Sign problem and the Worldvolume Hybrid Monte Carlo method

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"Challenges and opportunities in Lattice QCD simulations and related fields"

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Based on work with

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Issaku Kanamori (RIKEN R-CCS)

Today's talk

- What is the sign problem?
  - Difficulty for complex action
  - Why the naive method (reweighting) fails
- Overview of various approaches
- Argue that
  Worldvolume Hybrid Monte Carlo method
  is a promising method

Introduction

Basics of Monte Carlo methods

■ What we want: expectation values of observables

$$\begin{cases} x = (x^i) \in \mathbb{R}^N : \text{dynamical variable } (N\text{: DOF}) \\ S(x): \text{ action} \\ \mathcal{O}(x): \text{ observable} \\ dx = \prod_{i=1}^{N} dx^i \end{cases}$$

(e.g. scalar field

$$x^i \leftrightarrow \phi(t,\mathbf{x})$$

$$S(x) \leftrightarrow S[\phi] = \int dt\, d^3\mathbf{x} \left[\frac{1}{2}(\partial_t \phi)^2 + \cdots \right]$$

$$dx = \prod_i dx^i \leftrightarrow [d\phi] = \prod_{t,\mathbf{x}} d\phi(t,\mathbf{x})$$

)

$$\langle \mathcal{O} \rangle \equiv \int dx\, \rho(x) \mathcal{O}(x) \qquad \left(\rho(x) \equiv \frac{e^{-S(x)}}{\int dx\, e^{-S(x)}} \right)$$

When $N \gg 1$, numerical multiple integrals are unrealistic

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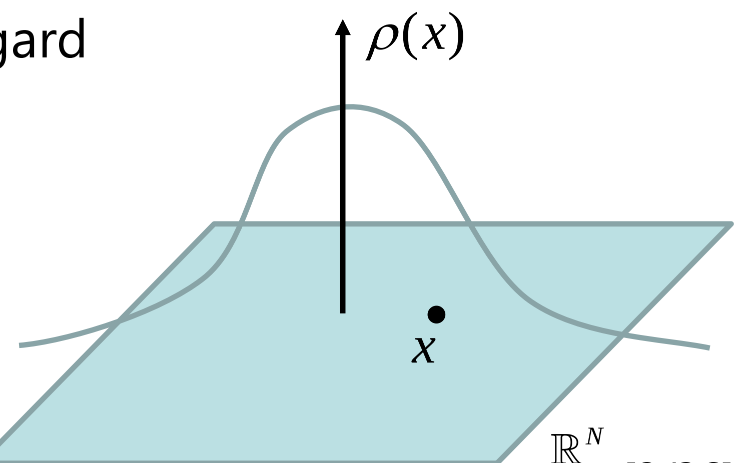
However, when $S(x)$ is real-valued, one can regard

$$\rho(x) = \frac{e^{-S(x)}}{\int dx\, e^{-S(x)}}$$

as a probability distribution $\left(\because \begin{array}{l} \rho(x) \geq 0 \quad (\forall x) \\ \int dx\, \rho(x) = 1 \end{array} \right)$

⇩

Markov chain Monte Carlo method



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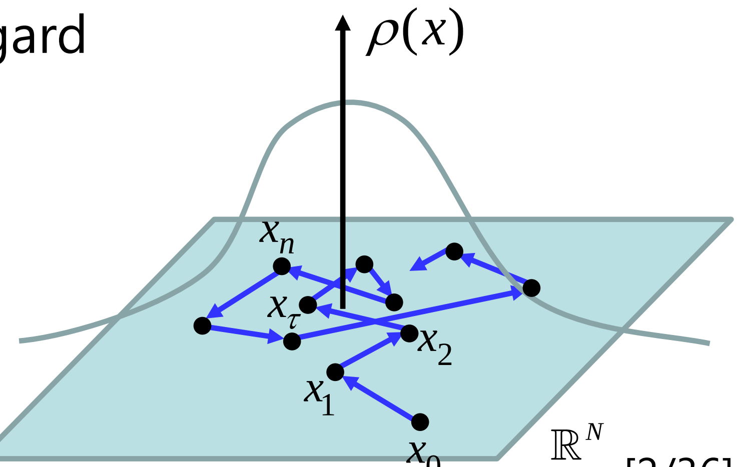


What if the action is complex-valued?

■ **complex action** $S(x) = \mathrm{Re}\, S(x) + i\, \mathrm{Im}\, S(x) \in \mathbb{C} \quad \big(\mathrm{Im}\, S(x) \neq 0\big)$

$\rho(x)$ cannot be regarded as a probability distribution $\left(\rho(x) = \dfrac{e^{-S(x)}}{\int dx\, e^{-S(x)}} \right)$

■ **Examples**

- finite-density QCD

Q: baryon number
μ: chemical potential

$$Z = \mathrm{tr}\, e^{-\beta(H-\mu Q)}$$

$$= \int [dA_\mu][d\psi d\bar{\psi}]\, e^{(1/2g^2)\int \mathrm{tr}\, F_{\mu\nu}^2 + \int \bar{\psi} D(A_\mu;\mu)\psi}$$

$$\left(\gamma_\mu = \gamma_\mu^\dagger \ (\mu = 1,2,3,0) \quad \{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu} 1_4 \right)$$

$$\big(D(A_\mu;\mu) = \gamma_\mu D_\mu + m + \mu\gamma_0 \big)$$

$$= \int [dA_\mu]\, e^{(1/2g^2)\int \mathrm{tr}\, F_{\mu\nu}^2} \boxed{\mathrm{Det}\, D(A_\mu;\mu)}$$

$$\in \mathbb{C} \quad \left(\because \left[\mathrm{Det}\, D(A_\mu;\mu)\right]^* = \mathrm{Det}\, D(A_\mu;-\mu^*) \right)$$

- Quantum Monte Carlo (QMC)

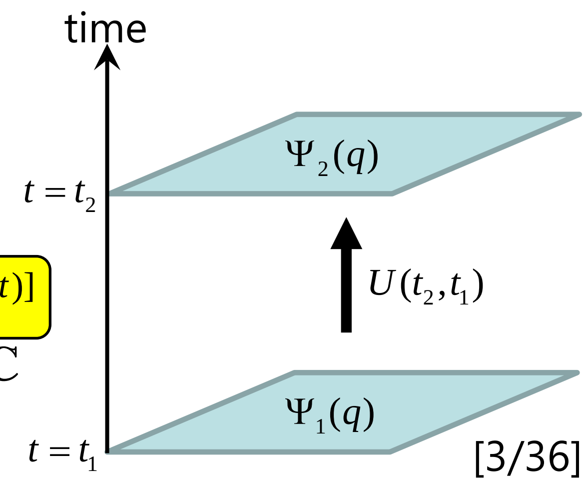
strongly correlated electron systems,
frustrated spin systems, ...

- real-time dynamics of QM/QFT

$$\langle \Psi_2 | U(t_2,t_1) | \Psi_1 \rangle = \int [dq(t)]\, \Psi_2^*\big(q(t_2)\big)\, \Psi_1\big(q(t_1)\big) \boxed{e^{iS[q(t)]}}$$

$$\in \mathbb{C}$$

$$\left(U(t_2,t_1) = T \exp\left[-i \int_{t_1}^{t_2} dt\, H(t) \right] \right)$$



Plan

1. Introduction (done)
2. Sign problem and various approaches
3. Complex Langevin method
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Sign problem

■ **reweighting method**: simplest prescription for the complex action

$$e^{-S(x)} = \underbrace{e^{-\mathrm{Re}\,S(x)}}_{\text{used for a wt}} \ \underbrace{e^{-i\,\mathrm{Im}\,S(x)}}_{\text{treated as part of obs}}$$

$$\langle \mathcal{O}(x) \rangle = \frac{\int dx\, e^{-S(x)} \mathcal{O}(x)}{\int dx\, e^{-S(x)}} = \frac{\int dx\, e^{-\mathrm{Re}\,S(x)} e^{-i\,\mathrm{Im}\,S_I(x)} \mathcal{O}(x) \Big/ \int dx\, e^{-\mathrm{Re}\,S(x)}}{\int dx\, e^{-\mathrm{Re}\,S(x)} e^{-i\,\mathrm{Im}\,S_I(x)} \Big/ \int dx\, e^{-\mathrm{Re}\,S(x)}}$$

highly oscillatory for $N \gg 1$

$$= \frac{\langle e^{-i\,\mathrm{Im}\,S_I(x)} \mathcal{O}(x) \rangle_{\text{rewt}}}{\langle e^{-i\,\mathrm{Im}\,S_I(x)} \rangle_{\text{rewt}}}$$

$$= \frac{e^{-O(N)}}{e^{-O(N)}} \quad \big(= O(1) \big)$$

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But, in numerical calc, the numer and denom are estimated with sample avgs

$$\langle \mathcal{O}(x)\rangle \approx \frac{e^{-O(N)} \pm O(1/\sqrt{N_{\text{conf}}})}{e^{-O(N)} \pm O(1/\sqrt{N_{\text{conf}}})} \qquad \begin{pmatrix} N \;:\; \text{DOF} \\ N_{\text{conf}} \;:\; \text{sample size} \end{pmatrix}$$

$\therefore$ small error $O(1/\sqrt{N_{\text{conf}}}) \le e^{-O(N)} \Leftrightarrow \boxed{N_{\text{conf}} \ge e^{O(N)}}$

SIGN PROBLEM!

Need an exponentially large sample

Example：Gaussian

$$\begin{cases} S(x) = \dfrac{\beta}{2}(x-i)^2 \equiv \mathrm{Re}\,S(x) + i\,\mathrm{Im}\,S(x) \\ \mathcal{O}(x) = x^2 \end{cases} \quad \left(\begin{array}{l} \mathrm{Re}\,S(x) = \dfrac{\beta}{2}(x^2-1) \\ \mathrm{Im}\,S(x) = -\beta x \end{array} \right)$$

$\boxed{\beta \gg 1}$ with $N=1$

large β mimics large DOF

$$\Rightarrow \quad \langle x^2 \rangle = \frac{\langle e^{-i\mathrm{Im}S(x)}\, x^2 \rangle_{\text{rewt}}}{\langle e^{-i\mathrm{Im}S(x)} \rangle_{\text{rewt}}} = \frac{\left(\beta^{-1}-1\right)e^{-\beta/2}}{e^{-\beta/2}}$$

$$\textbf{numerically} \approx \frac{\left(\beta^{-1}-1\right)e^{-\beta/2} \pm O(1/\sqrt{N_{\text{conf}}})}{e^{-\beta/2} \pm O(1/\sqrt{N_{\text{conf}}})}$$

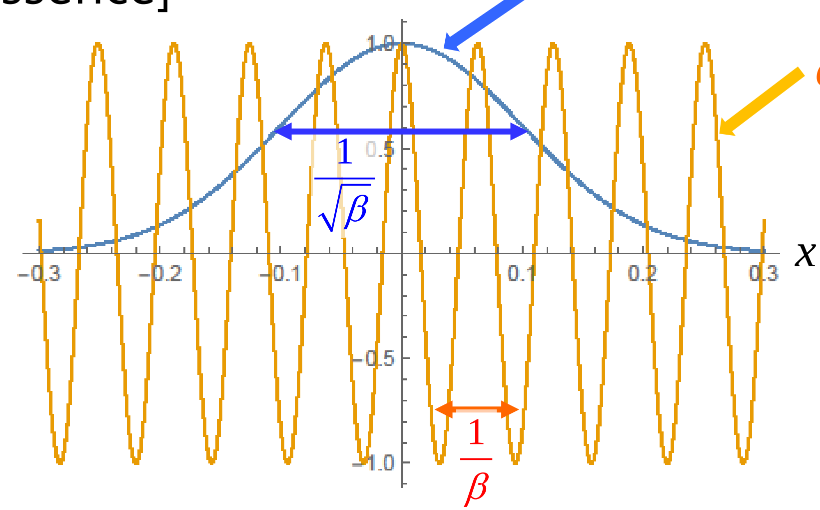
$\Rightarrow$ Necessary sample size:

$$1/\sqrt{N_{\text{conf}}} \lesssim O(e^{-\beta/2}) \quad \Leftrightarrow \quad \boxed{N_{\text{conf}} \gtrsim e^{O(\beta)}}$$

[Essence]

$e^{-\mathrm{Re}\,S(x)} \propto e^{-\beta x^2/2}$

$e^{-i\,\mathrm{Im}\,S(x)} \propto e^{i\beta x}$



In the limit $\beta \to \infty$ $\left(\because 1/\beta \ll 1/\sqrt{\beta}\right)$,
the integration becomes highly oscillatory

Various approaches

■ **method 1 : no use of reweighting**

▼ complex Langevin method **[Parisi 1983, Klauder 1983]**

(may show a wrong convergence problem) (⇐ wrong results w/ small stat errors)

■ **method 2 : deformation of the integration surface**

▼ Lefschetz thimble method **[Witten 2010] [Cristoforetti et al. 2012, Fujii et al. 2013]**

⇩

generalized thimble method **[Alexandru et al. 2015]**

⇩

tempered Lefschetz thimble method **[MF-Umeda 2017, Alexandru et al. 2017]**

⇩

Worldvolume Hybrid Monte Carlo method **[MF-Matsumoto 2020, Fujisawa et al. 2021, ...]**

▼ path optimization method **[Mori-Kashiwa-Ohnishi 2017, Alexandru et al. 2018]**

■ **method 3 : no use of MC in the first place**

▼ tensor network (e.g. TRG) **[Levin-Nave 2007, Shimizu-Kuramashi 2014, Kadoh et al. 2020, ...]**

- good at calculating the free energy (but not so much for correl fcns)
- direct treatement of Grassmann variables

⇨ Akiyama-san's talk

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Basic idea

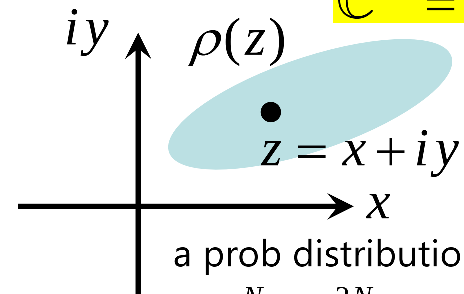
$$\frac{e^{-S(x)}}{\int_{\mathbb{R}^N} dx\, e^{-S(x)}} \in \mathbb{C}$$

does not define
a prob distribution on $\mathbb{R}^N$

$x \in \mathbb{R}^N$

$\to \ z = x + i\,y \in \mathbb{C}^N = \mathbb{R}^{2N}$

$\mathbb{C}^N = \mathbb{R}^{2N}$



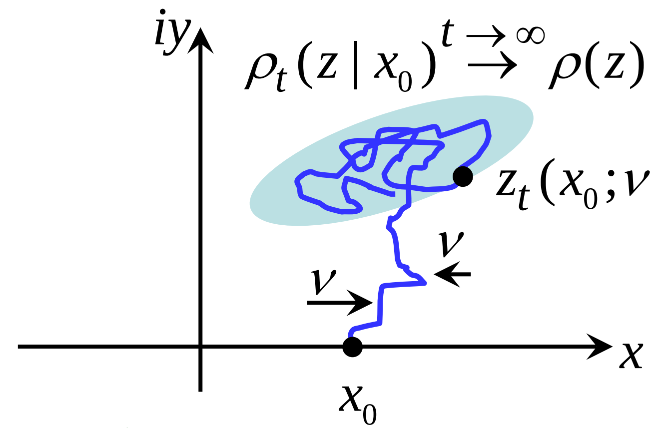
a prob distribution
in $\mathbb{C}^N = \mathbb{R}^{2N}$

