Sign problem and the Worldvolume HMC method I: basic algorithm

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Based on work with

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also with

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Issaku Kanamori (RIKEN R-CCS)
Takaaki Kuwahara (Kyoto Univ)

Introduction

Sign problem

A large system with a complex action:

$$\begin{cases} x=(x^i)\in\mathbb{R}^N \ \text{: dynamical variable } (N \text{ : \#DOF}) \\ S(x)=\operatorname{Re}S(x)+i\operatorname{Im}S(x)\in\mathbb{C} \text{ : complex action} \\ \mathcal{O}(x) \text{ : observable} \end{cases}$$

$$\left(\begin{array}{l} \text{e.g. scalar field} \\ x^i \leftrightarrow \phi(t,\mathbf{x}) \\ S(x)\leftrightarrow S[\phi]=\int dt\, d^3\mathbf{x}\left[\frac{1}{2}(\partial_t\phi)^2+\cdots\right] \\ dx=\prod_i dx^i \leftrightarrow [d\phi]=\prod_{t,\mathbf{x}} d\phi(t,\mathbf{x}) \end{array}\right)$$

$$\langle\mathcal{O}\rangle \equiv \frac{\int_{\mathbb{R}^N} dx\, e^{-S(x)}\,\mathcal{O}(x)}{\int_{\mathbb{R}^N} dx\, e^{-S(x)}} = \frac{\int_{\mathbb{R}^N} dx\, e^{-\operatorname{Re}S(x)} e^{-i\operatorname{Im}S(x)}\,\mathcal{O}(x)}{\int_{\mathbb{R}^N} dx\, e^{-\operatorname{Re}S(x)} e^{-i\operatorname{Im}S(x)}}$$

highly oscillatory

$$= \frac{\int_{\mathbb{R}^N} dx\, e^{-\operatorname{Re}S(x)} e^{-i\operatorname{Im}S(x)}\,\mathcal{O}(x) \Big/ \int_{\mathbb{R}^N} dx\, e^{-\operatorname{Re}S(x)}}{\int_{\mathbb{R}^N} dx\, e^{-\operatorname{Re}S(x)} e^{-i\operatorname{Im}S(x)} \Big/ \int_{\mathbb{R}^N} dx\, e^{-\operatorname{Re}S(x)}} = \frac{\langle e^{-i\operatorname{Im}S(x)}\,\mathcal{O}(x)\rangle_{\text{rewt}}}{\langle e^{-i\operatorname{Im}S(x)}\rangle_{\text{rewt}}} = \frac{e^{-O(N)}}{e^{-O(N)}}$$

$$\big(=O(1)\big)$$

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$$\langle e^{-i\,\mathrm{Im}\,S(x)}\rangle_{\text{rewt}} = \frac{\int dx\, e^{-\mathrm{Re}\,S(x)}e^{-i\,\mathrm{Im}\,S(x)}}{\int dx\, e^{-\mathrm{Re}\,S(x)}} = \frac{Z}{Z_{\text{pq}}} = \frac{e^{-Nf}}{e^{-Nf_{\text{pq}}}}$$ (assuming extensiveness)

Here,

$$|Z|\ \big(=e^{-N\,\mathrm{Re}\,f}\big) = \left|\int dx\, e^{-\mathrm{Re}\,S(x)}e^{-i\,\mathrm{Im}\,S(x)}\right| \le \int dx\, \left|e^{-\mathrm{Re}\,S(x)}e^{-i\,\mathrm{Im}\,S(x)}\right| = Z_{\text{pq}}\ \big(=e^{-Nf_{\text{pq}}}\big)$$

We thus have $\mathrm{Re}\,f \ge f_{\text{pq}}$, which means

$$\left|\langle e^{-i\,\mathrm{Im}\,S(x)}\rangle_{\text{rewt}}\right| = e^{-N(\mathrm{Re}\,f-f_{\text{pq}})} = e^{-O(N)}$$

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$\big(=O(1)\big)$

In MC calculations, the above estimates are accompanied by statistical errors:

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

⇨ neccesary sample size : $N_{\text{conf}} \gtrsim e^{O(N)}$ **sign problem!**

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⇒ neccesary sample size : $N_{\text{conf}} \gtrsim e^{O(N)}$ **sign problem!**

<u>thimble method</u> : reduces the coefficient of $O(N)$: $e^{-O(N)} \to e^{-e^{-\lambda t}O(N)}$

