Lefschetz-thimble path integral
and its physical application

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Introduction and Motivation
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:

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

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

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

How can we circumvent such oscillatory integrations?

⇒ **Lefschetz-thimble integrations**

[Witten, arXiv:1001.2933, 1009.6032]

Applications of this new technique for path integrals

▶ Study on phase transitions of matrix models.
▶ Lefschetz-thimble method elucidates Lee-Yang zeros.
  [Kanazawa, YT, JHEP 1503 (2015) 044]
▶ General theorem ensuring that $Z \in \mathbb{R}$.
  Sign problem in MFA can be solved.
▶ Application of the theorem to the $SU(3)$ matrix model
Introduction to Lefschetz-thimble integrations
Introduction to Lefschetz-thimble integrations
Oscillatory integrals with many variables can be evaluated using the "steepest descent" cycles $\mathcal{J}_\sigma$:

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

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

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

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Example: Airy integral

Airy integral:

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

The integrand is **holomorphic** w.r.t $x$

$\Rightarrow$ The contour can be deformed continuously without changing the value of the integration!
Rewrite the Airy integral

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

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

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

Figure: Lefschetz thimbles $\mathcal{J}$ and duals $\mathcal{K}$ ($a = \exp(0.1i), \exp(\pi i)$)
Tips: Airy integral & Airy equation

Let us consider the “equation of motion”:

\[ \int \frac{dz}{2\pi} \frac{d}{dz} e^{i(z^3/3 + az)} = 0. \]

This is nothing but the Airy equation:

\[ \left( \frac{d^2}{da^2} - a \right) Ai(a) = 0. \]

Two possible integration contours
= Two linearly independent solutions of eom.
Generalization to multiple integrals

Model integral:

\[ Z = \int_{\mathbb{R}^n} dx_1 \cdots dx_n \exp S(x_i). \]

What properties are required for Lefschetz thimbles \( \mathcal{I} \)?

1. \( \mathcal{I} \) should be an \( n \)-dimensional object in \( \mathbb{C}^n \).
2. \( \text{Im}[S] \) should be constant on \( \mathcal{I} \).
Complexified variables \((a = 1, \ldots, n)\): \(z_a = x_a + ip_a\).

Regard \(x_a\) as **coordinates** and \(p_a\) as **momenta**, so that **Poisson bracket** is given by

\[
\{f, g\} = \sum_{a=1,2} \left[ \frac{\partial f}{\partial x_a} \frac{\partial g}{\partial p_a} - \frac{\partial g}{\partial x_a} \frac{\partial f}{\partial p_a} \right].
\]
Short note on technical aspects

Hamilton equation with the Hamiltonian \( H = \text{Im}[S(z_\alpha)] \):

\[
\frac{df(x, p)}{dt} = \{H, f\} \quad \iff \quad \frac{dz_\alpha}{dt} = -\left(\frac{\partial S}{\partial z_\alpha}\right)
\]

This is Morse’s flow equation (= gradient flow):

\[
\frac{d}{dt} \text{Re}[S] = - \left| \left(\frac{\partial S}{\partial z}\right)^2 \right| \leq 0
\]

\[\Rightarrow \text{We can find } n \text{ good directions for } J \text{ around saddle points!} \]

(This is because a \( \pi/2 \)-rot. of coord. around a saddle point multiplies \((-1)\) to an eigenvalue. )

[Witten, 2010]
Oscillatory integrals with many variables can be evaluated using the “steepest descent” cycles $\mathcal{I}_\sigma$:

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

$\mathcal{I}_\sigma$ are called Lefschetz thimbles, and $\text{Im}[S]$ is constant on it.

$n_\sigma$: intersection numbers of duals $\mathcal{K}_\sigma$ and $\mathbb{R}^n$. 
Phase transition associated with symmetry
The partition function of our model study is the following:

\[ Z_N(G, m) = \int d\bar{\psi} d\psi \exp \left\{ \sum_{a=1}^{N} \bar{\psi}_a (i\phi + m) \psi_a + \frac{G}{4N} \left( \sum_{a=1}^{N} \bar{\psi}_a \psi_a \right)^2 \right\}. \]

\( \psi, \bar{\psi} \): 2-component Grassmannian variables with \( N \) flavors.
\( \phi = p_1 \sigma_1 + p_2 \sigma_2 \).
Hubbard–Stratonovich transformation

Bosonization ($\sigma \sim \langle \overline{\psi} \psi \rangle$):

$$Z_N(G, m) = \sqrt{\frac{N}{\pi G}} \int_{\mathbb{R}} d\sigma \, e^{-NS(\sigma)},$$

with

$$S(\sigma) \equiv \frac{\sigma^2}{G} - \log[p^2 + (\sigma + m)^2].$$

For simplicity, we put $m = 0$ in the following.