■ Algorithm **[Parisi 1983, Klauder 1983]**

$$\begin{cases} \dot{z}_t = -\partial S(z_t) + \nu_t \\ z_{t=0} = x_0 \end{cases} \Rightarrow z_t = z_t(x_0;\nu)$$

ν_t : Gaussian white noise

$$\left(\langle \nu_t \nu_{t'} \rangle_\nu = 2\delta(t-t') \right)$$



$$\left(\rho_t(z\,|\,x_0) \equiv \langle \delta^{2N}(z - z_t(x_0;\nu)) \rangle_\nu \right)$$

The following holds under a certain condition:

$$\int d^{2N}z\, \rho(z)\mathcal{O}(z) \overset{(*)}{=} \frac{\int_{\mathbb{R}^N} dx\, e^{-S(x)}\mathcal{O}(x)}{\int_{\mathbb{R}^N} dx\, e^{-S(x)}} \left(= \langle \mathcal{O}(x) \rangle \right)$$

Then, we have

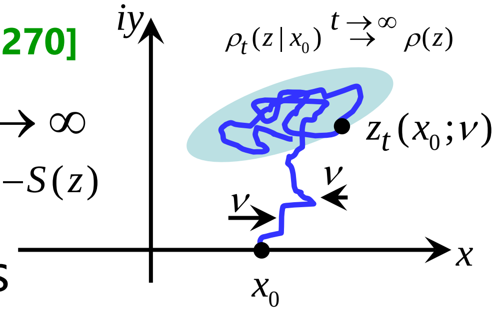
$$\langle \mathcal{O}(x) \rangle \approx \frac{1}{N_{\text{conf}}} \sum_{k=1}^{N_{\text{conf}}} \mathcal{O}(z_{\tau+k})$$

Wrong convergence problem

Condition for $(*)$ to hold : **[Aarts-James-Seiler-Stamatescu 1101.3270]**

$\rho_t(z\,|\,x_o)$: is not spread much in the direction $|\mathrm{Im}\, z| \to \infty$
(t : large) does not have large values near zeros of $e^{-S(z)}$

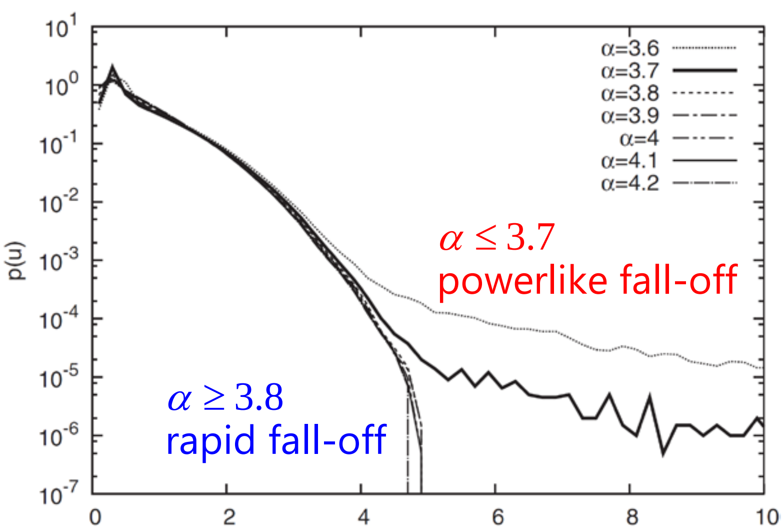
Otherwise, it gives wrong estimates with small stat errors



Explicit form **[Nagata-Nishimura-Shimasaki 1606.07627]**

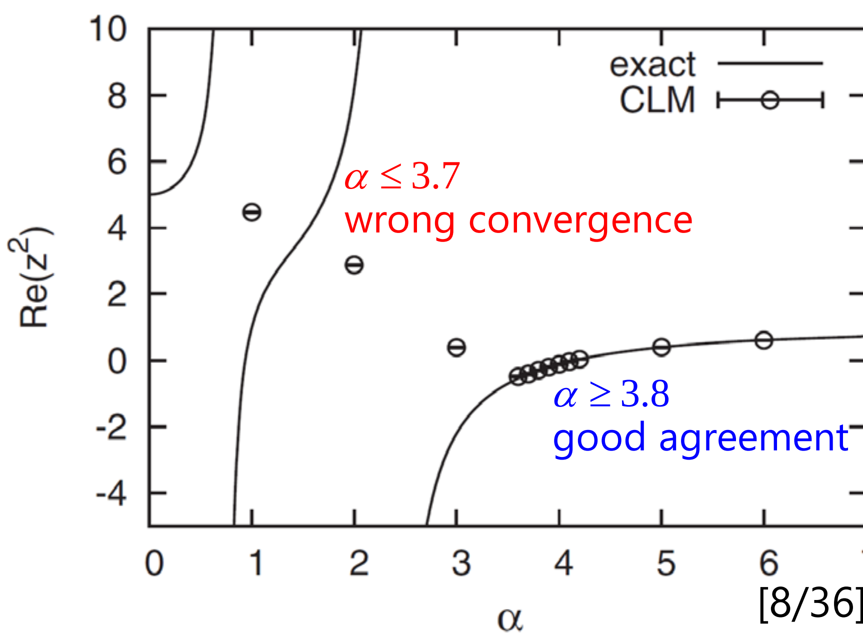
Histogram of $|\partial S(x+iy)|$ decreases rapidly (at least exponentially)

Example : $e^{-S(x)} = (x+i\alpha)^4 e^{-x^2/2}$ **[Nagata-Nishimura-Shimasaki 1606.07627]**



$u \equiv |S'(z)| \quad (z = x+iy)$

$p(u)$: normalized histogram



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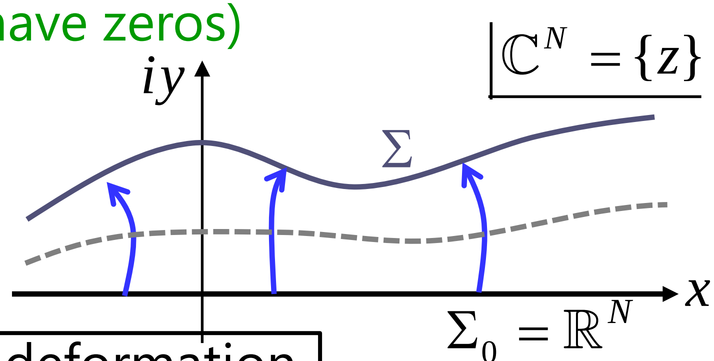
Basic idea of the thimble method (1/2)

■ Complexification of dyn variable: $x=(x^i)\in\mathbb{R}^N \;\Rightarrow\; z=(z^i=x^i+iy^i)\in\mathbb{C}^N$

assumption (satisfied for most cases) $\big(S(x)$: action, $\mathcal{O}(x)$: observable$\big)$

$e^{-S(z)}$, $e^{-S(z)}\mathcal{O}(z)$: entire fcns over $\mathbb{C}^N$ (can have zeros)

Cauchy's theorem



Integrals do not change under continuous deformation of integration surface : $\Sigma_0=\mathbb{R}^N \;\to\; \Sigma\,(\subset\mathbb{C}^N)$

(boundary at $|x|\to\infty$ kept fixed)

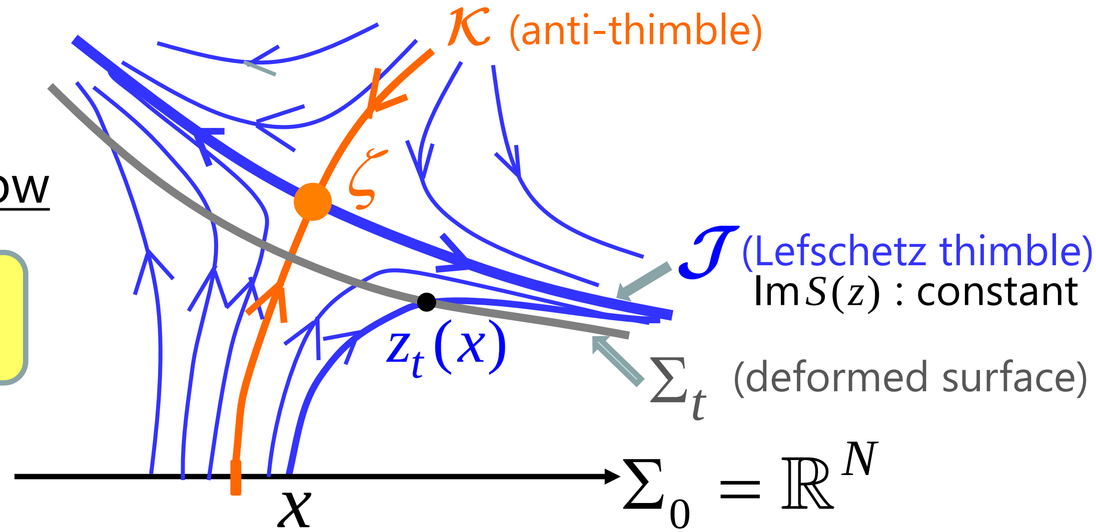
$$\langle\mathcal{O}(x)\rangle \equiv \frac{\int_{\Sigma_0} dx\, e^{-S(x)}\,\mathcal{O}(x)}{\int_{\Sigma_0} dx\, e^{-S(x)}} = \frac{\int_{\Sigma} dz\, e^{-S(z)}\,\mathcal{O}(z)}{\int_{\Sigma} dz\, e^{-S(z)}}$$

severe sign problem

sign problem will be significantly reduced if $\mathrm{Im}\,S(z)$ is almost constant on Σ

Basic idea of the thimble method (2/2)

■ Prescription for deformation



anti-holomorphic gradient flow

$$\dot{z}_t = \overline{\partial S(z_t)} \quad \text{with} \quad z_{t=0} = x$$

property

$$[S(z_t)]^{\cdot} = \partial S(z_t) \cdot \dot{z}_t = |\partial S(z_t)|^2 \geq 0 \quad \Rightarrow \quad \begin{cases} [\mathrm{Re}\, S(z_t)]^{\cdot} \geq 0 \\ [\mathrm{Im}\, S(z_t)]^{\cdot} = 0 \end{cases}$$

⇒ $\begin{cases} \mathrm{Re}\, S(z_t) \text{ : always increases except at crit pt } \zeta \\ \mathrm{Im}\, S(z_t) \text{ : always constant} \end{cases}$ $\left(\begin{array}{l} \zeta \text{ : crit pt} \\ \Leftrightarrow \ \partial S(\zeta) = 0 \end{array} \right)$

⇒ $\Sigma_t \xrightarrow{t \to \infty} \mathcal{J}$ (Lefschetz thimble) ≡ union of orbits starting from ζ

$\mathrm{Im}\, S(z)$: constant on $\mathcal{J}$ $(= \mathrm{Im}\, S(\zeta))$

⇒ Sign problem is expected to disappear on Σ_t at a sufficiently large t

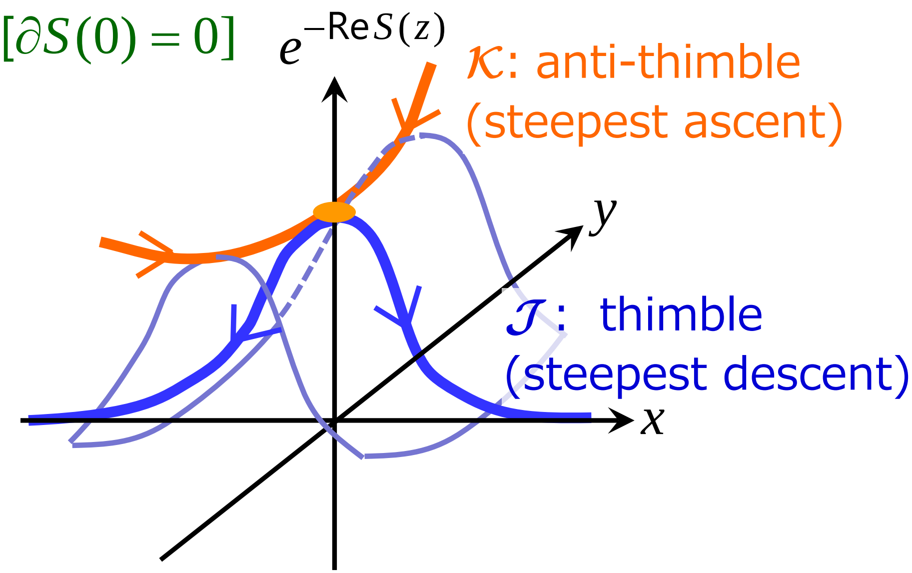
Digression：thimble＝YUBINUKI (指ぬき)

canonical form around a crit pt $\zeta = 0$ $[\partial S(0) = 0]$

■ complex dim 1 ($N = 1$)

$$S(z) = S(0) + \frac{\lambda}{2} z^2 + \cdots \quad (\lambda > 0)$$

⇨ $e^{-\mathrm{Re}\,S(z)} \propto e^{-\lambda(x^2 - y^2)/2}$ ⇨

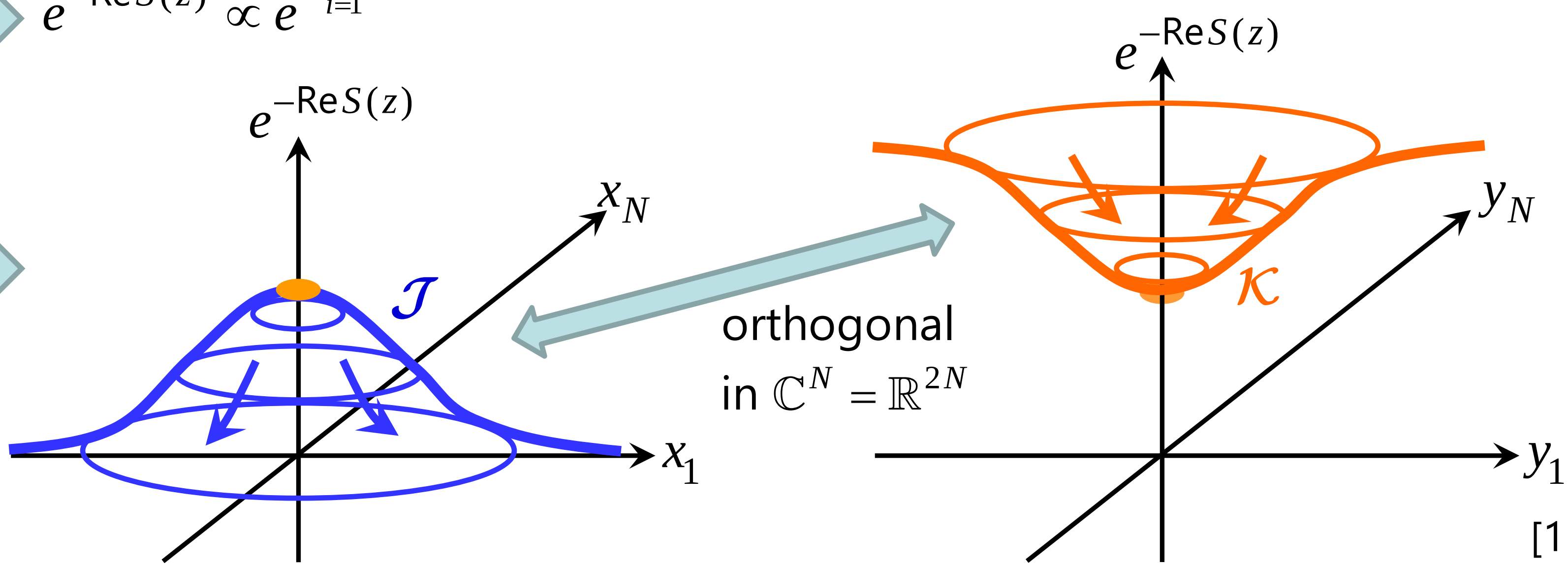


■ complex dim N

$$S(z) = S(0) + \sum_{i=1}^{N} \frac{\lambda_i}{2} z_i^2 + \cdots \quad (\lambda_i > 0)$$