Example : Gaussian

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

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

large β mimics large DOF

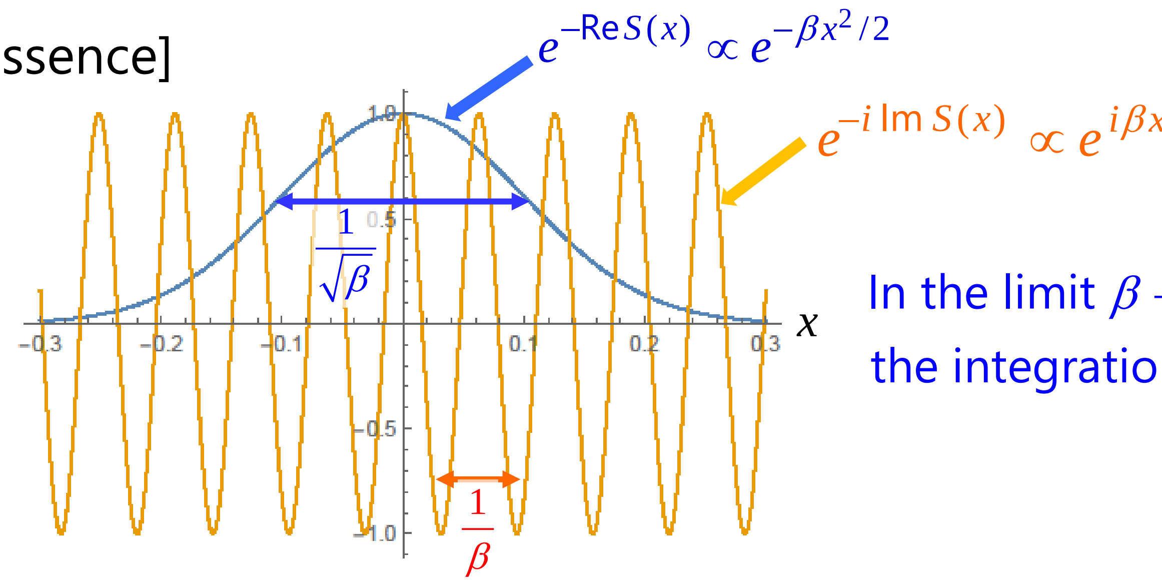
$$\Rightarrow \quad \langle x^2 \rangle = \frac{\langle e^{-i\,\mathrm{Im}\,S(x)}\, x^2 \rangle_{\text{rewt}}}{\langle e^{-i\,\mathrm{Im}\,S(x)} \rangle_{\text{rewt}}} = \frac{\left(\beta^{-1}-1\right)e^{-\beta/2}}{e^{-\beta/2}}$$

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

$\Rightarrow$ 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]



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

Various approaches

A major obstacle for first-principles calculations in various fields

examples: - finite-density QCD
- Quantum Monte Carlo of statistical systems
- real-time dynamics of quantum many-body systems

Various algorithms have been proposed:

- Complex Langevin **(CL)** method **[Parisi 1983, Klauder 1983]**
- Lefschetz thimble method
  - Original **(LT)** **[Witten 2010] [Cristoforetti et al. 2012, Fujii et al. 2013]**
  - Generalized thimble **(GT)** **[Alexandru et al. 2015]**
  - Tempered Lefschetz thimble **(TLT)** **[MF-Umeda 2017, Alexandru et al. 2017]**
  - Worldvolume HMC **(WV-HMC)** **[MF-Matsumoto 2020]**
- Path/sign optimization **[Mori-Kashiwa-Ohnishi 2017, Alexandru et al. 2018]**
- Tensor network **[Levin-Nave 2007, Xie et al. 2014, Adachi et al. 2019, ...]**
  [Gu et al. 2010, Shimizu-Kuramashi 2014, Akiyama-Kadoh 2020]

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Today's talk:

- **Explain the basics of the TLT and WV-HMC methods**
- **Extend the WV-HMC to group manifolds**

Plan

1. Introduction (done)
2. Lefschetz thimble (LT) method [Witten 2010, Cristoforetti et al. 2012, Fujii et al. 2013]
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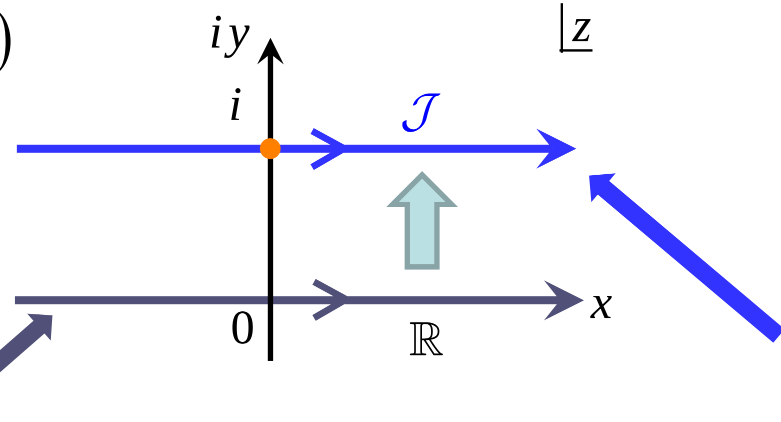
Warm-up: Gaussian (revisited)

$$\begin{cases} S(x) = \dfrac{\beta}{2}(x-i)^2 \quad (\beta \gg 1) \\ \mathcal{O}(x) = x^2 \end{cases}$$



$$\langle \mathcal{O}(x) \rangle = \frac{\int_{\mathbb{R}} dx\, e^{-S(x)}\, \mathcal{O}(x)}{\int_{\mathbb{R}} dx\, e^{-S(x)}} = \frac{\int_{-\infty}^{\infty} dx\, e^{-\beta(x-i)^2/2}\, x^2}{\int_{-\infty}^{\infty} dx\, e^{-\beta(x-i)^2/2}}$$

highly oscillatory

change of path

$x \to z = x + i$

$$\langle \mathcal{O}(x) \rangle_{\mathcal{J}} = \frac{\int_{\mathcal{J}} dz\, e^{-S(z)}\, \mathcal{O}(z)}{\int_{\mathcal{J}} dz\, e^{-S(z)}} = \frac{\int_{-\infty}^{\infty} dx\, e^{-\beta x^2/2}\, (x+i)^2}{\int_{-\infty}^{\infty} dx\, e^{-\beta x^2/2}}$$

oscillating factor disappears

Due to Cauchy's thm,
$\langle \mathcal{O}(x) \rangle = \langle \mathcal{O}(x) \rangle_{\mathcal{J}}$

$z = i$: saddle pt (critical pt)
$\mathcal{J}$: steepest descent (Lefschetz thimble)

