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

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Contents

Motivation: Sign problem, Silver Blaze problem

Method: Path integral on Lefschetz thimbles

Analysis: Semi-classical analysis of the one-site Hubbard model

Discussion: Speculation on Silver Blaze problem

Bonus: Complex Langevin method

Motivation: Sign problem, Silver Blaze problem

Finite-density QCD?

Neutron star

- Cold and dense nuclear matters
- $2m_{\mathrm{sun}}$ neutron star (2010)
- Gravitational-wave observations (2016$\sim$)

Reliable theoretical approach to equation of state must be developed!

$$Z(T,\mu)=\int \mathcal{D}A\ \underbrace{\mathrm{Det}(\not{D}(A,\mu)+m)}_{\text{quark}}\underbrace{\exp -S_{\mathrm{YM}}(A)}_{\text{gluon}}.$$

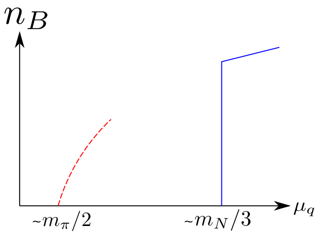
Sign problem in finite-density QCD

QCD & |QCD|

$$Z_{\mathrm{QCD}}=\int \mathcal{D}A\,(\det \not{D})\,\mathrm{e}^{-S_{\mathrm{YM}}},\ Z_{|\mathrm{QCD}|}=\int \mathcal{D}A\,|\det \not{D}|\,\mathrm{e}^{-S_{\mathrm{YM}}}.$$

If these two were sufficiently similar, we have no practical problems. However, it was observed in lattice QCD simulation that

(e.g., Barbour et. al. (PRD **56** (1998) 7063))



Baryon Silver Blaze problem

The curious incident of the dog in the night-time (Holmes, Silver Blaze).

Problem: It is of great importance for finite-density lattice QCD to understand $n_B = 0$ for $\mu_q < m_N/3$. (Cohen, PRL **91** (2003) 222001)

Current situation: For $\mu_q < m_\pi/2$, the problem is almost solved: Quark det. is (Adams, PRD **70** (2004) 045002)

$$\frac{\mathrm{Det}(\not{D}(A,\mu_q)+m)}{\mathrm{Det}(\not{D}(A,0)+m)} \simeq \prod_{\mathrm{Re}(\lambda_A)<\mu_q} \exp\beta\left(\mu_q-\lambda_A\right),$$

and $\text{ess-min}_A(\mathrm{Re}(\lambda_A)) = m_\pi/2$ (Nagata et. al., PTEP **2012** 01A103).

For $\mu_q > m_\pi/2$, no one knows how to understand this.

Method: Path integral on Lefschetz thimbles

Complexification of fields

There are two "new" approaches to the sign problem:

- Complex Langevin method: Solve the Langevin eq.

$$\frac{\mathrm{d}z}{\mathrm{d}\theta} = -\frac{\partial S}{\partial z} + \eta(\theta).$$

  η is a real stochastic noise, $\langle \eta(\theta)\eta(\theta') \rangle = 2\delta(\theta - \theta')$.

- Path integral on Lefschetz thimbles:

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

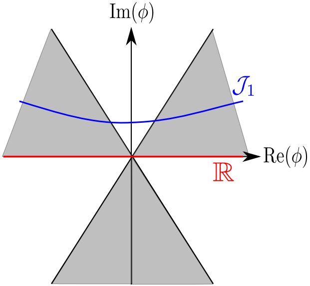
  Path integral is performed on steepest descent paths $\mathcal{J}_\sigma$. This is mathematically rigorous, and always true for finite dimensional integrals.

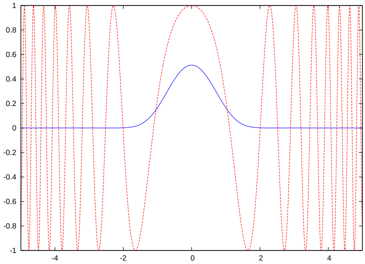
Lefschetz thimble for Airy integral

Airy integral is given as

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

Complexify the integration variable: $z = x + \mathrm{i}y$.





Integrand on $\mathbb{R}$, and on $\mathcal{J}_1$ $(a = 1)$

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 $\mathbb{R}$.