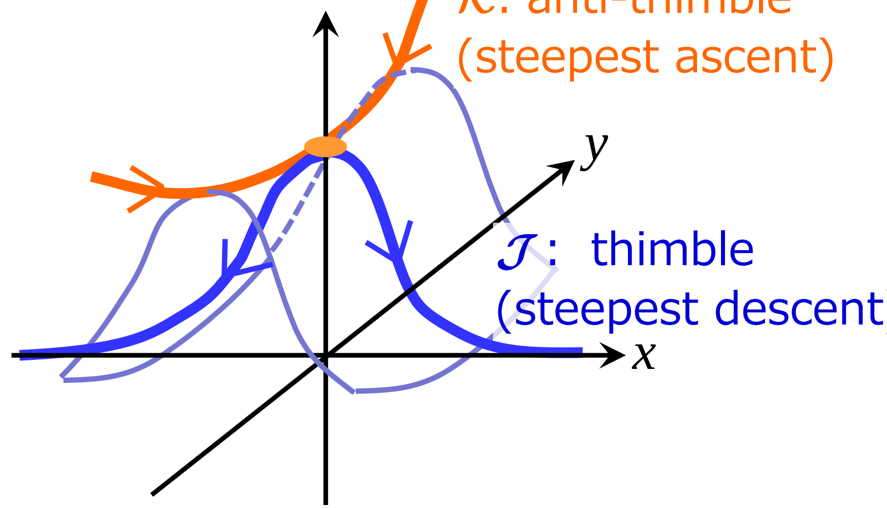
⇨ $e^{-\mathrm{Re}\,S(z)} \propto e^{-\sum_{i=1}^{N} \lambda_i (x_i^2 - y_i^2)/2}$

⇨



Digression：thimble＝YUBINUKI (指ぬき)

canonical form around a crit pt $\zeta = 0$ $[\partial S(0) = 0]$



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■ complex dim N

$$S(z) = S(0) + \sum_{i=1}^{N} \frac{\lambda_i}{2} z_i^2 + \cdots \quad (\lambda_i > 0)$$

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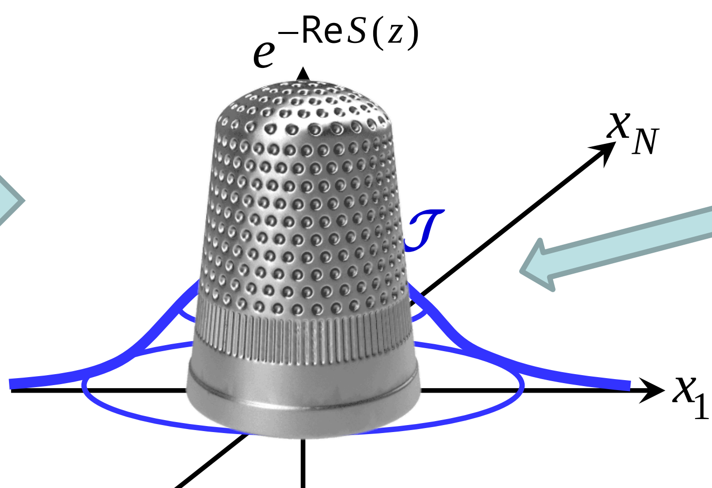
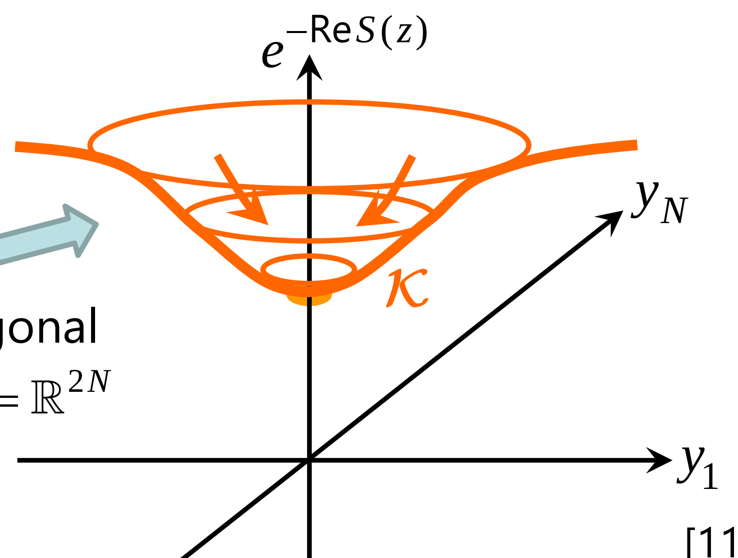
⇨



orthogonal
in $\mathbb{C}^N = \mathbb{R}^{2N}$



How does the sign problem disappear?

- Integration on the original surface $\Sigma_0 = \mathbb{R}^N$ (flow time $t=0$)

$$\langle \mathcal{O}(x) \rangle = \frac{\langle e^{-i\,\mathrm{Im}\,S(x)} \mathcal{O}(x) \rangle_{\Sigma_0(\mathrm{rewt})}}{\langle e^{-i\,\mathrm{Im}\,S(x)} \rangle_{\Sigma_0(\mathrm{rewt})}} \approx \frac{e^{-O(N)} \pm O(1/\sqrt{N_{\mathrm{conf}}})}{e^{-O(N)} \pm O(1/\sqrt{N_{\mathrm{conf}}})}$$

$\begin{pmatrix} N \text{ : DOF} \\ N_{\mathrm{conf}} \text{ : sample size} \end{pmatrix}$

⇒ need a huge size of sample : $N_{\mathrm{conf}} \simeq e^{O(N)}$ **sign problem**

flow

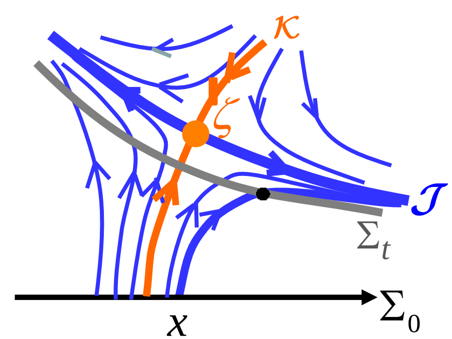
- Integration on a deformed surface Σ_t (flow time t)

$$\langle \mathcal{O}(x) \rangle = \frac{\langle e^{i\theta(z)} \mathcal{O}(z) \rangle_{\Sigma_t}}{\langle e^{i\theta(z)} \rangle_{\Sigma_t}} \approx \frac{e^{-e^{-\lambda t} O(N)} \pm O(1/\sqrt{N_{\mathrm{conf}}})}{e^{-e^{-\lambda t} O(N)} \pm O(1/\sqrt{N_{\mathrm{conf}}})}$$

$\left(e^{i\theta(z)} \equiv e^{-i\,\mathrm{Im}S(z)} \frac{dz}{|dz|} \right)$

$\left[e^{\lambda t} = O(N) \Leftrightarrow t = O(\log N) \right]$

$$= \frac{O(1) \pm O(1/\sqrt{N_{\mathrm{conf}}})}{O(1) \pm O(1/\sqrt{N_{\mathrm{conf}}})}$$

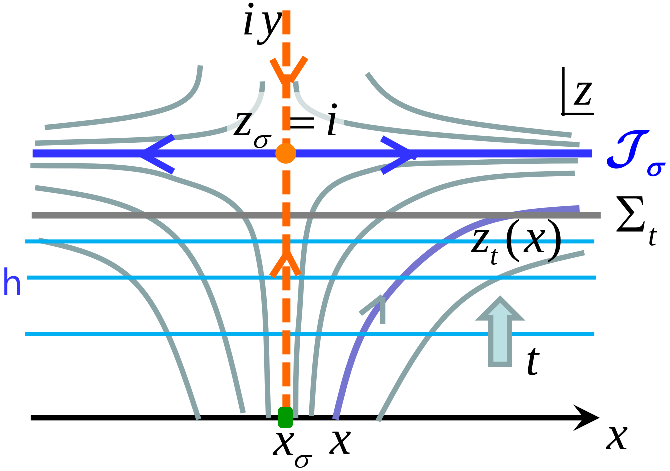


$\left[\lambda : \text{(typical) singular value of Hessian } \partial_i \partial_j S(\zeta) \right]$

⇒ **Sign problem disappears at flow time $t = O(\log N)$**

Example: Gaussian revisited

<u>Gradient flow</u>: $\left[S(z) = (\beta/2)(z-i)^2 \Rightarrow S'(z) = \beta(z-i) \right]$



$$\dot{z}_t = \overline{S'(z_t)} = \beta(\bar{z} + i) \ \text{with } z_{t=0} = x$$

$$\Rightarrow \ z_t(x) = x e^{\beta t} + i(1 - e^{-\beta t}) \quad \therefore |dz| = e^{\beta t} dx$$

exponential growth of coefficient

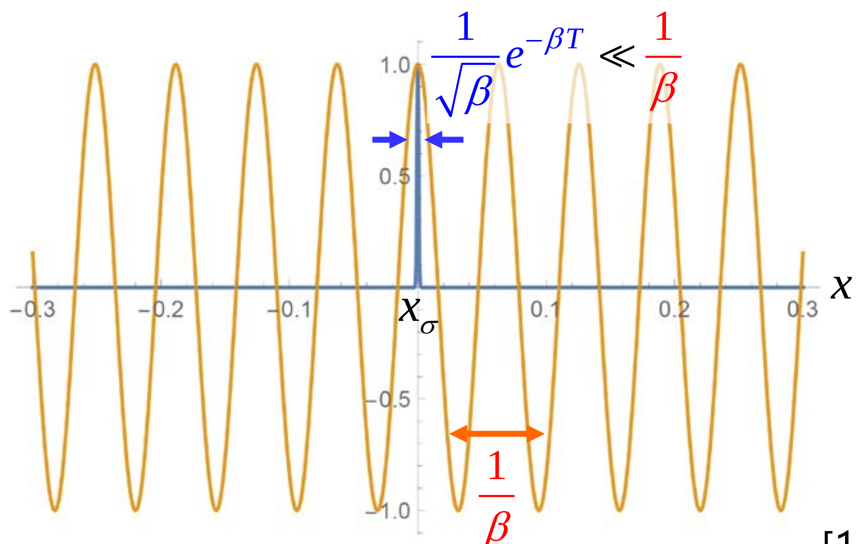
$$\Rightarrow \begin{cases} \mathrm{Re}\, S(z_t(x)) = \dfrac{1}{2} \beta e^{2\beta t} (x^2 - e^{-4\beta t}) \\ \mathrm{Im}\, S(z_t(x)) = -\beta x \ \therefore e^{i\theta(z_t(x))} = e^{i\beta x} \end{cases}$$

$$\Rightarrow \ \langle f(z) \rangle_{\Sigma_t} = \frac{\int_{\Sigma_t} |dz|\, e^{-\mathrm{Re}\, S(z)} f(z)}{\int_{\Sigma_t} |dz|\, e^{-\mathrm{Re}\, S(z)}} = \frac{\int dx\, e^{-(\beta/2) e^{2\beta t} x^2} f(z_t(x))}{\int dx\, e^{-(\beta/2) e^{2\beta t} x^2}}$$

No small numbers appear

if we take a large t $(\equiv T)$ s.t. $e^{-\beta T} \ll \dfrac{1}{\sqrt{\beta}}$

$$\langle x^2 \rangle = \frac{\langle e^{i\theta(z)} z^2 \rangle_{\Sigma_T}}{\langle e^{i\theta(z)} \rangle_{\Sigma_T}} = \frac{e^{-(\beta/2) e^{-2\beta T}} (\beta^{-1} - 1)}{e^{-(\beta/2) e^{-2\beta T}}} = \frac{O(1)}{O(1)}$$



<u>NB</u>. Logarithmic increase is enough:

$$T \sim O(\log \beta) \ (= O(\log N))$$

Appendix: Anti-holomorphic gradient flow

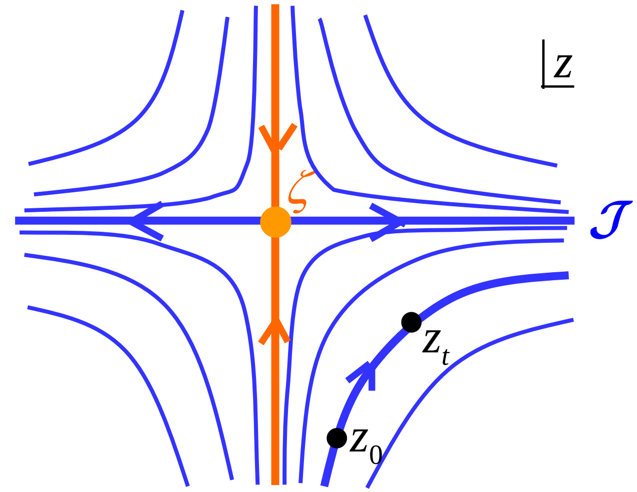
Behaviors around special points

(1) around a critical point $\zeta = \xi + i\eta$:

$$S(z) = \frac{\lambda}{2}(z-\zeta)^2 + \cdots \quad (\lambda > 0)$$

⇨ $\dot{z}_t = \overline{S'(z_t)} \simeq \lambda(\bar{z}_t - \bar{\zeta})$

⇨ $\begin{cases} x_t \simeq \xi + e^{\lambda t}(x_0 - \xi) \\ y_t \simeq \eta + e^{-\lambda t}(y_0 - \eta) \end{cases}$



ζ : critical point $\left(\partial S(\zeta) = 0\right)$

$\mathcal{J} \equiv \{z \mid z \to \zeta \ (t \to -\infty)\}$

: Lefschetz thimble associated with ζ

(2) around a zero z_* of $e^{-S(z)}$:

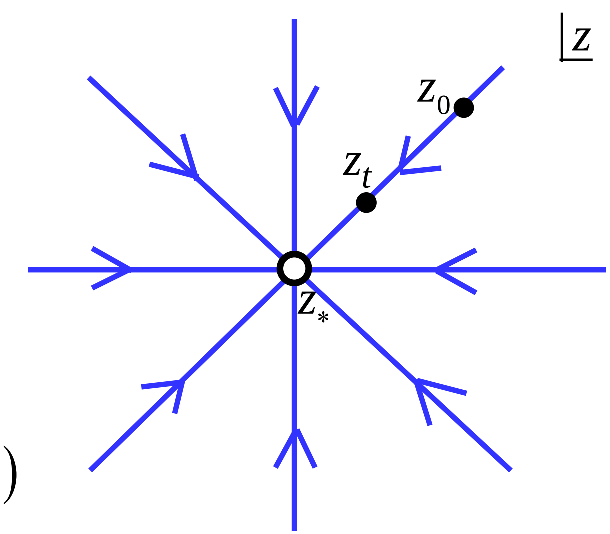
$$e^{-S(z)} = (z - z_*)^{\gamma} f(z) \quad \left(\gamma \in \mathbb{Z}_{>0}\right)$$

⇨ $S(z) = -\gamma \ln(z - z_*) + \cdots$

⇨ $\dot{z}_t = \overline{S'(z_t)} \simeq -\gamma(\bar{z}_t - \bar{z}_*)^{-1}$

⇨ $\begin{cases} |z_t - z_*|^2 \simeq |z_0 - z_*|^2 - 2\gamma t \\ \dfrac{z_t - z_*}{\bar{z}_t - \bar{z}_*} \simeq \text{const} \end{cases}$

(converges to z_* in finite flow time)



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Ergodicity problem in thimble methods

large flow time t ⇨ relaxation of oscillatory integral ⇨ **Sign problem** resolved?

