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 θ 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:

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

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

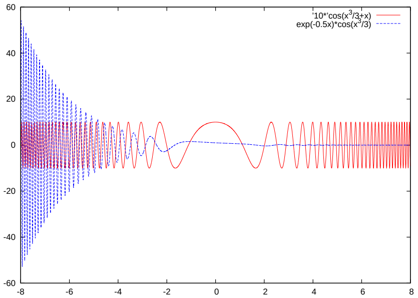


Figure: Real parts of integrands for $a = 1\ (\times 10)$ & $a = 0.5\mathrm{i}$

Contents

- How can we circumvent such oscillatory integrations?
  $\Rightarrow$ **Lefschetz-thimble integrations**

  [Witten, arXiv:1001.2933, 1009.6032]

  [YT, Koike, Ann. Physics 351 (2014) 250]

- 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

    [YT, Nishimura, Kashiwa, in preparation]

Introduction to Lefschetz-thimble integrations

Again Airy integral

Airy integral:

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

The integrand is **holomorphic** w.r.t x
$\Rightarrow$ The contour can be deformed continuously without changing the value of the integration!

Steepest descent contours for the Airy integral

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

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

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

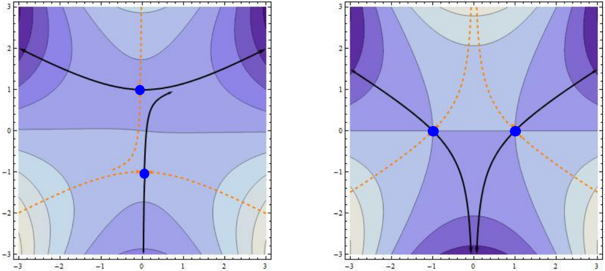


Figure: Lefschetz thimbles $\mathcal{J}$ and duals $\mathcal{K}$ $(a = \exp(0.1\mathrm{i}), \exp(\pi\mathrm{i}))$

Tips: Airy integral & Airy equation

Let us consider the "equation of motion":

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

This is nothing but the Airy equation:

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}a^2} - a\right) \mathrm{Ai}(a) = 0.$$

Two possible integration contours
= **Two** linearly independent solutions of eom.

Generalization to multiple integrals

Model integral:

$$Z = \int_{\mathbb{R}^n} \mathrm{d}x_1 \cdots \mathrm{d}x_n \exp S(x_i).$$

What properties are required for Lefschetz thimbles $\mathcal{J}$?

1. $\mathcal{J}$ should be an n-dimensional object in $\mathbb{C}^n$.
2. $\mathrm{Im}[S]$ should be constant on $\mathcal{J}$.

Short note on technical aspects

Complexified variables ($a = 1, \ldots, n$): $z_a = x_a + \mathrm{i} p_a$.

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 $H = \mathrm{Im}[S(z_a)]$:

$$\frac{\mathrm{d}f(x,p)}{\mathrm{d}t} = \{H, f\} \qquad \left(\Leftrightarrow \frac{\mathrm{d}z_a}{\mathrm{d}t} = -\overline{\left(\frac{\partial S}{\partial z_a}\right)}\right)$$

This is **Morse's flow equation (= gradient flow)**:

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

$\Rightarrow$ We can find n good directions for $\mathcal{J}$ around saddle points!

[Witten, 2010]

Multiple integral: Lefschetz-thimble method

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

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

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

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

Phase transition associated with symmetry

0-dim. Gross–Neveu-like model

The partition function of our model study is the following:

$$Z_N(G,m)=\int \mathrm{d}\bar{\psi}\mathrm{d}\psi\ \exp\left\{\sum_{a=1}^{N}\bar{\psi}_a(i\not{p}+m)\psi_a+\frac{G}{4N}\left(\sum_{a=1}^{N}\bar{\psi}_a\psi_a\right)^2\right\}.$$

Hubbard–Stratonovich transformation

Bosonization:

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

with

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

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

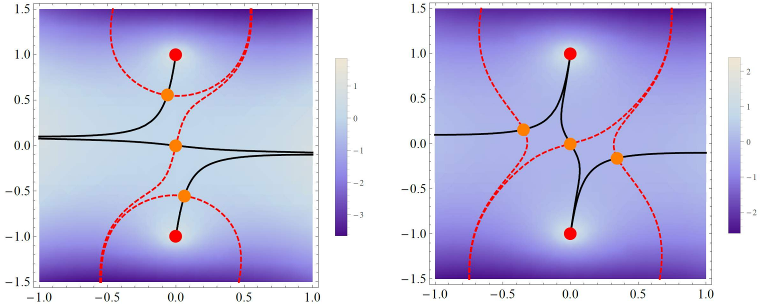
S has three saddle points:

$$0=\frac{\partial S(z)}{\partial z}=\frac{2z}{G}-\frac{2z}{p^2+z^2}\quad\Longrightarrow\quad z=0,\ \pm\sqrt{G-p^2}\,.$$

