Recent progresses of Lefschetz-thimble integral and refine complex Langevin method

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Aug 2, 2016 @ Plymouth University, UK

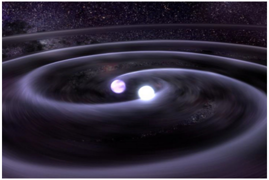
Finite-density quantum chromodynamics (QCD)

QCD

Fundamental theory for quarks and gluons

Neutron star

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



Neutron star merger

(image from NASA)

Path-integral expression of finite-density QCD:

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

Sign problem: $\mathrm{Det}(\not{D}(A,\mu_q)+m)\not\geq 0$ at $\mu_q\neq 0$.

Sign problem & Complexification of variables

Consider the path integral:

$$Z = \int \mathcal{D}x \exp(-S[x]).$$

- $S[x]$ is real $\Rightarrow$ No sign problem. Monte Carlo works.
- $S[x]$ is complex $\Rightarrow$ Sign problem appears!

If $S[x] \in \mathbb{C}$, eom $S'[x] = 0$ may have no real solutions $x(t) \in \mathbb{R}$.

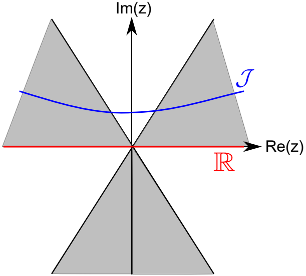
Idea: Complexify $x(t) \in \mathbb{C}$!

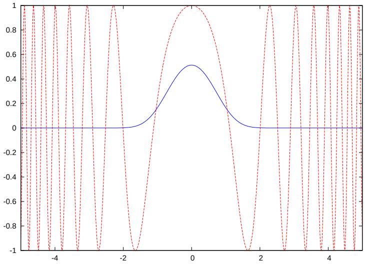
Lefschetz thimble for Airy integral

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 $\mathbb{R}$.

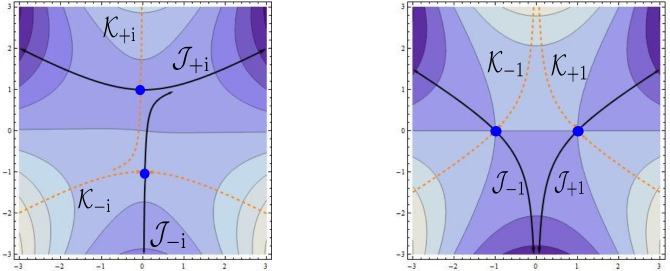


Figure: Lefschetz thimbles $\mathcal{J}$ and duals $\mathcal{K}$ $(a = 1\mathrm{e}^{0.1\mathrm{i}},\ -1)$

Gradient flow

Problem in the multi-dimension
$\mathrm{Im}(S) = \mathrm{const.}$ gives (2n-1)-dim. manifolds, instead of n-dim. ones.

Gradient flow Consider

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

This defines the steepest descent directions, since

$$\frac{\mathrm{d}}{\mathrm{d}t} S(z) = \sum_i \left| \left(\frac{\partial S(z)}{\partial z^i}\right) \right|^2 \geq 0.$$

The flow lines satisfies $\mathrm{Im}(S) = \mathrm{const.}$ [Witten, arXiv:1001.2933, 1009.6032]

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:

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

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

[Pham, '83, etc., Witten, arXiv:1001.2933, 1009.6032]

Monte Carlo simulation on one Lefschetz thimble

Most of the works before LATTICE 2015 are devoted to MC method with one-thimble ansatz.

$$Z = \int_{\mathbb{R}^n} \mathrm{d}^n x \, \mathrm{e}^{-S(x)} \Rightarrow Z' = \int_{\mathcal{J}_0} \mathrm{d}^n z \, \mathrm{e}^{-S(z)}.$$

[Christoforetti et al. (PRD(2012)), Fujii et al. (JHEP 1310), etc.]

Motivation

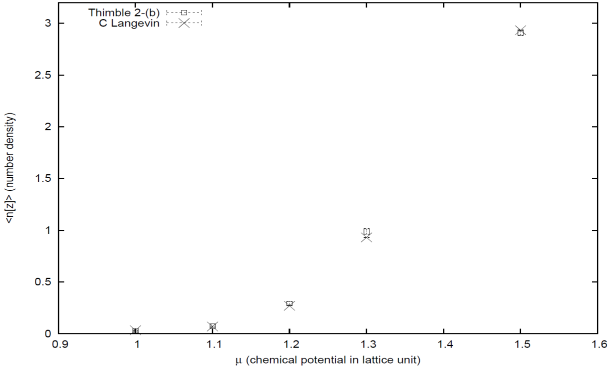
- Within the mean-field approx, this seems to be justified for bosonic theories.
- It was not known how to take the summation over thimbles.