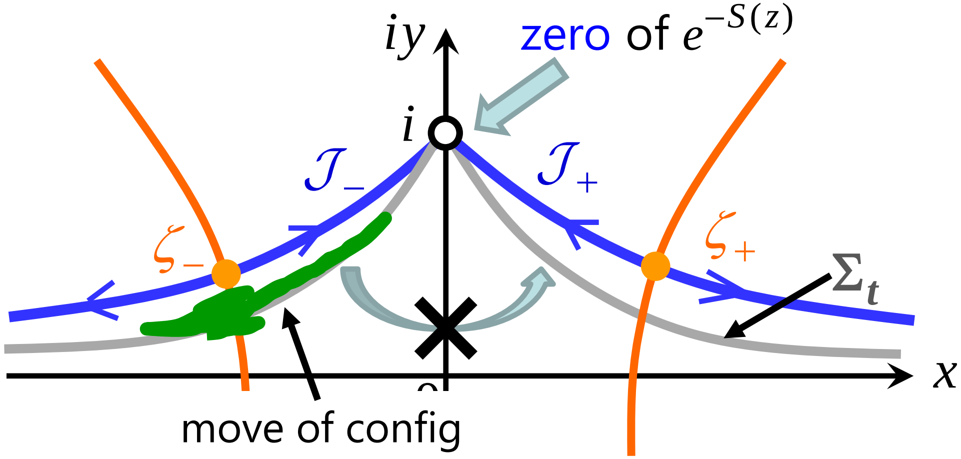
NO!

Ergodicity problem in thimble methods

large flow time t ⇒ relaxation of oscillatory integral ⇒ **Sign problem** resolved? **NO!**

Actually, there comes out another problem at large t : **Ergodicity problem**

E.g. $e^{-S(x)} = e^{-\beta x^2/2}(x-i)^\gamma \ \left(\beta \gg 1,\ \gamma \in \mathbb{Z}_{>0}\right)$ $\left(\begin{array}{l}\text{finite-density QCD :}\\ e^{-S[A]} = e^{-S_{\rm YM}[A]}\mathrm{Det}\,K[A]\end{array}\right)$



- 2 crit pts : $\zeta_\pm$
- 2 thimbles : $\mathcal{J}_\pm$

$\oplus$

- 1 zero of $e^{-S(z)}$: $z_* = i$

zero at $z_* = i$ ⇔ $\mathrm{Re}\,S(z) = +\infty$ at $z_* = i$

⇔ [∞ potential barrier on Σ_T] ⇔ configs cannot move

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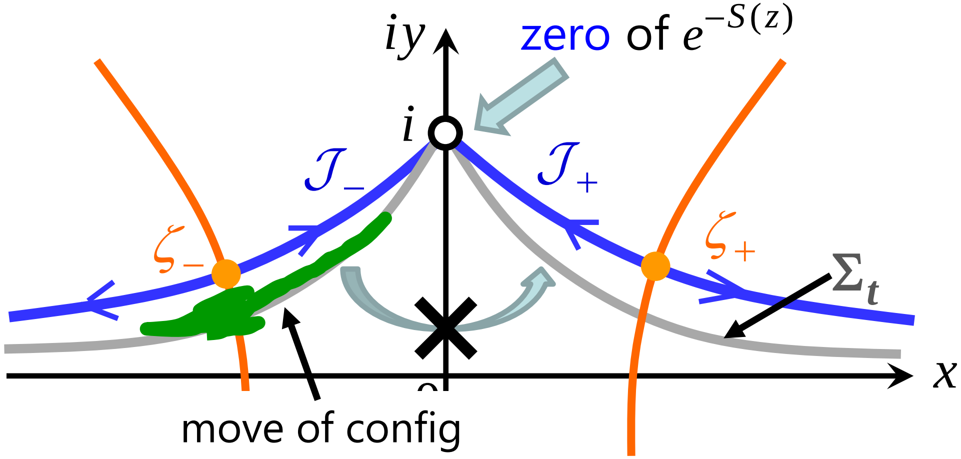

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⇔ [∞ potential barrier on Σ_T] ⇔ configs cannot move

[Marinari-Parisi 1992]
[Swendsen-Wang 1986, Geyer 1991
Hukushima-Nemoto 1996]

⇨ **solution :** **Implement the <u>tempering</u> to the thimble method**

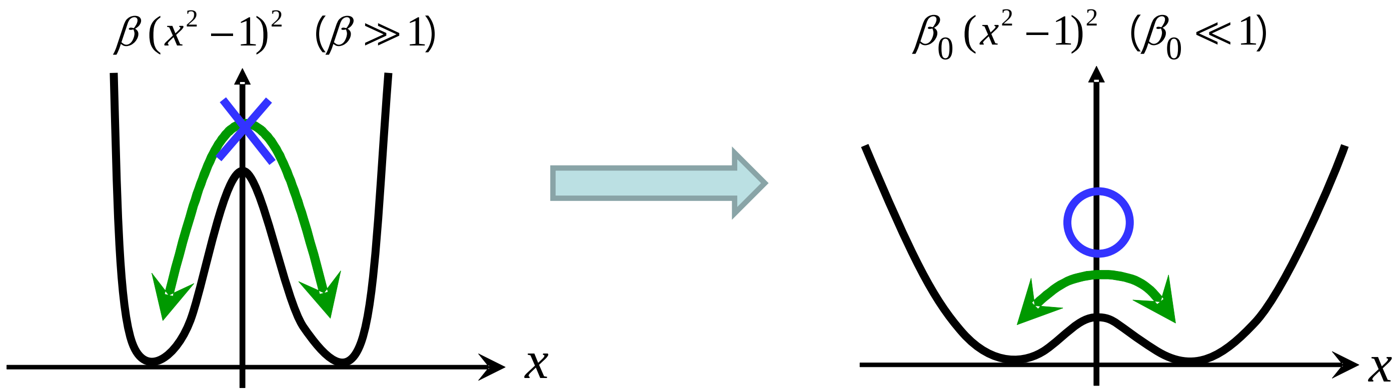
[MF-Umeda 2017] **using the flow time as a temp param**

Idea of tempering

[Marinari-Parisi 1992]

Suppose that the action $S(x;\beta)$ gives an ergodicity problem which disappears at a different value of β (say β_0)

Example： $S(x;\beta)=\beta\,(x^2-1)^2$ with $\beta \gg 1$



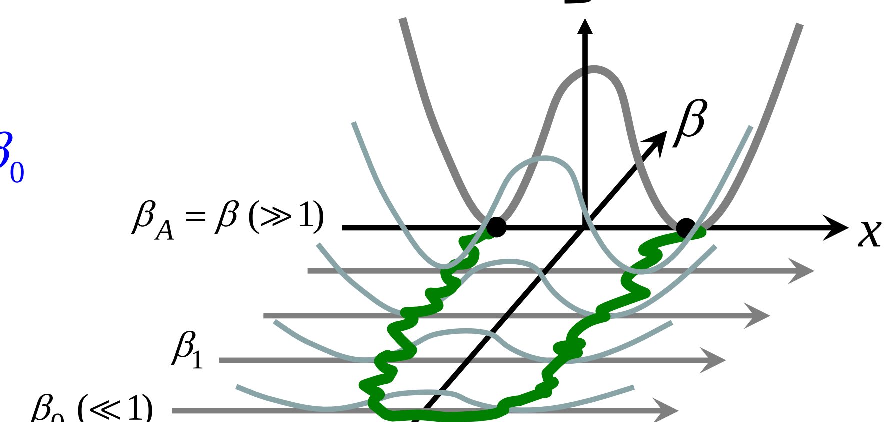
transition is difficult
due to the high potl barrier

transition is easy

Extend the config space by inserting multiple replicas between $\beta\,(\equiv \beta_A)$ and β_0

Easy transitions through detours

(Extended config space has AdS geometry **[MF-Matsumoto-Umeda 2018]**)



【parallelization】 "parallel tempering" or "replica exchange Monte Carlo"

[Swendsen-Wang 1986, Geyer 1991, Hukushima-Nemoto 1996]

Tempered Lefschetz thimble method

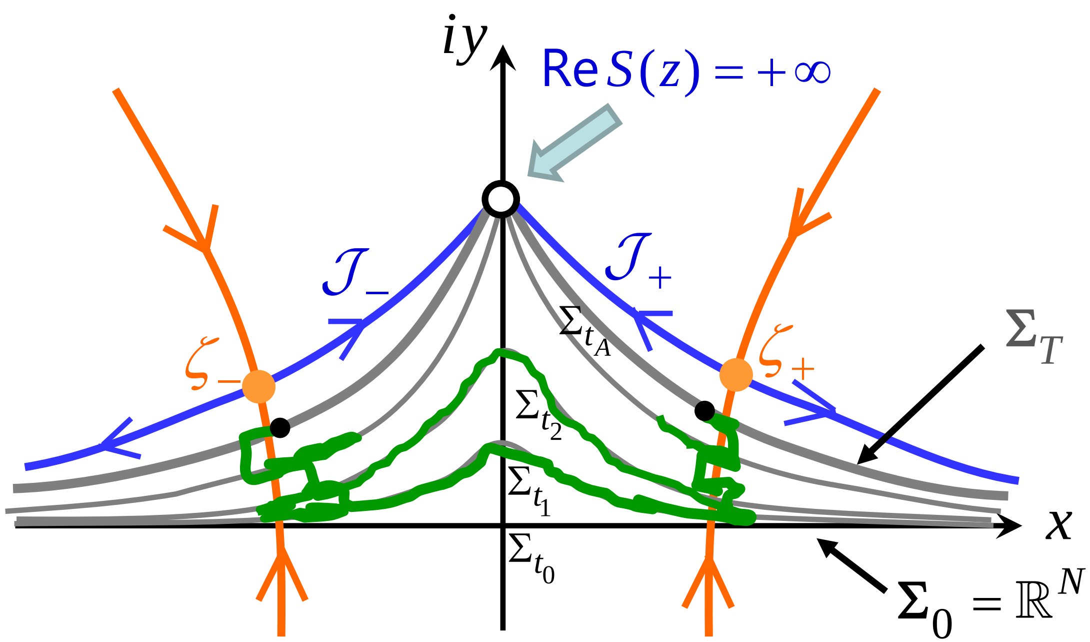
[Fukuma-Umeda 1703.00861]

■ TLT method

(1) Introduce replicas in between the initial integ surface $\Sigma_0 = \mathbb{R}^N$ and the target deformed surface Σ_T as $\left\{\Sigma_{t_0=0},\ \Sigma_{t_1},\ \Sigma_{t_2},\ \ldots,\ \Sigma_{t_A=T}\right\}$

(2) Setup a Markov chain for the extended config space $\{(t_a, x)\}$

(3) After equilibration, estimate observables with a subsample on Σ_T



Sign and ergodicity problems are solved simultaneously !

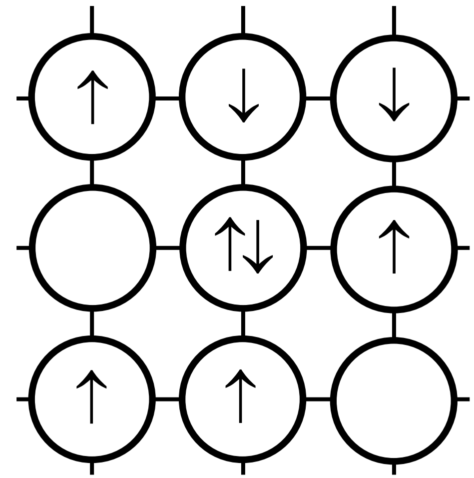
Hubbard model (1/4)

■ Hubbard model   toy model for electrons in a solid **[Hubbard 1963]**

- $c^\dagger_{\mathbf{x},\sigma},\ c_{\mathbf{x},\sigma}$: creation/annihilation of an electron (site $\mathbf{x}$, spin $\sigma(=\uparrow,\downarrow)$)
- Hamiltonian

$$H = -\kappa \sum_{\langle \mathbf{x},\mathbf{y}\rangle} \sum_{\sigma} c^\dagger_{\mathbf{x},\sigma} c_{\mathbf{y},\sigma} - \mu \sum_{\mathbf{x}} \left(n_{\mathbf{x},\uparrow} + n_{\mathbf{x},\downarrow}\right) + U \sum_{\mathbf{x}} n_{\mathbf{x},\uparrow} n_{\mathbf{x},\downarrow}$$

$$\begin{cases} n_{\mathbf{x},\sigma} \equiv c^\dagger_{\mathbf{x},\sigma} c_{\mathbf{x},\sigma} \\ \kappa\,(>0) : \text{hopping parameter} \\ \mu : \text{chemical potential} \\ U\,(>0) : \text{on-site repulsive potential} \end{cases}$$



$(N_S$: # of sites$)$

- Quantum Monte Carlo (discretized imaginary time : $\beta = N_\tau \epsilon$)