$\mathrm{Im}\, S(z)$: const $(=0)$ on $\mathcal{J}$

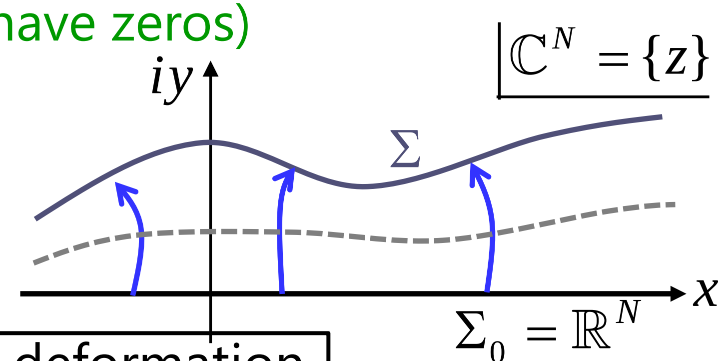
Basic idea of the thimble method (1/2)

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

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 : $\Sigma_0 = \mathbb{R}^N \;\rightarrow\; \Sigma \; (\subset \mathbb{C}^N)$

(boundary at $|x| \rightarrow \infty$ 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

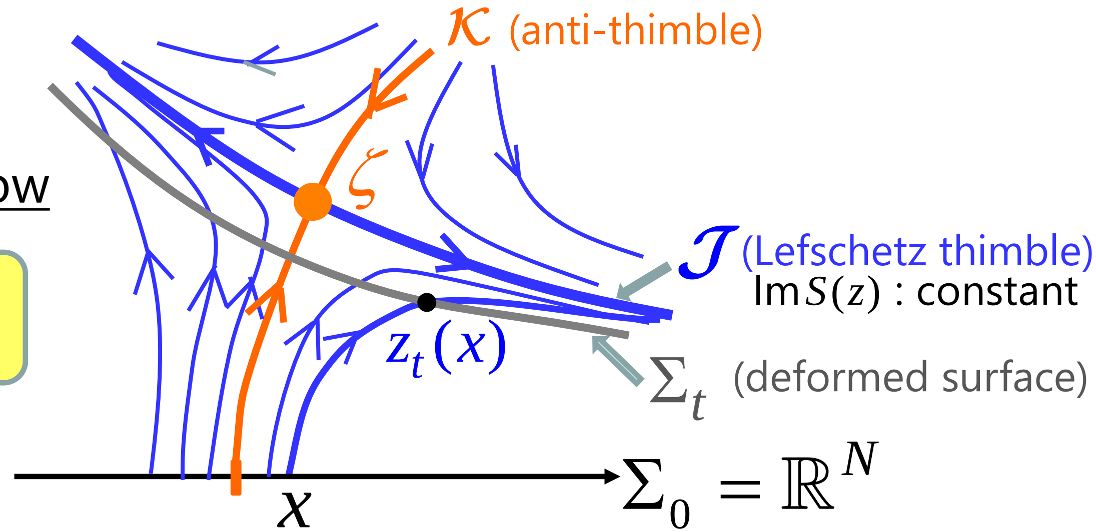
sign problem will be significantly reduced if $\mathrm{Im}\,S(z)$ is almost constant on Σ

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

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

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

Def $\boxed{\mathcal{J} \text{ (Lefschetz thimble)} \equiv \text{ union of flows out of crit pt } \zeta}$

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

$\Rightarrow$ If $\Sigma_t \xrightarrow{t\to\infty} \mathcal{J}$, then the oscillatory behavior of integral over Σ_t must be reduced significantly by taking t to be sufficiently large

How the sign problem disappears

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

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

(N : DOF, N_{conf} : sample size)

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

flow

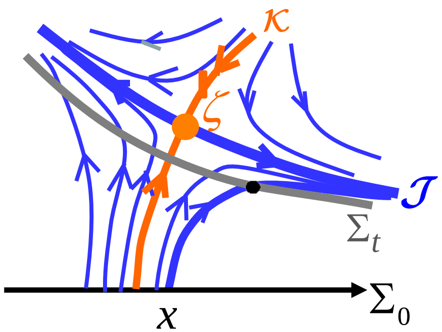
- Integration on a deformed surface Σ_t (flow time t)

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

$$\left(\langle g(z)\rangle_{\Sigma_t} \equiv \frac{\int_{\Sigma_t}|dz|\,e^{-\mathrm{Re}\,S(z)}g(z)}{\int_{\Sigma_t}|dz|\,e^{-\mathrm{Re}\,S(z)}}, \quad e^{i\theta(z)} \equiv e^{-i\,\mathrm{Im}S(z)}\frac{dz}{|dz|}\right)$$

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

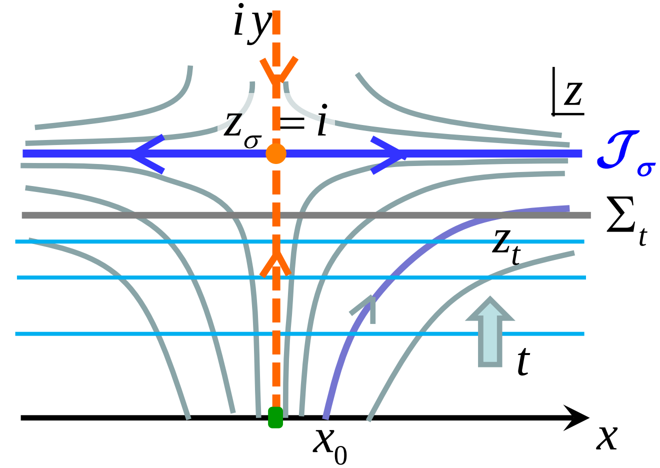
$$= \frac{O(1) \pm O(1/\sqrt{N_{\mathrm{conf}}})}{O(1) \pm O(1/\sqrt{N_{\mathrm{conf}}})}$$



[λ: (typical) singular value of Hessian $\partial_i\partial_j S(\zeta)$]