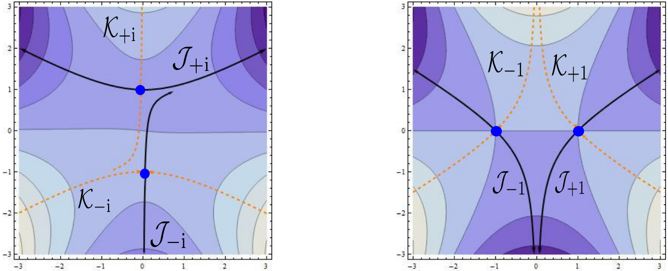


Figure: Lefschetz thimbles $\mathcal{J}$ and duals $\mathcal{K}$ $(a = 1\mathrm{e}^{0.1\mathrm{i}},\ -1)$

Lefschetz decomposition formula

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

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

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

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

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

[Witten, arXiv:1001.2933, 1009.6032]

Analysis: Semi-classical analysis of the one-site Hubbard model

One-site Fermi Hubbard model

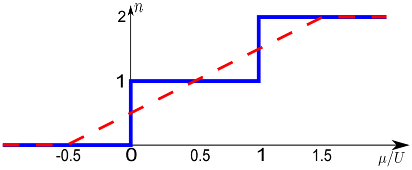
One-site Hubbard model:

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

Fock state gives the number density immediately:

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

In the zero-temperature limit,



(YT, Hidaka, Hayata, 1509.07146)(cf. Monte Carlo with 1-thimble approx. gives a wrong result: Fujii, Kamata, Kikukawa,1509.08176, 1509.09141; Alexandru, Basar, Bedaque,1510.03258.)

Path integral for one-site model

The path-integral expression for the one-site Hubbard model: :

$$Z=\sqrt{\frac{\beta}{2\pi U}}\int_{\mathbb{R}}\mathrm{d}\varphi\,\underbrace{\left(1+\mathrm{e}^{\beta(\mathrm{i}\varphi+\mu+U/2)}\right)^2}_{\text{Fermion Det}}\mathrm{e}^{-\beta\varphi^2/2U}.$$

Integrand has complex phases causing the sign problem.

φ is an auxiliary field for the number density:

$$\langle\hat{n}\rangle=\mathrm{Im}\langle\varphi\rangle/U.$$

Flows at $\mu/U < -0.5$ (and $\mu/U > 1/5$)

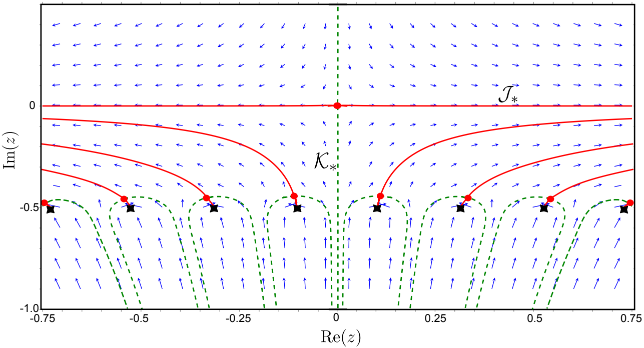


Figure: Flow at $\mu/U = -1$. $\mathcal{J}_* \simeq \mathbb{R}$.

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

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

(YT, Hidaka, Hayata, 1509.07146)

Flows at $-0.5 < \mu/U < 1.5$

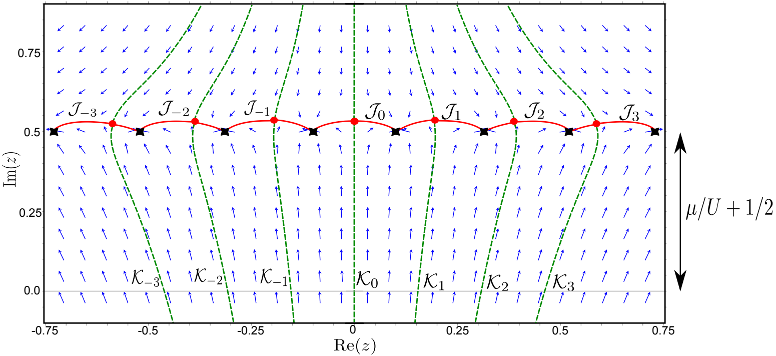


Figure: Flow at $\mu/U = 0$

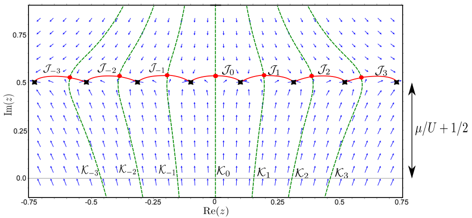
Complex saddle points lie on $\mathrm{Im}(z_m)/U \simeq \mu/U + 1/2$.

