Quantum tunneling in the real-time path integral by the Lefschetz thimble method

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Workshop on Noncommutative and generalized geometry in string theory, gauge theory and related physical models

in Corfu Summer Institute

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Ref.)   JN, Katsuta Sakai, Atis Yosprakob, in preparation

Quantum tunneling

- Described by instantons in the imaginary-time path integral
  - decay rate of a false vacuum in QFT Coleman ('77)
  - bubble nucleation in 1st order phase transitions,
  - domain wall fusions etc.

$$Z = \int \mathcal{D}x(t)\, e^{i\int dt L}$$

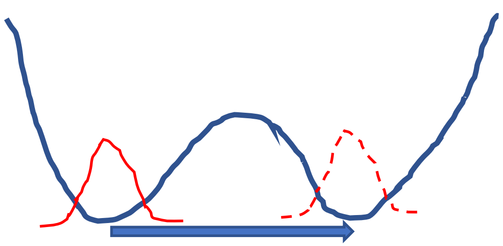
$$L = \left(\frac{dx}{dt}\right)^2 - (x^2-1)^2$$

$$t = -i\tau$$

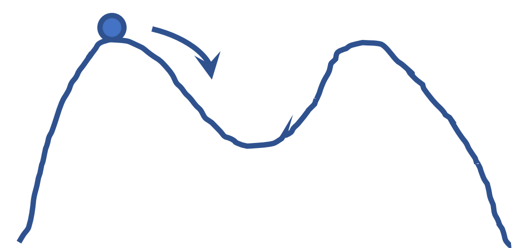
imaginary time

$$Z = \int \mathcal{D}x(\tau)\, e^{-\int d\tau \tilde{L}}$$

$$\tilde{L} = \left(\frac{dx}{d\tau}\right)^2 + (x^2-1)^2$$



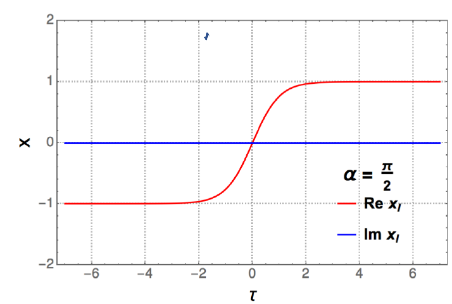
quantum tunneling



Classical solution :

$$x(\tau) = \tanh\tau$$

instanton



Tunneling amplitude can be calculated within the semi-classical approximation.

$\sim \exp(-S_0/\hbar)$ nonperturbative phenomenon

How can we describe quantum tunneling directly in the real-time path integral ?

- Motivations :
  - In reality, there are also contributions from classical motion over the barrier (c.f., sphalerons in QFT)
  - To obtain the wave function after tunneling and its subsequent time-evolution.

- However, a naïve analytic continuation of instantons leads to singular complex trajectories.

Cherman-Ünsal ('14)

We clarify this issue completely by explicit Monte Carlo calculations.

Sign problem in Monte Carlo methods

The basic idea of Monte Carlo calculations

$$Z = \int \prod_{i=1}^{N} dx_i \, w(x_1, \cdots, x_N)$$

$$\langle O \rangle = \frac{1}{Z} \int \prod_{i=1}^{N} dx_i \, O(x_1, \cdots, x_N) \, w(x_1, \cdots, x_N)$$

$w(x_1, \cdots, x_N) \geq 0$

- Generate configurations $(x_1, \cdots, x_N)$ with the probability distribution $\frac{1}{Z} w(x_1, \cdots, x_N)$
- Calculate $\langle O \rangle$ as expectation values of $O(x_1, \cdots, x_N)$

Real-time evolution of the wave function :

$$\Psi(x_{\mathsf{f}}, t_{\mathsf{f}}) = \int \mathcal{D}x(t) \, \Psi(x(t_{\mathsf{i}}), t_{\mathsf{i}}) \, e^{iS[x(t)]}$$

complex weight !

cannot be identified as the probability distribution

sign problem !

We use the Lefschetz thimble method to overcome this problem.

Plan of the talk

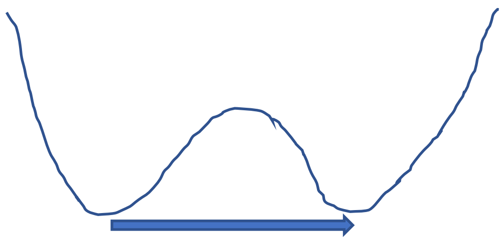
1. Brief review of previous works
2. Lefschetz thimble method
3. Backpropagating HMC algorithm
4. Optimizing the flow equation
5. Quantum tunneling in the real-time path integral
6. Summary and discussions

1.Brief review of previous works

Analytically continuation of instantons

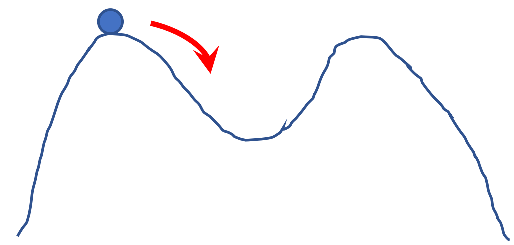
Cherman-Ünsal ('14)

$$L = \left(\frac{dx}{dt}\right)^2 - (x^2-1)^2$$



quantum tunneling

$$L = \left(\frac{dx}{d\tau}\right)^2 + (x^2-1)^2$$



Wick rotation : $t \mapsto \tau e^{-i\alpha}$

$x(t) \mapsto x(\tau)$

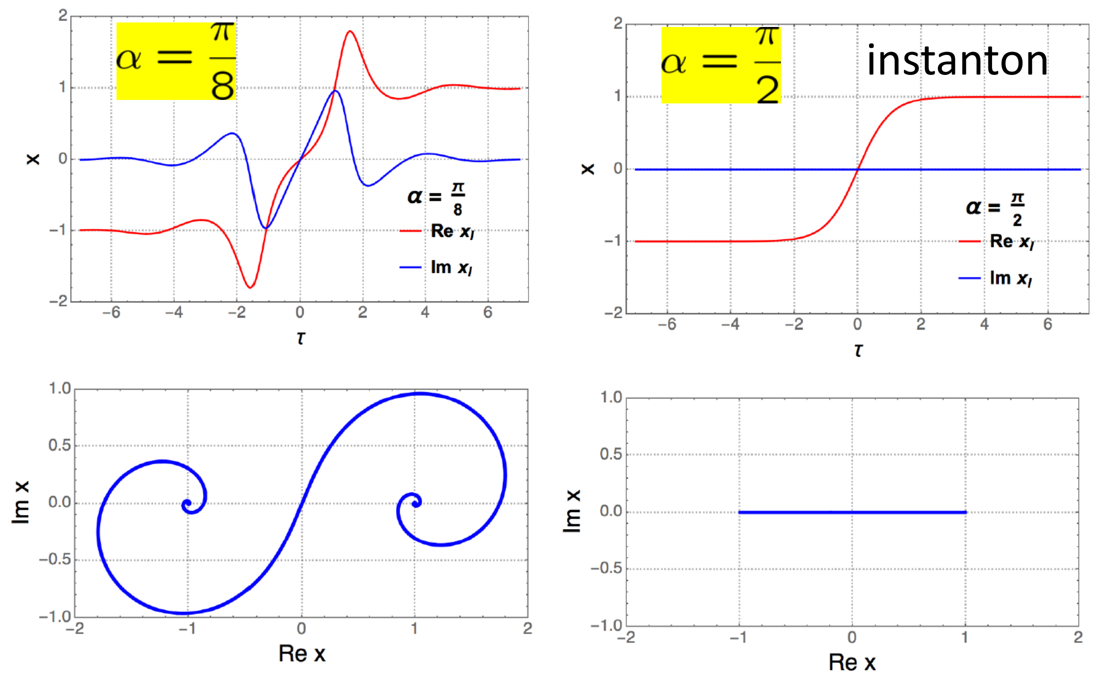
$$L = e^{2i\alpha}\left(\frac{dx}{d\tau}\right)^2 - (x^2-1)^2$$

$\alpha = \frac{\pi}{2} \Leftrightarrow$ imag. time

$x(\tau) = \tanh\tau$

classical solution for general α

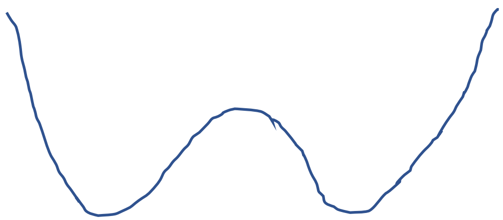
$$x(\tau) = \tanh\left(\tau e^{-i(\alpha - \frac{\pi}{2})}\right)$$



