
\langle \ell \rangle, \langle \overline{\ell} \rangle \in \mathbb{R}.
\]

Since \(\text{Im}(z_2) < 0\) and

\[
\ell \simeq \frac{1}{3} (2e^{iz_2} \cos \theta_1 + e^{-2iz_2}),
\]

we can confirm that

\[
\overline{\ell} > \ell.
\]

(YT, Nishimura, Kashiwa, PRD91, 101701)
General set up

Consider the oscillatory multiple integration,

\[ Z = \int_{\mathbb{R}^n} d^n x \exp(-S(x)). \]

To ensure \( Z \in \mathbb{R} \), suppose the existence of a linear map \( L \), satisfying

- \( \overline{S(x)} = S(L \cdot x) \).
- \( L^2 = 1 \).

Let’s construct a systematic computational scheme of \( Z \) with \( Z \in \mathbb{R} \).
Flow eq. and Complex conjugation

Morse’s downward flow:

\[
\frac{dz_i}{dt} = \left( \frac{\partial S(z)}{\partial z_i} \right).
\]

Complex conjugation of the flow:

\[
\frac{d\bar{z}_i}{dt} = \left( \frac{\partial S(z)}{\partial \bar{z}_i} \right) = \left( \frac{\partial S(L \cdot \bar{z})}{\partial \bar{z}_i} \right),
\]

therefore \(z' = L \cdot \bar{z}\) satisfy the same flow equation:

\[
\frac{dz'_i}{dt} = \left( \frac{\partial S(z')}{\partial z'_i} \right).
\]
General Theorem: Saddle points & thimbles

Let us decompose the set of saddle points into three parts, $\Sigma = \Sigma_0 \cup \Sigma_+ \cup \Sigma_-$, where

$$\Sigma_0 = \{ \sigma \mid z^\sigma = L \cdot \overline{z^\sigma} \},$$
$$\Sigma_\pm = \{ \sigma \mid \text{Im} S(z^\sigma) \geq 0 \}.$$

The antilinear map gives $\Sigma_+ \simeq \Sigma_-$. This correspondence also applies to Lefschetz thimbles.

(YT, Nishimura, Kashiwa, PRD91, 101701)
General Theorem

The partition function:

\[ Z = \sum_{\sigma \in \Sigma_0} n_{\sigma} \int_{\mathcal{J}_{\sigma}} d^n z \exp -S(z) \]
\[ + \sum_{\tau \in \Sigma_+} n_{\tau} \int_{\mathcal{J}_{\tau} + \mathcal{J}_{\tau}^K} d^n z \exp -S(z). \]

Each term on the r.h.s. is real.

(YT, Nishimura, Kashiwa, PRD91, 101701)

Consequence

Charge conjugation ensures the reality of physical observables manifestly in the Lefschetz-thimble decomposition.
The QCD partition function at finite density

The QCD partition function:

\[ Z_{\text{QCD}} = \int \mathcal{D}A \, \det M(\mu_{qk}, A) \exp -S_{\text{YM}}[A], \]

w./ the Yang-Mills action \( S_{\text{YM}} = \frac{1}{2} \text{tr} \int_0^\beta d^4x \int d^3x |F_{\mu\nu}|^2 (>0) \), and

\[ \det M(\mu, A) = \det \left[ \gamma^\nu (\partial_\nu + igA_\nu) + \gamma^4 \mu_{qk} + m_{qk} \right]. \]

is the quark determinant.
Charge conjugation

If \( \mu_{qk} \neq 0 \), the quark determinant takes complex values
\[ \Rightarrow \text{Sign problem} \text{ of QCD}. \]

However, \( Z_{\text{QCD}} \in \mathbb{R} \) is ensured thanks to the charge conjugation
\[ A \mapsto -A^t: \]

\[ \det \mathcal{M}(\mu_{qk}, A) = \det \mathcal{M}(-\mu_{qk}, A^\dagger) = \det \mathcal{M}(\mu_{qk}, -A). \]

(First equality: \( \gamma_5 \)-transformation, Second one: charge conjugation)

Consequence

Our theorem applies to the (lattice) QCD: The thimble decomposition manifestly ensures the reality of physical observables.
Lefschetz-thimble integral is a useful tool to treat multiple integrals.

Saddle point approximation can be applied without violating $Z \in \mathbb{R}$.

Sign problem of effective models of QCD is (partly) explored.