  Trotter decomposition + bosonization (HS transformation)

$$\Rightarrow \quad Z_{\beta,\mu} \equiv \mathrm{tr}\, e^{-\beta H}$$

$$\approx \int [d\phi] e^{-S[\phi_{\ell,\mathbf{x}}]} \equiv \int \prod_{\ell=1}^{N_\tau} \prod_{\mathbf{x}} d\phi_{\ell,\mathbf{x}}\ e^{-(1/2)\sum_{\ell,\mathbf{x}} \phi_{\ell,\mathbf{x}}{}^2} \det M_a[\phi] \det M_b[\phi]$$

$$M_{a/b}[\phi] \equiv 1_{N_S} + e^{\pm\beta\mu} \prod_{\ell} \left(e^{\epsilon\kappa K}\, \mathrm{diag}[e^{\pm i\sqrt{\epsilon U}\phi_{\ell,\mathbf{x}}}] \right) : N_S \times N_S \text{ matrix}$$

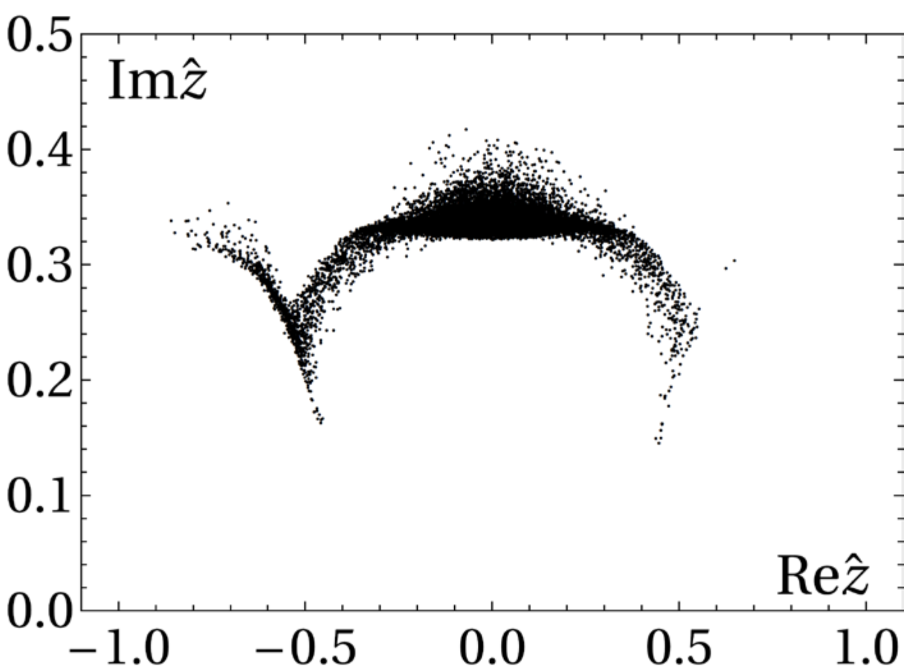
Hubbard model (2/4)

[MF-Matsumoto-Umeda 1906.04243]

scattered plot of flowed configs at $T = 0.5$ $(\beta\mu = 5)$

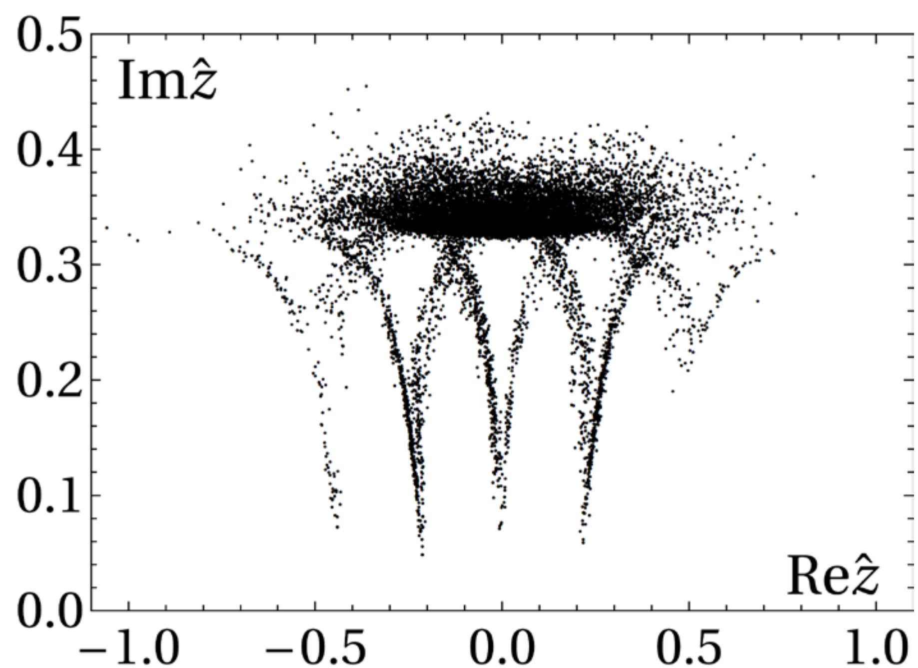
(projected on a plane $\hat{z} = (1/N)\sum_i z^i$)

w/o temp



stuck to a small # of thimbles

w/ temp

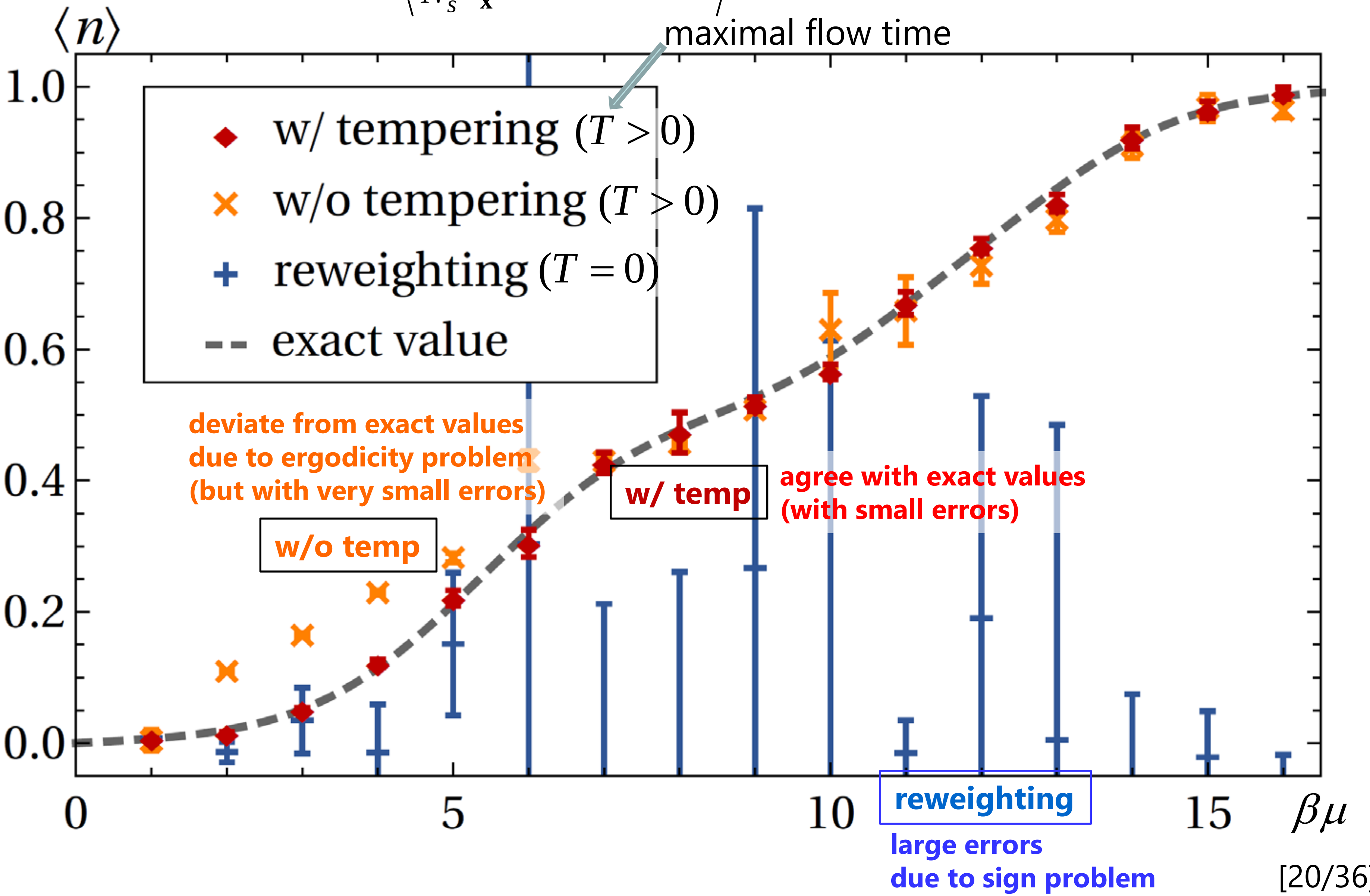


distributed widely
over many thimbles

Hubbard model (3/4)

[MF-Matsumoto-Umeda 1906.04243]

$$\begin{bmatrix} N_\tau = 5, N_S = 2\times 2 \\ \beta\kappa = 3, \quad \beta U = 13 \end{bmatrix} \qquad \langle n \rangle = \left\langle \frac{1}{N_S} \sum_{\mathbf{x}} \left(n_{\mathbf{x},\uparrow} + n_{\mathbf{x},\downarrow} - 1 \right) \right\rangle$$



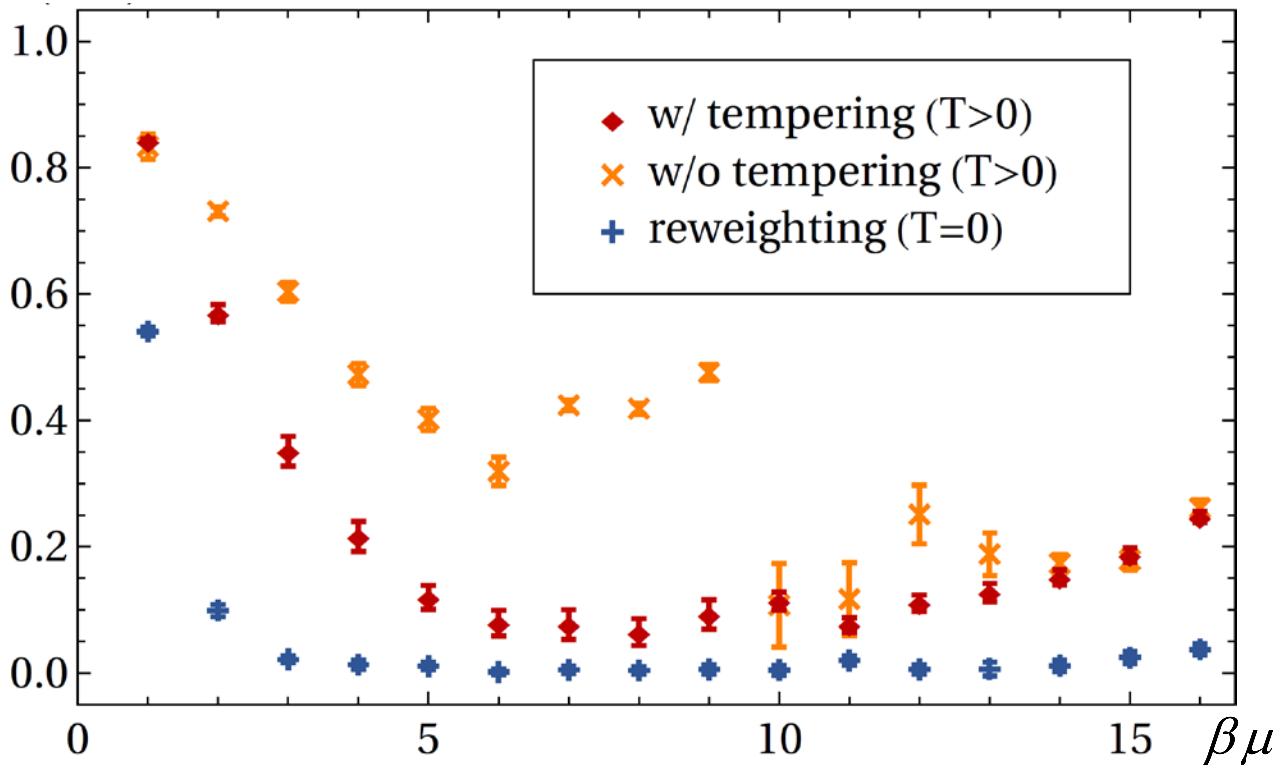
Hubbard model (4/4)

[MF-Matsumoto-Umeda 1906.04243]

average phase factor

$$\left(\langle \mathcal{O}(x) \rangle = \frac{\langle e^{i\theta(z)}\, \mathcal{O}(z) \rangle_{\Sigma_T}}{\langle e^{i\theta(z)} \rangle_{\Sigma_T}} \right)$$

$$\left| \langle e^{i\theta(z)} \rangle_{\Sigma_T} \right|$$



When only a single (or very few) thimble is sampled by mistake, the average phase factor can take a larger value (due to the lack of cancellations among different thimbles)

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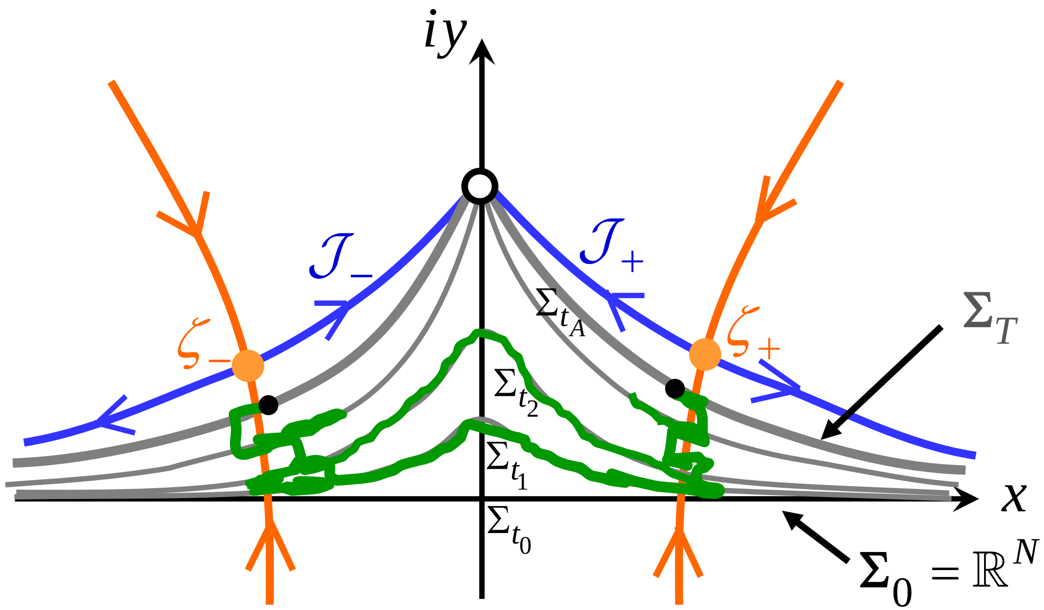
Pros and cons of the original TLT method

■ <u>TLT method</u> **[MF-Umeda 2017]**

Introduce replicas in between Σ_0 and Σ_T : $\left\{\Sigma_{t_0=0},\ \Sigma_{t_1},\ \Sigma_{t_2},\ \ldots,\ \Sigma_{t_A=T}\right\}$