This value is far away from $n = \mathrm{Im}\langle z\rangle/U$=0, 1, or 2.

Complex classical solutions

If $\beta U \gg 1$, the classical sol. for $-0.5 < \mu/U < 1.5$ are labeled by $m \in \mathbb{Z}$:

$$z_m \simeq \mathrm{i}\left(\mu + \frac{U}{2}\right) + 2\pi m T.$$



At these solutions, the classical actions become

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

Semiclassical partition function

Using complex classical solutions z_m, let us calculate

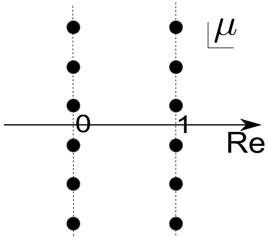
$$Z_{\mathrm{cl}} := \sum_{m=-\infty}^{\infty} \mathrm{e}^{-S_m}.$$

This expression is valid for $-1/2 \lesssim \mu/U \lesssim 3/2$.
This is calculable using the elliptic theta function:

$$\begin{aligned} Z_{\mathrm{cl}} &\simeq \mathrm{e}^{-S_0}\left(1+2\sum_{m=1}^{\infty} \cos 2\pi m\left(\frac{\mu}{U}+\frac{1}{2}\right)\mathrm{e}^{-2\pi^2 m^2/\beta U}\right) \\ &= \mathrm{e}^{-S_0}\theta_3\left(\pi\left(\frac{\mu}{U}+\frac{1}{2}\right), \mathrm{e}^{-2\pi^2/\beta U}\right). \end{aligned}$$

Number density & Lee–Yang zeros

Lee–Yang zeros of $Z_{\rm cl}$:



Semiclassical study gives the correct transition!

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

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

Important interference among multiple thimbles

Let us consider a "phase-quenched" multi-thimble approximation:

$$Z_{|\mathrm{cl.}|} = \sum_m \left| \mathrm{e}^{-S_m} \right| = \mathrm{e}^{-S_0(\mu)} \theta_3(0, \mathrm{e}^{-2\pi^2/\beta U}).$$

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

Consequence

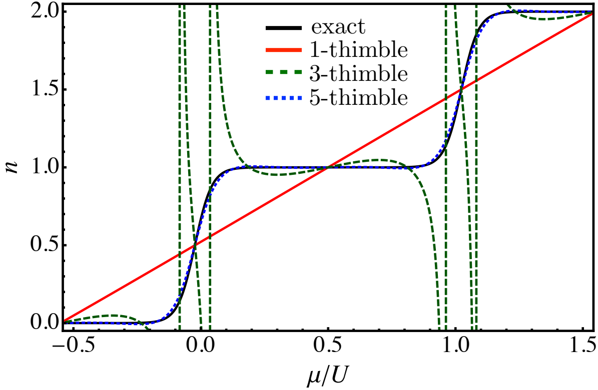
In order to describe the step functions, we need interference of complex phases among different Lefschetz thimbles.

(cf. Particle Productions: Dumulu, Dunne, PRL 104 250402)

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

Numerical results

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



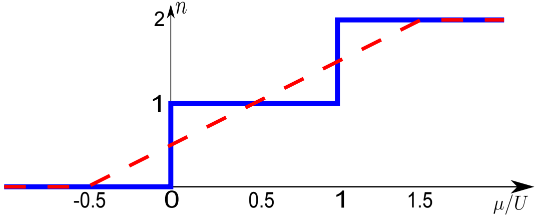
Necessary number of Lefschetz thimbles $\simeq \beta U/(2\pi)$.

(YT, Hidaka, Hayata, NJP 18 (2016) 033002, arXiv:1509.07146[hep-th])

Discussion: Speculation on Silver Blaze problem

Curious incident of n in the one-site model

We have a big difference bet. the exact result and naive expectation:



Naive guess: This is similar to what happens for QCD and |QCD|.
$\mu/U = -0.5 \Leftrightarrow \mu_q = m_\pi/2$.