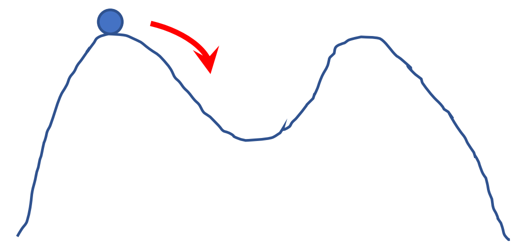
Analytically continuation of instantons

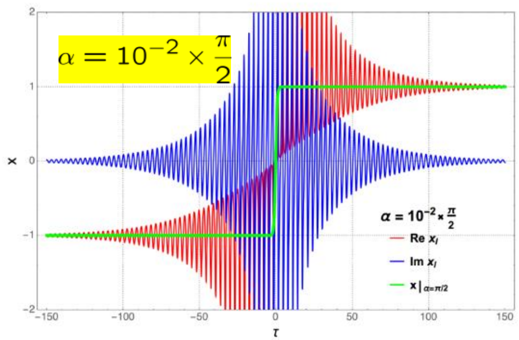
Cherman-Ünsal ('14)

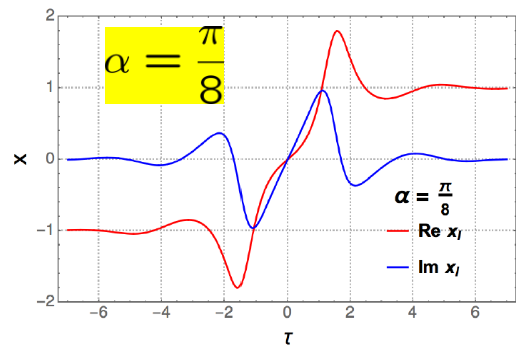
$$L = \left(\frac{dx}{dt}\right)^2 - (x^2-1)^2$$

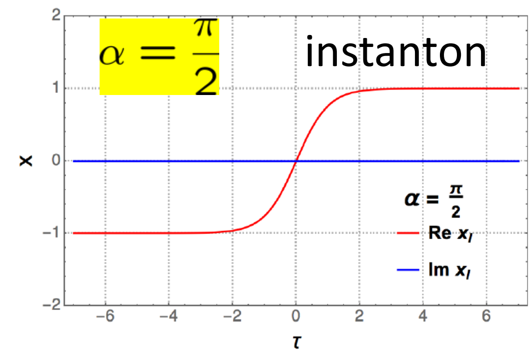


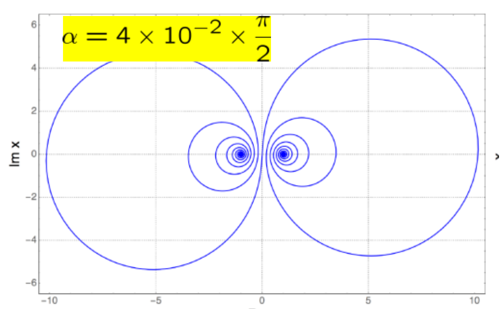
$$L = \left(\frac{dx}{d\tau}\right)^2 + (x^2-1)^2$$

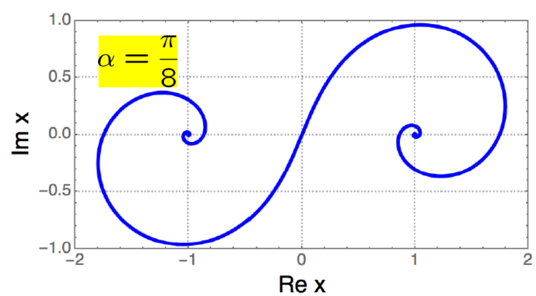


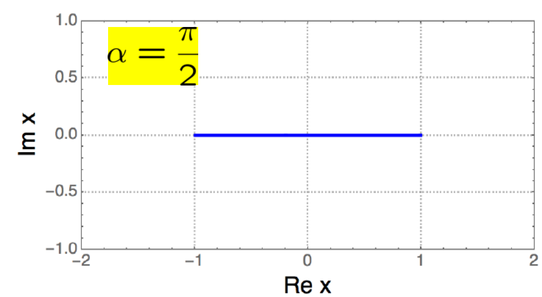












singular for $\alpha \to 0$

What kind of path is responsible for quantum tunneling ?

Exact classical solutions in the double-well potiential

Koike-Tanizaki ('14)

conservation of energy : $\left(\frac{dz}{dt}\right)^2 + (z^2-1)^2 = p^2$

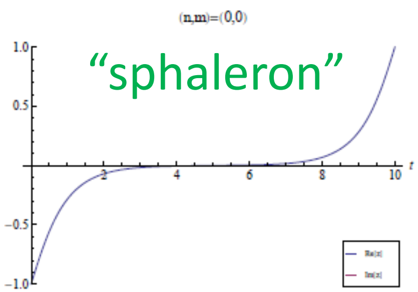
$$z(t) = \sqrt{\frac{p^2-1}{2p}}\, \mathrm{sd}\left(\sqrt{2p}\,t + c\,, \sqrt{\frac{1+p}{2p}}\right)$$

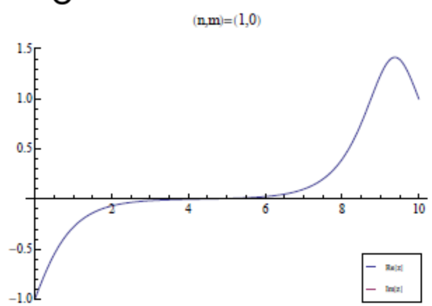
Jacobi elliptic function

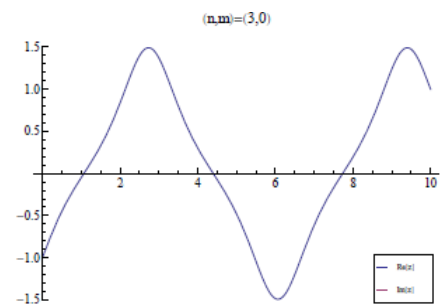
integration constants : $c\ ,p$ ⬅ boundary conditions $\begin{cases} z\left(-\frac{T}{2}\right) = -1 \\ z\left(\frac{T}{2}\right) = 1 \end{cases}$

There are infinitely many solutions labeled by integers (n,m).

real solutions : $n=0$ or $m=0$

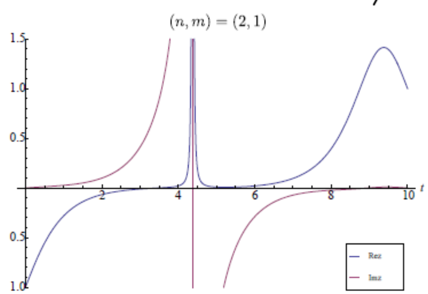






$T=10$

complex solutions : $n \neq 0$ and $m \neq 0$



The solutions become highly oscillating as the integers *n, m* become large.

$\mathrm{Re}(S) = S_0$ for $T \to \infty$

$\Leftrightarrow \exp(-S_0/\hbar)$ suppression ➡ responsible for quantum tunneling ?

