Application of Lefschetz thimbles to fermionic sign problem

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Motivation: Monte Carlo simulation and Sign problem

Exponential complexity to solve QFTs

Quantum systems: the Hilbert space $\mathcal{H}$ and the Hamiltonian $\hat{H}$.

Accept the lattice model of QFTs, then

$$\dim\mathcal{H} = \#^{\mathrm{Volume}}.$$

$\Rightarrow$ Solving QFT completely ($=$ diagonalization of $\hat{H}$) is exponentially hard.

Notice: We do not always need to know about all the states precisely. We are usually interested in
Vacuum and several excitations, Thermal states, etc.

Path integral and Monte Carlo simulation

To characterize the thermal state, we can use path integral,

$$Z = \mathrm{tr}_{\mathcal{H}}\left[\mathrm{e}^{-\beta\hat{H}}\right] = \int_M \mathcal{D}A \exp(-S[A]).$$

The integration domain M (of an $SU(N)$ gauge theory) is

$$M = SU(N)^{\beta\cdot\mathrm{Volume}}.$$

We want a tool to evaluate Z without exponential complexity.

Monte Carlo method: Consider the case $\mathrm{e}^{-S[A]} \geq 0$.
Generate an ensemble $\{A_i\}_i$ following $\frac{1}{Z}\mathrm{e}^{-S[A]}$, and evaluate

$$\langle O(A)\rangle \simeq \frac{1}{N}\sum_{i=1}^{N} O(A_i).$$

More about Monte Carlo simulation

Do we really circumvent exponential complexity using MC method?

$$\text{Error of } \frac{1}{N}\sum_{i=1}^{N} O(A_i) = \frac{\text{Typical values of } |O(A_i)|}{\sqrt{N}}.$$

It indeed solves the exponential complexity for operators satisfying

$$\frac{\langle O(A)\rangle}{\text{Typical values of } |O(A_i)|} \sim (\beta \cdot \mathrm{Volume})^{-\#}.$$

It has been quite successful to understand Hadron structures, thermodynamics of finite-temperature QCD, etc.

Sign problem

What happens if $S[A]$ takes complex values so that $\mathrm{e}^{-S[A]} \not\geq 0$?

Reweighting: To use Monte Carlo method, we generate the ensemble $\{A_i\}_i$ following the phase-quenched distribution $\mathrm{e}^{-\mathrm{Re}(S[A])}$:

$$\langle O(A)\rangle = \frac{\langle O(A)\mathrm{e}^{-\mathrm{i}\,\mathrm{Im}(S[A])}\rangle_{\mathrm{p.q.}}}{\langle \mathrm{e}^{-\mathrm{i}\,\mathrm{Im}(S[A])}\rangle_{\mathrm{p.q.}}} \simeq \frac{\frac{1}{N}\sum_{i=1}^{N} O(A_i)\mathrm{e}^{-\mathrm{i}\,\mathrm{Im}(S[A])}}{\frac{1}{N}\sum_{i=1}^{N} \mathrm{e}^{-\mathrm{i}\,\mathrm{Im}(S[A])}}.$$

Since $S[A] \propto \beta \cdot \mathrm{Volume}$, $\langle \mathrm{e}^{-\mathrm{i}\,\mathrm{Im}(S[A])}\rangle_{\mathrm{p.q.}} = \mathrm{e}^{-\beta\cdot\mathrm{Volume}\,\Delta f}$. Thus,

$$\text{Necessary } N \text{ of configurations} \gtrsim \mathrm{e}^{2\beta\cdot\mathrm{Volume}\,\Delta f}.$$

Exponential complexity revives due to the sign problem.

Example of sign problem: Finite-density QCD

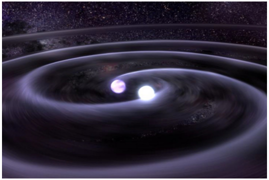
Partition function of QCD is

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

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

Neutron star

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



Binary NS merger (NASA)

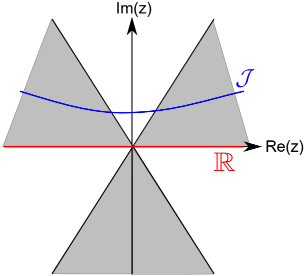
Method: Path integral on Lefschetz thimbles

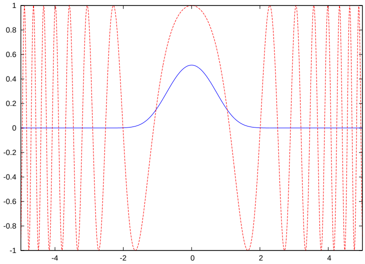
Lefschetz thimble for Airy integral

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 $\mathbb{R}$.

