Worldvolume Hybrid Monte Carlo algorithm in the generalized Lefschetz thimble method

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Journal club at KEK, February 19, 2021

Ref.) Masafumi Fukuma, Nobuyuki Matsumoto, arXiv:2012.08468

The sign problem in Monte Carlo methods

- E.g., in finite density QCD

$$
\begin{aligned}
Z &= \int dU \, d\Psi \, \mathrm{e}^{-S[U,\Psi]} \\
&= \int dU \, \mathrm{e}^{-S_{\mathrm{g}}[U]} \det \mathcal{M}[U]
\end{aligned}
$$

The fermion determinant becomes complex in general.

$$
\det \mathcal{M}[U] = |\det \mathcal{M}[U]| \, \mathrm{e}^{i\Gamma[U]}
$$

Generate configurations *U* with the probability $\mathrm{e}^{-S_{\mathrm{g}}[U]} \, |\det \mathcal{M}[U]|$
and calculate

$$
\langle \mathcal{O}[U] \rangle = \frac{\langle \mathcal{O}[U] \, \mathrm{e}^{i\Gamma[U]} \rangle_0}{\langle \mathrm{e}^{i\Gamma[U]} \rangle_0}
$$

(reweighting)

become exponentially small as the volume increases
due to violent fluctuations of the phase Γ

Number of configurations needed to evaluate <O> increases exponentially.

"sign problem"

Sign problem occurs also in many other interesting cases

- finite density QCD
- gauge theories with a theta term
- IKKT matrix model for superstring theory
- real-time evolution of quantum systems
- Yukawa interactions
- supersymmetric theories
- chiral fermions
- systems of strongly coupled electrons etc.

fermionic origin

Solving the sign problem will be a great breakthrough in theoretical physics !

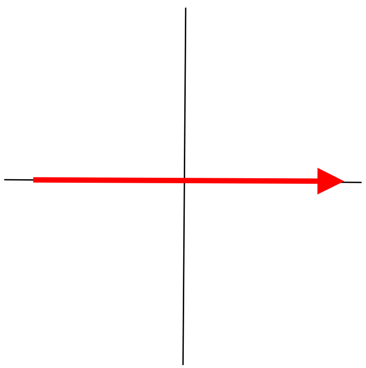
A new development toward solution to the sign problem

2011～

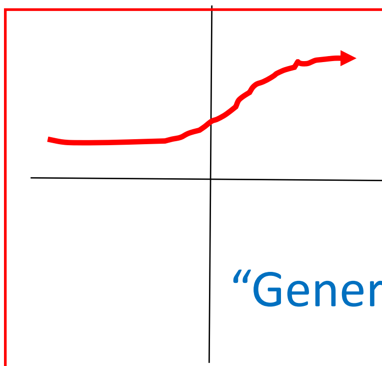
Key : complexification of dynamical variables

The original path integral

$$Z = \int dx\, w(x)$$



The phase of $w(x)$ oscillates violently (sign problem)

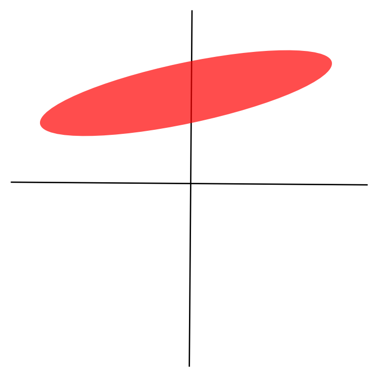


$$Z = \int dz\, w(z)$$

Minimize the sign problem by deforming the integration contour

“Generalized Lefschetz Thimble Method”

This paper



An equivalent stochastic process of the complexified variables (no sign problem !)

“Complex Langevin Method”

The equivalence to the original path integral holds under certain conditions.

Two big problems in generalized Lefschetz thimble method (GLTM)

- Numerically costly

  In order to obtain the deformed contour, which minimizes the sign problem, one has to solve the holomorphic gradient flow eq. at each Metropolis updates. In particular, one has to calculate the Jacobian, which is time-consuming.

- Ergodicity problem

  The ergodicity problem occurs when there are more than one thimbles that contribute to the path integral.

Both these problems can be solved by the worldvolume approach. Moreover, the standard Hybrid Monte Carlo (HMC) algorithm is applicable.

⇒ This makes the GLTM much more powerful.

Plan of the talk

1. Brief review of the GLTM
2. Worldvolume approach to the GLTM
3. Brief review of HMC algorithm
4. HMC on the worldvolume
5. Results for Random Matrix Theory
6. Summary and discussions