2.Lefschetz thimble method

We consider a general model defined by a multi-variable integral

$$Z = \int_{\mathbb{R}^N} dx \, e^{-S(x)}$$

$$x = (x_1, \cdots, x_N) \in \mathbb{R}^N$$

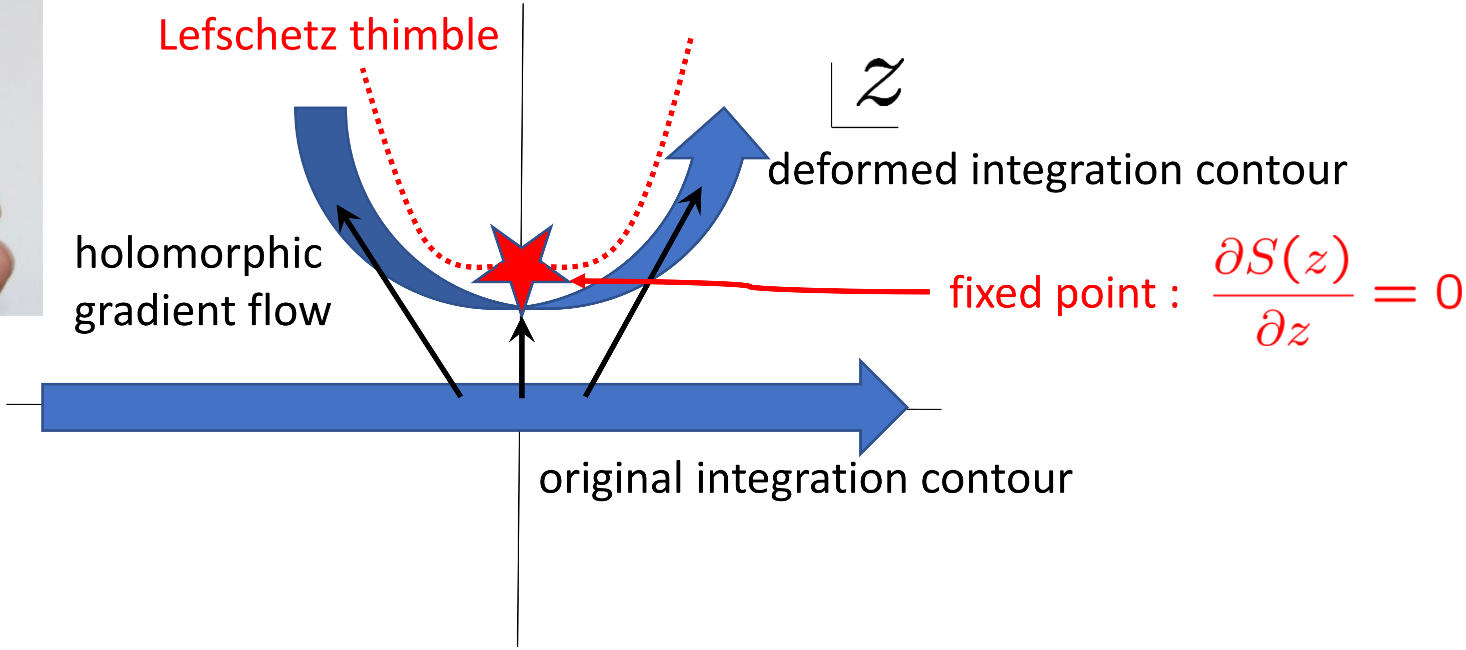
$$S(x) \in \mathbb{C}$$

$$\langle \mathcal{O}(x) \rangle = \frac{1}{Z} \int_{\mathbb{R}^N} dx \, \mathcal{O}(x) \, e^{-S(x)}$$

Difficult to evaluate due to the sign problem.

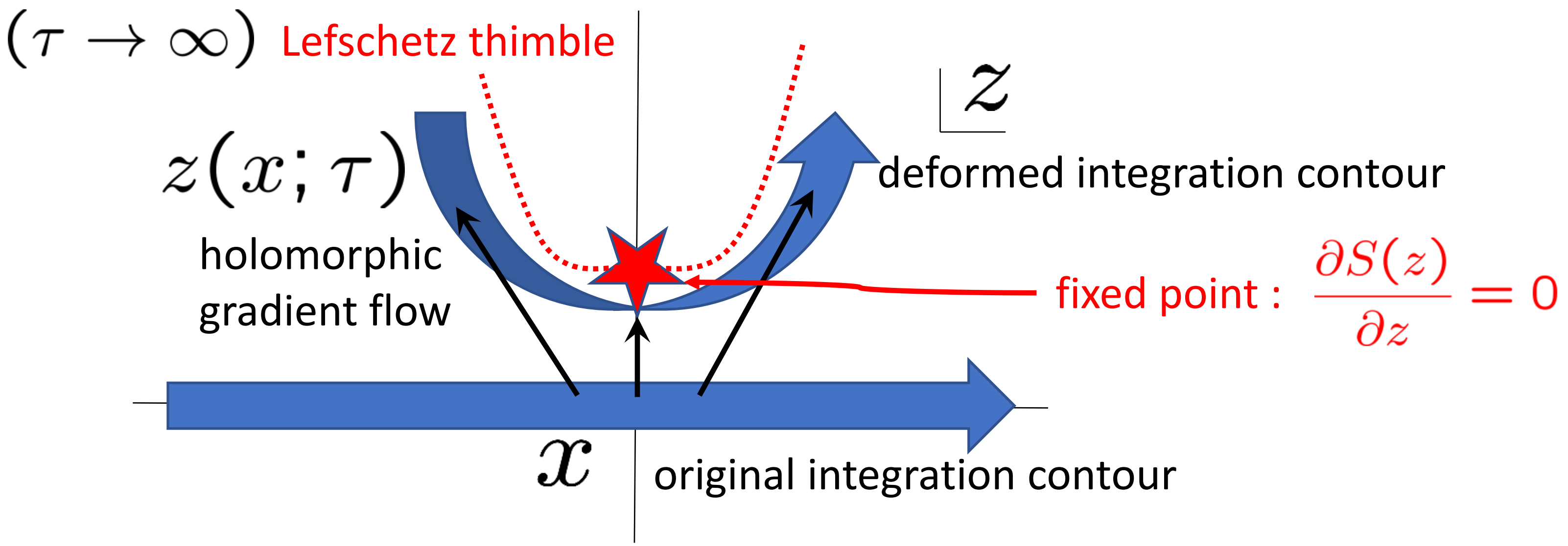
The generalized thimble method (GTM)

A.Alexandru, G.Basar, P.F.Bedaque, G.W.Ridgway and N.C.Warrington, JHEP 1605 (2016) 053



As a result of the property of the holomorphic gradient flow, the sign problem becomes milder on the deformed contour !

The holomorphic gradient flow



solve $\quad \frac{\partial}{\partial \sigma} z_k(x;\sigma) = \overline{\frac{\partial S(z(x;\sigma))}{\partial z_k}}$

from $\sigma = 0$ to $\sigma = \tau$

with the initial condition $z(x;0) = x \in \mathbb{R}^N$

One obtains a one-to-one map from x to $z(x;\tau)$

An important property of the holomorphic gradient flow

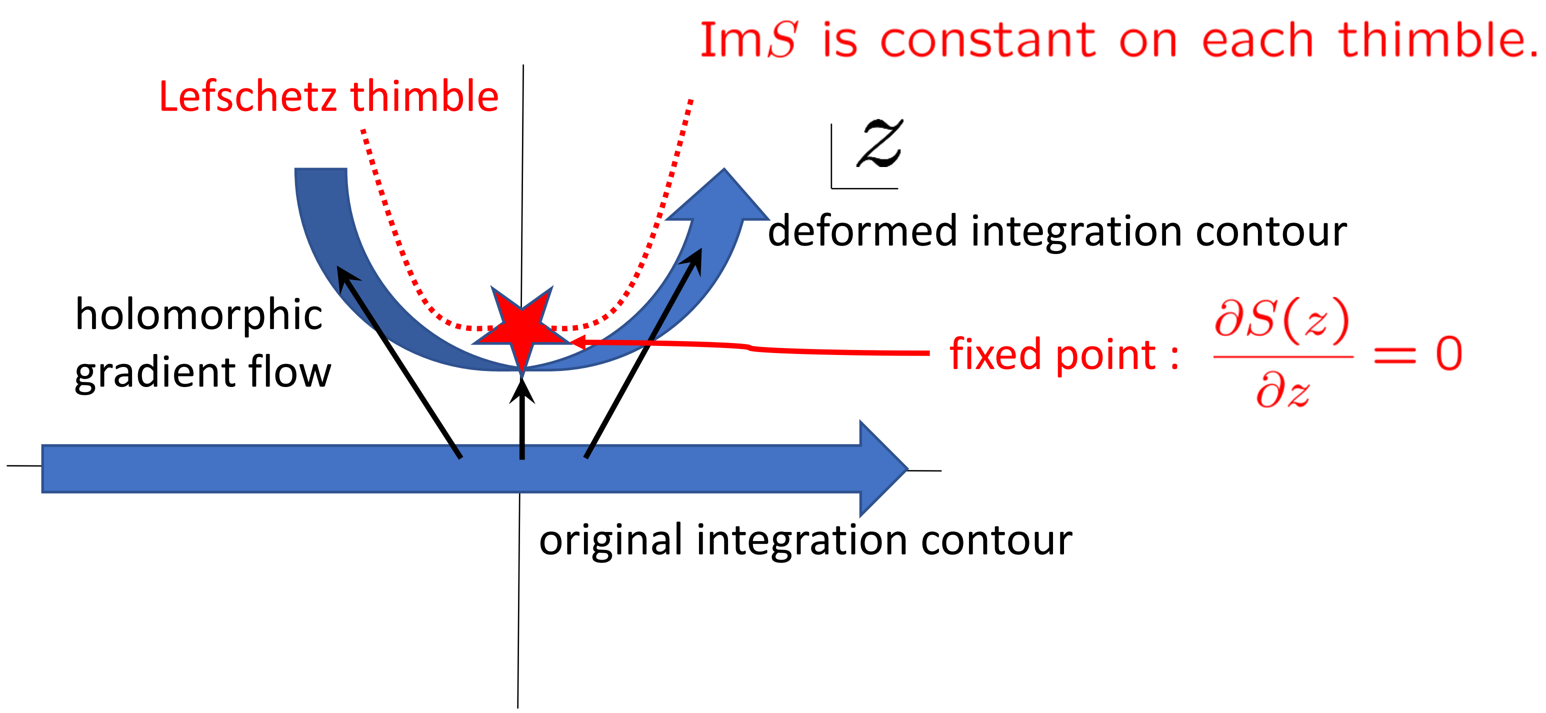
Note that $S(x)$ is complex!

$$\frac{d}{d\sigma}S(z(x;\sigma)) = \frac{\partial S(z(x;\sigma))}{\partial z_k}\frac{\partial z_k(x;\sigma)}{\partial \sigma}$$
$$= \frac{\partial S(z(x;\sigma))}{\partial z_k}\overline{\frac{\partial S(z(x;\sigma))}{\partial z_k}}$$
$$= \left|\frac{\partial S(z(x;\sigma))}{\partial z_k}\right|^2$$

real positive !