Sign problem should be alleviated at flow time $t = O(\log N)$

Example: Gaussian (re-revisited)



gradient flow $\left[S(z)=(\beta/2)(z-i)^2 \Rightarrow S'(z)=\beta(z-i)\right]$

$\dot{z}_t = \overline{S'(z_t)} = \beta(\bar{z}+i)$ with $z_{t=0}=x_0$

⇨ $z_t = x_0 e^{\beta t} + i(1-e^{-\beta t})$

⇨ $\Sigma_t = \{z \in \mathbb{C} \mid \mathrm{Im}\, z = 1-e^{-\beta t}\}$

⇨ change of integration path $z = x + i(1-e^{-\beta t}) \in \Sigma_t$

⇨ $e^{-S(z)} \propto e^{-\beta x^2/2} e^{i e^{-\beta t}\beta x}$ $\begin{cases} \text{width of distribution : } 1/\sqrt{\beta} \\ \text{width of oscillation : } e^{\beta t}/\beta \end{cases}$

$$\left(\langle g(z) \rangle_{\Sigma_t} \equiv \frac{\int_{\Sigma_t} |dz|\, e^{-\mathrm{Re}\, S(z)} g(z)}{\int_{\Sigma_t} |dz|\, e^{-\mathrm{Re}\, S(z)}} \qquad e^{i\theta(z)} \equiv e^{-i\,\mathrm{Im}\, S(z)} \frac{dz}{|dz|} \right)$$

⇨ By taking t to be large $\left(\text{s.t. } e^{\beta t}/\beta \gtrsim 1/\sqrt{\beta}\right)$,
the integral is not oscillatory any more!

$$\left(\text{In fact, } \langle x^2 \rangle = \frac{\langle e^{i\theta(z)} z^2 \rangle_{\Sigma_t}}{\langle e^{i\theta(z)} \rangle_{\Sigma_t}} = \frac{e^{-(\beta/2)e^{-2\beta t}} \left(\beta^{-1}-1\right)}{e^{-(\beta/2)e^{-2\beta t}}} = \frac{O(1)}{O(1)} \approx \frac{O(1) \pm O(1/\sqrt{N_{\mathrm{conf}}})}{O(1) \pm O(1/\sqrt{N_{\mathrm{conf}}})} \right)$$

NB: logarithm increase is sufficient:

$t \sim O(\log \beta)$ $\left(\Leftrightarrow t \sim O(\log N)\right)$

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Ergodicity problem in thimble methods

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

NO!

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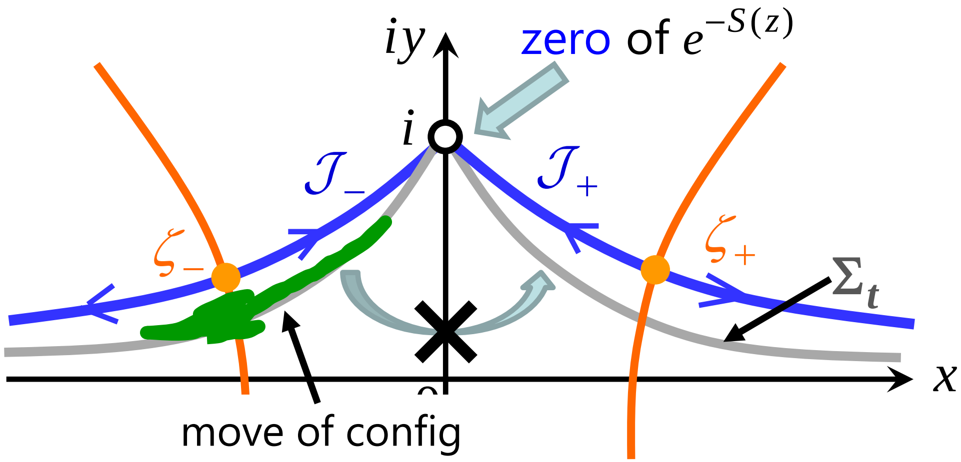
Actually, there comes out another problem at large t : **Ergodicity problem**

E.g. $e^{-S(x)} = e^{-\beta x^2/2}(x-i)^\gamma \ \ (\beta \gg 1,\ \gamma \in \mathbb{Z}_{>0})$ $\left(\text{finite-density QCD : } e^{-S(A)} = e^{-S_{\rm YM}(A)} \det D(A)\right)$



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

$\oplus$

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

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

$\Leftrightarrow$ [∞ potential barrier on Σ_T] $\Leftrightarrow$ configs cannot move

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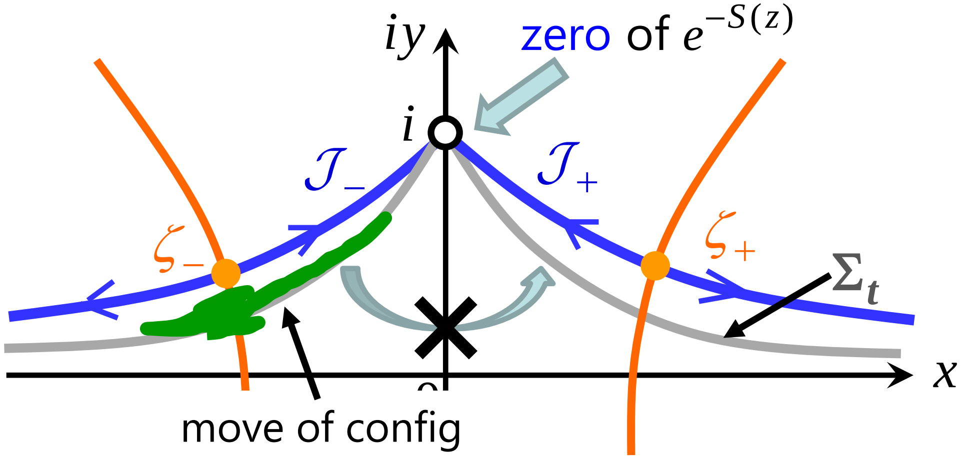

