Lefschetz-thimble path integral for studying the sign problem and Silver Blaze phenomenon

Yuya Tanizaki

Department of Physics, The University of Tokyo
Theoretical Research Division, Nishina Center, RIKEN

Oct. 26, 2015 @ University of Connecticut

Collaborators: Yoshimasa Hidaka, Tomoya Hayata (RIKEN)
Introduction and Motivation
Motivation

QCD phase diagram

Schematic figure:

(Fukushima, Hatsuda, Rept. Prog. Phys. 74 (2011) 014001)

- Finite temperatures ··· Lattice simulation works well!
- Finite density ··· No \textit{ab initio} calculations.
Where is the finite-density QCD?

Neutron star
- Cold and dense nuclear matters
- $2m_{\text{sun}}$ neutron star (2010)
- Gravitational-wave observations (2017~)

Heavy-ion collision
- Low-energy scan of heavy-ion collisions are planned and run in many facilities (RHIC, SIS, J-PARC)

Reliable theoretical approach to equation of state must be developed!

$$Z(T, \mu) = \int \mathcal{D}A \, \text{Det}(D(A) + m) \exp -S_{\text{YM}}(A).$$
**Silver Blaze problem in finite-density QCD**

QCD & $|\text{QCD}|$

\[
Z_{\text{QCD}} = \int DA (\det \gamma_\nu D_\nu) e^{-S_{\text{YM}}}, \quad Z_{|\text{QCD}|} = \int DA |\det \gamma_\nu D_\nu| e^{-S_{\text{YM}}}.
\]

At $\mu = 0$, these two are the same! But,

At $T = 0$, the state must be equal to the QCD vac. for $|\mu| \lesssim m_N/3$.

Can we describe this “trivial” behavior using path integral?
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:

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

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

Figure: Real parts of integrands for $a = 1 \times 10$ & $a = 0.5i$
Lefschetz decomposition formula

Oscillatory integrals with many variables can be evaluated using the “steepest descent” cycles $\mathcal{J}_\sigma$: (classical eom $S'(z_\sigma) = 0$)

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

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

$$\mathcal{J}_\sigma = \left\{ z(0) \left| \lim_{t \to -\infty} z(t) = z_\sigma \right. \right\}, \quad \frac{d z^i(t)}{d t} = \left( \frac{\partial S(z)}{\partial z^i} \right).$$

$n_\sigma$: intersection numbers of duals $\mathcal{K}_\sigma$ and $\mathbb{R}^n$ ($\mathcal{K}_\sigma = \left\{ z(0) \left| z(\infty) = z_\sigma \right. \right\}$).

[Witten, arXiv:1001.2933, 1009.6032]
Lefschetz thimble for Airy integral

Airy integral is given as

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

Complexify the integration variable: $z = x + iy$.

Integrand on $\mathbb{R}$, and on $J_1$ ($a = 1$)
Rewrite the Airy integral

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

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

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

Figure: Lefschetz thimbles $\mathcal{J}$ and duals $\mathcal{K}$ ($a = 1e^{0.1i}, -1$)
Simplest model study to understand the sign problem
One-site Fermi Hubbard model

Hubbard model (\(\hat{c}:\) annihilation op., \(\hat{n} = \hat{c}^\dagger \hat{c}\)):

\[
\hat{H}_F = -t \sum_{\langle i,j \rangle, \sigma} \hat{c}_{\sigma,i}^\dagger \hat{c}_{\sigma,j} + U \sum_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} - \mu \sum_i (\hat{n}_{i,\uparrow} + \hat{n}_{i,\downarrow}).
\]

This is too difficult as a toy model.