Real part of the action increases along the flow,
while the imaginary part is kept constant.

The integration is dominated by a small region of x as the flow-time increases.



As a result, the sign problem becomes milder !

The deformed integration contour

$$\Sigma_\tau = \{z(x;\tau) | x \in \mathbb{R}^N\}$$

N-dimensional real manifold in $\mathbb{C}^N$

$$Z = \int_{\mathbb{R}^N} dx\, e^{-S(x)}$$

$$= \int_{\Sigma_\tau} dz\, e^{-S(z)}$$

$$= \int_{\mathbb{R}^N} dx\, \det J(x;\tau)\, e^{-S(z(x;\tau))}$$

Cauchy's theorem

HMC on the deformed contour

HMC on the original contour

$$J_{kl}(x;\tau) \equiv \frac{\partial}{\partial x_l} z_k(x;\tau)$$

reweighting for the residual sign problem is necessary

$$\langle \mathcal{O}(x) \rangle = \frac{\langle e^{i\theta} \mathcal{O}(z(x;\tau)) \rangle_0}{\langle e^{i\theta} \rangle_0} \qquad \theta = -\mathrm{Im} S(z) + \arg(\det J)$$

Problems in the GTM

- One has to solve the holomorphic gradient flow

$$\frac{\partial}{\partial\sigma} z_k(x;\sigma) = \overline{\frac{\partial S(z(x;\sigma))}{\partial z_k}}$$

to sample each point on Σ_τ

HMC algorithm

Fukuma-Matsumoto-Umeda ('19)

The Jacobian $J_{kl}(x;\tau) \equiv \frac{\partial}{\partial x_l} z_k(x;\tau)$
has to be calculated by solving the corresponding flow eq.,
which is the most time-consuming part.

- When there are more than one thimbles,
the tunneling from one thimble region to another
does not occur very frequently for large τ.

➡ ergodicity problem

integrating over the flow time

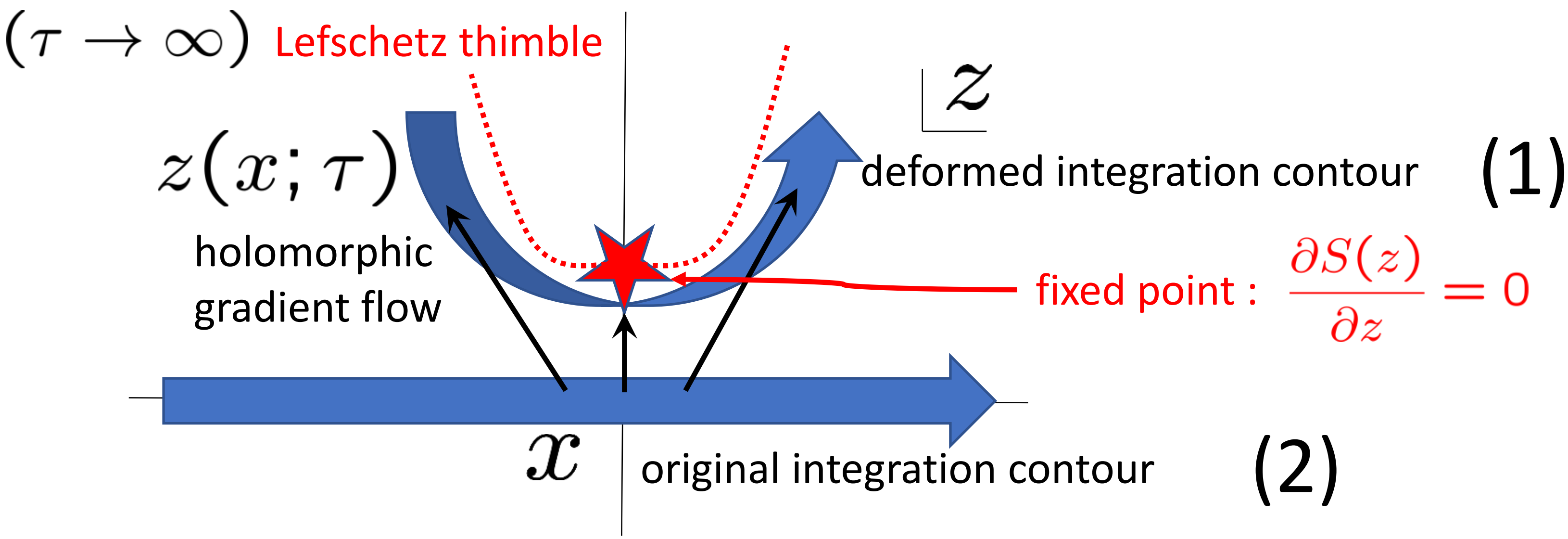
Fukuma-Matsumoto('20)

3. Backpropagating HMC algorithm

Fujisawa, JN, Sakai, Yosprakob, JHEP 04 (2022) 179

arXiv : 2112.10519 [hep-lat]

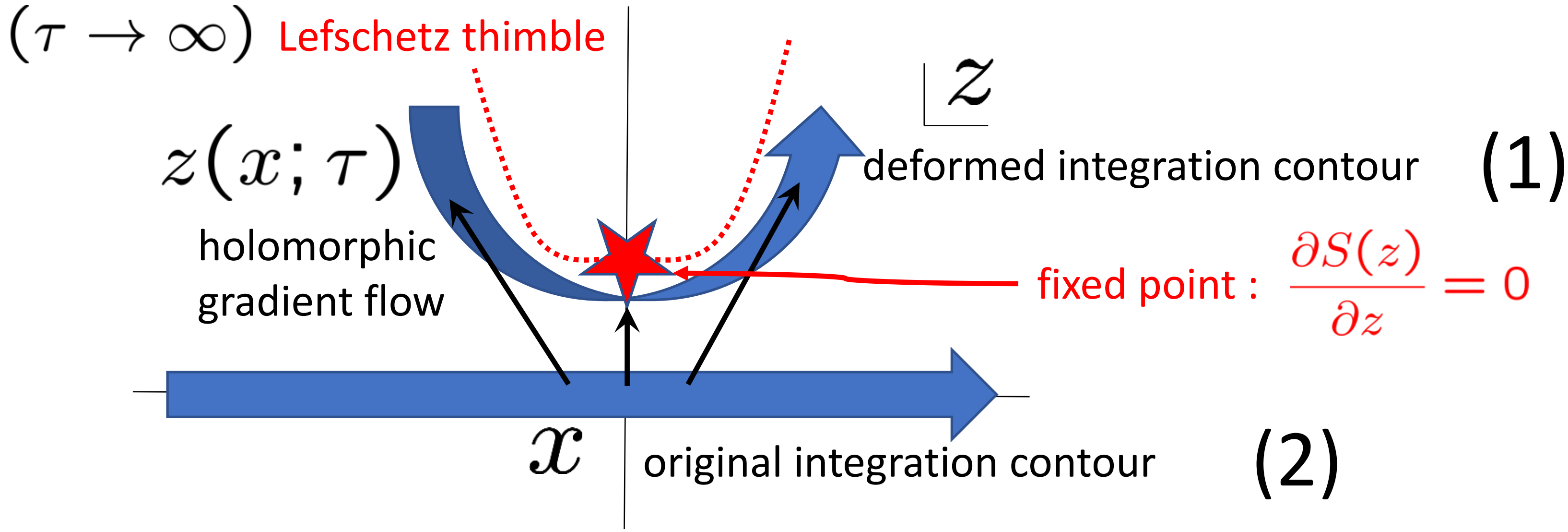
Two possibilities for HMC algorithm



$$
\begin{aligned}
Z &= \int_{\mathbb{R}^N} dx\, e^{-S(x)} \\
&= \int_{\Sigma_\tau} dz\, e^{-S(z)} && (1) \\
&= \int_{\mathbb{R}^N} dx\, \det J(x;\tau)\, e^{-S(z(x;\tau))} && (2)
\end{aligned}
$$