It is successful for several models, and a lot of numerical techniques are developed.

Relativistic Bose gas:

$$S = \int \mathrm{d}^4 x \left[|\partial \phi|^2 + (m^2 - \mu^2)|\phi|^2 + \mu \phi^* \partial_0 \phi + \lambda |\phi|^4 \right]$$

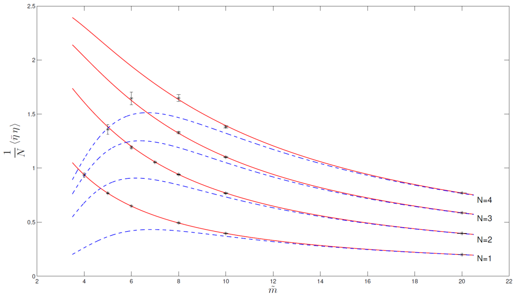
(Cristoforetti et al., PRD 88 (2013) 051501; Fujii et al., JHEP 1310 (2013) 147; Cristoforetti et al., PRD 89 (2014) 114505; Alexandru et al. 1606.02742)



Fujii et al. (JHEP 1310)

Chiral Random Matrix model

$$S = N\mathrm{tr}(X^\dagger X + Y^\dagger Y) - \ln\det\begin{pmatrix} m & \mathrm{i}\,\mathrm{ch}(\mu)X + \mathrm{sh}(\mu)Y \\ \mathrm{i}\,\mathrm{ch}(\mu)X^\dagger + \mathrm{sh}(\mu)Y^\dagger & m \end{pmatrix}^{N_f}$$



CRMT with 1-thimble ansatz with $N_f = 2$, $\mu/\sqrt{N} = 2$. (Di Renzo, Eruzzi, PRD(2015))

(cf. Naive CL gives the phase-quenched result. (Mollgaard, Splittorff, 1309.4335)

Some gauge cooling extends applicability of CL until $\mu/\sqrt{N} \lesssim 3$ (Nagata et al. 1604.07717))

(0+1)-dimensional fermion model

List

- Tanizaki, Hidaka, Hayata, 1509.07146
- Fujii, Kamata, Kikukawa, 1509.08176, 1509.09141
- Alexandru, Basar, Bedaque, 1510.03258
- Alexandru, Basar, Bedaque, Ridgway, Warrington, 1512.08764

Related studies

- 2-dim Hubbard on 1-thimble (Mukherjee, Cristoforetti, 1403.5680)
- 0-dim models (Tanizaki, 1412.1891, Kanazawa, Tanizaki, 1412.2802)
- Ch. RMT on 1-thimble (Eruzzi, Di Renzo, 1507.03858)

One-site Fermi Hubbard model

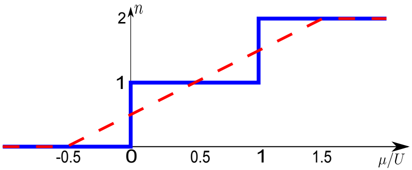
One-site Hubbard model:

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

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)

Path integral for one-site model

Effective Lagrangian of the one-site Hubbard model:

$$\mathcal{L} = \frac{\varphi^2}{2U} + \psi^* \left[\partial_\tau - (U/2 + \mathrm{i}\varphi + \mu)\right] \psi.$$

The path-integral expression is

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

Integrand has complex phases causing the sign problem.

φ is an auxiliary field for the number density:

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

Sign problem and Gradient flows at $\mu/U < -0.5$

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

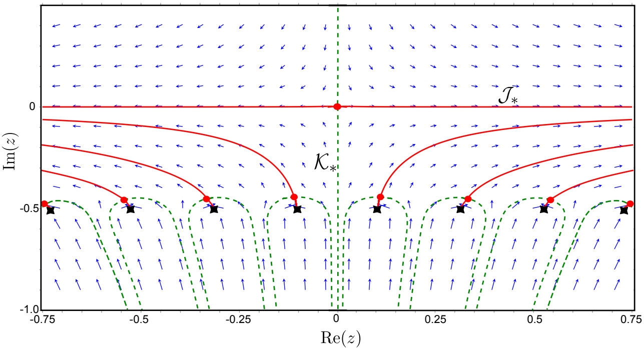


Figure: Flow at $\mu/U = -1$. $\mathcal{J}_* \simeq \mathbb{R}$.