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⇔ [∞ potential barrier on Σ_T] ⇔ configs cannot move

⇨ **solution : Tempered Lefschetz thimble method**

[MF-Umeda 2017]

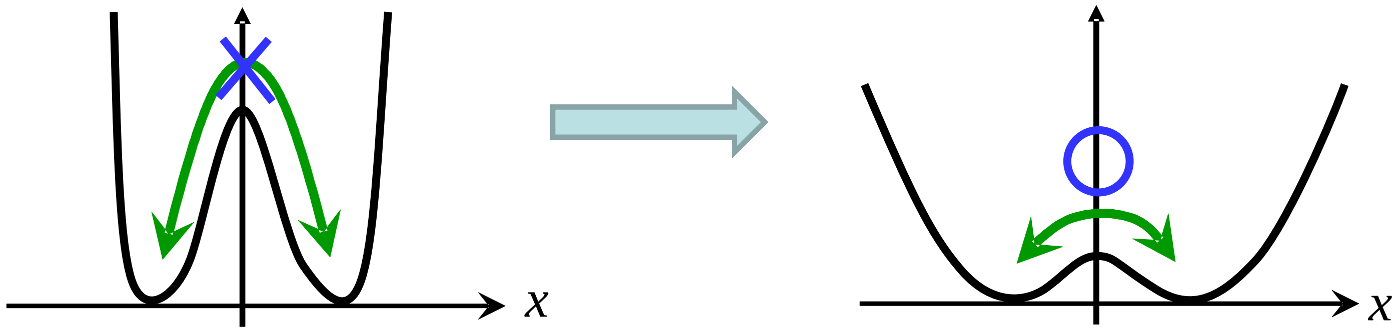
Idea of tempering

[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 $\beta \gg 1$

$\beta(x^2-1)^2 \quad (\beta \gg 1)$ $\qquad\qquad$ $\beta_0(x^2-1)^2 \quad (\beta_0 \ll 1)$



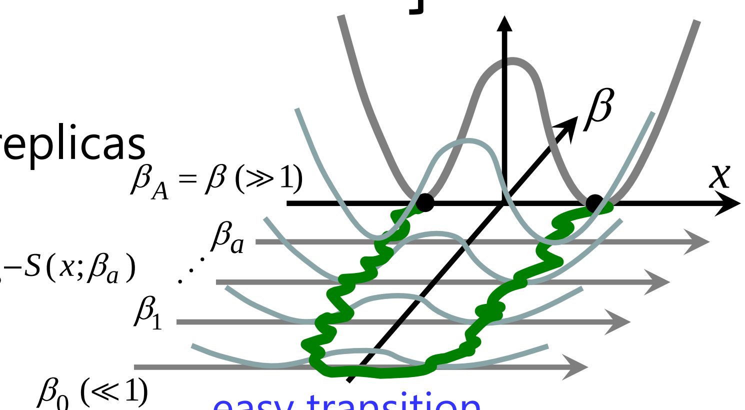
transition is difficult due to the high potl barrier

transition is easy

Algorithm :

① Extend the config space by introducing multiple replicas $\{\beta_0,\ldots,\beta_A\}$ in betwenen $\beta(=\beta_A)$ and β_0, and introduce a Markov chain s.t. $p_{\rm eq}(x,\beta_a)=w_a\, e^{-S(x;\beta_a)}$

② After thermalization, estimate observables by using the subsample at $\beta_A=\beta$



easy transition passing through a detour

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

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

Tempered Lefschetz thimble method

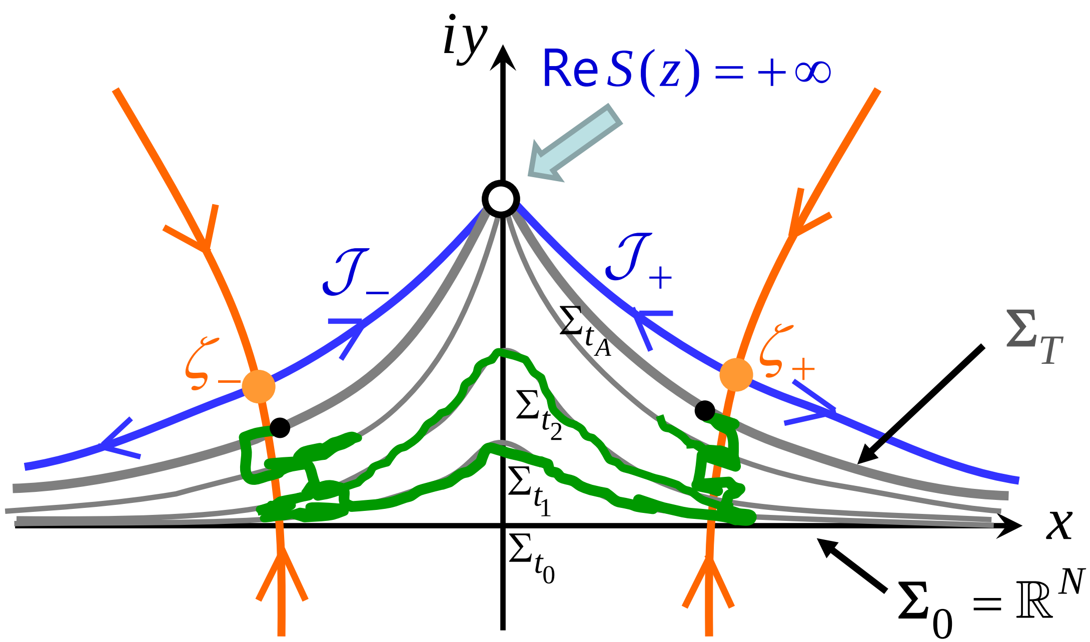
[Fukuma-Umeda 1703.00861]

■ <u>TLT method</u>

(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 thermalization, estimate observables with a subsample on Σ_T



Sign and ergodicity problems are solved simultaneously !