Turn off the hopping, \(t = 0\):

\[
\hat{H} = U \hat{n}_{\uparrow} \hat{n}_{\downarrow} - \mu (\hat{n}_{\uparrow} + \hat{n}_{\downarrow}).
\]

Fock state gives the partition function immediately!

\[
Z = \text{tr} \left[ \exp - \beta \hat{H} \right] = 1 + 2e^{\beta \mu} + e^{\beta (2\mu - U)}.
\]
One-site Fermi Hubbard model

The number density is given as

$$\langle \hat{n} \rangle = \frac{1}{\beta} \frac{\partial}{\partial \mu} \ln Z = \frac{2(e^{\beta \mu} + e^{\beta(2\mu - U)})}{1 + 2e^{\beta \mu} + e^{\beta(2\mu - U)}}.$$

In the zero-temperature limit,

$$n(\beta = \infty) = \begin{cases} 
2 & (1 < \mu/U), \\
1 & (0 < \mu/U < 1), \\
0 & (\mu/U < 0). 
\end{cases}$$

Question

*How can we describe these step functions using the path-integral formalism?*
Path integral for one-site model

The partition function reads

\[
Z = \lim_{N \to \infty} \sqrt{\frac{\beta/N}{2\pi U}} \int \prod_{k=1}^{N} d\varphi_k \exp \left( -\frac{\beta}{N} \sum_{k=1}^{N} \frac{\varphi_k^2}{2U} \right) \\
\times \int \prod_{k=1}^{N} d\psi_k^* d\psi_k \exp \left( \sum_{k=1}^{N} \psi_{k+1}^* \left( \psi_{k+1} - e^{\frac{\beta}{N} (i\varphi_k + \mu + U/2)} \psi_k \right) \right),
\]

with the antiperiodic boundary condition \( \psi_{N+1} = -\psi_1 \).

\( \varphi \) is an auxiliary field for the number density:

\[
\langle \hat{n} \rangle = \langle \psi_{k+1}^* e^{\frac{\beta}{N} (i\varphi_k + \mu + U/2)} \psi_k \rangle = -\frac{i}{U} \langle \varphi_k \rangle.
\]
Integrate out fermions

Fermion spectrum:

\[ \lambda_\ell(\varphi, \mu) = 1 - e^{(2\ell-1)\pi i/N} \exp \frac{\beta}{N^2} \sum_{k=1}^{N} (i\varphi_k + \mu + U/2). \]

It couples only to the Matsubara zero mode of \( \varphi \).

The path integral reduces to the zero-mode integral:

\[ Z = \sqrt{\frac{\beta}{2\pi U}} \int d\varphi \left( 1 + e^{\beta(i\varphi + \mu + U/2)} \right)^2 e^{-\frac{\beta\varphi^2}{2U}}. \]

Integrand has complex phases causing the sign problem.
Effective action:

\[ S(z) = \frac{\beta}{2U} z^2 - 2 \ln \left( 1 + \exp \beta \left( iz + \mu + \frac{U}{2} \right) \right). \]

It has a charge conjugation symmetry:

\[ \overline{S(z)} = S(-\bar{z}), \]

This ensures the manifest reality of observables.

(YT, Nishimura, Kashiwa, PRD 91, 101701(R) (2015))

The flow equation reads

\[ \frac{dz}{dt} = \frac{\beta}{U} \bar{z} + \frac{2i \beta \exp \beta \left( -i\bar{z} + \mu + \frac{U}{2} \right)}{1 + \exp \beta \left( -i\bar{z} + \mu + \frac{U}{2} \right)}. \]
Flows at $\mu/U < -0.5$ and $\mu/U > 1/5$

Figure: Flow at $\mu/U = 2$

$$Z = \int_{\mathcal{J}_*} dz \ e^{-S(z)}.$$ 

Number density: $n_* = 0$ for $\mu/U < -0.5$, $n_* = 2$ for $\mu/U > 1.5$. 

(YT, Hidaka, Hayata, 1509.07146)
Flows at $-0.5 < \mu/U < 1.5$

Behaviors of the flow become totally different!