<u>Pros</u> : can be applied to any systems
once formulated by path integrals with continuous variables

<u>Cons</u> : large comput cost at large DOF

- necessary # of replicas $\propto O(N^{0-1})$
- need to calculate Jacobian $J_t(x) = \partial z_t(x) / \partial x \propto O(N^3)$
  everytime we exchange configs between adjacent replicas

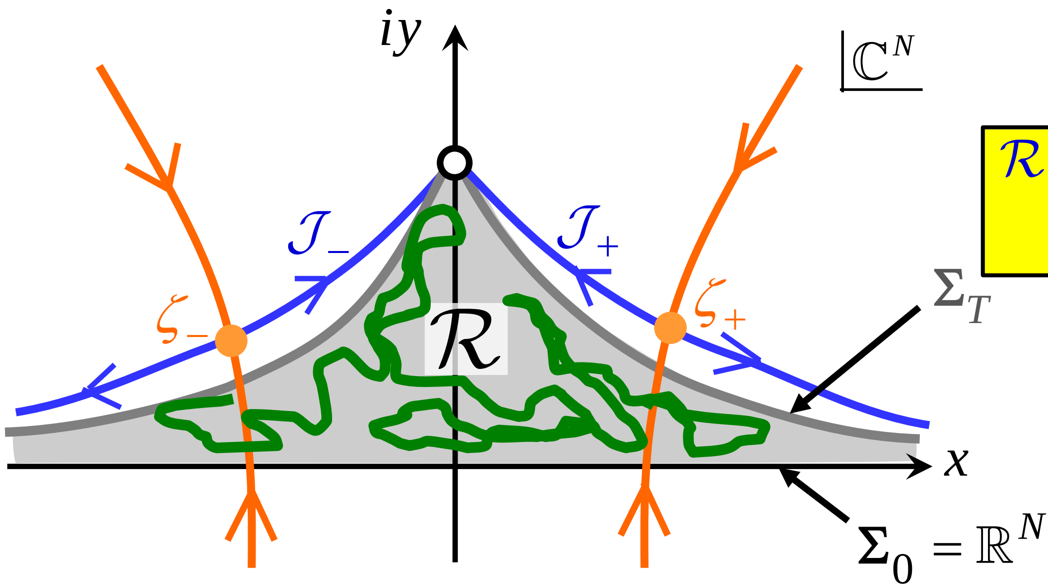
Worldvolume HMC (1/2)

[MF-Matsumoto 2012.08468]

■ <u>Worldvolume Hybrid Monte Carlo</u> (WV-HMC)

HMC on a continuous accumulation of integ surfaces, $\mathcal{R} \equiv \bigcup_{0\le t\le T} \Sigma_t$

"**worldvolume**"



$\mathcal{R}$: orbit of integration surface in the "target space" $\mathbb{C}^N = \mathbb{R}^{2N}$

$$\begin{pmatrix} \text{orbit of particle} & \to & \text{worldline} \\ \text{orbit of string} & \to & \text{worldsurface} \\ \text{orbit of surface (membrane)} & \to & \text{worldvolume} \end{pmatrix}$$

<u>Pros</u> : can be applied to any systems once formulated by path integrals with continuous variables

$\oplus$ major reduction of comput cost at large DOF

- No need to introduce replicas explicitly
- No need to calculate Jacobian $J_t(x) = \partial z_t(x) / \partial x$ in MD process
- Configs can move largely due to the use of HMC

Worldvolume HMC (2/2)

[MF-Matsumoto 2012.08468]

■ mechanism

$$\langle \mathcal{O}(x) \rangle \equiv \frac{\int_{\Sigma_0} dx\, e^{-S(x)} \mathcal{O}(x)}{\int_{\Sigma_0} dx\, e^{-S(x)}} = \frac{\int_{\Sigma_t} dz_t\; e^{-S(z_t)} \mathcal{O}(z_t)}{\int_{\Sigma_t} dz_t\; e^{-S(z_t)}}$$

⇦ t-independent

⇦ t-independent

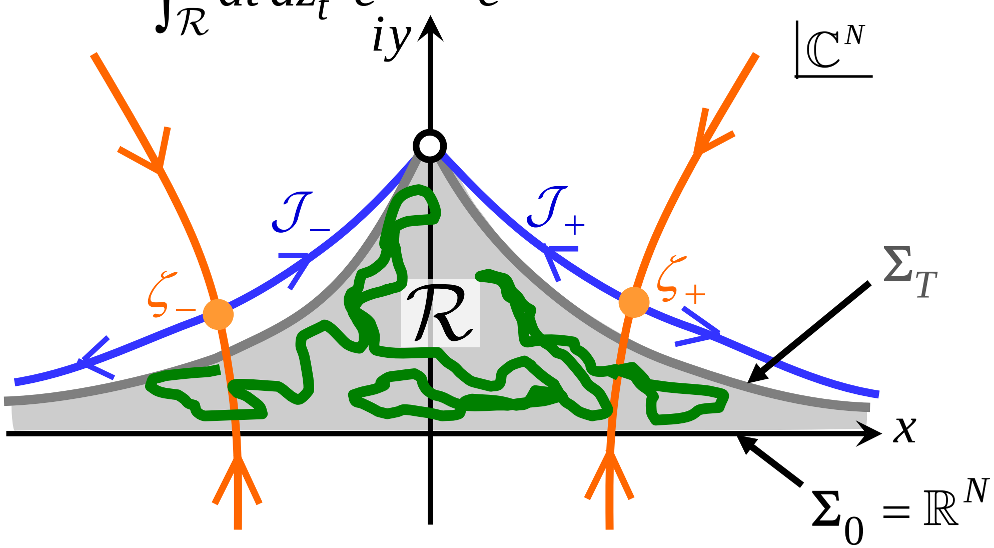
$$= \frac{\int_0^T dt\, e^{-W(t)} \int_{\Sigma_t} dz_t\; e^{-S(z_t)} \mathcal{O}(z_t)}{\int_0^T dt\, e^{-W(t)} \int_{\Sigma_t} dz_t\; e^{-S(z_t)}}$$

$(W(t)$: arbitrary fcn$)$

(chosen s.t. the appearance prob at different t are almost the same)

$$= \frac{\int_{\mathcal{R}} dt\, dz_t\;\, e^{-W(t)} e^{-S(z_t)} \mathcal{O}(z_t)}{\int_{\mathcal{R}} dt\, dz_t\;\, e^{-W(t)} e^{-S(z_t)}}$$

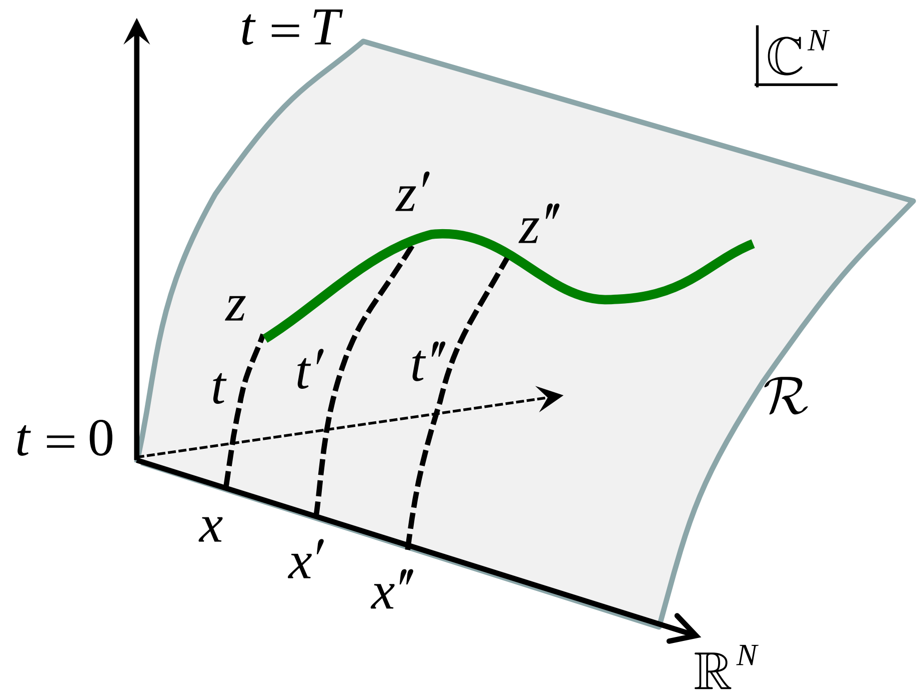
$\Leftarrow$ path integral over the worldvolume $\mathcal{R}$



Statistical analysis method for the WV-TLTM is established in **[MF-Matsumoto-Namekawa 2107.06858]**

Two pictures in WV-HMC

[MF-Matsumoto 2012.08468]



(1) **<u>Target-space picture</u>**

[MF-Matsumoto 2012.08468]

sample: $\{z, z', z'', \ldots\}$

(2) **<u>Parameter-space picture</u>**

[MF-Matsumoto 2012.08468]

[Fujisawa et al. 2112.10519]

sample: $\{(t, x), (t', x'), (t'', x''), \ldots\}$

At first sight, (2) may seem simpler,
but actually (1) is faster and more solid as an algorithm

We employ (1) <u>target-space picture</u>

Computational cost of WV-HMC

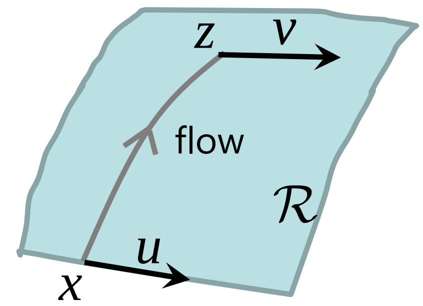
[MF-Matsumoto 2012.08468]
[MF-Matsumoto-Namekawa, Lattice2022]

$z=(z^i)\in\mathbb{C}^N \quad (N\propto V$: DOF)

<u>Configuration flow</u> $\quad \dot{z}_i=\overline{\partial_i S(z)} \quad \Rightarrow O(N)$

<u>Vector flow</u> $\quad \dot{v}_i=\overline{\partial_i\partial_j S(z)\,v_j} \quad \Rightarrow O(N^2)$ [when $\partial_i\partial_j S(z)$ is dense]

$\Rightarrow O(N)$ [when $\partial_i\partial_j S(z)$ is sparse (local field case)]



<u>RATTLE</u>
$$\begin{cases} z'=z+\Delta s\,\pi-\Delta s^2\,\overline{\partial V(z)}-\lambda \\ \pi_{1/2}=(z'-z)/\Delta s \\ \tilde{\pi}'=\pi_{1/2}-\Delta s\,\overline{\partial V(z')} \\ \pi'=\Pi'_{\mathcal{R}}\tilde{\pi}' \end{cases}$$

$\big(V(z)=\mathrm{Re}S(z)+W(t(z))\big)$

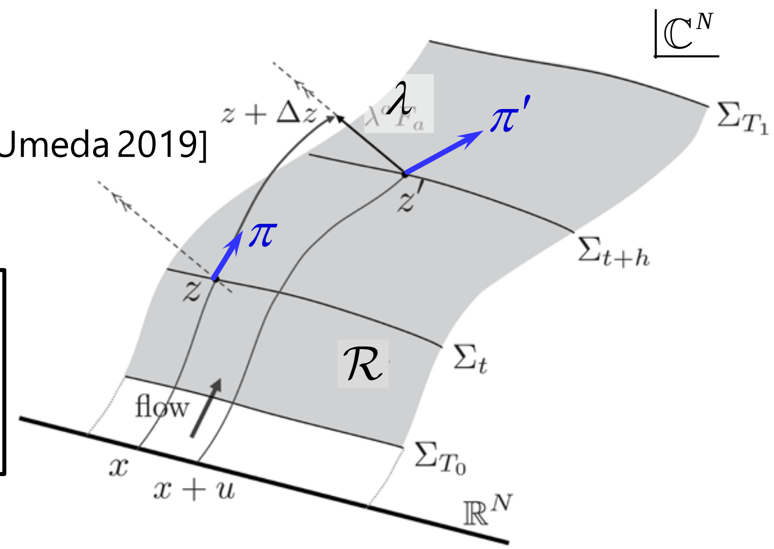
cf) RATTLE on a single thimble $\mathcal{J}=\Sigma_\infty$ [Fujii et al. 2013]
RATTLE on Σ_t [Alexandru@Lattice2019, MF-Matsumoto-Umeda 2019]

$\lambda\in N_z\mathcal{R}$ is determined s.t. $z'\in\mathcal{R}$

⇔

For given $z=z_t(x)$ and π,
find $h\in\mathbb{R}$, $u\in\mathbb{R}^N$, $\lambda\in N_z\mathcal{R}$
s.t. $z_t(x)+\Delta s\,\pi-\Delta s^2\,\overline{\partial V(z)}-\lambda=z_{t+h}(x+u)$

This can be solved by Newton's method
with BiCGStab for linear inversion
(which requires only config/vector flows) $\Rightarrow O(N)$



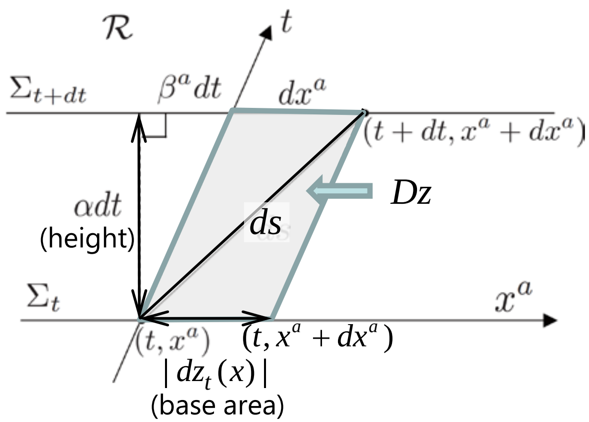
Comput cost at each MD step is expected to be $O(N)$ for local field theory (with the absence of fermion determinant)

Appendix: Details of WV-HMC (1/2)

[MF-Matsumoto 2012.08468]