Hubbard model (1/4)

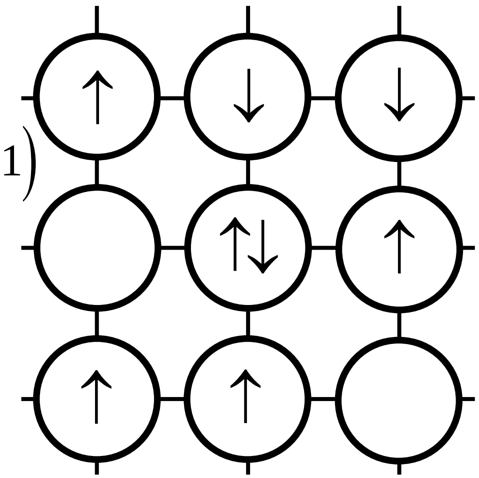
■ Hubbard model   toy model for electrons in a solid **[Hubbard 1963]**

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

- Hamiltonian

$$H = -\kappa \sum_{\langle \mathbf{x},\mathbf{y}\rangle} \sum_{\sigma} c^\dagger_{\mathbf{x},\sigma} c_{\mathbf{y},\sigma} + U \sum_{\mathbf{x}} \left(n_{\mathbf{x},\uparrow} - \frac{1}{2}\right)\left(n_{\mathbf{x},\downarrow} - \frac{1}{2}\right) - \mu \sum_{\mathbf{x}} \left(n_{\mathbf{x},\uparrow} + n_{\mathbf{x},\downarrow} - 1\right)$$

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



$(N_s$: # of sites$)$

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

Trotter decomposition + bosonization (HS transformation)

$$Z_{\beta,\mu} \equiv \operatorname{tr} e^{-\beta H}$$

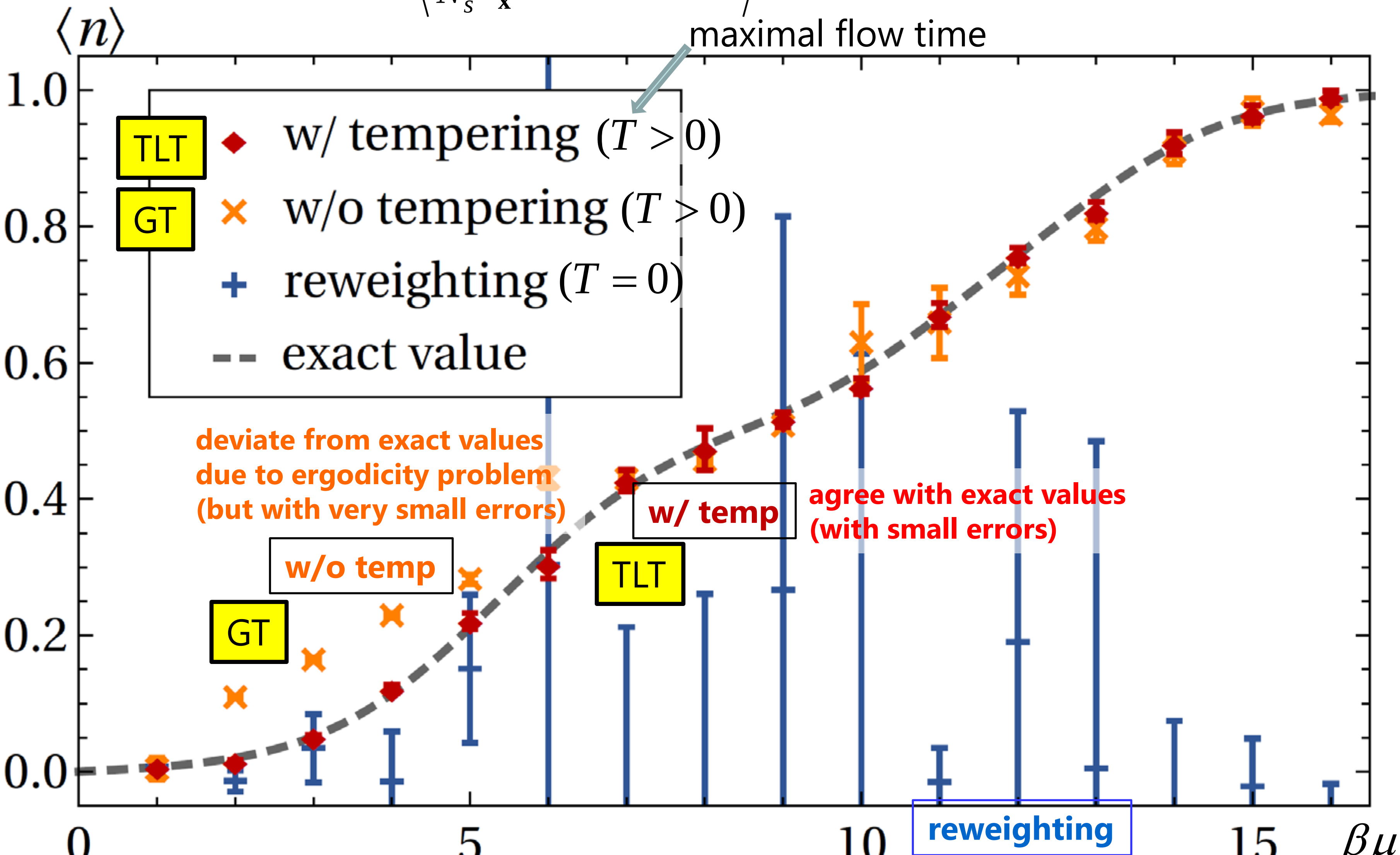
$$\approx \int [d\phi]\, e^{-S[\phi_{\ell,\mathbf{x}}]} \equiv \int \prod_{\ell=1}^{N_t} \prod_{\mathbf{x}} d\phi_{\ell,\mathbf{x}}\ e^{-(1/2)\sum_{\ell,\mathbf{x}} \phi_{\ell,\mathbf{x}}{}^2} \det M_a[\phi] \det M_b[\phi]$$