Cauchy's theorem

Two possibilities for HMC algorithm



(1) Fukuma-Matsumoto-Umeda ('19), Fukuma-Matsumoto('20)

constrained Hamilton dynamics on Σ_τ — cumbersome

force : $F_k = \frac{\partial \mathrm{Re} S(z)}{\partial z_k}$ — straightforward

$|\det J|$ included in the measure

(2) Fujisawa-JN-Sakai-Yosprakob ('21)

unconstrained Hamilton dynamics on $\mathbb{R}^N$ — straightforward

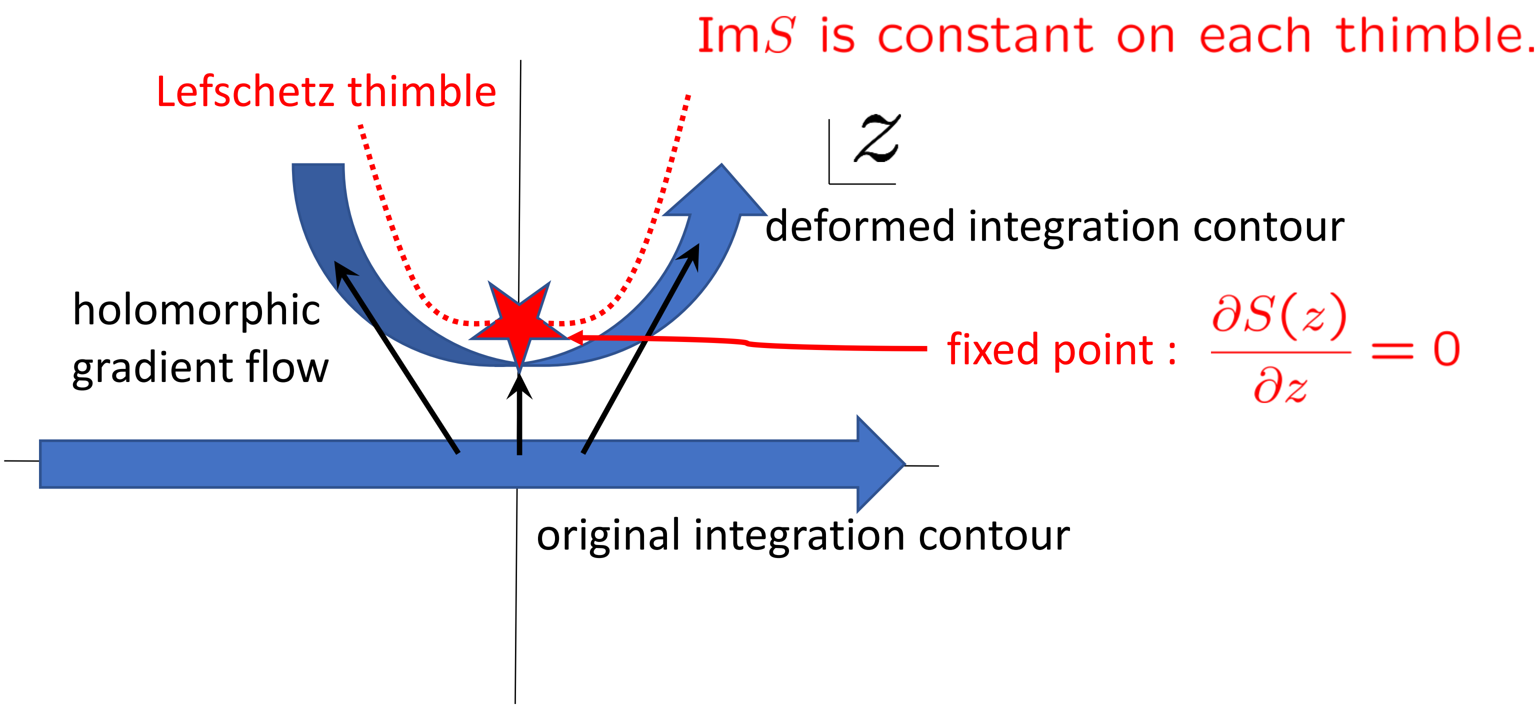
force : $f_k = \frac{\partial \mathrm{Re} S(z(x))}{\partial x_k}$ — Use "backpropagation"

$|\det J|$ has to be reweighted — overlap problem ?

4. Optimizing the flow equation

JN-Sakai-Yosprakob, in preparation

Diverging problem in flow eq.

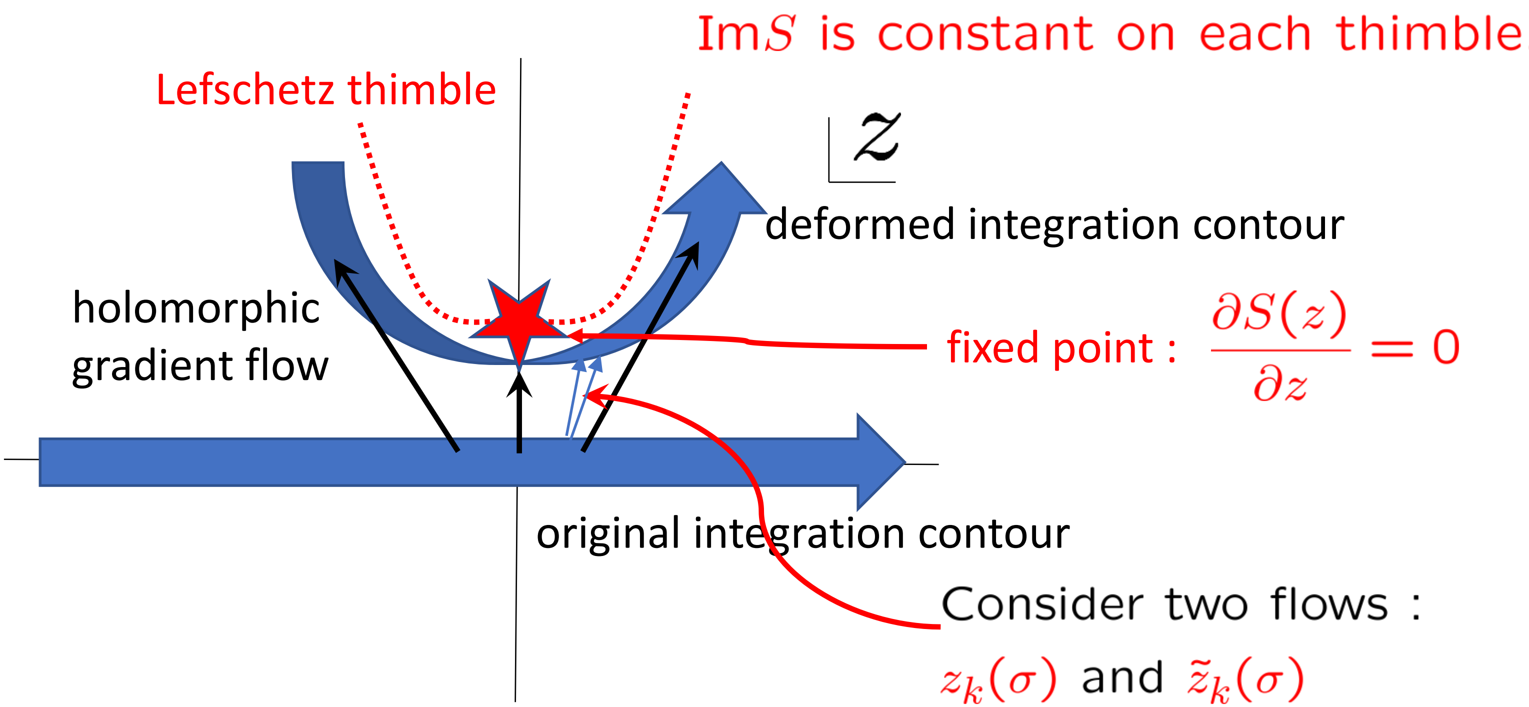


small region on the original contour

➡ exponentially expands with the flow

Expansion rate depends on the fluctuation mode !

Expansion rate



$$\frac{\partial}{\partial \sigma} z_k(\sigma) = \overline{\frac{\partial S(z(\sigma))}{\partial z_k}}$$

$$\tilde{z}_k(\sigma) = z_k(\sigma) + \zeta_k(\sigma)$$

$$\frac{\partial}{\partial \sigma} \zeta_k(\sigma) = \overline{H_{kl}(z(\sigma))}\ \overline{\zeta_l(\sigma)}$$

$$H_{kl}(z) = \frac{\partial^2 S(z)}{\partial z_k \partial z_l}$$

expansion rate = singular values of H_{kl} (Hessian)

Singular value decomposition

general complex matrix A

$$A = U \Lambda V \qquad U,\ V\ :\ \text{unitary}$$

$$\Lambda = \text{diag}(\lambda_1, \lambda_2, \cdots, \lambda_N)$$

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_N \geq 0$$

$$\frac{\partial}{\partial \sigma} \zeta_k(\sigma) = \overline{H_{kl}(z(\sigma))}\ \overline{\zeta_l(\sigma)}$$

$$H = U^{\top} \Lambda U$$

$$U \frac{\partial}{\partial \sigma} \zeta(\sigma) = \Lambda\ \overline{U \zeta(\sigma)}$$

condition number : $\eta(H) = \dfrac{\lambda_1}{\lambda_N}$

If the condition number is $\eta(H) \gg 1$,
the expansion rates have a huge hierarchy !

In order to solve the sign problem, $\tau \gtrsim O\left(\dfrac{1}{\lambda_N}\right)$

$$\lambda_1 \tau \gtrsim \frac{\lambda_1}{\lambda_N} \gg 1$$

The flow diverges !