(YT, Hidaka, Hayata, 1509.07146)

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

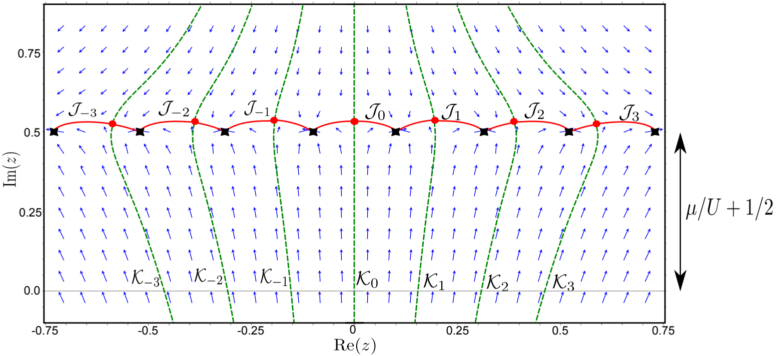


Figure: Flow at $\mu/U = 0$

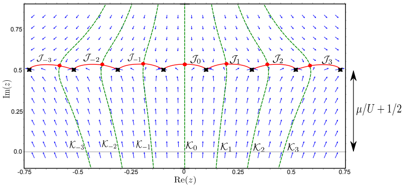
Complex saddle points lie on $n_{\mathrm{MF}} = \mathrm{Im}(z_m)/U \simeq \mu/U + 1/2$.

(YT, Hidaka, Hayata, 1509.07146)

Complex classical solutions

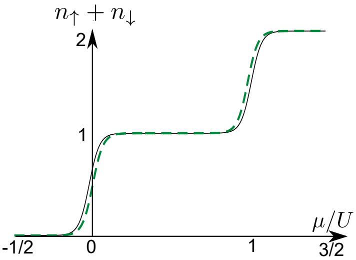
Classical solutions:

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



At these solutions, the classical actions become

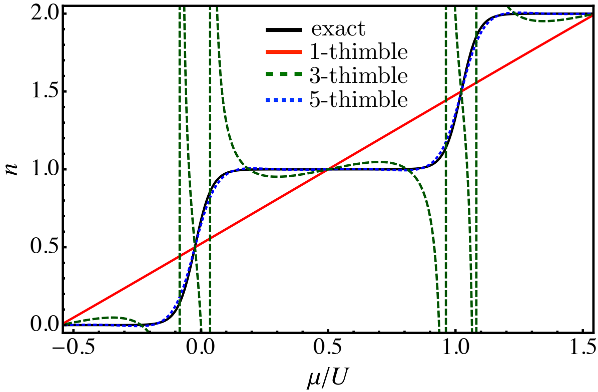
$$S_0 \simeq -\frac{\beta U}{2}\left(\frac{\mu}{U} + \frac{1}{2}\right)^2,$$
$$\mathrm{Re}\,(S_m - S_0) \simeq \frac{2\pi^2}{\beta U} m^2,$$
$$\mathrm{Im}\, S_m \simeq 2\pi m \left(\frac{\mu}{U} + \frac{1}{2}\right).$$



Classically, $Z_{\text{classical}} = \sum_m \mathrm{e}^{-S_m}$.

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,1509.07146)

Relation with complex Langevin method

List

- Aarts, 1308.4811, Aarts, Bongiovanni, Seiler, Sexty, 1407.2090
- Tsutsui, Doi, 1508.04231
- Fukushima, Tanizaki, 1507.07351
- Hayata, Hidaka, Tanizaki, 1511.02437
- Abe, Fukushima, 1607.05436

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

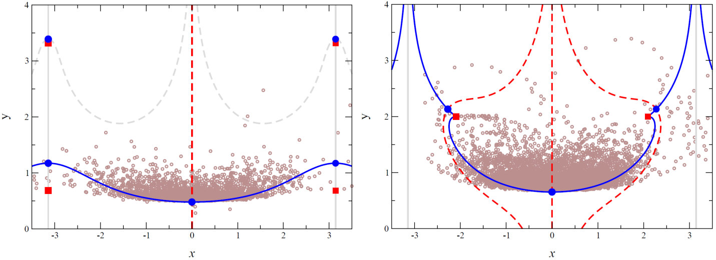
$$\frac{\mathrm{d}}{\mathrm{d}\theta}\langle O(z_\eta(\theta))\rangle_\eta = \hbar\langle O''(z_\eta(\theta))\rangle_\eta - \langle O'(z_\eta(\theta))S'(z_\eta(\theta))\rangle_\eta.$$

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

Relation between CL and LT?