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

Hubbard model (2/4)

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

[MF-Matsumoto-Umeda 1906.04243]



large errors
due to sign problem

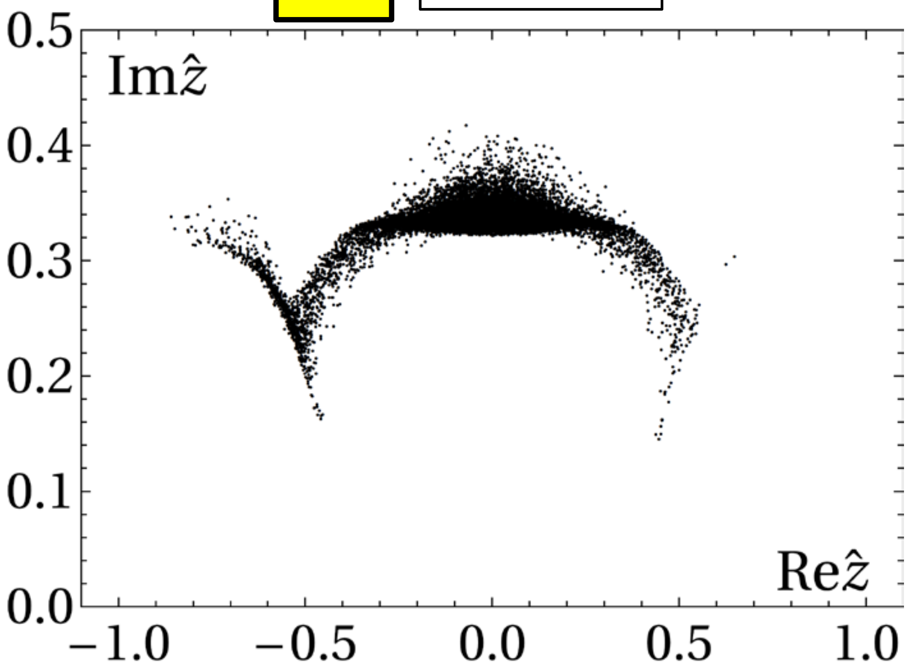
Hubbard model (3/4)

[MF-Matsumoto-Umeda 1906.04243]

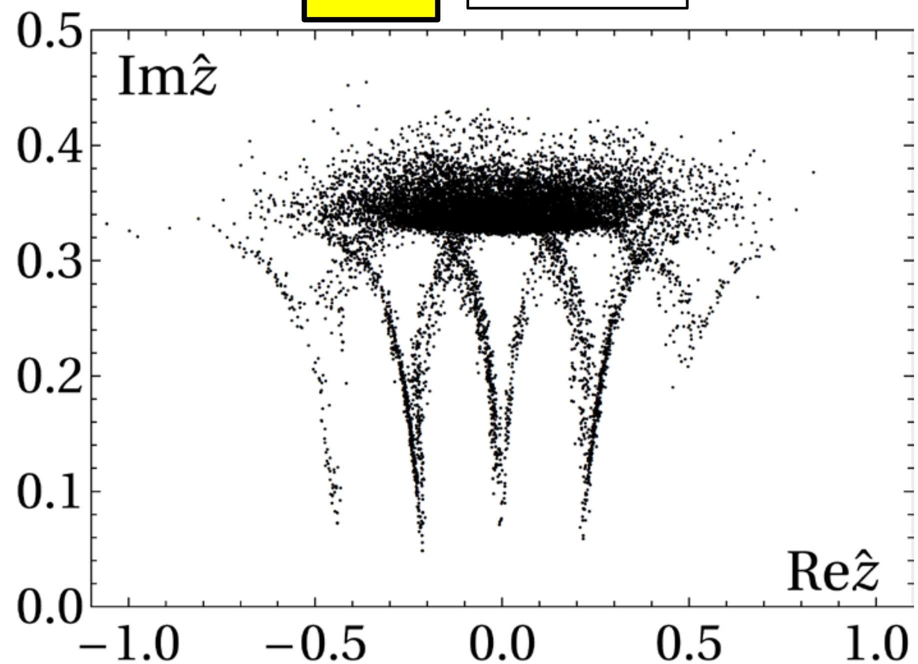
scattered plot of flowed configs at $T = 0.5$ ($\beta\mu = 5$)

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

GT w/o temp



TLT w/ temp



stuck to a small # of thimbles

distributed widely over many thimbles

(cf. dominant-thimble approach : [Ulybyshev-Valgushev 1712.02188, 1906.02726] [Ulybyshev,Assaad 2407.09452])

