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

Yuya Tanizaki

Department of Physics, The University of Tokyo

Theoretical Research Division, Nishina Center, RIKEN

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Collaborators: Kouji Kashiwa (YITP, Kyoto), Hiromichi Nishimura (Bielefeld)

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**.

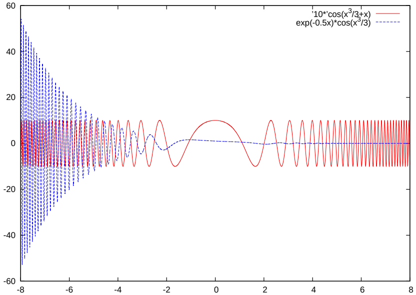

Figure: Real parts of integrands for $a = 1$ $(\times 10)$ & $a = 0.5\mathrm{i}$

First thing first
Lefschetz decomposition formula

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

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

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

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

n_σ: 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:

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

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

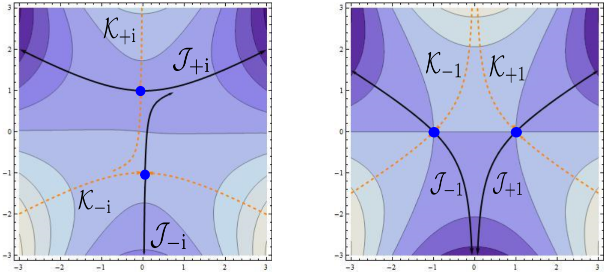

Figure: Lefschetz thimbles $\mathcal{J}$ and duals $\mathcal{K}$ $(a = \exp(0.1\mathrm{i}), \exp(\pi \mathrm{i}))$

Sign problem in MFA: Motivation

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

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

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 $\boldsymbol{L}$:

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

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

Charge conjugation in the Polyakov loop model

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

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

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

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

Behaviors of the flow

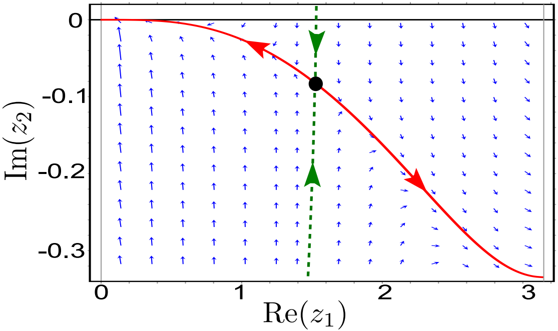

Figure: Flow at $h = 0.1$ and $\mu = 2$ in the $\mathrm{Re}(z_1)$-$\mathrm{Im}(z_2)$ plane.

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

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

we can confirm that

$$\overline{\ell} > \ell.$$

(YT, Nishimura, Kashiwa, PRD91, 101701)

General 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 $Z \in \mathbb{R}$.

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:

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

therefore $z' = L\cdot \overline{z}$ satisfy the same flow eqation:

$$\frac{\mathrm{d}z'_i}{\mathrm{d}t} = \overline{\left(\frac{\partial S(z')}{\partial z'_i}\right)}.$$

General Theorem: Saddle points & thimbles

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

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

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

(YT, Nishimura, Kashiwa, PRD91, 101701)

General Theorem

The partition function:

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

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

(YT, Nishimura, Kashiwa, 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:

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

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

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

is the quark determinant.

Charge conjugation

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

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

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

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

Consequence

Our theorem applies to the (lattie) QCD: The thimble decomposition manifestly ensures the reality of physical observables.

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.