1.Brief review of the GLTM

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

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

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

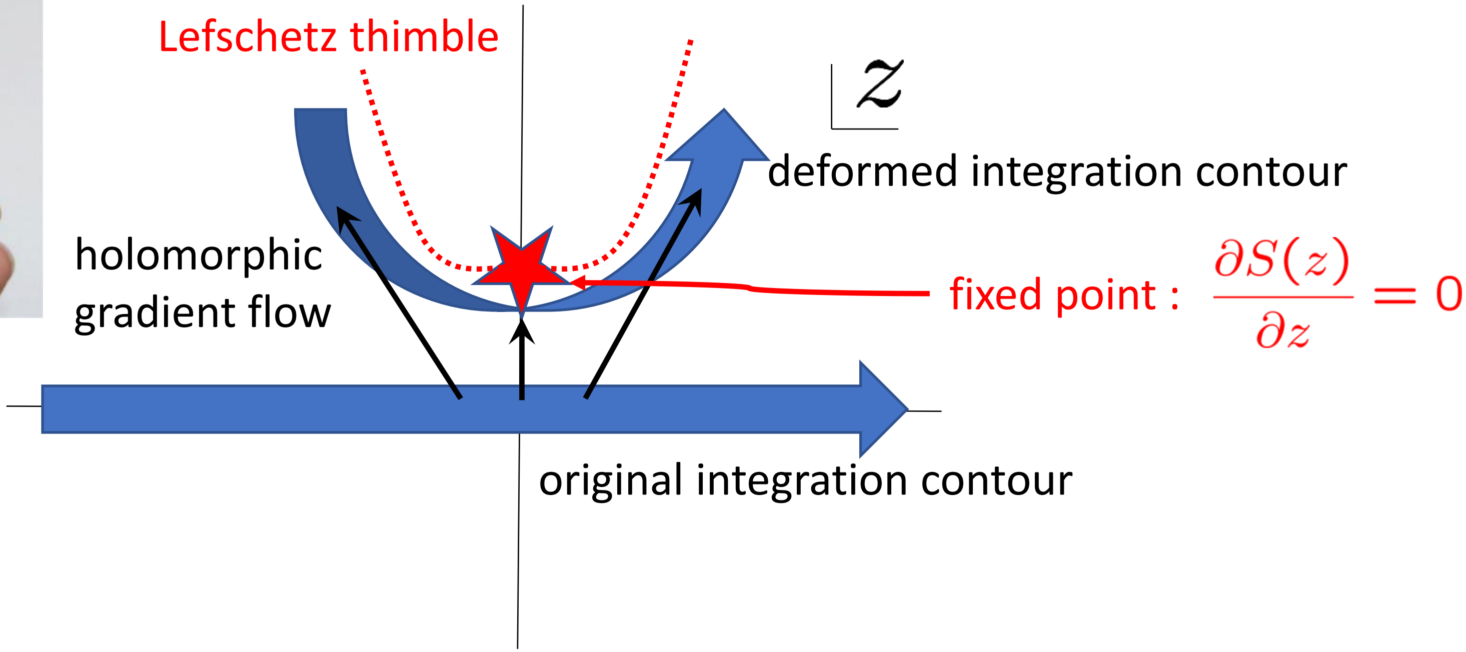
$$S(x) \in \mathbb{C}$$

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

Difficult to evaluate due to the sign problem.

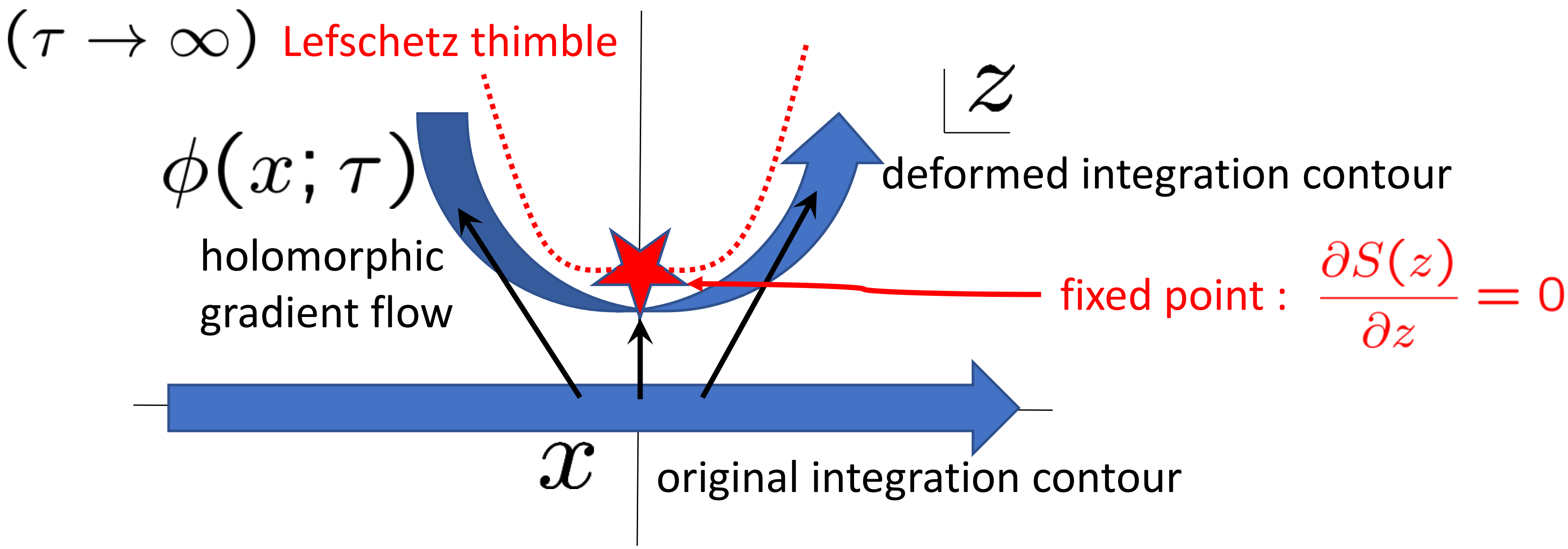
The generalized Lefschetz thimble method (GLTM)

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 $\quad \dfrac{\partial}{\partial \sigma}\phi_k(x;\sigma) = \overline{\left(\dfrac{\partial S(\phi(x;\sigma))}{\partial \phi_k}\right)}$