Furthermore, saddle points lie around $\text{Im}(z_m)/U \simeq \mu/U + 1/2$. This value is far away from $n = \text{Im} \langle z \rangle/U = 0, 1, \text{or } 2$. 
Numerical results

Results for $\beta U = 30$: (1, 3, 5-thimble approx.: $\mathcal{I}_0$, $\mathcal{I}_0 \cup \mathcal{I}_{\pm 1}$, and $\mathcal{I}_0 \cup \mathcal{I}_{\pm 1} \cup \mathcal{I}_{\pm 2}$)

(YT, Hidaka, Hayata, arXiv:1509.07146[hep-th])

(cf. Fujii, Kamata, Kikukawa, 1509.08176, 1509.09141; Alexandru, Basar, Bedaque, 1510.03258)

Question

Multiple thimbles can solve the discrepancy. But how?
Semiclassical study of the sign problem
Complex classical solutions

Let us solve, for $-0.5 < \mu/U < 1.5$,

$$
\frac{\beta}{U} iz + \frac{2\beta \exp \beta (iz + \mu + \frac{U}{2})}{1 + \exp \beta (iz + \mu + \frac{U}{2})} = 0.
$$

If $\beta U \gg 1$, the solutions are labeled by $m \in \mathbb{Z}$:

$$
z_m = i \left( \mu + \frac{U}{2} \right) + T \left( 2\pi m + i \ln \frac{\frac{3}{2}U - \mu}{\frac{U}{2} + \mu} \right) + O(T^2).
$$

At these solutions, the classical actions become

$$
S_0 \simeq -\frac{\beta U}{2} \left( \frac{\mu}{U} + \frac{1}{2} \right)^2,
\text{Re} \left( S_m - S_0 \right) \simeq \frac{2\pi^2}{\beta U} m^2,
\text{Im} S_m \simeq 2\pi m \left( \frac{\mu}{U} + \frac{1}{2} \right).
$$
Semiclassical partition function

Using complex classical solutions $z_m$, let us calculate

$$Z_{\text{cl}} := \sum_{m=-\infty}^{\infty} e^{-S_m}.$$ 

This expression is valid for $-1/2 \lesssim \mu/U \lesssim 3/2$.

This is calculable using the elliptic theta function:

$$Z_{\text{cl}} \simeq e^{-S_0} \left(1 + 2 \sum_{m=1}^{\infty} \cos 2\pi m \left(\frac{\mu}{U} + \frac{1}{2}\right)e^{-2\pi^2 m^2/\beta U}\right)$$

$$= e^{-S_0} \theta_3 \left(\pi \left(\frac{\mu}{U} + \frac{1}{2}\right), e^{-2\pi^2/\beta U}\right).$$
Semiclassical analysis

Number density & Lee–Yang zeros

Semiclassical study gives the correct transition!

\[ n_{cl} := \frac{1}{\beta} \frac{\partial}{\partial \mu} \ln Z_{cl} \rightarrow \begin{cases} 2 & (1 < \mu/U < 3/2), \\ 1 & (0 < \mu/U < 1), \\ 0 & (-1/2 < \mu/U < 0). \end{cases} \]

Using the infinite-product form of the elliptic theta function,

\[ \theta_3(z, q) = \prod_{\ell=1}^{\infty} \left\{ (1 - q^{2\ell}) \left( 1 + 2q^{2\ell-1} \cos(2z) + q^{4\ell-2} \right) \right\}. \]

Zeros of \( Z_{cl} \) are

\[ \mu = \pm i\pi T(2\ell - 1), \quad \mu = U \pm i\pi T(2\ell - 1). \]

\[ \Rightarrow \text{1st order transition at } \mu = 0, \ U \text{ as } T \rightarrow 0. \]
Important interference among multiple thimbles

Let us consider a “phase-quenched” multi-thimble approximation:

\[ Z_{\text{cl.}} = \sum_{m} |e^{-S_m}| = e^{-S_0(\mu)} \theta_3(0, e^{-2\pi^2/\beta U}). \]

- Lee–Yang zeros cannot appear at \( \mu/U = 0, 1 \).
- One-thimble, or “phase-quenched”, result: \( n \simeq \mu/U + 1/2 \).

Consequence

In order to describe the step functions, we need interference of complex phases among different Lefschetz thimbles.

(cf. Hidden Topological Angles: Behtash, Sulejmanpasic, Schäfer, Ünsal, PRL 115 041601)
Numerical results

Let us remind the result for $n$:

We need five thimbles to describe the transition at $\beta U = 30$.