$S$ has three saddle points:

$$0 = \frac{\partial S(z)}{\partial z} = \frac{2z}{G} - \frac{2z}{p^2 + z^2} \implies z = 0, \pm \sqrt{G - p^2}.$$
Behaviors of the flow

Figures for $G = 0.7 e^{-0.1i}, 1.1 e^{-0.1i}$ at $p^2 = 1$

[Kanazawa, YT, arXiv:1412.2802]:

- $z = 0$ is the unique critical point contributing to $Z$ if $G < p^2$.
- All three critical points contribute to $Z$ if $G > p^2$.
Stokes phenomenon

The difference of the way of contribution can be described by \textbf{Stokes phenomenon}. [Witten, arXiv:1001.2933, 1009.6032]

Figures of $G$-plane for $\text{Im} S(0) = \text{Im} S(z_\pm)$ [Kanazawa, YT, arXiv:1412.2802]:

\[
\begin{array}{c}
\begin{matrix}
\begin{array}{c}
\begin{array}{c}
\text{$G$-plane figure for $\text{Im} S(0) = \text{Im} S(z_\pm)$} \\
\text{[Kanazawa, YT, arXiv:1412.2802]} \\
\end{array}
\end{array}
\end{matrix}
\end{array}
\]
Dominance of contribution

The Stokes phenomenon tells us the number of Lefschetz thimbles contributing to $Z_N$. However, it does not tell which thimbles give main contribution.

$$Z_N \sim \# \exp(-NS(0)) + \# \exp(-NS(z_\pm))$$

In order to obtain $\langle \sigma \rangle \neq 0$ in the large-$N$ limit, $z_\pm$ should dominate $z = 0$.

$$\Rightarrow \quad \text{Re}S(z_\pm) \leq \text{Re}S(0)$$
Blue line: $\text{Im} S(z_{\pm}) = \text{Im} S(0)$.
Green line: $\text{Re} S(z_{\pm}) = \text{Re} S(0)$.
Red points: Lee-Yang zeros at $\mathcal{N} = 40$. [Kanazawa, YT, arXiv:1412.2802]
Conclusions for studies with GN-like models

1. Decomposition of the integration path in terms of Lefschetz thimbles is useful to visualize different phases.
2. The possible link between Lefschetz-thimble decomposition and Lee–Yang zeros is indicated.
Preliminary comments on a recent paper [Nishimura, Shimasaki, arXiv:1504.08359] from the Lefschetz-thimble viewpoint
Singularity of the drift term

Model:

\[ Z = \int \mathrm{d}x (x + i\alpha) \sqrt{\pi} e^{-x^2/2}. \]

Drift term in the complex Langevin equation:

\[ \frac{\partial S}{\partial z} = z - \frac{p}{z + i\alpha}. \]

The singularity of the drift term breaks the formal proof for the correctness of CLE at the stage of integration by parts.

[Nishimura, Shimasaki, arXiv:1504.08359]
Expectation values of $x^2$ for various $\alpha$

CLE breaks down for $\alpha \lesssim 14$ at $p = 50$. 

[Nishimura, Shimasaki, arXiv:1504.08359]
The Stokes phenomenon happens at $\alpha = \sqrt{4p}$.

Is this phenomenon related to the breakdown of CLE?

Looks interesting. No one can answer yet, though...
Sign problem in MFA and its solution: Formal discussion
At finite-density QCD (in the heavy-dense limit), the Polyakov-loop effective action looks like

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

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)
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

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

Let’s construct a \textbf{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:

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

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

\[
\begin{align*}
\Sigma_0 &= \{ \sigma \mid z^\sigma = L \cdot \bar{z}^\sigma \}, \\
\Sigma_\pm &= \{ \sigma \mid \text{Im} S(z^\sigma) \gtrless 0 \}.
\end{align*}
\]

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

(YT, Nishimura, Kashiwa, arXiv:1504.02979[hep-th])
The partition function:

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

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

(YT, Nishimura, Kashiwa, arXiv:1504.02979[hep-th])
Sign problem in MFA and its solution: Application to QCD-like theories
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 $S_{\text{YM}} = \frac{1}{2} \text{tr} \int_0^\beta dx^4 \int d^3 \mathbf{x} |F_{\mu\nu}|^2$ ($> 0$), and

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

is the quark determinant.
If $\mu_{qk} \neq 0$, the quark determinant takes complex values
⇒ **Sign problem** 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 equality: charge conjugation)
Polyakov-loop effective model

The Polyakov line \( L \):

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

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 acts as $L \leftrightarrow L^\dagger$:

$$V_{\text{eff}}(z_1, z_2) = V_{\text{eff}}(\overline{z_1}, \overline{z_2}).$$

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

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

Figure: Flow at $h = 0.1$ and $\mu = 2$ in the $\Re(z_1)$-$\Im(z_2)$ 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, arXiv:1504.02979[hep-th])
**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

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

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

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

(YT, Nishimura, Kashiwa, arXiv:1504.02979[hep-th])
Summary for the sign problem in MFA

- 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.