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

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

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

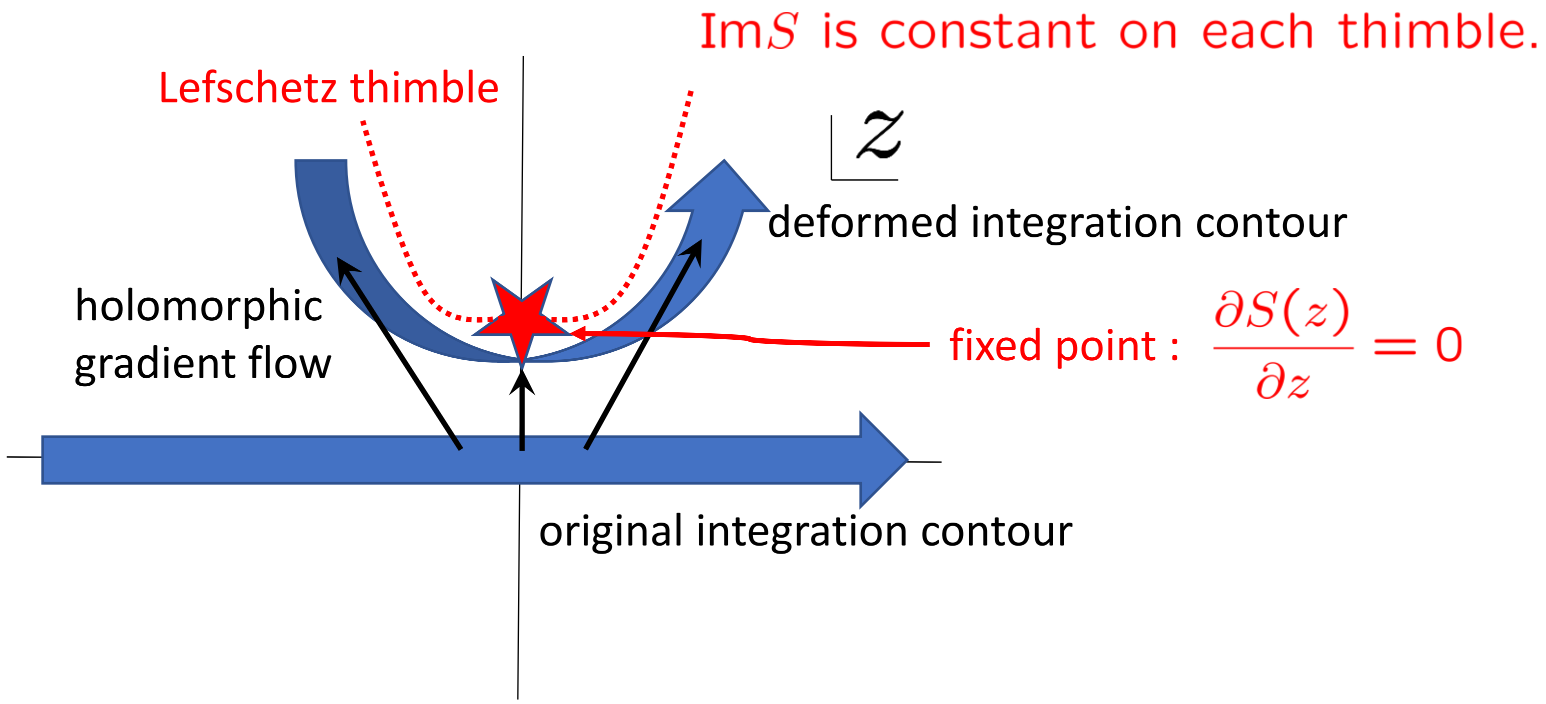
An important property of the holomorphic gradient flow

$$\begin{aligned}\frac{d}{d\sigma}S(\phi(x;\sigma)) &= \frac{\partial S(\phi(x;\sigma))}{\partial \phi_k}\frac{\partial \phi_k(x;\sigma)}{\partial \sigma} \\ &= \frac{\partial S(\phi(x;\sigma))}{\partial \phi_k}\overline{\left(\frac{\partial S(\phi(x;\sigma))}{\partial \phi_k}\right)} \\ &= \left|\frac{\partial S(\phi(x;\sigma))}{\partial \phi_k}\right|^2\end{aligned}$$

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

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

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

$$\begin{aligned} Z &= \int_{\mathbb{R}^N} dx\, e^{-S(x)} \\ &= \int_{\Sigma_\tau} d\phi\, e^{-S(\phi)} \\ &= \int_{\mathbb{R}^N} dx\, \det J(x;\tau)\, e^{-S(\phi(x;\tau))} \\ &= \int_{\mathbb{R}^N} dx\, e^{-S_{\text{eff}}(x;\tau)} \end{aligned}$$

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

$$S_{\text{eff}}(x;\tau) \equiv S(\phi(x;\tau)) - \log\det J(x;\tau)$$

$$\langle \mathcal{O}(x) \rangle = \frac{\langle e^{-i\,\text{Im}S_{\text{eff}}(x;\tau)}\mathcal{O}(\phi(x;\tau))\rangle_{\text{Re}S_{\text{eff}}}}{\langle e^{-i\,\text{Im}S_{\text{eff}}(x;\tau)}\rangle_{\text{Re}S_{\text{eff}}}} \qquad \text{(reweighting)}$$

Problems in the GLTM

- One has to solve the holomorphic gradient flow

$$\frac{\partial}{\partial \sigma}\phi_k(x;\sigma) = \overline{\left(\frac{\partial S(\phi(x;\sigma))}{\partial \phi_k}\right)}$$

to sample each point on Σ_τ

In particular, the Jacobian $J_{kl}(x;\tau) \equiv \frac{\partial}{\partial x_l}\phi_k(x;\tau)$
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.