Optimizing the flow equation

flow eq. $$\frac{\partial}{\partial\sigma} z_k(x;\sigma) = A_{kl} \overline{\frac{\partial S(z(x;\sigma))}{\partial z_l}}$$

The crucial property of the flow eq. is maintained

$$\frac{d}{d\sigma} S(z(x;\sigma)) = \frac{\partial z_k(x;\sigma)}{\partial\sigma} \frac{\partial S(z(x;\sigma))}{\partial z_k}$$
$$= \overline{\frac{\partial S(z(x;\sigma))}{\partial z_l}} A_{kl} \frac{\partial S(z(x;\sigma))}{\partial z_k}$$

real positive !

if A is Hermitian with positive EVs.

$$A = V^\dagger \Omega V$$
$$\Omega = \mathrm{diag}(\omega_1, \omega_2, \cdots, \omega_N)$$
$$\omega_k > 0$$

Optimal flow equation

$$\frac{\partial}{\partial\sigma} z_k(x;\sigma) = A_{kl} \overline{\frac{\partial S(z(x;\sigma))}{\partial z_l}}$$

preconditioner

$$\tilde{z}_k(\sigma) = z_k(\sigma) + \zeta_k(\sigma)$$

$$\frac{\partial}{\partial\sigma} \zeta_k(\sigma) = A_{kl} \overline{H_{lm}(z(\sigma))}\ \overline{\zeta_m(\sigma)}$$

$$\frac{\partial}{\partial\sigma} \zeta(\sigma) = A\overline{H}\ \overline{\zeta(\sigma)}$$

$$= V^\dagger \Omega\, V\, U^\dagger \Lambda\, \bar{U}\ \overline{\zeta(\sigma)}$$

$$H = U^\top \Lambda\, U$$

$$A = V^\dagger\, \Omega\, V$$

Optimal choice for A : $V = U$, $\Omega = \Lambda^{-1}$

$$A = (\overline{H}\, \overline{H}^\dagger)^{-1/2} = (H^\dagger H)^{-1/2}$$

$$U \frac{\partial}{\partial\sigma} \zeta(\sigma) = \overline{U\zeta(\sigma)}$$

The expansion rates become **equal**.

5. Quantum tunneling in the real-time path integral

JN-Sakai-Yosprakob, work in progress

Time-evolution of the wave function

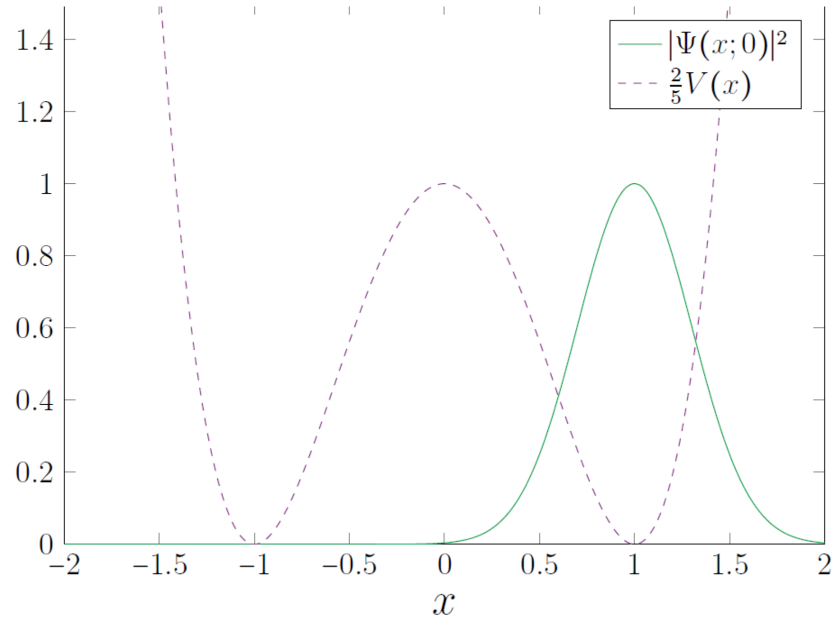
$$\Psi(x_{\mathsf{f}}, t_{\mathsf{f}}) = \int_{x(t_{\mathsf{f}}) = x_{\mathsf{f}}} \mathcal{D}x(t)\, \Psi(x(t_{\mathsf{i}}), t_{\mathsf{i}})\, e^{iS[x(t)]}$$

$$S[x(t)] = \int dt \left\{ \frac{1}{2} m \left(\frac{dx}{dt} \right)^2 - V(x) \right\}$$

$$V(x) = \alpha (x^2 - 1)^2$$

$$\Psi(x, t_{\mathsf{i}}) = \exp\left\{ -\frac{1}{4\sigma^2} (x-1)^2 \right\}$$

$$\alpha = 2.5 \,, \qquad \sigma = 0.3$$



Discretize the time as:

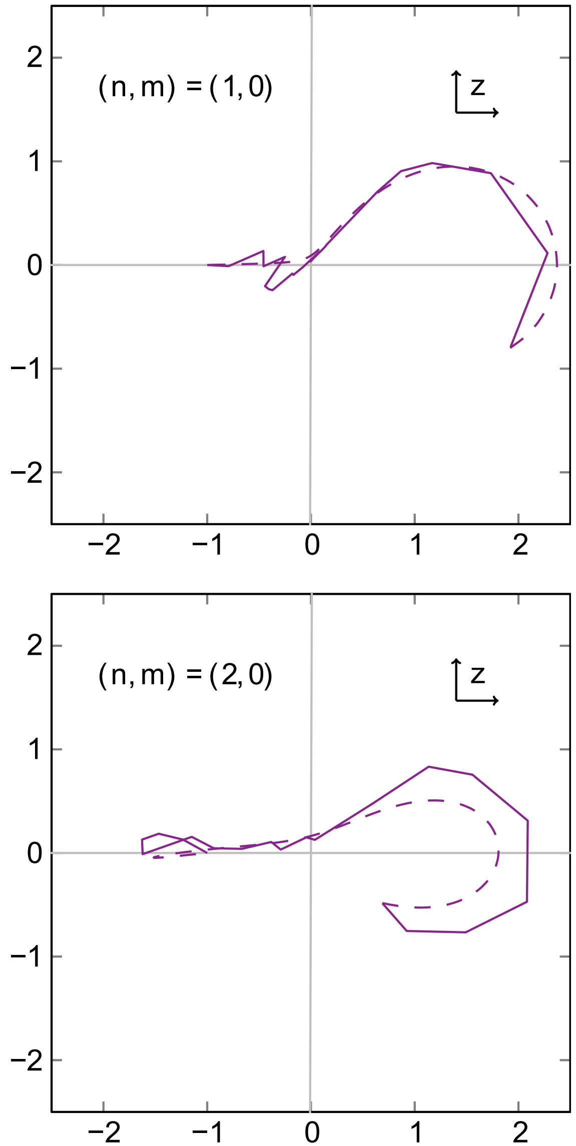
$$x_n = x(t_n)$$

$$t_n = \frac{n-1}{N} T \qquad (n = 1, \cdots, N)$$

$$N = 20 \,, \qquad T = 2$$

Results of GTM with the optimal flow

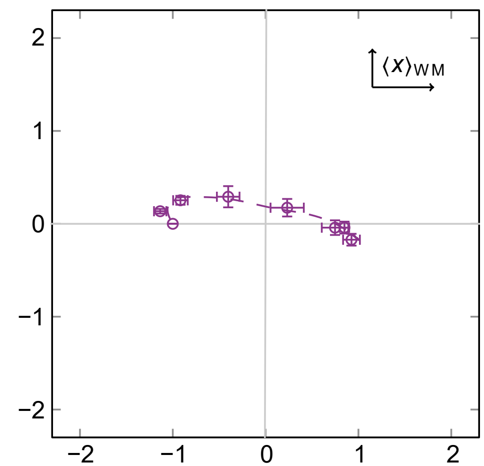
typical configs. at large τ



$$N_\tau = 10\ , \quad 0.2 < \tau < 4$$
$$t_{\mathrm{HMC}} = 1.0\ , \quad N_{\mathrm{HMC}} = 10$$

ensemble average
("weak value" of $x(t)$)

$$\frac{\langle x_{\mathrm{f}} | e^{-i\hat{H}(T-t)} \hat{x} e^{-i\hat{H}t} | \Psi_{\mathrm{i}} \rangle}{\langle x_{\mathrm{f}} | e^{-i\hat{H}(T-t)} e^{-i\hat{H}t} | \Psi_{\mathrm{i}} \rangle}$$



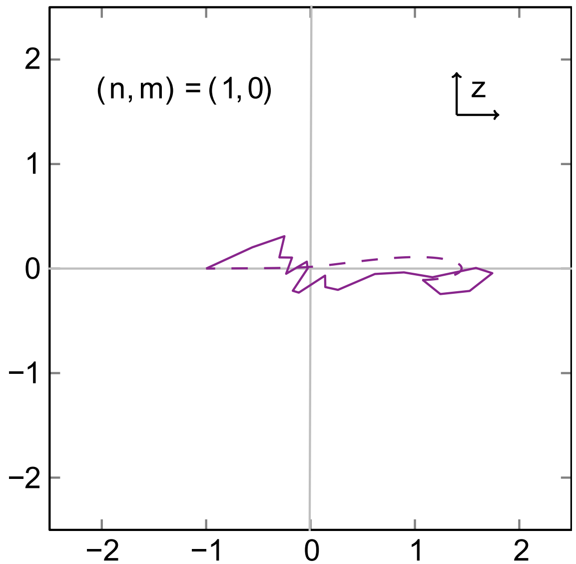
agreement with results obtained by solving Schödinger eq.

