Studying the Silver Blaze Problem based on Picard-Lefschetz Theory

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Motivation: Sign problem, Silver Blaze problem

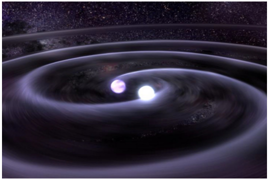
Finite-density quantum chromodynamics (QCD)

QCD

Fundamental theory for quarks and gluons

Neutron star

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



Neutron star merger

(image from NASA)

Reliable theoretical approach to equation of state must be developed!

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

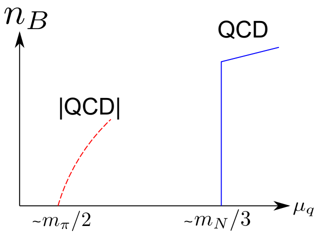
Sign problem: $\mathrm{Det}(\not{D}(A,\mu_q)+m)\not\geq 0$ at $\mu_q\neq 0$.

Sign problem 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 at $T = 0$
(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: Explain why $n_B = 0$ for $\mu_q < m_N/3$ using path integral.
(Cohen, PRL **91** (2003) 222001)

Current situation: For $\mu_q < m_\pi/2$, the problem is solved.
For $\mu_q > m_\pi/2$, however, no one knows how to understand this.

Method: Path integral on Lefschetz thimbles

Sign problem of path integrals

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 $x(t) \in \mathbb{R}$.

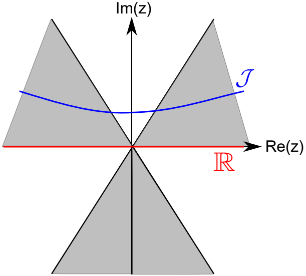
Idea: Complexify $x(t) \in \mathbb{C}$!

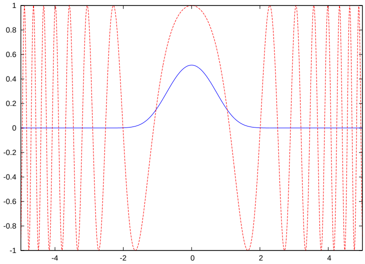
Lefschetz thimble for Airy integral

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 $\mathbb{R}$.

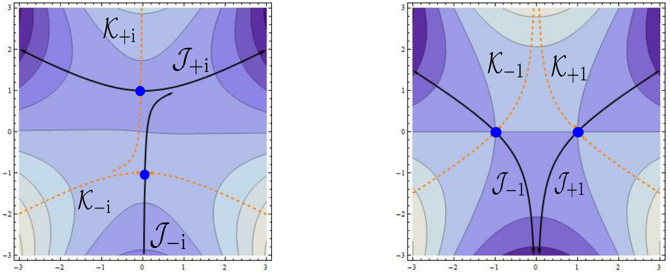


Figure: Lefschetz thimbles $\mathcal{J}$ and duals $\mathcal{K}$ $(a = 1\mathrm{e}^{0.1\mathrm{i}}, -1)$

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, 1967; Kaminski, 1994; Witten, arXiv:1001.2933, 1009.6032]

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

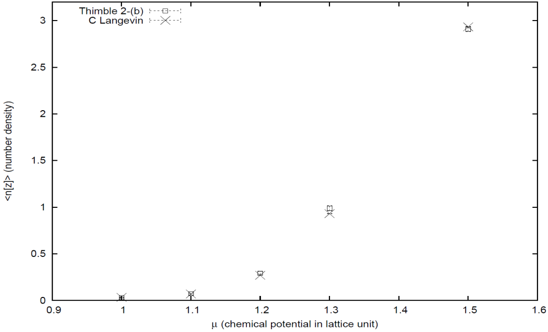
Previous studies: MC with one-thimble ansatz

In previous studies, one has been used one-thimble ansatz:

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

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

Relativistic Bose gas:



Fujii et al. (JHEP 1310)

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

One-site Fermi Hubbard model

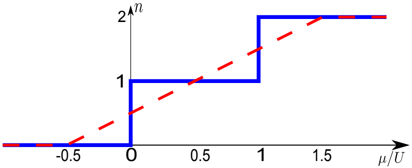
One-site Hubbard model:

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

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

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 fermion determinant

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:

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

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

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

Minimal value of $\varepsilon(A) = m_\pi/2$.

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 $\mu < m_\pi/2$,

$$\frac{\mathrm{Det}\left[\gamma_4(\not{D}_A + m) - \mu\right]}{\mathrm{Det}\left[\gamma_4(\not{D}_A + m)\right]} = \prod_{\mathrm{Re}\lambda_j > 0} \frac{\left(1 + \mathrm{e}^{-\beta(\lambda_j - \mu)}\right)\left(1 + \mathrm{e}^{-\beta(\lambda_j + \mu)}\right)}{\left(1 + \mathrm{e}^{-\beta\lambda_j}\right)\left(1 + \mathrm{e}^{-\beta\lambda_j}\right)} \to 1.$$

(Cohen PRL **91** (2003), Adams, PRD **70** (2004), Nagata et. al. PTEP **2012**)

The sign problem disappears by the reweighting method.