■ Preparation

$$\langle \mathcal{O}(x)\rangle = \frac{\int_{\mathcal{R}} dt\, dz_t\; e^{-W(t)} e^{-S(z_t)} \mathcal{O}(z_t)}{\int_{\mathcal{R}} dt\, dz_t\; e^{-W(t)} e^{-S(z_t)}}$$



natural measure to appear in HMC on $\mathcal{R}$

= vol element Dz of the induced metric

ADM decomposition

$$ds^2 = \alpha^2 dt^2 + \gamma_{ab}(dx^a + \beta^a dt)(dx^b + \beta^b dt) \quad (\alpha : \text{lapse})$$

$$\Rightarrow \quad Dz = \alpha\, dt\, |dz_t(x)| = \alpha\, |\det J|\, dt\, dx \qquad \left(J = \frac{\partial z_t(x)}{\partial x} \right)$$

$$\Rightarrow \quad dt\, dz_t(x) = Dz \frac{dt\, dz_t(x)}{Dz} = Dz \frac{dt\, dx \det J}{dt\, dx\, \alpha\, |\det J|} = Dz\, \alpha^{-1}(z) e^{i\varphi(z)} \qquad \left(e^{i\varphi(z)} \equiv \frac{\det J}{|\det J|} \right)$$

$$\Rightarrow \quad \langle \mathcal{O}(x)\rangle = \frac{\int_{\mathcal{R}} dt\, dz_t\; e^{-W(t)} e^{-S(z)} \mathcal{O}(z)}{\int_{\mathcal{R}} dt\, dz_t\; e^{-W(t)} e^{-S(z)}} = \frac{\int_{\mathcal{R}} Dz\, \alpha^{-1}(z) e^{i\varphi(z)}\, e^{-W(t)} e^{-\mathrm{Re}\, S(z) - i\, \mathrm{Im}\, S(z)} \mathcal{O}(z)}{\int_{\mathcal{R}} Dz\, \alpha^{-1}(z) e^{i\varphi(z)}\, e^{-W(t)} e^{-\mathrm{Re}\, S(z) - i\, \mathrm{Im}\, S(z)}}$$

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

$$= \frac{\int_{\mathcal{R}} Dz\, \boxed{e^{-V(z)}}\, \boxed{A(z)}\, \mathcal{O}(z)}{\int_{\mathcal{R}} Dz\, \boxed{e^{-V(z)}}\, \boxed{A(z)}} \equiv \frac{\langle A(z) \mathcal{O}(z)\rangle_{\mathcal{R}}}{\langle A(z)\rangle_{\mathcal{R}}} \qquad \left(\langle f(z)\rangle_{\mathcal{R}} \equiv \frac{\int_{\mathcal{R}} Dz\, e^{-V(z)} f(z)}{\int_{\mathcal{R}} Dz\, e^{-V(z)}} \right)$$

Appendix: Details of WV-HMC (2/2)

[MF-Matsumoto 2012.08468]

■ Algorithm

$$\boxed{\langle \mathcal{O}(x)\rangle = \frac{\langle A(z)\mathcal{O}(z)\rangle_{\mathcal{R}}}{\langle A(z)\rangle_{\mathcal{R}}}}$$

$$\left(\langle f(z)\rangle_{\mathcal{R}} \equiv \frac{\int_{\mathcal{R}} Dz\, e^{-V(z)} f(z)}{\int_{\mathcal{R}} Dz\, e^{-V(z)}} \right)$$

$$\begin{cases} V(z) = \mathrm{Re}\, S(z) + W(t(z)) & \text{: potential} \\ A(z) = \alpha^{-1}(z)\, e^{i\varphi(z)} e^{-i\,\mathrm{Im}\, S(z)} & \text{: reweighting factor} \end{cases}$$

$$\left(e^{i\varphi(z)} \equiv \frac{\det J}{|\det J|} \right)$$

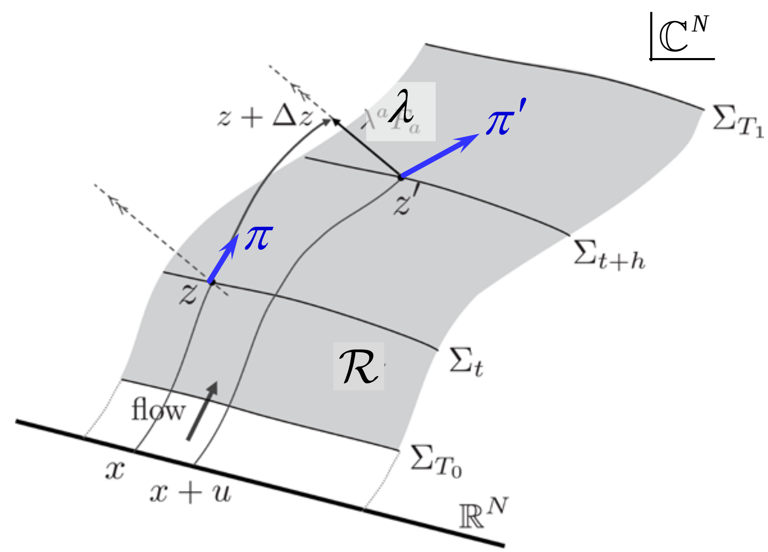
HMC on a constrained space **[Andersen 1983, Leimkuhler-Skeel 1994]**

$\langle f(z)\rangle_{\mathcal{R}}$ is estimated with RATTLE

$$\begin{cases} \pi_{1/2} = \pi - \Delta s\, \overline{\partial V(z)} - \lambda \\ z' = z + \Delta s\, \pi_{1/2} \\ \pi' = \pi - \Delta s\, \overline{\partial V(z')} - \lambda' \end{cases}$$

$\lambda \in N_z\mathcal{R}$ and $\lambda' \in N_{z'}\mathcal{R}$ are determined s.t.

$$\begin{cases} z' \in \mathcal{R} \\ \pi' \in T_{z'}\mathcal{R} \end{cases}$$



cf) RATTLE on $\mathcal{J} = \Sigma_\infty$ [Fujii et al. 2013]
RATTLE on Σ_t [Alexandru@Lattice2019, MF-Matsumoto-Umeda 2019]

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8. Summary and outlook

Successfully applied to ...

— (0+1)dim massive Thirring model **[MF-Umeda 1703.00861]** **(TLT)**

— 2dim Hubbard model **[MF-Matsumoto-Umeda 1906.04243, 1912.13303]** **(TLT)**

— chiral random matrix model (a toy model of finite-density QCD) **[MF-Matsumoto 2012.08468]** **(WV-HMC)**

— anti-ferro Ising on triangular lattice **[MF-Matsumoto 2020, JPS meeting]** **(WV-HMC)**

— complex scalar field at finite density **[MF-Namekawa 2022, in preparation]** **(WV-HMC)**

So far always successful for any models when applied,
though the system sizes are not yet very large (DOF $N \lesssim 10^4$)

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Chiral random matrix model (1/2)

[MF-Matsumoto 2012.08468]

■ finite density QCD

$$\left(\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}, \ \gamma_\mu = \gamma_\mu^\dagger = \begin{pmatrix} 0 & \sigma_\mu \\ \sigma_\mu^\dagger & 0 \end{pmatrix} \right)$$

$$\begin{aligned} Z_{\text{QCD}} &= \operatorname{tr} e^{-\beta(H-\mu N)} \\ &= \int [dA_\mu][d\psi d\bar{\psi}]\, e^{(1/2g^2)\int \operatorname{tr} F_{\mu\nu}^2 + \int [\bar{\psi}(\gamma_\mu D_\mu + m)\psi + \mu \psi^\dagger \psi]} \\ &= \int [dA_\mu]\, e^{(1/2g^2)\int \operatorname{tr} F_{\mu\nu}^2} \operatorname{Det} \begin{pmatrix} m & \sigma_\mu(\partial_\mu + A_\mu) + \mu \\ \sigma_\mu^\dagger(\partial_\mu + A_\mu) + \mu & m \end{pmatrix} \end{aligned}$$

⇩ toy model

■ chiral random matrix model **[Stephanov 1996, Halasz et al. 1998]**

$$Z_{\text{Steph}} = \int d^2 W\, e^{-n \operatorname{tr} W^\dagger W} \det \begin{pmatrix} m & iW + \mu \\ iW^\dagger + \mu & m \end{pmatrix}$$

(quantum field replaced by a matrix incl spacetime DOF)

$(T = 0,\ N_f = 1)$

$W = (W_{ij}) = (X_{ij} + i Y_{ij}) : n \times n$ complex matrix

$\left(\text{DOF} : N = 2n^2 \ \Leftrightarrow\ 4L^4 (N_c^2 - 1)\right)$

■ role as an important benchmark model

- well approximates the qualitative behavior of QCD at large n
- complex Langevin suffers from wrong convergence **[Bloch et al. 2018]**

Chiral random matrix model (2/2)

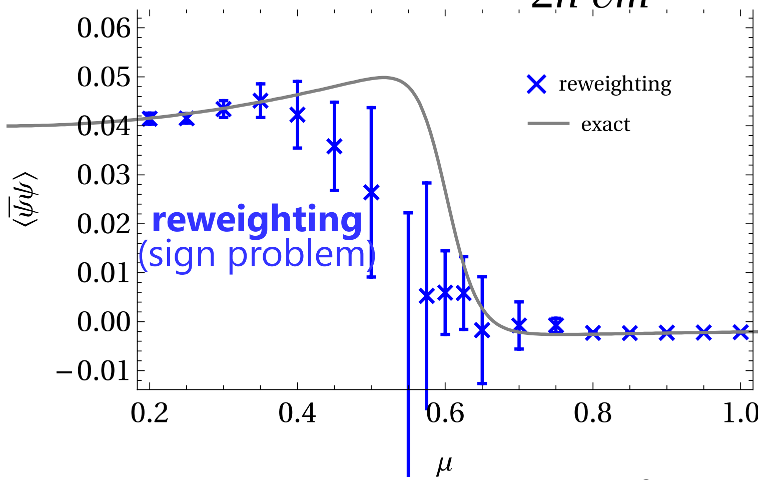
[MF-Matsumoto 2012.08468]

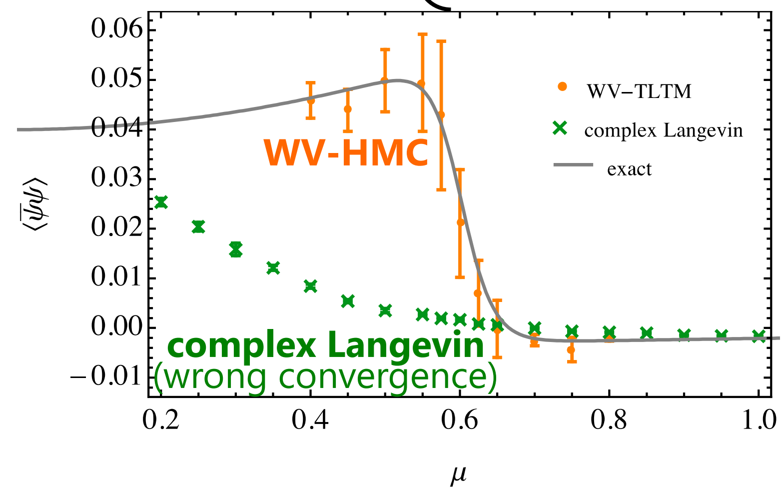
matrix size : $n=10$ (DOF : $N=200$)

(now easy at large DOF compared to the original TLTM)

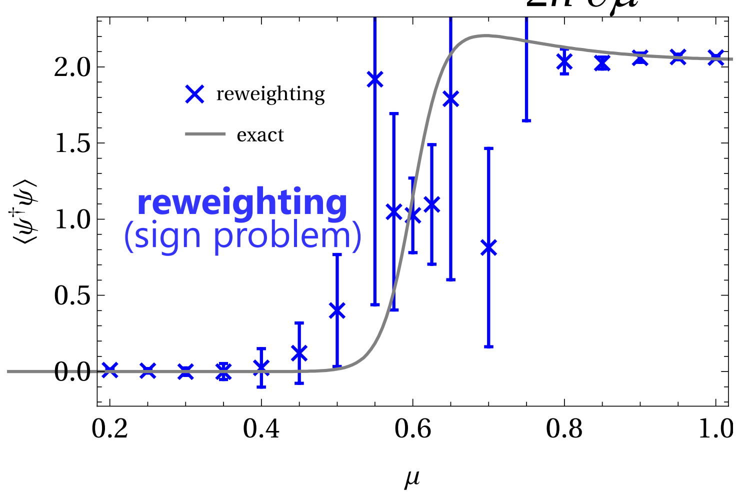
sample size
reweighting : 10k
complex Langevin :10k
WV-TLTM : 4k-17k

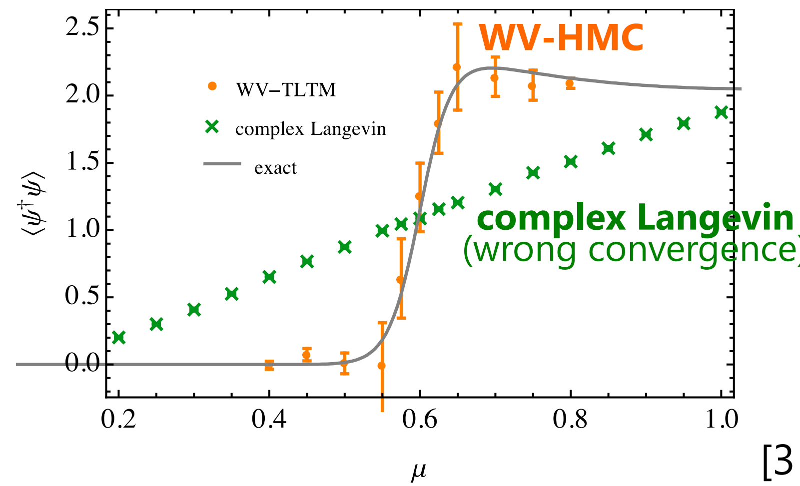
chiral condensate $\langle\bar{\psi}\psi\rangle \equiv \dfrac{1}{2n}\dfrac{\partial}{\partial m}\ln Z_{\text{Steph}}$ $[m=0.004,\ T=0]$





baryon # density $\langle\psi^{\dagger}\psi\rangle \equiv \dfrac{1}{2n}\dfrac{\partial}{\partial \mu}\ln Z_{\text{Steph}}$





Finite-density complex scalar field (1/3)

$\varphi(x) = \frac{1}{\sqrt{2}}[\varphi_1(x) + i\varphi_2(x)]$: complex scalar field

Continuum action

(x_0 : Euclidean time)

$$S(\varphi) = \int d^d x \left[\partial_\nu \varphi^* \partial_\nu \varphi + m^2 \varphi^* \varphi + \lambda (\varphi^* \varphi)^2 + \mu (\varphi^* \partial_0 \varphi - \partial_0 \varphi^* \varphi) \right]$$
$$\simeq \int d^d x \left[(\partial_\nu \varphi^* + \mu \delta_{\nu,0} \varphi^*)(\partial_\nu \varphi - \mu \delta_{\nu,0} \varphi) + m^2 |\varphi|^2 + \lambda |\varphi|^4 \right]$$

Lattice action [Aarts 0810.2089]

$$S(\varphi) = \sum_n \left[(2d + m^2) |\varphi_n|^2 + \lambda |\varphi_n|^4 - \sum_{\nu=0}^{d-1} (e^{\mu \delta_{\nu,0}} \varphi_n^* \varphi_{n+\nu} + e^{-\mu \delta_{\nu,0}} \varphi_n \varphi_{n+\nu}^*) \right]$$

Introducing (ξ_n, η_n) with $\varphi_n = \frac{1}{\sqrt{2}}(\xi_n + i\eta_n)$, we have