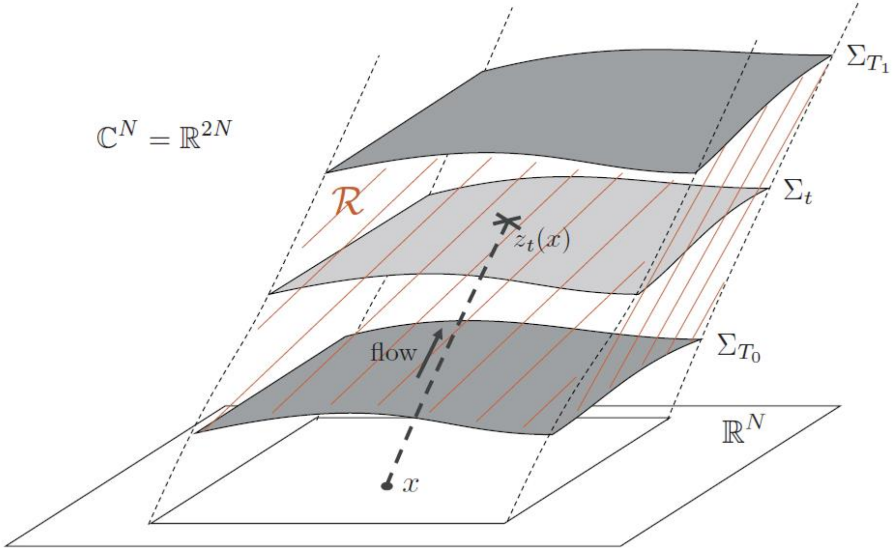
⇨ ergodicity problem

2. Worldvolume approach to the GLTM

The basic idea of the worldvolume approach

$$Z = \int_{\Sigma_\tau} d\phi \, e^{-S(\phi)}$$

$$Z_W = \int d\tau e^{-W(\tau)} \int_{\Sigma_\tau} d\phi \, e^{-S(\phi)}$$



Consider Monte Carlo simulation on the "worldvolume" $\mathcal{R}$ obtained by the one-parameter family of the deformed contour.

- Choose the potential W in such a way that one can sample configurations from a wide region of τ

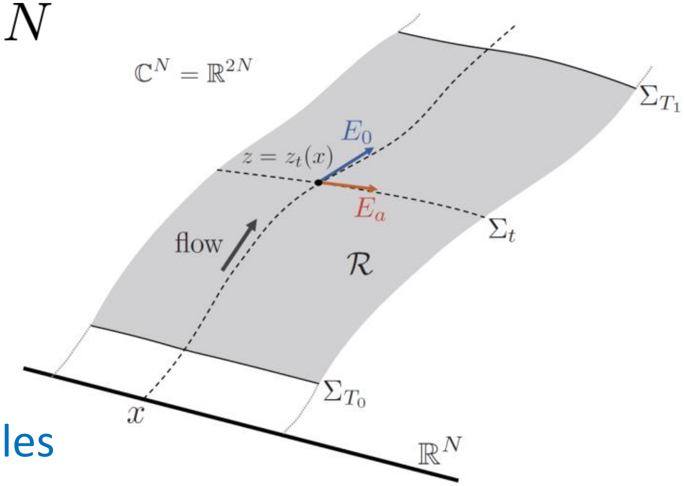
  small τ region : no problem with ergodicity
  large τ region : sign problem becomes weaker

  Measurements should be done here.

The measure for sampling points on the worldvolume

The worldvolume $\mathcal{R}$ is $(N+1)$-dimensional mfd embedded in $\mathbb{C}^N$ and each point is parametrized by $\{\xi^\mu\} = \{(\tau, x_i)\} \in \mathbb{R}^{N+1}$

$$\mathbb{C} \ni z^i(\xi) = \phi^i(x;\tau) \qquad i = 1, \cdots, N$$



<u>tangent vectors :</u> $E^i_\mu = \dfrac{\partial z^i(\xi)}{\partial \xi^\mu}$

$$\begin{cases} E^i_0 = \dfrac{\partial}{\partial \tau}\phi_i(x;\tau) = \overline{\dfrac{\partial S}{\partial z^i}} \\ E^i_j = \dfrac{\partial}{\partial x_j}\phi_i(x;\tau) = J_{ij}(x;\tau) \end{cases}$$

Jacobian for the change of variables

<u>induced metric on the worldvolume</u>

$$\begin{aligned} ds^2 &= g_{\mu\nu} d\xi^\mu d\xi^\nu \\ &= \overline{E^i_\mu d\xi^\mu}\, E^i_\nu d\xi^\nu \end{aligned} \quad \Rightarrow \quad g_{\mu\nu} = \mathrm{Re}(\overline{E^i_\mu}\, E^i_\nu)$$

<u>the volume element on the world volume :</u> $\mathcal{D}z = \sqrt{g}\, d^{N+1}\xi$

This is the measure that is used effectively when sampling the points $z^i(\xi)$ on the worldvolume.

Explicit results for the volume element

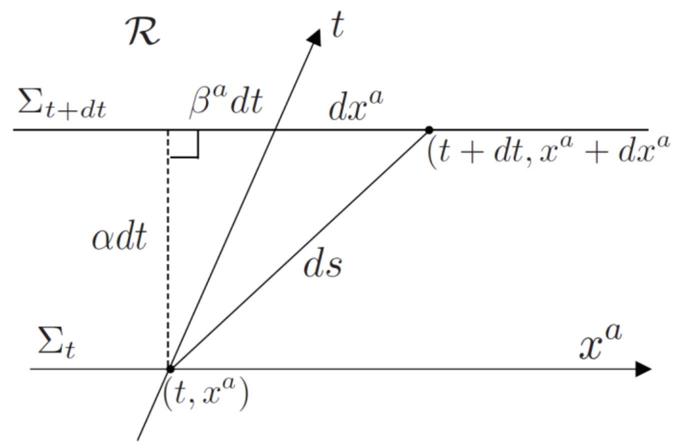
$$\xi^\mu = (\tau, x_i)$$

$$\begin{aligned} ds^2 &= g_{\mu\nu} d\xi^\mu d\xi^\nu \\ &= \alpha^2 d\tau^2 + \gamma_{ij}(dx^i + \beta^i d\tau)(dx^j + \beta^j d\tau) \end{aligned}$$

ADM decomposition (well-known in GR)

$$\gamma_{ij} = \mathrm{Re}(\overline{E_i} E_j) = (J^\dagger J)_{ij}$$

$$\begin{aligned} \mathcal{D}z &= \sqrt{g}\, d^{N+1}\xi \\ &= \alpha \sqrt{\det \gamma}\, d^{N+1}\xi \\ &= \alpha |\det J|\, d\tau\, d^N x \end{aligned}$$



Modulus of the Jacobian is naturally taken into account !!!