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

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

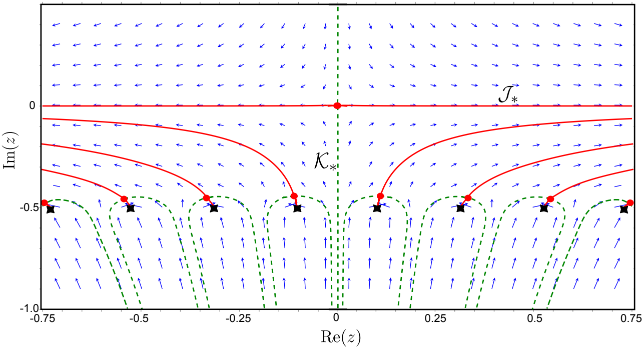


Figure: Flow at $\mu/U = -1$. $\mathcal{J}_* \simeq \mathbb{R}$.

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

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

(YT, Hidaka, Hayata, 1509.07146)

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 $n = 0$.

Finite density QCD: The situation is almost the same, since

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

but $n_B = 0$ for $\mu_q \lesssim m_N/3$.

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

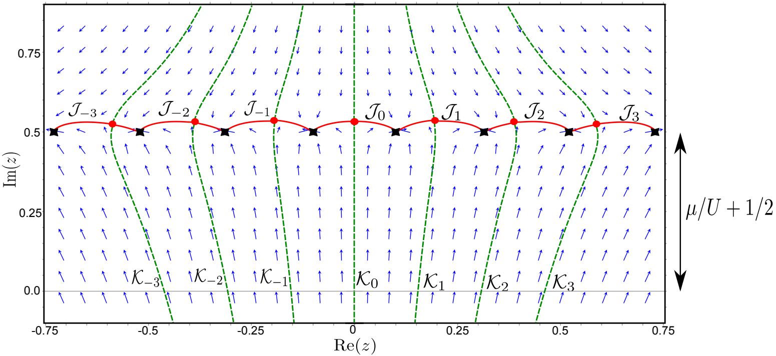


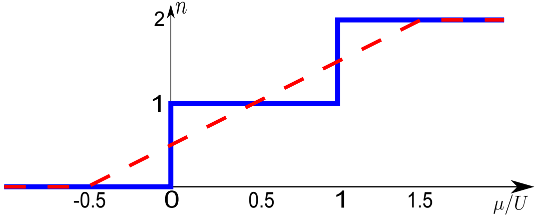
Figure: Flow at $\mu/U = 0$

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.

Curious incident of n in one-site Hubbard model

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

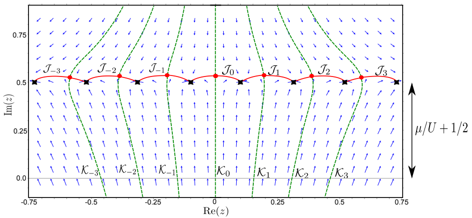


This is similar to what happens for QCD and |QCD|.
$\mu/U = -0.5 \Leftrightarrow \mu_q = m_\pi/2$.

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

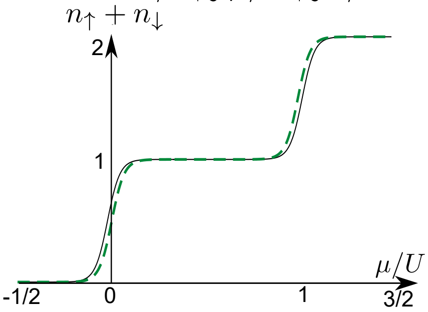
$$S_0 \simeq -\frac{\beta U}{2}\left(\frac{\mu}{U} + \frac{1}{2}\right)^2,$$
$$\mathrm{Re}\left(S_m - S_0\right) \simeq \frac{2\pi^2}{\beta U} m^2,$$
$$\mathrm{Im}\, S_m \simeq 2\pi m \left(\frac{\mu}{U} + \frac{1}{2}\right).$$

Semiclassical partition function

Using complex classical solutions z_m, let us calculate

$$Z_{\mathrm{cl}} := \sum_{m=-\infty}^{\infty} \mathrm{e}^{-S_m} = \mathrm{e}^{-S_0(\mu)} \theta_3 \left(\pi \left(\frac{\mu}{U} + \frac{1}{2} \right), \mathrm{e}^{-2\pi^2/\beta U} \right).$$