Question

How many thimbles are necessary for practical purpose?
**Necessary number of complex classical solutions**

Criterion to neglect the Lefschetz thimbles $\mathcal{J}_m$ for large $|m|:

$$\left| \frac{Z_{cl}^{(m)} - Z_{cl}^{(m-1)}}{Z_{cl}^{(m)}} \right| \ll 1.$$  

Assuming $|m| \gg 1$, we can write this as

$$\frac{2|\exp - S_m|}{Z_{cl}} \lesssim \varepsilon.$$  

Here $\varepsilon \ll 1$ is a controlling parameter of an error. We can solve this inequality with respect to $m$:

$$|m| \gtrsim \sqrt{-\frac{\beta U}{2\pi^2} \ln \frac{\varepsilon}{2} \theta_3 \left( \pi \left( \frac{\mu}{U} + \frac{1}{2} \right), e^{-2\pi^2/\beta U} \right)}.$$
Necessary number of complex classical solutions

If the sign problem is severe, \( \theta_3 \left( \frac{\pi}{2}, e^{-2\pi^2/\beta U} \right) \approx \sqrt{\frac{2\beta U}{\pi}} e^{-\beta U/8} \).

The criterion gives

\[
|m| \gtrsim \frac{\beta U}{4\pi}
\]

If the sign problem is mild, \( \frac{Z_{cl}}{e^{-S_0}} \approx \theta_3 \left( \pi, e^{-2\pi^2/\beta U} \right) \approx \sqrt{\frac{\beta U}{2\pi}}. \)

We only need

\[
|m| \gtrsim \sqrt{\frac{\beta U}{2\pi^2}} \ln \frac{\sqrt{8\pi}}{\varepsilon \sqrt{\beta U}}
\]

Necessary number of thimbles depends on the region which one wants to study.

For most severe cases, it is proportional to \( \beta U (\to \infty) \).

(YT, Hidaka, Hayata, 1509.07146)
Relation between complex Langevin and Lefschetz thimbles
(to appear soon. In collaboration with Y. Hidaka, and T. Hayata)
Complex Langevin method

Complex Langevin has been regarded as a sign-problem solver via stochastic quantization (Klauder, PRA 29, 2036 (1984), Parisi, PLB 131, 393 (1983)):

\[
\frac{dz_\eta(\theta)}{d\theta} = - \frac{\partial S}{\partial z}(z_\eta(\theta)) + \sqrt{\hbar}\eta(\theta).
\]

\(\theta\): Stochastic time, \(\eta\): Random force satisfying
\[\langle \eta(\theta)\eta(\theta') \rangle_\eta = 2\delta(\theta - \theta').\]

Itô calculus shows that
\[\frac{d}{d\theta}\langle O(z_\eta(\theta)) \rangle_\eta = \hbar\langle O''(z_\eta(\theta)) \rangle_\eta - \langle O'(z_\eta(\theta)) S'(z_\eta(\theta)) \rangle_\eta.\]

If the l.h.s becomes zero as \(\theta \to \infty\), this is nothing but the Dyson–Schwinger eq.
Complex Langevin and Lefschetz thimbles

For any solutions of the DS eq,

\[ \langle O(z_\eta) \rangle_\eta = \frac{1}{Z} \sum_\sigma \exists d_\sigma \int_{\mathcal{J}_\sigma} dz \, e^{-S(z)/\hbar} O(z), \]

in \( d_\sigma \in \mathbb{C} \). To reproduce physics, \( d_\sigma = \langle K_\sigma, \mathbb{R} \rangle \).

So far, we ONLY assume the convergence of the complex Langevin method.
Semiclassical limit

Let us take $\hbar \ll 1$ for computing

$$
\langle O(z_\eta) \rangle_\eta = \frac{1}{Z} \sum_\sigma d_\sigma \int_{\mathcal{J}_\sigma} dz \, e^{-S(z)/\hbar} O(z).
$$

I have NO idea how to compute the LHS. However, positivity of the probability density and its localization around $z_\sigma$’s imply that

$$
\exists c_\sigma \geq 0 \text{ s.t. } \langle O(z_\eta) \rangle_\eta \simeq \sum_\sigma c_\sigma O(z_\sigma).
$$