Behaviors of the flow

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

[Kanazawa, YT, arXiv:1412.2802]:

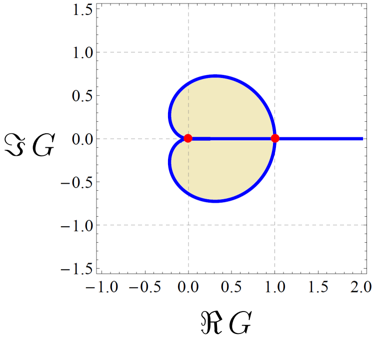


- $z = 0$ is the unique critical point contributing to Z if $G < p^2$.
- All three critical points contribute to Z if $G > p^2$.

Stokes phenomenon

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

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



Dominance of contribution

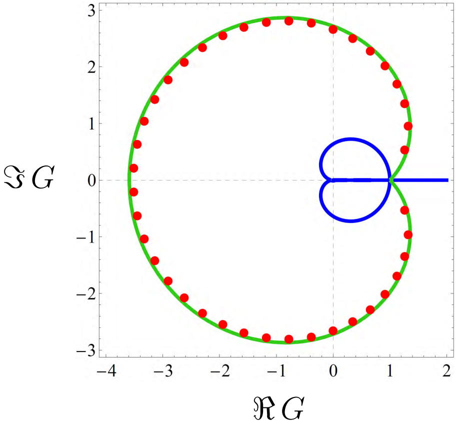
The Stokes phenomenon tells us the **number** of Lefschetz thimbles contributing to Z_N.
However, it does **not** tell which thimbles give main contribution.

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

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

$$\Rightarrow \qquad \mathrm{Re}S(z_\pm) \leq \mathrm{Re}S(0)$$

Connection with Lee–Yang zero



Blue line: $\mathrm{Im} S(z_\pm) = \mathrm{Im} S(0)$.
Green line: $\mathrm{Re} S(z_\pm) = \mathrm{Re} S(0)$.
Red points: Lee-Yang zeros at $N = 40$. [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.

Sign problem in MFA and its solution: Formal discussion

Airy integral with real a

If $a \in \mathbb{R}$, the following partition function is real:

$$Z_{\mathrm{Airy}}(a) = \frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{d}x \exp \mathrm{i} \left(\frac{x^3}{3} + ax \right).$$

However, the integrand is **complex-valued**.

Why does this happen?
What is the mean-field approximation of this partition function?

Airy integral: Antilinear symmetry

The system have an antilinear symmetry:

$$\overline{S(x)} = -\mathrm{i}\left(\frac{x^3}{3} + ax\right) = S(-x).$$

By summing up in pairs $\pm x$, the result becomes **manifestly real**!

Airy integral: Lefschetz thimble

Extend the linear map $x \mapsto -x$ to the antilinear map $z \mapsto -\overline{z}$.

The Lefschetz thimbles form invariants under the antiliner map:

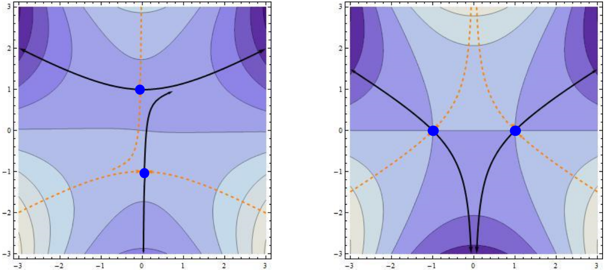


Figure: Lefschetz thimbles $\mathcal{J}$ and duals $\mathcal{K}$ ($a = \exp(0.1\mathrm{i})$, $\exp(\pi \mathrm{i})$)

Generalization: Set up

Consider the oscillatory multiple integration,

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

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 $Z \in \mathbb{R}$.