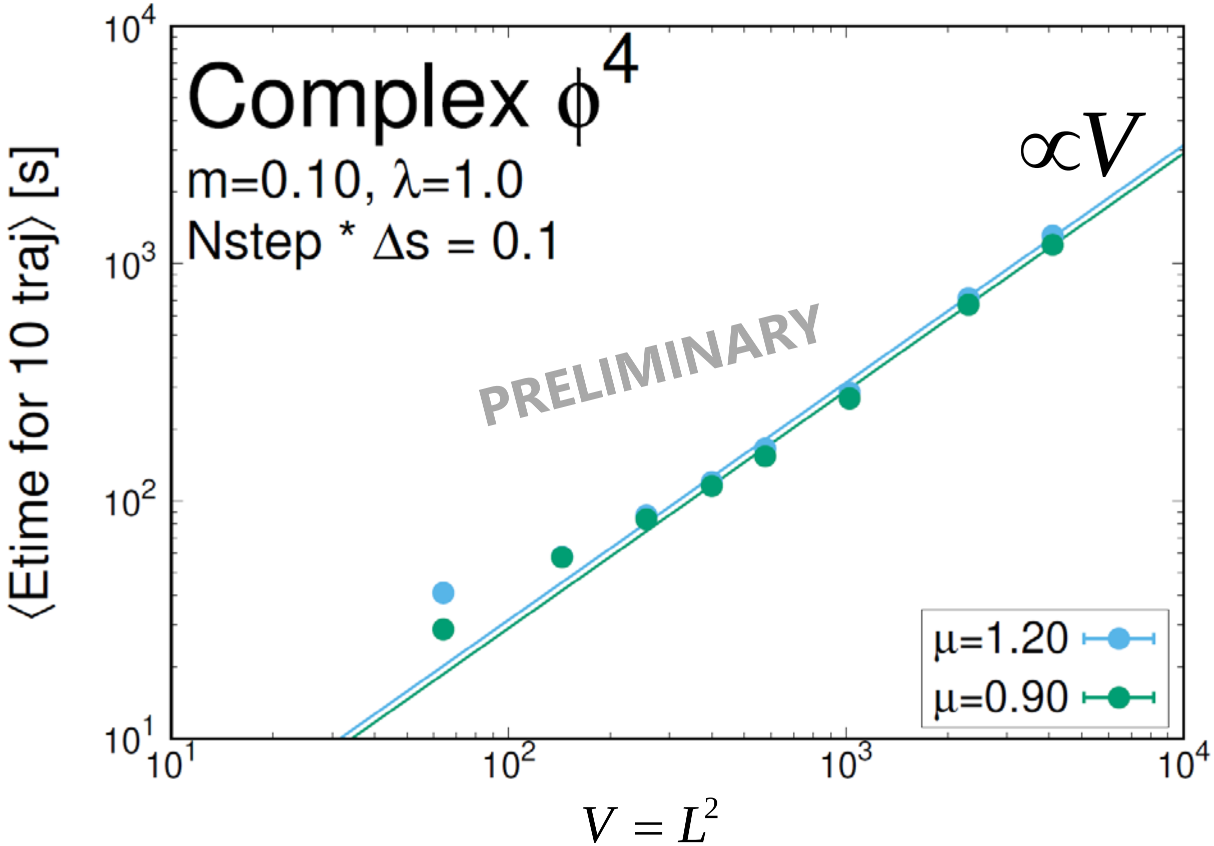
$$S(\xi,\eta) = \sum_n \left[\begin{array}{l} \frac{2d + m^2}{2}(\xi_n^2 + \eta_n^2) + \frac{\lambda}{4}(\xi_n^2 + \eta_n^2)^2 - \sum_{i=1}^{d-1} (\xi_{n+i}\xi_n + \eta_{n+i}\eta_n) \\ - \cosh\mu (\xi_{n+0}\xi_n + \eta_{n+0}\eta_n) - i \sinh\mu (\xi_{n+0}\eta_n - \eta_{n+0}\xi_n) \end{array} \right]$$

We complexify $(\xi,\eta) \in \mathbb{R}^{2V}$ to $(z,w) \in \mathbb{C}^{2V}$ with the flow equation

$$\dot{z}_n = [\partial S(z,w)/\partial z_n]^*, \quad \dot{w}_n = [\partial S(z,w)/\partial w_n]^* \quad \left(\begin{array}{l} V: \text{ lattice volume} \\ \quad \Rightarrow N = 2V \end{array} \right)$$

■ Computational scaling in 2D

[MF-Matsumoto-Namekawa, Lattice2022]



computed on Yukawa21
(@YITP, Kyoto Univ)

⇨ to be run on Fugaku

The figure clearly shows that the comput cost scales as $O(V) = O(N)$
$(N = 2V)$

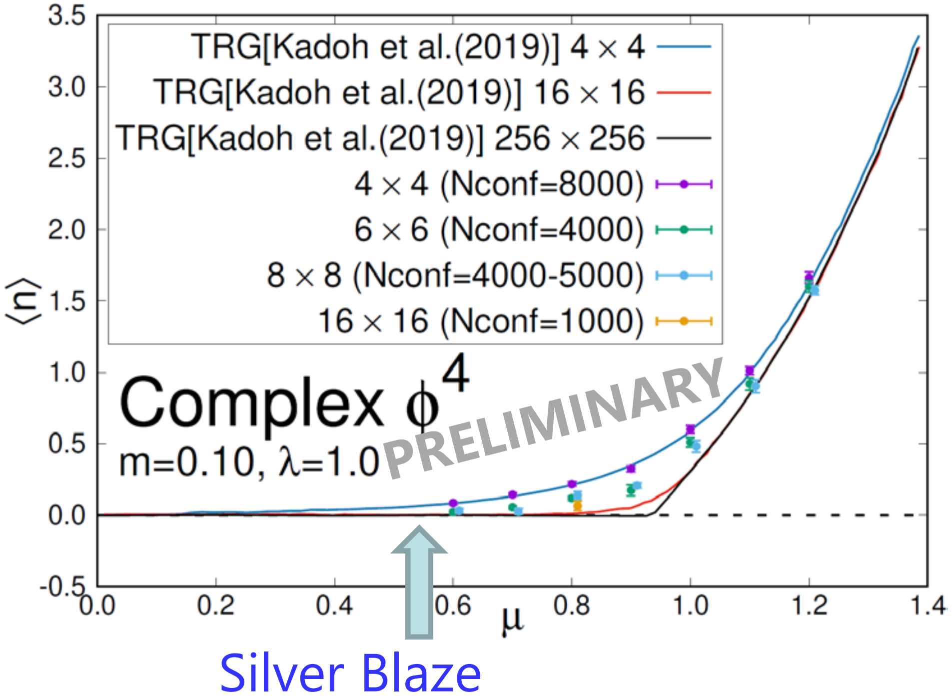
(NB: The scaling will become $O(V^{1.25})$
if we reduce the MD stepsize as $\Delta s \propto V^{-1/4}$
to keep the same amount of acceptance for increasing volume)

Finite-density complex scalar field (3/3)

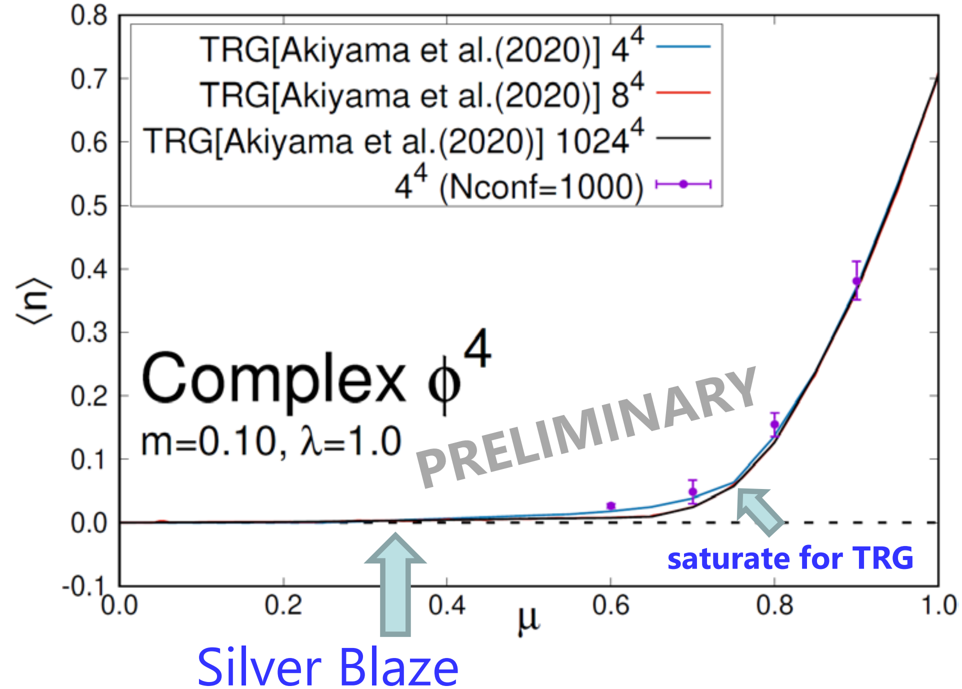
[MF-Namekawa, in preparation]

■Comparison with TRG method **[TRG (2D): Kadoh et al. 1912.13092]**
[TRG (4D): Akiyama et al. 2005.04645]

2D



4D



- WV-HMC gives results consistent with TRG at small volumes
- It should be interesting to investigte behaviors at large 4D volumes where TRG starts suffering from the systematic errors due to the introduction of D_{cut}

Yang-Mills theory has become a target

WV-HMC also works for group manifolds

[MF, in preparation]

[MF, in preparation]

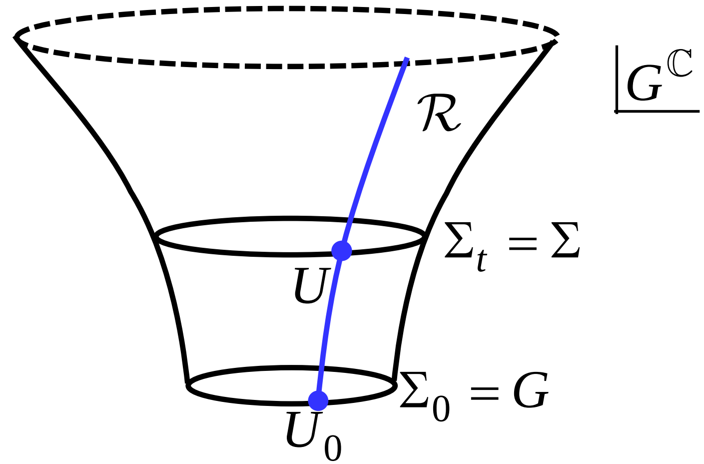
[MF-Kanamori-Namekawa, ongoing]

[Example]

1-site model with a pure imaginary coupling:

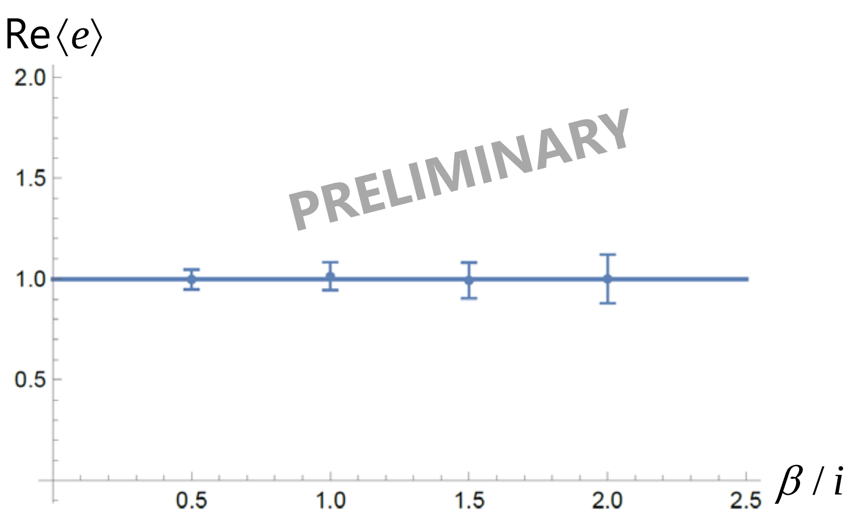
$$S(U) \equiv \beta\, e(U) \equiv \frac{\beta}{2N}\,\mathrm{tr}\left(2 - U - U^{-1}\right)$$

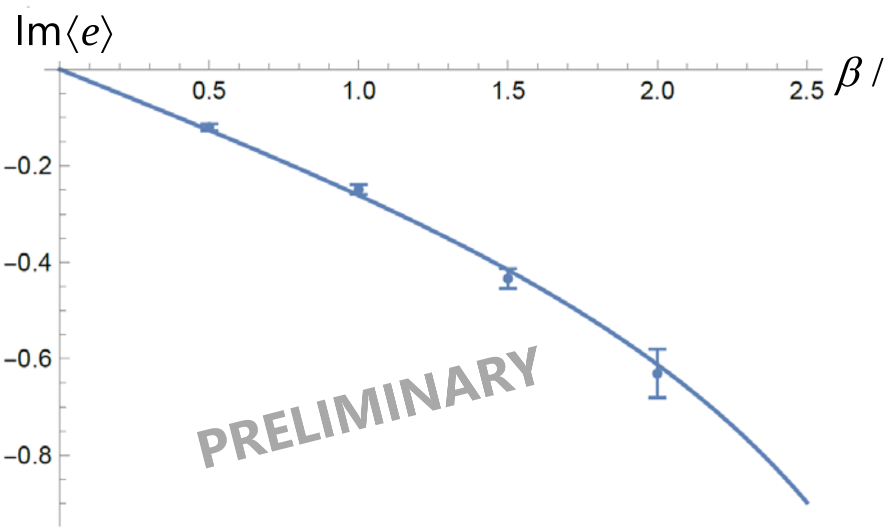
$$\left(U \in G = SU(2)\,;\;\; \beta \in i\,\mathbb{R}\right)$$



analytic result: $\langle e \rangle = 1 - I_2(\beta) / I_1(\beta)$

numerical result (WV-HMC):





This algorithm can be applied to Yang-Mills theory straightforwardly

[MF-Kanamori-Namekawa, ongoing]

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Summary and outlook

■ Summary

▼ WV-HMC seems to be a promising method esp. for local field theories

- Allows a coding such as to enjoy the locality
- Does not have a wrong convergence problem (as in the complex Langevin)
- Can increase the precision to arbitrarily high order by increasing the sample size

  (No systematic errors such as those caused by introducing D_{cut} in TRG)

"Power of Monte Carlo"

■ Outlook

▼ Application to QCD

- WV-HMC for a path integration on a group manifold **[MF, in preparation]**
- WV-HMC for pure Yang-Mills with finite θ **[MF-Kanamori-Namekawa, ongoing]**
- WV-HMC for finite-density QCD **[MF-Kanamori-Namekawa-..., ongoing]**

▼ Further improvement of algorithm **[MF, MF-Matsumoto-Namekawa-..., ongoing]**

▼ Combining various algorithms

(e.g.) path optimization method and/or TRG (non-MC) **cf) TRG for 2D YM: [MF-Kadoh-Matsumoto 2107.14149]**

▼ Particularly important: MC calc for time-dependent systems

⇨ first-principles calc of nonequilibrium processes
such as those in the early universe, heavy ion collision experiments, ...

Thank you.