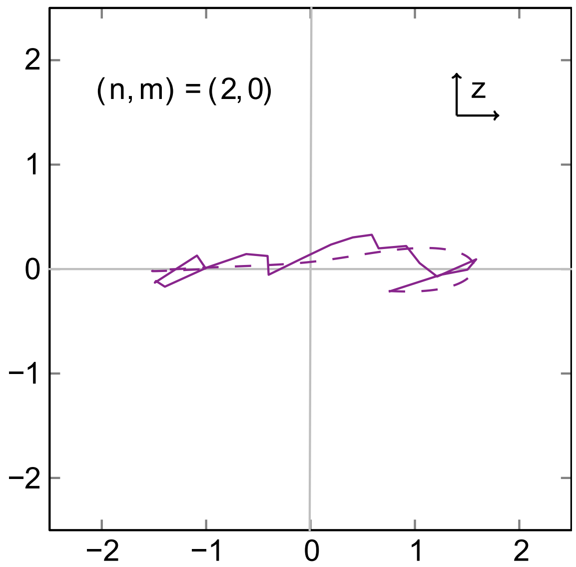
Quantum tunneling is represented by complex trajectories.

(But not the ones speculated by Koike-Tanizaki.)

Introducing momentum in the initial state

a typical config. at large τ





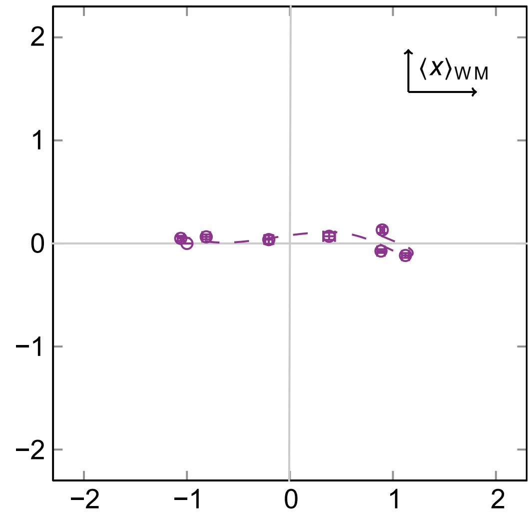
$$\Psi(x, t_{\mathrm{i}}) = \exp\left\{-\frac{1}{4\sigma^2}(x-1)^2 + i\,p\,x\right\}$$

$$p = 2$$

ensemble average

("weak value" of $x(t)$)

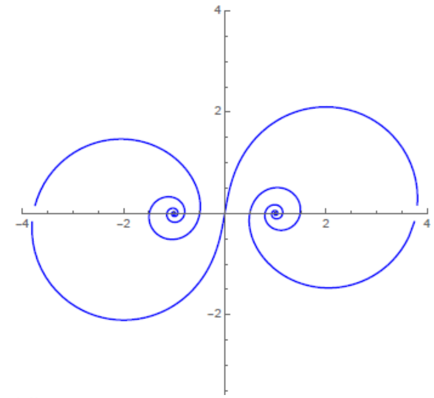
$$\frac{\langle x_{\mathrm{f}}|e^{-i\hat{H}(T-t)}\hat{x}e^{-i\hat{H}t}|\Psi_{\mathrm{i}}\rangle}{\langle x_{\mathrm{f}}|e^{-i\hat{H}(T-t)}e^{-i\hat{H}t}|\Psi_{\mathrm{i}}\rangle}$$



Classical motion over the barrier becomes dominant.

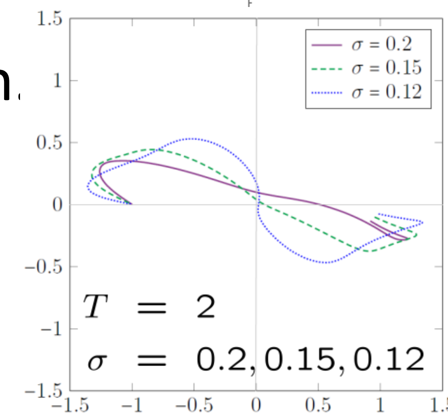
→ almost real trajectories

Relationship to the previous works



- Previous works considered the propagator. (fixed end points)

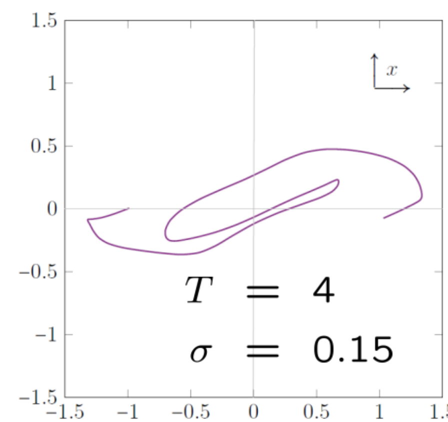
  Koike-Tanizaki ('14), Cherman-Ünsal ('14)



- We have introduced the initial wave function.

$$\Psi(x, t_{\mathrm{i}}) = \exp\left\{-\frac{1}{4\sigma^2}(x-1)^2\right\}$$

As σ decreases,
the weak value of $x(t)$
shows spiral behaviors.



- In the long-time limit,
  → singular trajectories
  (analytic continuation of instantons)

6. Summary and Discussions

Summary and discussions

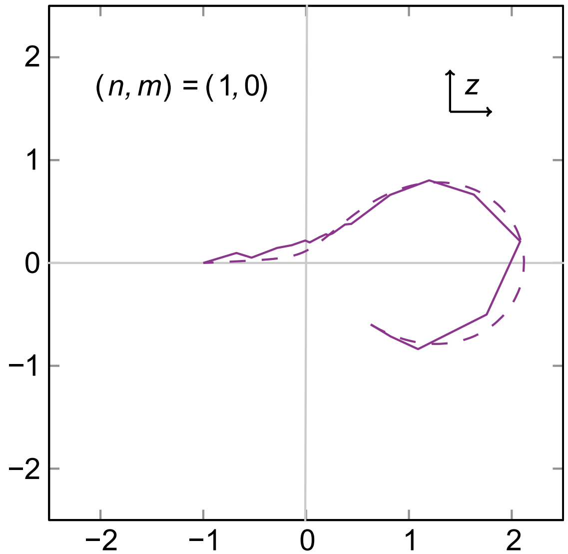
- Quantum tunneling in the real-time path integral
  important applications in QFT, quantum cosmology etc..
- Unlike the previous work, we performed explicit MC calculations based on the Lefschetz thimble method.
- By introducing the initial wave function, we found :
  - Complex trajectories are responsible for quantum tunneling.
  - Introducing momentum makes the trajectories closer to real.
- HMC on the real axis (v.s. HMC on the deformed contour)
  - Calculation of the force by backpropagation is a breakthrough.
  - Optimizing the flow eq. is also important.
    No overlap problem due to reweighting |det J|

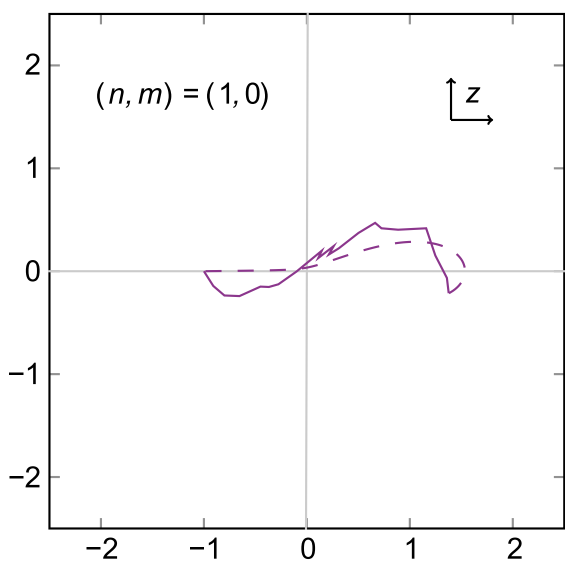
Useful for studying various systems with the sign problem.
(finite density QCD, IKKT matrix model,…)