Generalization: Flow eq. and Complex conjugation

Morse's downward flow:

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

Complex conjugation of the flow:

$$\frac{\mathrm{d}\overline{z_i}}{\mathrm{d}t} = \overline{\left(\frac{\partial S(L\cdot\overline{z})}{\partial \overline{z_i}}\right)},$$

and thus $z' := L\cdot\overline{z}$ satisfies Morse's flow equation .

Generalization: Immediate conclusion

Denote the antilinear map as $K(z) := L \cdot \overline{z}$.

1. When z^σ is a saddle point, so is $K(z^\sigma)$.
2. Let $\mathcal{J}_\sigma$ is the Lefschetz thimble around z^σ.
   $\Rightarrow \mathcal{J}_\sigma^K := \{K(z) \mid z \in \mathcal{J}_\sigma\}$ coincides with the Lefschetz thimble around $K(z^\sigma)$ (up to orientation).
3. Intersection numbers are the same: $\langle \mathcal{K}_\sigma, \mathbb{R}^n \rangle = \langle \mathcal{K}_\sigma^K, \mathbb{R}^n \rangle$ under appropriate choice of the orientation.
4. The contributing thimbles always form an invariant pair $\mathcal{J}_\sigma \cup \mathcal{J}_\sigma^K$.

General Theorem

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

$$\begin{aligned} \Sigma_0 &= \{\sigma \mid z^\sigma = L \cdot \overline{z^\sigma}\}, \\ \Sigma_+ &= \{\sigma \mid \mathrm{Im} S(z^\sigma) > 0\}, \\ \Sigma_- &= \{\sigma \mid \mathrm{Im} S(z^\sigma) < 0\}. \end{aligned}$$

The antilinear map gives $\Sigma_+ \simeq \Sigma_-$.

General Theorem

The partition function:

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

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

(YT, Nishimura, Kashiwa, in preparation)

Sign problem in MFA and its solution: Application to QCD-like theories

The QCD partition function at finite density

The QCD partition function:

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

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

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

is the quark determinant.

Charge conjugation

If $\mu_{\mathrm{qk}} \neq 0$, the quark determinant takes complex values
$\Rightarrow$ **Sign problem** of QCD.

However, $Z_{\mathrm{QCD}} \in \mathbb{R}$ is ensured thanks to the charge conjugation $A \mapsto -A^t$:

$$\begin{aligned} \overline{\det \mathcal{M}(\mu_{\mathrm{qk}}, A)} &= \det \mathcal{M}(-\mu_{\mathrm{qk}}, A^\dagger) \\ &= \det \mathcal{M}(\mu_{\mathrm{qk}}, -\overline{A}). \end{aligned}$$

(First equality: γ_5-transformation,
Second equality: charge conjugation)

Polyakov-loop effective model

The Polyakov line $\boldsymbol{L}$:

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

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

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

where $H = \sin^2\theta_1 \sin^2(\theta_1 + 3\theta_2)/2 \sin^2(\theta_1 - 3\theta_2)/2$.

Charge conjugation in the Polyakov loop model

Charge conjugation acts as $\boldsymbol{L} \leftrightarrow \boldsymbol{L}^\dagger$:

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

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

$$V_{\mathrm{eff}} \;=\; -h\frac{(3^2-1)}{2}\Big(e^{\mu}\ell_{\mathbf{3}}(\theta_1,\theta_2) + e^{-\mu}\ell_{\overline{\mathbf{3}}}(\theta_1,\theta_2)\Big)$$

Behaviors of the flow

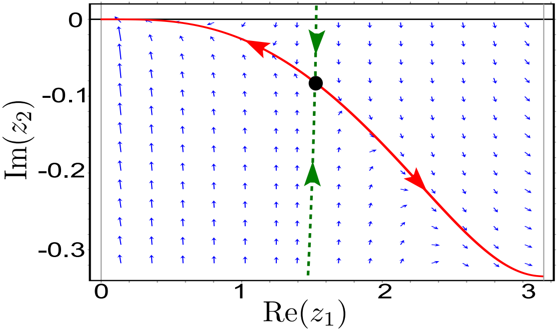


Figure: Flow at $h = 0.1$ and $\mu = 2$ in the $\mathrm{Re}(z_1)$-$\mathrm{Im}(z_2)$ plane.

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, in preparation)

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 $\mathrm{Im}(z_2) < 0$ and

$$\ell \simeq \frac{1}{3}(2e^{\mathrm{i}z_2}\cos\theta_1 + e^{-2\mathrm{i}z_2}),$$

we can confirm that

$$\bar{\ell} > \ell.$$

(YT, Nishimura, Kashiwa, in preparation)

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.