Dimensionally reduced expression of fermion det.

One-site Hubbard model:

$$\mathrm{Det}\left[\partial_\tau - \left(\mu + \frac{U}{2} + \mathrm{i}\varphi\right)\right] = \left(1 + \mathrm{e}^{-\beta(-U/2-\mu)}\mathrm{e}^{\mathrm{i}\beta\varphi}\right)^2 .$$

Quark determinant in QCD:

$$\mathrm{Det}\left[\gamma_4(\not{D}_A + m) - \mu\right] = \mathcal{N}(A)\prod_{\varepsilon_j>0}\left(1+\mathrm{e}^{-\beta(\varepsilon_j-\mu-\mathrm{i}\phi_j)}\right)\left(1+\mathrm{e}^{-\beta(\varepsilon_j+\mu+\mathrm{i}\phi_j)}\right),$$

where the spectrum of $\gamma_4(\not{D}_A + m)$ is

$$\lambda_{(j,n)} = \varepsilon_j(A) - \mathrm{i}\phi_j(A) + (2n+1)\mathrm{i}\pi T.$$

Formal correspondence: $-U/2 \leftrightarrow \text{ess-min}(\varepsilon_j) = m_\pi/2$, $\varphi \leftrightarrow \phi_j$.

(YT, Hidaka, Hayata, NJP 18 (2016) 033002, arXiv:1509.07146[hep-th])

Silver Blaze problem for $\mu < -U/2$, $\mu < m_\pi/2$

One-site Hubbard model: As $\beta U \gg 1$ and $-U/2 - \mu > 0$,

$$\mathrm{Det}\left[\partial_\tau - \left(\mu + \frac{U}{2} + \mathrm{i}\varphi\right)\right] = \left(1 + \mathrm{e}^{-\beta(-U/2-\mu)}\mathrm{e}^{\mathrm{i}\beta\varphi}\right)^2 \simeq 1.$$

The sign problem almost disappears, so that $\mathcal{J}_* \simeq \mathbb{R}$.

Finite-density QCD: As $\beta \to \infty$ and $\mu < m_\pi/2$,

$$\frac{\mathrm{Det}\left[\gamma_4(\not{D}_A + m) - \mu\right]}{\mathrm{Det}\left[\gamma_4(\not{D}_A + m)\right]} \to 1.$$

The sign problem disappears by the reweighting method.

$\Rightarrow$ Lefschetz thimbles $\simeq$ Original integration regions

Silver Blaze problem for $\mu > -U/2$, $\mu > m_\pi/2$

One-site Hubbard model: At each real config., the magnitude is exponentially large:

$$\mathrm{Det}\left[\partial_\tau - \left(\mu + \frac{U}{2} + \mathrm{i}\varphi\right)\right] = O\left(\mathrm{e}^{\beta(U+\mu/2)}\right)$$

This large contributions must be canceled exactly in order for $n = 0$.

In the Lefschetz-thimble method, this is realized by interference among multiple thimbles.

Question

Does the same thing happens for QCD?

We guess that it would, but we do not yet know how severe it is.

Bonus: Complex Langevin method

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)):

$$\frac{\mathrm{d}z_\eta(\theta)}{\mathrm{d}\theta} = -\frac{\partial S}{\partial z}(z_\eta(\theta)) + \sqrt{\hbar}\eta(\theta).$$

θ: Stochastic time, η: Random force $\langle \eta(\theta)\eta(\theta')\rangle_\eta = 2\delta(\theta-\theta')$.

Itô calculus shows that

$$\frac{\mathrm{d}}{\mathrm{d}\theta}\langle O(z_\eta(\theta))\rangle_\eta = \hbar\langle O''(z_\eta(\theta))\rangle_\eta - \langle O'(z_\eta(\theta))S'(z_\eta(\theta))\rangle_\eta.$$

If the l.h.s becomes zero as $\theta\to\infty$, this is the Dyson–Schwinger eq.

Complex Langevin and Lefschetz thimbles

For any solutions of the DS eq,

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

in $d_\sigma \in \mathbb{C}$. To reproduce physics, $d_\sigma = \langle \mathcal{K}_\sigma, \mathbb{R}\rangle \in \mathbb{Z}$.