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

$$Z_W = \int d\tau\, e^{-W(\tau)} \int_{\Sigma_\tau} d\phi\, e^{-S(\phi)}$$

$$\det J\, d^N x = |\det J| e^{i\varphi}\, d^N x$$

$$= \int_{\mathcal{R}} \mathcal{D}z \boxed{\alpha^{-1} e^{i\varphi}\, e^{-i\,\mathrm{Im} S(z)}} e^{-\mathrm{Re} S(z) - W(\tau)}$$

treated as a reweighting factor in measurements

No need to calculate J during MC simulation !

3. Brief review of HMC algorithm

What does Monte Carlo algorithms do ?

$$Z = \int dx\, e^{-S(x)} \qquad S(x) \in \mathbb{R}$$

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

"configurations"

generate $\{x^{(k)}\}$ $(k = 1, 2, \cdots, n)$ "ensemble"

with the probability $\propto e^{-S(x)}$

$$\langle \mathcal{O}(x) \rangle = \lim_{n\to\infty} \boxed{\frac{1}{n} \sum_{k=1}^{n} \mathcal{O}(x^{(k)})}$$

"ensemble average"

finite $n \longrightarrow$ statistical error

Markov chain:

$$x^{(0)} \to x^{(1)} \to \cdots \to x^{(n-1)} \to x^{(n)}$$

Define transition prob. $P(x^{(k)} \to x^{(k+1)})$ s.t. "algorithm"

$$e^{-S(x)} P(x \to x') = e^{-S(x')} P(x' \to x)$$

"detailed balance"

Metropolis algorithm

$$x^{(k)} \to x^{(k+1)}$$

Metropolis algorithm

1) Propose a new configuration x'

2) Calculate $\Delta S = S(x') - S(x^{(k)})$

3) Accept x' with probability $\min(1, e^{-\Delta S})$

$$x^{(k+1)} = x'$$

Otherwise reject it, and keep the previous one.

$$x^{(k+1)} = x^{(k)}$$

The most basic algorithm applicable to any system.

One can make only small updates in Step 1) in order to keep reasonable acceptance rate.

Hybrid Monte Carlo algorithm

Duane, Kennedy, Pendleton, Roweth, Phys.Lett.B 195 (1987) 216

The idea : Use the information of $S(x)$ in Step 1) of Metropolis algorithm.

Introduce new variable p — "momentum" conjugate to x

$$Z = \int dx\, e^{-S(x)} = \int dx\, dp\, e^{-H(x,p)}$$

$$H(x,p) = \frac{1}{2}p^2 + S(x)$$ "Hamiltonian"

a) generate p with probability $\propto e^{-\frac{1}{2}p^2}$ needed for ergodicity

b) solve a fictitious time evolution using $H(x,p)$.

$$(x^{(k)}, p) \longrightarrow (x', p')$$

$$\Delta H \approx 0$$

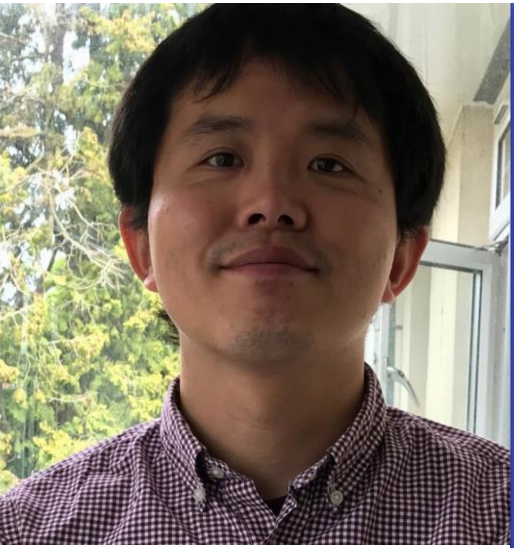
Hamiltonian conservation
not exact due to errors from discretizing time

absorbed completely by Step c)

c) accept x' with probability $\min(1, e^{-\Delta H})$

One can make large updates within reasonable acceptance rate.

If you want to learn more about Monte Carlo methods,...



Masanori Hanada
花田　政範
（Univ. of Surrey, UK）

So Matsuura
松浦　壮
(Keio Univ.)

4. HMC on the worldvolume

HMC algorithm on the worldvolume

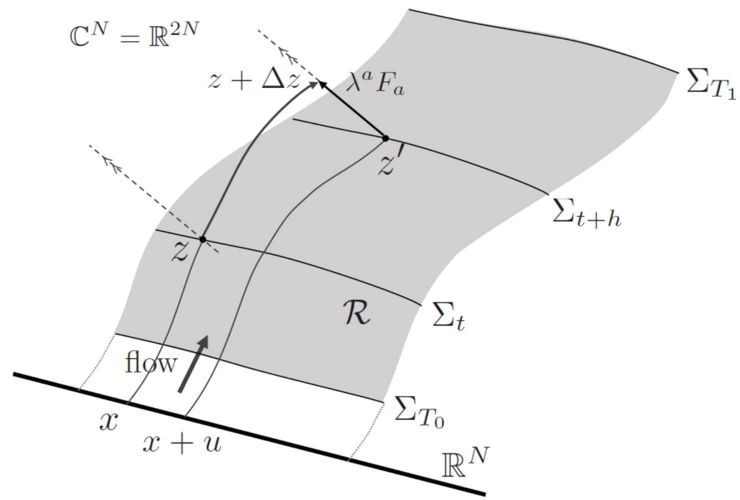
the Hamiltonian dynamics constrained on the worldvolume

"The normal force" has to be taken into account.