Both methods relies on complexification, but not much is known for their relations.
CL and LT looks similar, but they are still different:
($U(1)$ link model , $S = -\beta\cos(z) - \ln[1 + \kappa\cos(z - \mathrm{i}\mu)]$)

$\beta = 1, \mu = 2$



$\kappa = 1/2$ $\kappa = 2$

(Aarts, Bongiovanni, Seiler, Sexty, 1407.2090)

Semiclassical incorrectness of CL method

If $\hbar$ is small enough, we can show a sufficient condition for incorrect behaviors of CL method.

(Hayata, Hidaka, YT, 1511.02437)

Assume that CL method is correct, then

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

Since $\hbar \ll 1$,

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

Semiclassical inconsistency

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

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

The right hand side can be complex, which contradicts with $c_\sigma \geq 0$!
(Hayata, Hidaka, YT, 1511.02437)

We show that the complex Langevin is wrong if

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

Open question Connection with the histogram test on CL method?

Refine Complex Langevin via thimbles (1)

Deform the theory so that only one thimble contributes, and apply CL (Tsutsui, Doi, 1508.04231)

$$Z=\int f(x)\mathrm{e}^{-S(x)}\mathrm{d}x \ \Rightarrow Z_{\mathrm{new}}=\int (f(x)+\mathrm{i}g(x))\mathrm{e}^{-S(x)}\mathrm{d}x.$$

One can compute VEV of the original theory using the new one as

$$\langle O\rangle_{\mathrm{original}}=\mathrm{Re}\langle O\rangle_{\mathrm{new}}-\frac{\langle g\rangle_{\mathrm{quench}}}{\langle f\rangle_{\mathrm{quench}}}\mathrm{Im}\langle O\rangle_{\mathrm{new}}.$$

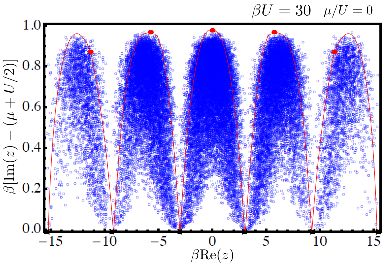
$\langle g\rangle_{\mathrm{quench}}/\langle f\rangle_{\mathrm{quench}}$ is common for any observables.
Compute $\langle O\rangle_{\mathrm{new}}$ using CL with "appropriate" g.

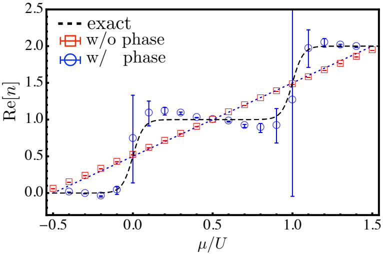
Open question What g should be chosen?

Refine Complex Langevin via thimbles (2)

Perform the reweighting by attaching complex phases of thimbles to CL distribution (Hayata, Hidaka, YT, 1511.02437)

Test on one-site fermion model





Clear improvement, but there's unknown systematic error.

Open question Can we justify and make it rigorous?

Simulation on multiple thimbles

List

- Alexandru, Basar, Bedaque, Ridgway, Warrington, 1512.08764
- Alexandru,Basar, Bedaque, Vartak, Warrington, 1605.08040

Related studies

- Alexandru, Basar, Bedaque, Ridgway, Warrington, 1604.00956
- Alexandru, Basar, Bedaque, Ridgway, Warrington, 1606.02742

Possible concerns for practical applications

Interference among Lefschetz thimbles is very important for our interest (especially when fermion exists).

This means that we must ...