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

Semiclassical limit

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

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

I have NO idea how to compute the LHS. However, positivity of the probability density and its localization around z_σ's imply that

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

RHS is

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

Semiclassical inconsistency

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

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

$c_\sigma \geq 0$. And, $d_\sigma = \langle K_\sigma, \mathbb{R}\rangle$ to get physics. $\Rightarrow$ Inconsistent!
(Hayata, Hidaka, YT, arXiv:1511.02437[hep-lat])

We show that the complex Langevin is wrong if

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

Open question: Recently, our knowledge on the CL method is developing (Aarts, Seiler, and Stamatesc, 2009; Nishimura, Shimasaki, 2015, etc.). Can one understand our result from this viewpoint?

Proposal for modification

Assume that

$$c_\sigma = \frac{\langle \mathcal{K}_\sigma, \mathbb{R} \rangle}{Z} \left| \sqrt{\frac{2\pi\hbar}{S''(z_\sigma)}} \mathrm{e}^{-S(z_\sigma)/\hbar} \right|.$$

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

$$P = \sum_\sigma c_\sigma P_\sigma, \quad \mathrm{supp}(P_\sigma) \cap \mathrm{supp}(P_\tau) = \emptyset.$$

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

$$\langle O(z_\eta) \rangle_\eta \simeq \sum_\sigma \frac{\langle \mathcal{K}_\sigma, \mathbb{R} \rangle}{Z} \left| \sqrt{\frac{2\pi\hbar}{S''(z_\sigma)}} \mathrm{e}^{-S(z_\sigma)/\hbar} \right| O(z_\sigma).$$

Proposal for modification (conti.)

If so, defining the phase function

$$\Phi(z,\overline{z}) = \sum_{\sigma} \sqrt{\frac{|S''(z_\sigma)|}{S''(z_\sigma)}} \mathrm{e}^{-\mathrm{i}\,\mathrm{Im}\,S(z_\sigma)/\hbar} \chi_{\mathrm{supp}(\mathrm{P}_\sigma)}(z,\overline{z}),$$

we can compute

$$\langle O(z_\eta)\rangle^{\mathrm{new}} := \frac{\langle \Phi(z_\eta,\overline{z}_\eta) O(z_\eta)\rangle_\eta}{\langle \Phi(z_\eta,\overline{z}_\eta)\rangle_\eta}.$$

This new one is now consistent within the semiclassical analysis.

(Hayata, Hidaka, YT, arXiv:1511.02437[hep-lat])

Caution: Our proposal evades inconsistency, but is not necessarily correct. Can we improve the proposal?

Complex Langevin study of one-site Hubbard model

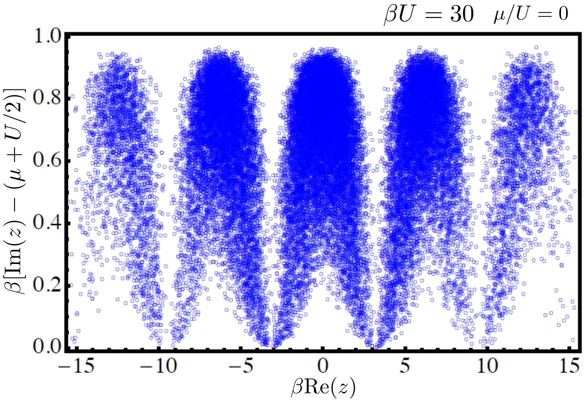
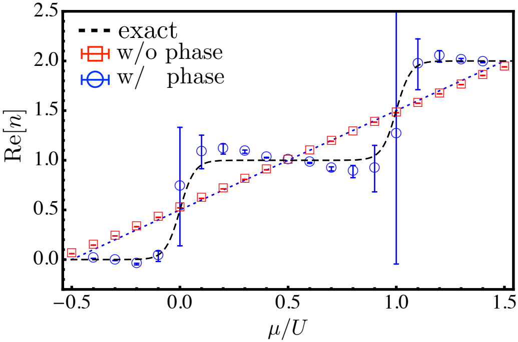


Figure: CL distribution at $\mu/U = 0$

It looks quite similar to Lefschetz thimbles.

Complex Langevin simulation

One-site Fermi Hubbard model:



(Hayata, Hidaka, YT, arXiv:1511.02437[hep-lat])

Consequence

Modified complex Langevin is not perfect yet, but it seems to point a correct way.

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