（垂直抗力）　$\mathcal{N}^i \in \mathbb{C} \quad (i = 1, \cdots, N)$

It has to be orthogonal to
all the tangent vectors : $E^i_\mu = \dfrac{\partial z^i(\xi)}{\partial \xi^\mu}$

$$\begin{cases} E^i_0 = \dfrac{\partial}{\partial \tau}\phi_i(x;\tau) = \overline{\dfrac{\partial S}{\partial z^i}} \\ E^i_j = \dfrac{\partial}{\partial x_j}\phi_i(x;\tau) = J_{ij}(x;\tau) \end{cases}$$



$$\mathrm{Re}(\overline{\mathcal{N}^i} E^i_0) = 0 \cdots\cdots\cdots\cdots (\#)$$

$$\boxed{\mathrm{Re}(\overline{\mathcal{N}^i} E^i_j) = 0 \quad (j = 1, \cdots, N)}$$

$$\mathcal{N}^i = \sum_{k=1}^{N} \lambda_k F^i_k \,, \quad \lambda_k \in \mathbb{R} \,, \quad F^i_k = i E^i_k$$

$$\begin{aligned} \mathrm{Re}(\overline{F^i_k}\, E^i_j) &= \mathrm{Im}(\overline{E^i_k}\, E^i_j) \\ &= \mathrm{Im}(J^\dagger J)_{kj} \\ &= 0 \end{aligned}$$

λ_k should be chosen to satisfy (#).

Hamilton eq. on the worldvolume

$$Z_W = \int d\tau \, e^{-W(\tau)} \int_{\Sigma_\tau} d\phi \, e^{-S(\phi)}$$
$$= \int_{\mathcal{R}} \mathcal{D}z \boxed{\alpha^{-1} e^{i\varphi} \, e^{-i\,\mathrm{Im}S(z)}} \, e^{-\mathrm{Re}S(z) - W(\tau)}$$

treated as a reweighting factor in measurements

$$V(z, \bar{z}) = \mathrm{Re}(S(z)) + W(\tau(z, \bar{z}))$$

$$H = \overline{\pi^i} \pi^i + V(z, \bar{z})$$

Hamilton eq. $\begin{cases} \dfrac{dz^i}{dt} = \pi^i \\ \dfrac{d\pi^i}{dt} = -\dfrac{\partial}{\partial \bar{z}^i} V(z, \bar{z}) + \mathcal{N}^i \end{cases}$

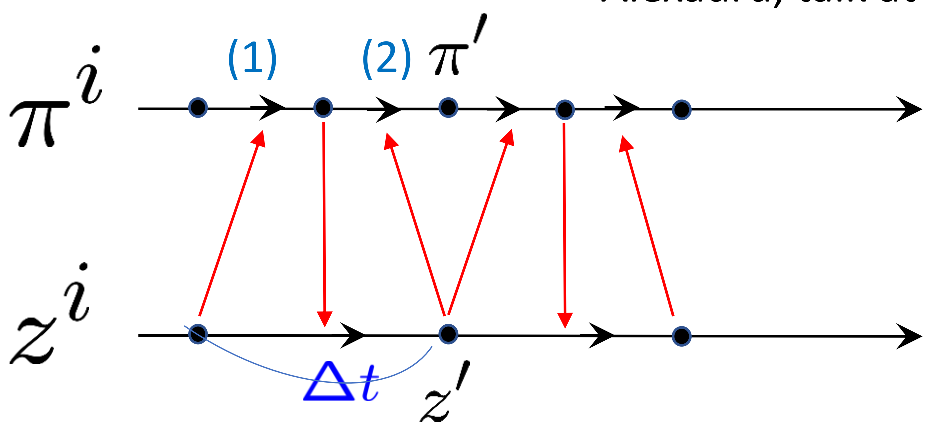
"normal force"

should be determined s.t.
$\pi^i \in \mathcal{T}_z$ (tangent space)

Discretizing the Hamilton eq.

“RATTLE” H.C.Anderson(’83)

c.f.) Fujii et al. JHEP 10 (2013) 147,
Fukuma, Matsumoto, Umeda, arXiv:1912.13303
Alexadru, talk at LATTICE2019, Wuhan



$$\frac{d\pi^i}{dt} = -\frac{\partial}{\partial \bar{z}^i} V(z, \bar{z}) + \mathcal{N}^i$$

$$\frac{dz^i}{dt} = \pi^i$$

How to determine the normal force $\mathcal{N}^i$ at each step.

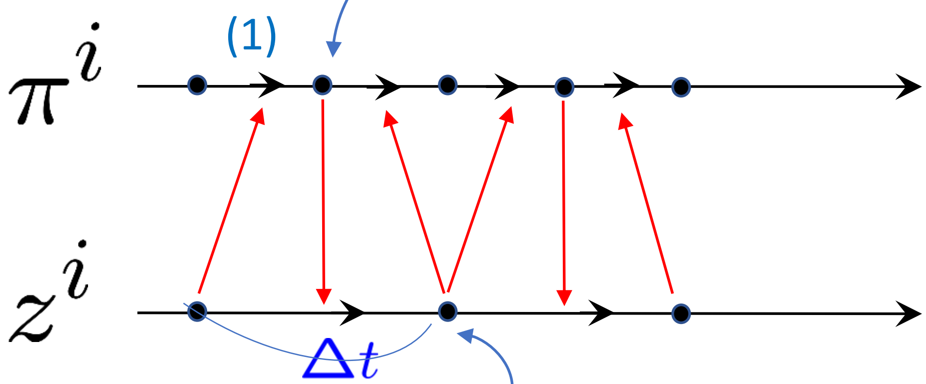
(1) Require z' to lie on the worldvolume.
(2) Require π' to lie on $\mathcal{T}_{z'}$ (tangent space at z')

⇒ $z^i(n\Delta t)$: on the worldvolume
$\pi^i(n\Delta t)$: on the tangent space at $z^i(n\Delta t)$

exact at the discretized level !