RHS is

$$
\int_{\mathcal{J}_\sigma} dz \, e^{-S(z)/\hbar} O(z) \simeq \sqrt{\frac{2\pi \hbar}{S''(z_\sigma)}} \, e^{-S(z_\sigma)/\hbar} O(z_\sigma).
$$
**Semiclassical inconsistency**

In the semiclassical analysis, one obtains (for dominant saddle points)

\[ c_\sigma = \frac{d_\sigma}{Z} \sqrt{\frac{2\pi \hbar}{S''(z_\sigma)}} e^{-S(z_\sigma)/\hbar}. \]

\[ c_\sigma \geq 0. \text{ And, } d_\sigma = \langle K_\sigma, \mathbb{R} \rangle \text{ to get physics. } \Rightarrow \text{ Inconsistent!} \]

(Hayata, Hidaka, YT, to appear)

We show that the complex Langevin is wrong if

- There exist several dominantly contributing saddle points.
- Those saddle points have different complex phases.

**Consequence**

*Naive complex Langevin method cannot explain the Silver Blaze phenomenon.*
Proposal for modification

Assume that

\[
c_\sigma = \frac{\langle K_\sigma, \mathbb{R} \rangle}{Z} \left| \sqrt{\frac{2\pi \hbar}{S''(z_\sigma)}} e^{-S(z_\sigma)/\hbar} \right|.
\]

Because of the localization of probability distribution \( P \), it would be given as

\[
P = \sum_\sigma c_\sigma P_\sigma, \quad \text{supp}(P_\sigma) \cap \text{supp}(P_\tau) = \emptyset.
\]

Assumption means “CL = phase quenched multi-thimble approx.”:

\[
\langle O(z_\eta) \rangle_\eta \simeq \sum_\sigma \frac{\langle K_\sigma, \mathbb{R} \rangle}{Z} \left| \sqrt{\frac{2\pi \hbar}{S''(z_\sigma)}} e^{-S(z_\sigma)/\hbar} \right| O(z_\sigma).
\]
Proposal for modification (conti.)

If so, defining the phase function

\[ \Phi(z, \bar{z}) = \sum_{\sigma} \sqrt{|S''(z_{\sigma})|} \frac{e^{-i \text{Im} S(z_{\sigma})/\hbar}}{S''(z_{\sigma})} \chi_{\text{supp}(P_{\sigma})}(z, \bar{z}), \]

we can compute

\[ \langle O(z_\eta) \rangle^{\text{new}} := \frac{\langle \Phi(z_\eta, \bar{z}_\eta) O(z_\eta) \rangle_\eta}{\langle \Phi(z_\eta, \bar{z}_\eta) \rangle_\eta}. \]

This new one is now consistent within the semiclassical analysis.
Possible questions on the proposal

Our prescription would work well if $P$ is a sum of “well localized” distributions and $c_\sigma$ can be well understood.

This prescription has the sign problem because $\Phi$ is complex, but it can be less severe compared with the original one.

Possible questions are

- Is the assumption on $c_\sigma$ valid? How can we compute it?
- Can we go beyond the semiclassical analysis?
  If not, what is an error estimate?

I have no answers....

Anyway, let’s try!
Numerical test 1

\[ S(x) = \frac{x^4}{4} - \frac{x^2}{2} + i\alpha x \] (Semiclassical limit is \( \alpha \to \infty \)):

(Preliminary)

(Hayata, Hidaka, YT, to appear)
Numerical test 2

One-site Fermi Hubbard model: (Preliminary)

Consequence

Modified complex Langevin is not perfect yet, but it seems to point a correct way. I hope this can attack the Silver Blaze phenomenon.
Summary and conclusion
Picard–Lefschetz theory gives a suitable framework for saddle-point analysis even if $S(\phi)$ takes complex values.

One-site Hubbard model is a nice toy model to play with the sign problem.

Destructive interference among complex phases of Lefschetz thimbles play a pivotal role for the baryon Silver Blaze.

Naive complex Langevin method is incorrect for generic cases and cannot explain baryon Silver Blaze.

Modified complex Langevin may become a multi-thimble simulator, which has not been achieved in any other algorithms.