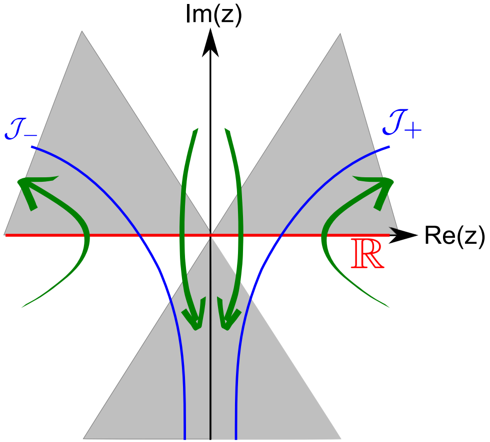
- Find all contributing complex saddle points,
- Construct Lefschetz thimbles around those saddle points,
- Evaluate integration on each Lefschetz thimbles, and
- Sum up those results.

We need some machinery to do them *automatically*.

Idea for multiple thimble simulation

Deform the original cycle $\mathbb{R}^n$ by the gradient flow, $\dfrac{\mathrm{d}z}{\mathrm{d}t} = \overline{\left(\dfrac{\partial S}{\partial z}\right)}$:

(Alexandru, Basar, Bedaque, Ridgway, Warrington, JHEP (2016))



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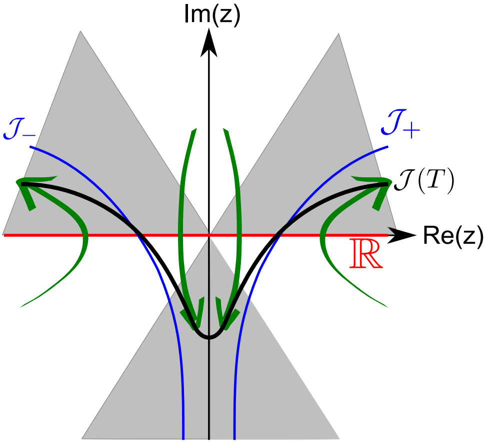


Formulation

Let us fix a flow time T, and define

$$\mathcal{J}(T) := \left\{ z(T;x) \in \mathbb{C}^n \,\middle|\, \frac{\mathrm{d}z(t;x)}{\mathrm{d}t} = \overline{\left(\frac{\partial S}{\partial z}\right)},\ z(0;x) = x \in \mathbb{R}^n \right\}.$$

By construction, $z(T;\cdot) : \mathbb{R}^n \xrightarrow{\sim} \mathcal{J}(T)$ and

$$\begin{aligned} \int_{\mathbb{R}^n} \mathrm{d}^n x\, \mathrm{e}^{-S(x)} &= \int_{\mathcal{J}(T)} \mathrm{d}^n z\, \mathrm{e}^{-S(z)} \\ &= \int_{\mathbb{R}^n} \mathrm{d}^n x \det\left(\frac{\partial z^i(T,x)}{\partial x^j}\right) \mathrm{e}^{-S(z(T;x))}. \end{aligned}$$

⇒One can do usual Monte Carlo + reweighting by regarding

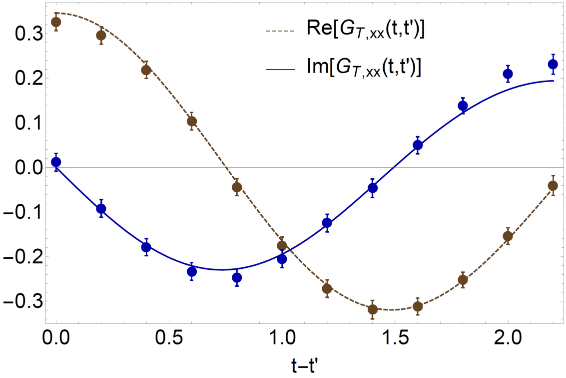
$$S_{\mathrm{eff},T}(x) := S(z(T;x)) - \ln\left[\det\left(\frac{\partial z^i(T,x)}{\partial x^j}\right)\right]$$

as the effective classical action.

Real-time dynamics

This method is applied to Schwinger-Keldysh path integral for

$$S = \int \mathrm{d}t \left(\frac{1}{2}\dot{x}^2 - \frac{1}{2}x^2 - x^4 \right).$$



Feynman propagators at $\beta = 0.8$. $T_{\text{flow}} = 0.2$. (Alexandru,Basar, Bedaque, Vartak, Warrington, arXiv:1605.08040)

Summary and Conclusion

- Lefschetz-thimble method is helpful to analyze structures of sign problems.
- Many Lefschetz thimbles can contribute. Especially, interference among them will play an important role for physical observables.
- Dynamics in complexified space is complicated.
  Comparison among one-thimble ansatz, complex Langevin, and saddle point analysis gives us a good insight.
- Recent developments may enable us to study nonperturbative field theories with the sign problem.