Determining the normal force (1)

$$\pi^i\left(\frac{\Delta t}{2}\right) = \pi^i(0) - \frac{\Delta t}{2}\frac{\partial V(z,\bar{z})}{\partial \bar{z}^i}\bigg|_{z(0)} + \mathcal{N}^i$$



$$\frac{d\pi^i}{dt} = -\frac{\partial}{\partial \bar{z}^i}V(z,\bar{z}) + \mathcal{N}^i$$

$$\frac{dz^i}{dt} = \pi^i$$

$$z^i(\Delta t) = z^i(0) + \Delta t\, \pi^i\left(\frac{\Delta t}{2}\right)$$

Require $z^i(\Delta t)$ to lie on the worldvolume. c.f.) $z^i(0) = \phi^i(x;\tau)$

i.e., $\exists (u,h)$ s.t. $z^i(\Delta t) = \phi^i(x+u;\tau+h)\cdots\cdots\cdots(\flat)$

The normal force
$$\begin{cases} \mathcal{N}^i = \sum_{k=1}^{N} \lambda_k F_k^i\ , \quad \lambda_k \in \mathbb{R}\ , \quad F_k^i = iE_k^i \\ \mathrm{Re}(\overline{\mathcal{N}^i}E_0^i) = 0\cdots\cdots\cdots(\#) \end{cases}$$

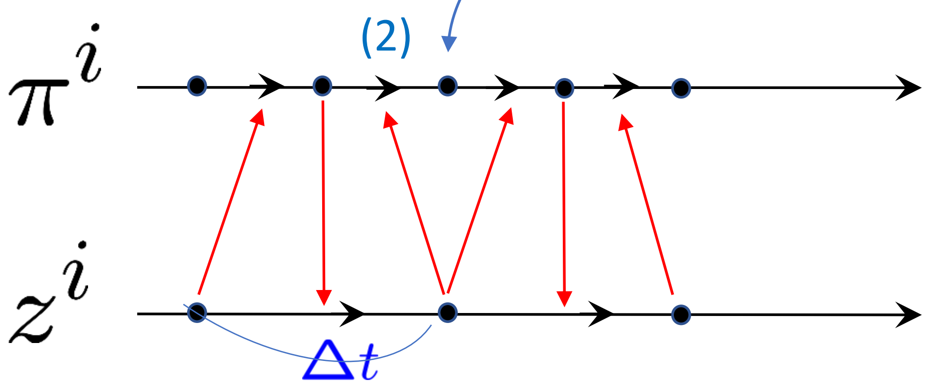
$(2N+1)$ unknowns : $u^i,\ h,\ \lambda_k$

$(2N+1)$ equations : $(\flat)$, $(\#)$

Can be solved by iterative methods like the Newton method.

Determining the normal force (2)

$$\pi^i(\Delta t) = \overbrace{\boxed{\pi^i\left(\frac{\Delta t}{2}\right) - \frac{\Delta t}{2}\,\frac{\partial V(z,\bar{z})}{\partial \bar{z}^i}\bigg|_{z(\Delta t)}}}^{\tilde{\pi}^i} + \mathcal{N}^i$$



$$\frac{d\pi^i}{dt} = -\frac{\partial}{\partial \bar{z}^i} V(z,\bar{z}) + \mathcal{N}^i$$

$$\frac{dz^i}{dt} = \pi^i$$

Require $\pi^i(\Delta t)$ to lie on $\mathcal{T}_{z(\Delta t)}$.

$$\Downarrow$$

$$\begin{aligned} \pi^i(\Delta t) &= \text{projection of } \tilde{\pi}^i \text{ onto } \mathcal{T}_{z(\Delta t)} \\ &= g^{\mu\nu} E^i_\mu \, \mathrm{Re}(\overline{E^j_\nu}\, \tilde{\pi}^j) \end{aligned}$$

tangent vectors :

$$E^i_\mu = \frac{\partial z^i(\xi)}{\partial \xi^\mu}$$

$$g_{\mu\nu} = \mathrm{Re}(\overline{E^i_\mu}\, E^i_\nu)$$

$$g^{\mu\nu} = (g^{-1})_{\mu\nu}$$

appearance of the Jacobian

Note: $\begin{cases} E^i_0 = \dfrac{\partial}{\partial \tau}\phi_i(x;\tau) = \overline{\dfrac{\partial S}{\partial z^i}} \\ E^i_j = \dfrac{\partial}{\partial x_j}\phi_i(x;\tau) = J_{ij}(x;\tau) \end{cases}$

In solving the Hamilton eq. on the worldvolume,
the Jacobian J appears only in the form : $J_{ij}(x;\tau)\, v^j$

$$\frac{\partial}{\partial \sigma} J_{ij}(x;\sigma) = \overline{H_{ik}(\phi(x;\sigma)) J_{kj}(x;\sigma)}$$

$\mathcal{O}(N^3)$ calculations

$$H_{ij}(z) \equiv \frac{\partial}{\partial z^i}\frac{\partial}{\partial z^j} S(z) \qquad J(x;0) = 1$$

$$v^i(\sigma) \equiv J_{ij}(x;\sigma)\, v^j \qquad v^j \in \mathbb{R}$$

$$\frac{\partial}{\partial \sigma} v^i(\sigma) = \overline{H_{ij}(\phi(x;\sigma)) v^j(\sigma)}$$

$\mathcal{O}(N^2)$ calculations

(For local field theories, $\mathcal{O}(N)$ calculations)

5. Results for Random Matrix Theory

Random Matrix Theory for finite density QCD

$$\boxed{Z_n(m,\mu) = \int dX \; \det(D+m)\, e^{-n\,\mathrm{tr}(X^\dagger X)}}$$

$$D = \begin{pmatrix} 0 & iX+\mu \\ iX^\dagger+\mu & 0 \end{pmatrix}$$

M.A.Stephanov, PRL 76 (1996) 4472 [hep-lat/9604003]

$$\mathbb{C} \ni X_{ij} = x_{ij} + i\, y_{ij}$$

general $n \times n$ matrix

flow these variables into complex plane!