Backup slides

Reducing $\hbar \mapsto \frac{\hbar}{2}$ in $\exp(iS/\hbar)$

a typical config. at large τ



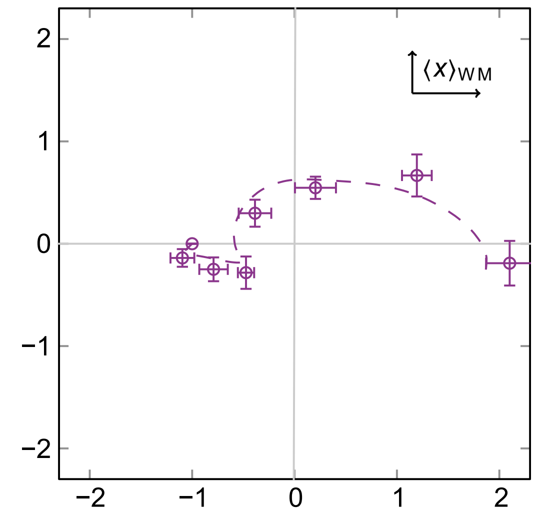


$$\Longleftrightarrow \begin{cases} T & \mapsto & \frac{T}{2} \\ V(x) & \mapsto & 4\,V(x) \end{cases}$$

ensemble average

(“weak value” of $x(t)$)

$$\frac{\langle x_{\rm f}|e^{-i\hat{H}(T-t)}\hat{x}e^{-i\hat{H}t}|\Psi_{\rm i}\rangle}{\langle x_{\rm f}|e^{-i\hat{H}(T-t)}e^{-i\hat{H}t}|\Psi_{\rm i}\rangle}$$



quantum tunneling + classical motion

→ first complex and then real trajectories

Good effects of the optimized flow on the Jacobian

$$J_{kl}(x;\tau) \equiv \frac{\partial}{\partial x_l} z_k(x;\tau)$$

$$\frac{\partial}{\partial \sigma} z_k(x;\sigma) = \overline{\frac{\partial S(z(x;\sigma))}{\partial z_k}}$$

flow eq. for the Jacobian :

$$\begin{aligned} \frac{\partial}{\partial \sigma} J_{kl}(x;\sigma) &= \frac{\partial}{\partial x_l} \overline{\frac{\partial S(z(x;\sigma))}{\partial z_k}} \\ &= \overline{\frac{\partial^2 S(z(x;\sigma))}{\partial z_k \partial z_m} \frac{\partial}{\partial x_l} z_m(x;\sigma)} \\ &= \overline{H_{km}(x;\sigma) J_{ml}(x;\sigma)} \end{aligned}$$

$$H_{kl}(z) = \frac{\partial^2 S(z)}{\partial z_k \partial z_l}$$

$$\frac{\partial}{\partial \sigma} z_k(x;\sigma) = A_{kl} \overline{\frac{\partial S(z(x;\sigma))}{\partial z_l}}$$

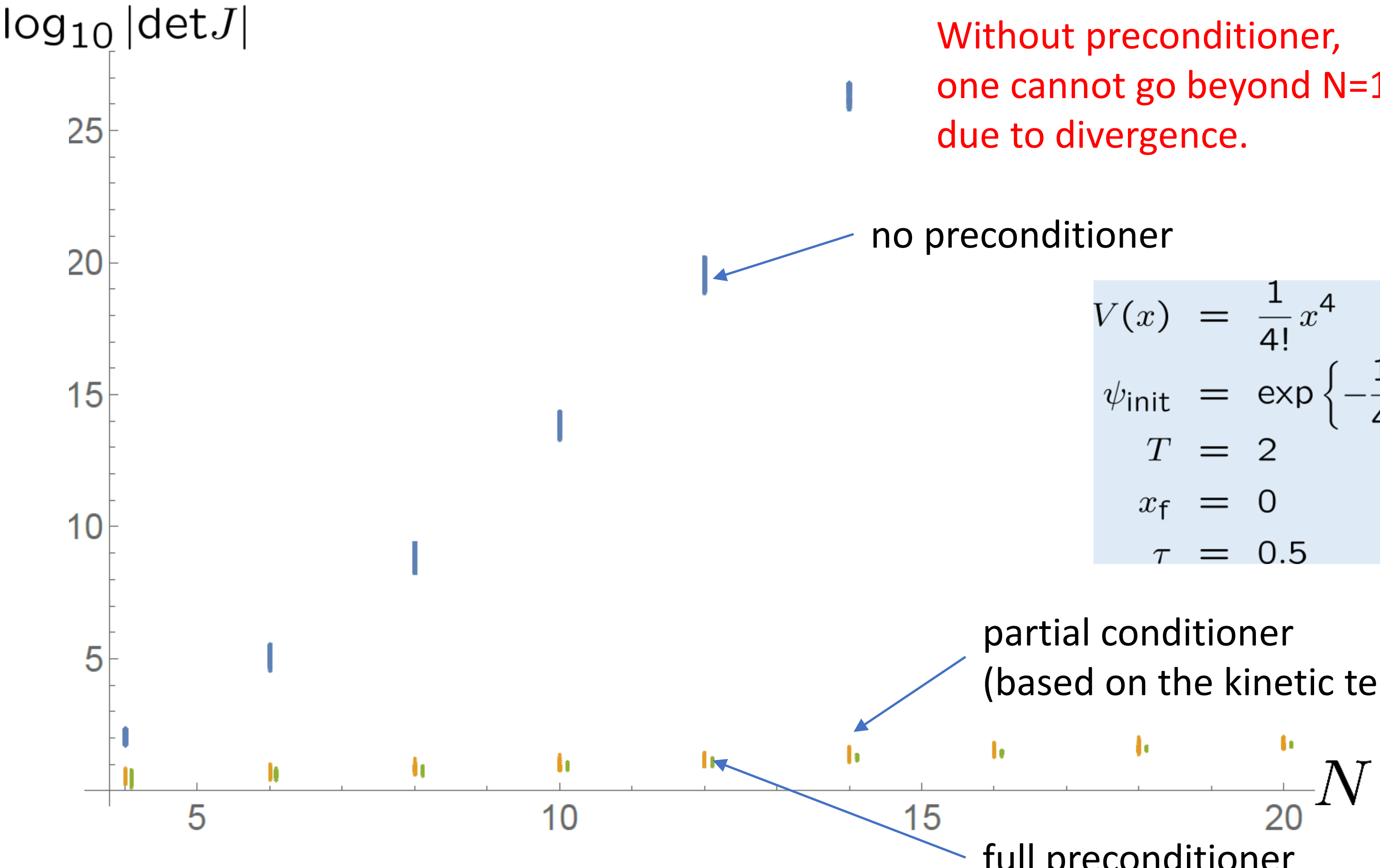
$$\begin{aligned} A &= (\overline{H}\,\overline{H}^\dagger)^{-1/2} \\ &= (H^\dagger H)^{-1/2} \end{aligned}$$

$$\begin{aligned} \frac{\partial}{\partial \sigma} J_{kl}(x;\sigma) &= \frac{\partial}{\partial x_l} A_{kp} \overline{\frac{\partial S(z(x;\sigma))}{\partial z_p}} \\ &\sim A_{kp} \overline{H_{pm}(x;\sigma) J_{ml}(x;\sigma)} \end{aligned}$$

$$U \frac{\partial}{\partial \sigma} J(x;\sigma) \sim \overline{UJ((x;\sigma)}$$

Rapid growth of |det J| is avoided.

Results from applications to real-time evolution in quantum mechanics



Without preconditioner, one cannot go beyond N=16 due to divergence.

$$V(x) = \frac{1}{4!}x^4$$
$$\psi_{\text{init}} = \exp\left\{-\frac{1}{4}(x-1)^2\right\}$$
$$T = 2$$
$$x_{\text{f}} = 0$$
$$\tau = 0.5$$

Overlap problem is NOT seen for the optimal flow !

How to deal with the preconditioner

Optimal choice for A :

$$A = (\overline{H}\,\overline{H}^\dagger)^{-1/2} = (H^\dagger H)^{-1/2}$$

strange quark

We use a well-known technique for simulating QCD with (2+1)-flavor.

$$|\det D_s| = \det(D_s^\dagger D_s)^{1/2} = \int dF d\bar{F}\, e^{-\bar{F}(D_s^\dagger D_s)^{-1/2} F}$$

Rational Hybrid Monte Carlo (RHMC) algorithm

Clark-Kennedy ('05)

rational approximation :

$$x^{-1/2} \sim \sum_{i=1}^{Q} \frac{c_i}{x + m_i}$$

$$(H^\dagger H)^{-1/2} \sim \sum_{i=1}^{Q} \frac{c_i}{H^\dagger H + m_i}$$

multi-mass CG solver :

$$(H^\dagger H + m_i)\, x = b$$

Need to solve this only for the smallest m_i.

The numerical cost for the optimal flow eq. is still O(N) !

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  - Complex trajectories are responsible for quantum tunneling.
  - Introducing momentum makes the trajectories closer to real.
  - Reducing $\hbar$ leads to (complex + real) trajectories.

- HMC on the real axis (v.s. HMC on the deformed contour)
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