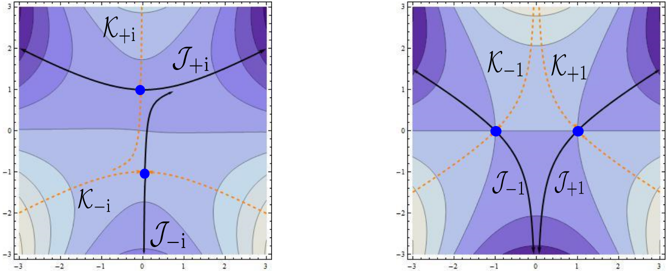


Figure: Lefschetz thimbles $\mathcal{J}$ and duals $\mathcal{K}$ ($a = 1\mathrm{e}^{0.1\mathrm{i}}$, -1)

Multiple integrals on Lefschetz thimbles

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

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

Unlike one-dimensional case, the steepest descent manifold is not uniquely defined.
$\Rightarrow$ Use of the homology $H_n(M_\mathbb{C}, \{\mathrm{e}^{-\mathrm{Re}(S)} \ll 1\})$ becomes quite essential:

$$\begin{aligned} H_n(M_\mathbb{C}, \{\mathrm{e}^{-\mathrm{Re}(S)} \ll 1\}) &\simeq \sum_\sigma \mathbb{Z}\,[\mathcal{J}_\sigma], \\ H_n(M_\mathbb{C} \setminus \{\mathrm{e}^{-\mathrm{Re}(S)} \ll 1\}) &\simeq \sum_\sigma \mathbb{Z}\,[\mathcal{K}_\sigma]. \end{aligned}$$

[Pham, 1967; Kaminski, 1994; Howls, 1997]

Multiple integrals on Lefschetz thimbles

Concrete construction Pick up the Kähler metric $\mathrm{d}s^2 = g_{i\bar{j}}\mathrm{d}z^i \otimes \mathrm{d}\overline{z^j}$, and consider the gradient flow:

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

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

$$\mathcal{J}_\sigma = \left\{ z(0) \middle| \lim_{t\to-\infty} z(t) = z_\sigma \right\}.$$

Similarly, $\mathcal{K}_\sigma = \{z(0)|z(\infty) = z_\sigma\}$.

[Pham, 1967; Kaminski, 1994; Howls, 1997, Witten, arXiv:1001.2933, 1009.6032]

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

Monte Carlo algorithm on Lefschetz thimbles

Monte Carlo algorithms on $\mathcal{J}_\sigma$ has been developing since 2012.

- Langevin on $\mathcal{J}_\sigma$ Cristoforetti, Di Renzo, Scorzato, 1205.3996
- Hybrid MC on $\mathcal{J}_\sigma$ Fujii, Honda, Kato, Kikukawa, Komatsu, Sano, 1309.4371
- Contraction algorithm Alexandru, Basar, Bedaque, 1510.03258

These methods generate ensembles $\{z_i\}_i$ on $\mathcal{J}_\sigma$ following $\mathrm{e}^{-S(z)}$:

$$\frac{1}{Z}\int_{\mathcal{J}_\sigma} \mathrm{d}^n z O(z) \exp(-\hbar^{-1} S(z)) \simeq \frac{\frac{1}{N}\sum_{i=1}^N \frac{\mathrm{d}^n z_i}{|\mathrm{d}^n z_i|} O(z_i)}{\frac{1}{N}\sum_{i=1}^N \frac{\mathrm{d}^n z_i}{|\mathrm{d}^n z_i|}}.$$

Comment: $\int_{\mathcal{J}_\sigma}$ satisfies resurgence (Berry, Howls, '91, Howls '97).
This numerical technique will allow to access analytic properties in the Borel plane for QFTs.

Lefschetz thimbles with fermionic determinant

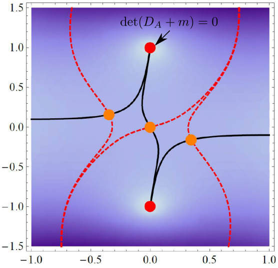
We would like to apply Lefschetz thimbles to treat the sign problem of

$$Z = \int_M \mathcal{D}A\, \mathrm{e}^{-S_{\mathrm{YM}[A]} + \ln \mathrm{Det}(\not{D}(A,\mu_q)+m)}.$$

Because of fermionic determinant, $\mathcal{J}_\sigma$ have their boundaries at

$$\mathrm{Det}(\not{D}(A,\mu_q)+m) = 0, \quad \text{or} \quad \mathrm{Re}(S_{\mathrm{YM}}[A]) = +\infty.$$

The formula, $[M] = \sum_\sigma \langle M, \mathcal{K}_\sigma \rangle [\mathcal{J}_\sigma]$, still holds (1412.1891, 1412.2802 with Kanazawa).