exact results :

$$Z_n(m,\mu) = n\, e^{n(\mu^2-m^2)} \int_0^\infty d\rho\, e^{-n\rho}\, I_0(2nm\sqrt{\rho})\,(\rho-\mu^2)^n$$

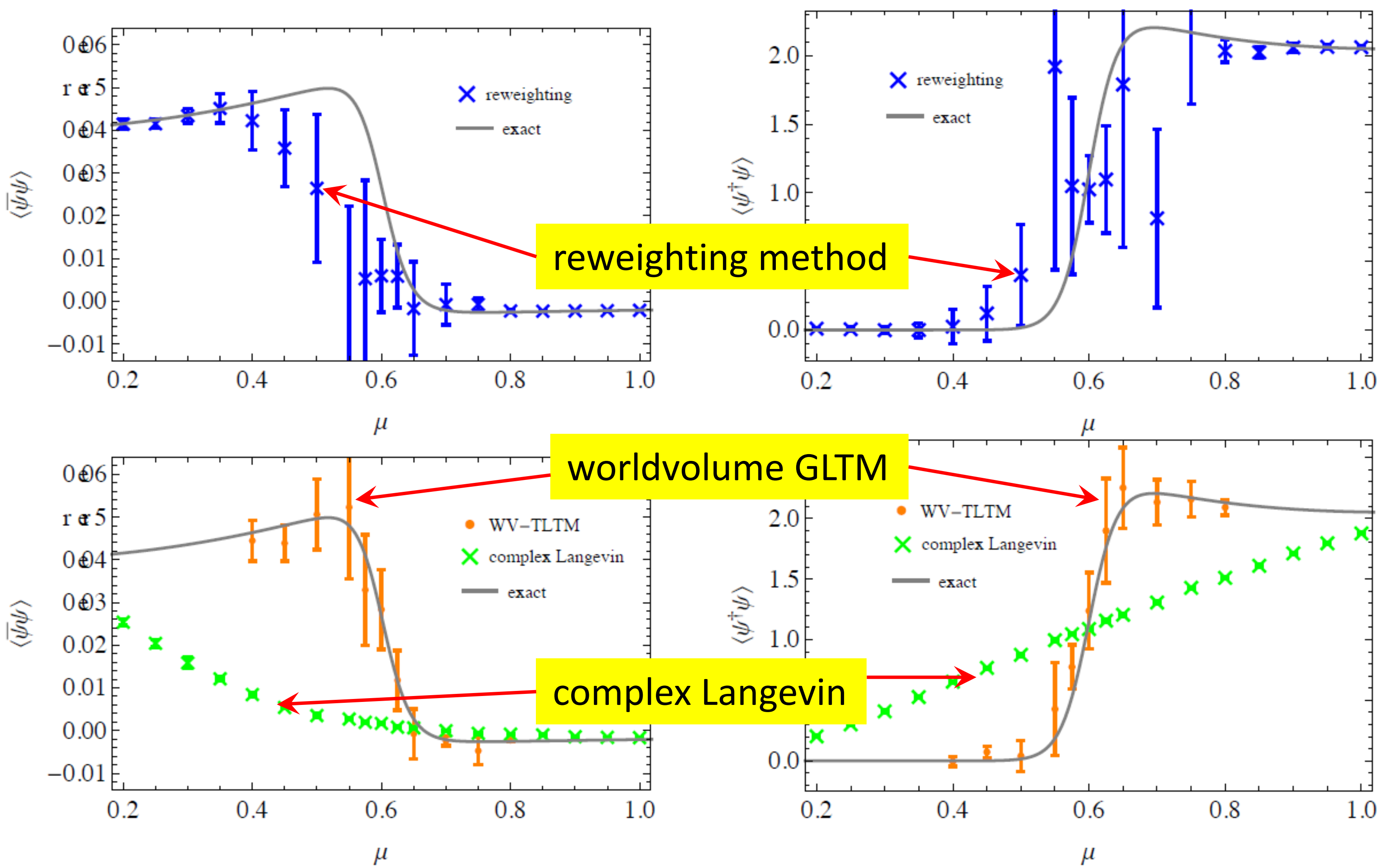
$$\left\{ \begin{array}{lcl} \langle\bar\psi\psi\rangle & = & \dfrac{1}{2n}\dfrac{\partial}{\partial m}\log Z_n(m,\mu) \\ \langle\psi^\dagger\psi\rangle & = & \dfrac{1}{2n}\dfrac{\partial}{\partial \mu}\log Z_n(m,\mu) \end{array} \right.$$

"chiral condensate"

"fermion number density"

Results for $n = 10, \ m = 0.004$

chiral condensate　　　　fermion number density



Worldvolume GLTM works even near the phase transition ! (c.f., reweighting)
Complex Langevin method fails for this model because of the singular drift problem.

6. Summary and Discussions

Summary and discussions

- Solving the sign problem in Monte Carlo methods is extremely important in theoretical physics.

- Many methods are being developed in recent years.

  - density of state method — conventional MC
  - complex Langevin method
  - generalized Lefschetz thimble method
  - path optimization method

  complex Langevin, generalized Lefschetz thimble, path optimization: complexifying variables using holomorphicity

  - tensor renormalization group method — non-stochastic method
  - quantum computing — different hardware

my opinion

Choose the best method depending on the system.

As for approaches based on complexifying variables

- Complex Langevin method is the best whenever it is applicable.
  (easy to write a code and computationally less demanding)

  $\mathcal{O}(N)$ calculations !

  as in ordinary Monte Carlo methods

  So, try it first!
  It may fail in some parameter regions, though.

- In that case, use the generalized Lefschetz thimble method !
  (It is expected to work even in cases where the CLM fails.)

  $\mathcal{O}(N^3)$ calculations

  needed to calculate Jacobian at measurements.

The worldvolume hybrid Monte Carlo algorithm is really the key to application of the GLTM to many interesting systems !