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



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

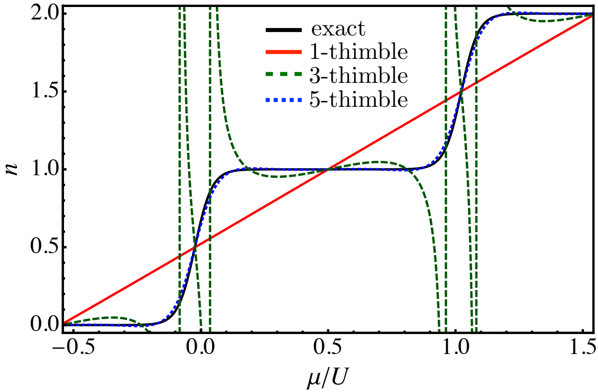
In order to describe the step functions, we need interference of complex phases among different Lefschetz thimbles.

(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])

Review: Practical algorithm for simulating multiple Lefschetz thimbles

Possible concerns for practical applications

In this study, we *emphasized* the importance of interference among Lefschetz thimbles.

Then, the following becomes important:

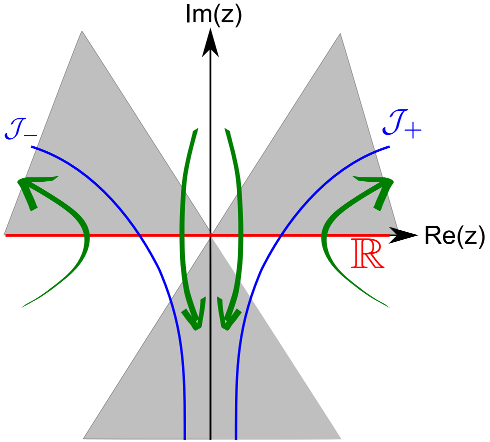
- Find all contributing complex saddle points,
- Construct Lefschetz thimbles around those saddle points,
- Evaluate integration on each Lefschetz thimbles, and
- Sum up those results.

We need some machinery to do them *automatically*.

Neat idea for multiple thimble simulation

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

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



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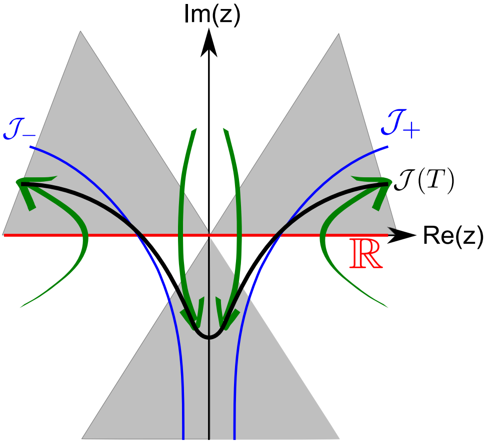

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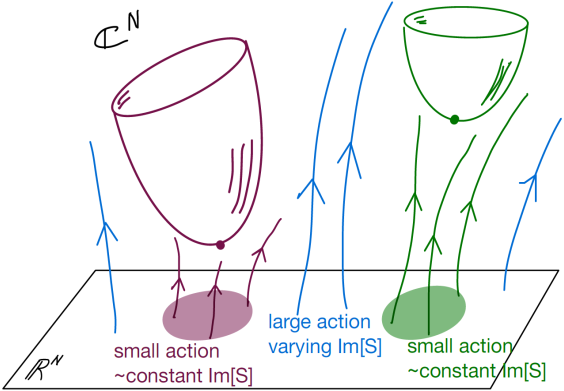


Thanks to Gokce for nice figure!

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

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

$\Rightarrow$One can do usual Monte Carlo + reweighting by regarding

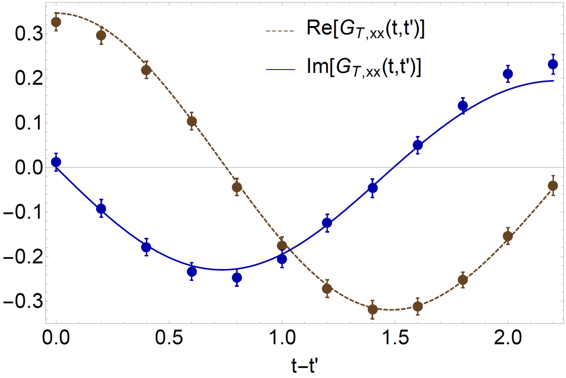
$$S_{\mathrm{eff},T}(x) := S(z(T;x)) - \ln\left[\det\left(\frac{\partial z^i(T,x)}{\partial x^j}\right)\right]$$

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

Summary and conclusion

Summary and Conclusion

- Lefschetz-thimble method 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.
- Interference of complex phases among Lefschetz thimbles plays a pivotal role for the (baryon) Silver Blaze problem.
- Recent developments may enable us to study nonperturbative field theories with the sign problem.