Applications: Case studies of fermionic sign problem

- One-site Hubbard model (1509.07146, with Tomoya Hayata, Yoshimasa Hidaka)
- Multi-flavor massless QED_2 (to appear, with Motoi Tachibana)

Path integral for one-site Hubbard model

We consider the $(0+1)$-dimensional fermion model,

$$S=\int_0^\beta \mathrm{d}\tau\left(\frac{\phi(\tau)^2}{2U}+\psi^*[\partial_\tau+(-U/2-\mu-\mathrm{i}\phi(\tau))]\psi\right).$$

The path-integral expression for the one-site Hubbard model $(\varphi=\frac{1}{\beta}\int_0^\beta \mathrm{d}\tau\phi(\tau))$:

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

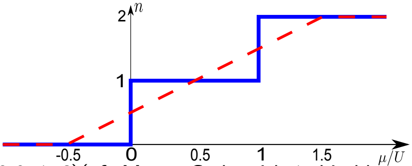
Integrand has complex phases causing the sign problem.

φ is an auxiliary field for the fermion number density:

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

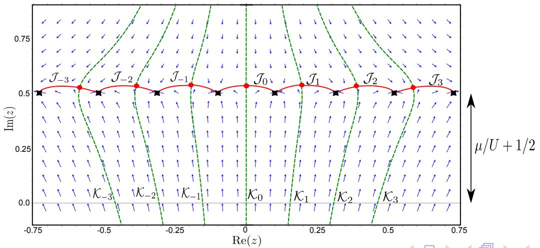
Behaviors of number density and Lefschetz thimbles

Number density n with exact result and one-thimble result:



(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.)

Lefschetz thimbles with $-0.5U < \mu < 1.5\mu$:

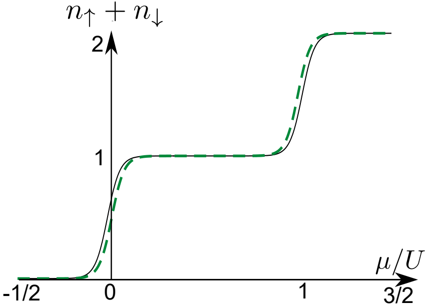


Semiclassical partition function

Using complex classical solutions z_m, let us calculate

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

This expression is a good approximation for $-1/2 \lesssim \mu/U \lesssim 3/2$.



Sign problem after Lefschetz-thimble deformation

This computation means that the sign problem exists after the Lefschetz-thimble deformation.
Compute the reweighting factor:

$$\frac{\int_{\sum_m \mathcal{J}_m} \mathrm{d}z \mathrm{e}^{-S(z)}}{\int_{\sum_m \mathcal{J}_m} |\mathrm{d}z| \mathrm{e}^{-\mathrm{Re}(S(z))}} \simeq \frac{\sum_m \mathrm{e}^{-S_m}}{\sum_m \mathrm{e}^{-\mathrm{Re}(S_m)}} = \frac{\theta_3\left(\pi\left(\frac{\mu}{U}+\frac{1}{2}\right), \mathrm{e}^{-2\pi^2/\beta U}\right)}{\theta_3\left(0, \mathrm{e}^{-2\pi^2/\beta U}\right)}.$$

At $\mu = 0$, for example,

$$\frac{\int_{\sum_m \mathcal{J}_m} \mathrm{d}z \mathrm{e}^{-S(z)}}{\int_{\sum_m \mathcal{J}_m} |\mathrm{d}z| \mathrm{e}^{-\mathrm{Re}(S(z))}} \simeq \exp\left(-\beta \frac{U}{8}\right).$$

Lefschetz-thimble method reduces $\Delta f = 2U$ to $\Delta f = U/8$ in the one-site Hubbard model.

Multi-flavor massless QED$_2$

2-dimensional $U(1)$ gauge theories with N_f massless fermions:

$$Z = \int \mathcal{D}A\, \mathrm{e}^{-S_{\mathrm{ph}}[A]} \int \mathcal{D}\overline{\psi}\mathcal{D}\psi \exp\left(-\sum_{a=1}^{N_f}\int \mathrm{d}^2x\, \overline{\psi}_a \left[D_A - \mu_a\gamma^0\right]\psi_a\right)$$

Since the fermions are massless, the nonzero topological sectors do not appear:

$$A = \underbrace{\frac{2\pi}{\beta}h_0 \mathrm{d}x^0 + \frac{2\pi}{L}h_1 \mathrm{d}x^1}_{\text{toron}} + \underbrace{*\mathrm{d}\phi}_{\text{photon}} + \underbrace{\mathrm{d}\lambda}_{\text{gauge}} .$$

ϕ-dependence is computable using the anomaly equation, and does not have the sign problem.

Toron-field integral of multi-flavor massless QED$_2$

The toron-field integration becomes ($\tau = L/\beta$: temperature)

$$Z = \int_0^1 \mathrm{d}h_0 \mathrm{d}h_1 \exp\left[-\frac{2\pi}{\tau} F(h_0, h_1)\right],$$

where F is the fermion one-loop free energy ($\mu'_a = L\mu_a/(2\pi)$),

$$F = N_f \left(h_1 - \frac{1}{2}\right)^2 - \frac{\tau}{2\pi} \sum_{a=1}^{N_f} \sum_{n=1}^{\infty} \Big\{ \ln\left(1 + \mathrm{e}^{-\frac{2\pi}{\tau}(n + h_1 - 1 - \mu'_a) - 2\pi \mathrm{i} h_0}\right)$$
$$+ \ln\left(1 + \mathrm{e}^{-\frac{2\pi}{\tau}(n - h_1 + \mu'_a) + 2\pi \mathrm{i} h_0}\right) + \ln\left(1 + \mathrm{e}^{-\frac{2\pi}{\tau}(n + h_1 - 1 + \mu'_a) + 2\pi \mathrm{i} h_0}\right)$$
$$+ \ln\left(1 + \mathrm{e}^{-\frac{2\pi}{\tau}(n - h_1 - \mu'_a) - 2\pi \mathrm{i} h_0}\right) \Big\}.$$

In the limit $\tau \to 0$, we can use the mean-field approximation with complex saddle points (to appear, with Motoi Tachibana) (cf.1504.02979, with Hiromichi Nishimura, Kouji Kashiwa).

Gradient flow for massless QED$_2$

All the relevant complex saddle points have real F:

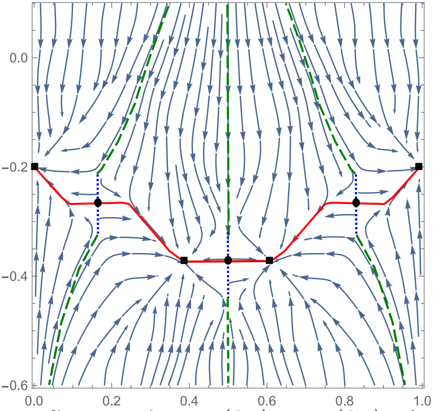
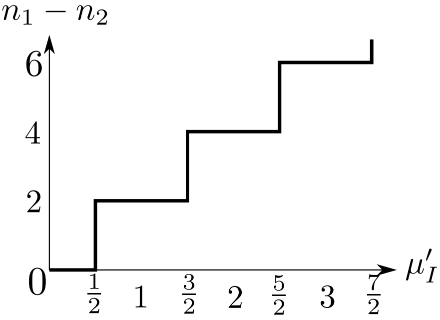


Figure: Gradient flow in the $\mathrm{Re}(h_1)$-$\tau\mathrm{Im}(h_0)$ plane at $N_f = 3$

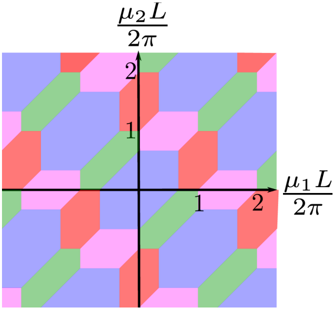
(to appear, with Motoi Tachibana)

Phase structure of multi-flavor massless QED$_2$

At the zero-temperature with finite L, $\tau = 0$, the first-order transition occurs in this model:



(a) Fermion number at $N_f = 2$



(b) Phase boundary at $N_f = 3$

Since the mean-field approx. is good, one can show that

$$\frac{\int_{\sum_m \mathcal{J}_m} \mathrm{d}^2 h\, \mathrm{e}^{-S(h)}}{\int_{\sum_m \mathcal{J}_m} |\mathrm{d}^2 h| \mathrm{e}^{-\mathrm{Re}(S(h))}} \simeq 1.$$

Summary

- The sign problem is reviewed from the viewpoint of exponential complexity.
- Using Cauchy's theorem, one can deform the oscillatory integral into the sum of steepest descent integrals on Lefschetz thimbles
- Monte Carlo method on Lefschetz thimble is developing.
  This has a potential to study not only the sign problem but also resurgence relation of QFTs numerically.
- We consider two examples of the fermionic sign problem.
  In the one-site model, the exponential complexity is not solved, but Δf is reduced.
  In massless QED_2, the exponential complexity is circumvented by using Lefschetz thimbles.