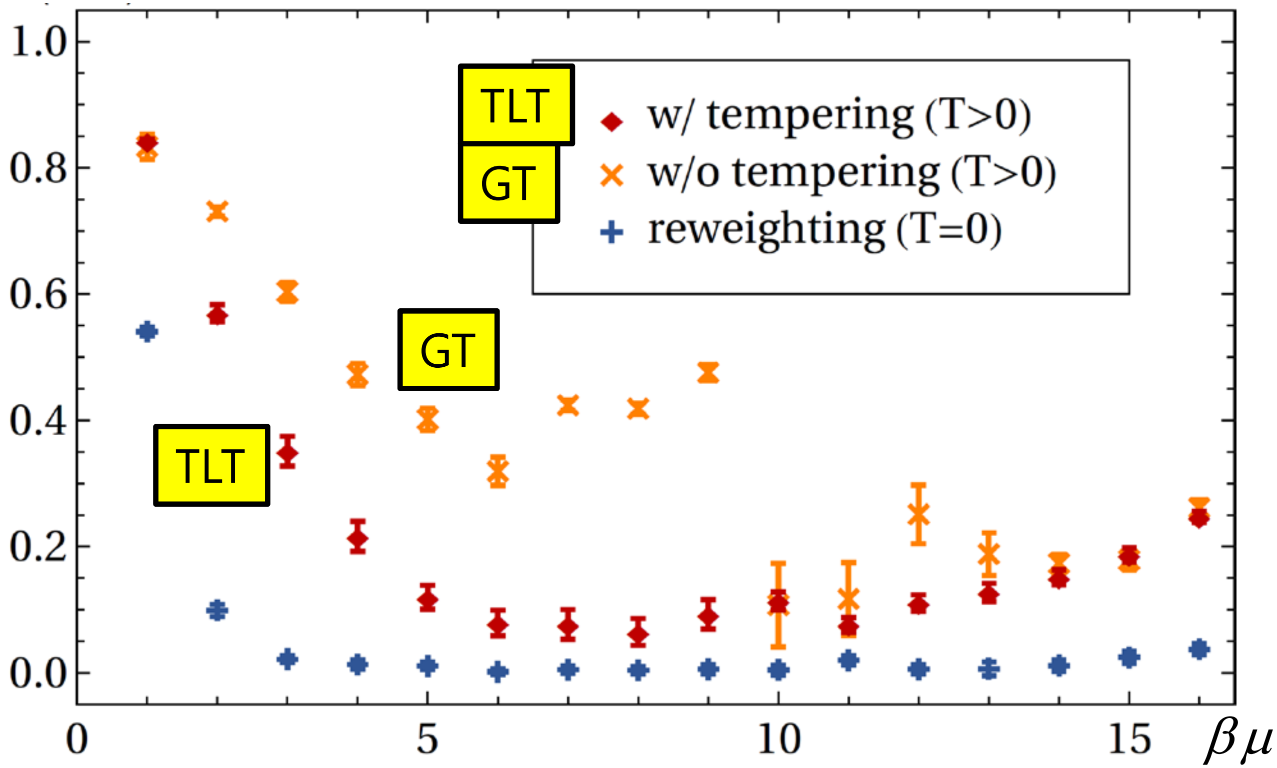
Hubbard model (4/4)

[MF-Matsumoto-Umeda 1906.04243]

average phase factor

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

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



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)

Generalized Thimble method vs TLT method (1/2)

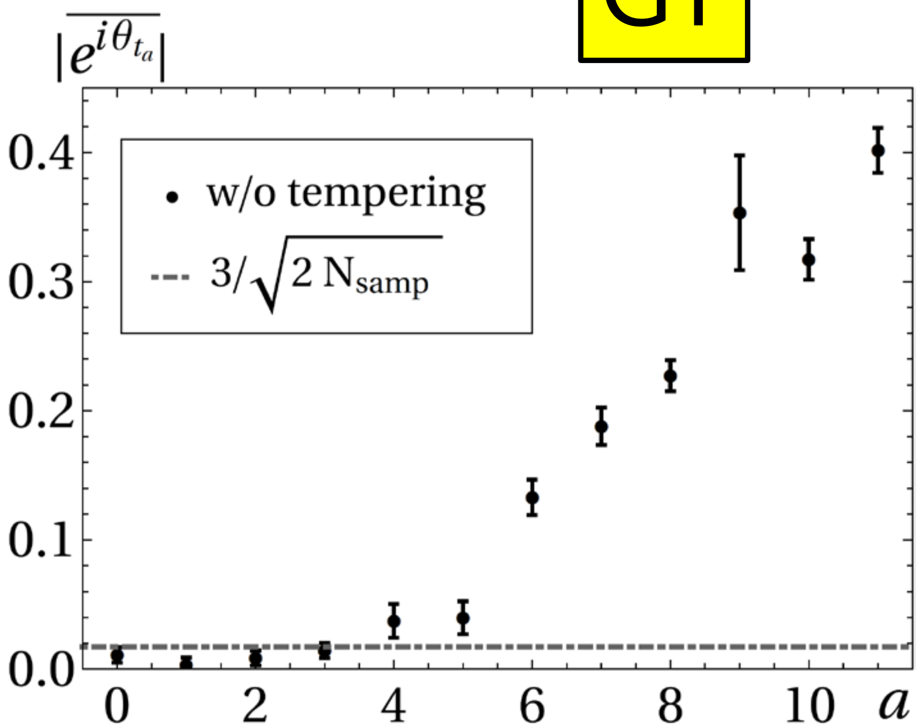
[MF-Matsumoto-Umeda 1906.04243]

- imaginary time : 5 steps ($N_\tau = 5$)
- spatial lattice: 2D periodic lattice with $N_s = 2\times 2$
- $\beta\kappa = 3,\ \ \beta U = 13,\ \ 0 \le T \le 0.5 (\Leftrightarrow 0 \le a \le 11)$
- sample size: 5,000~25,000 depending on $\beta\mu$

$$\left(\langle n \rangle = \frac{\langle e^{i\theta(z)} n(z) \rangle_{\Sigma_{t_a}}}{\langle e^{i\theta(z)} \rangle_{\Sigma_{t_a}}} \approx \overline{n}_a \right)$$

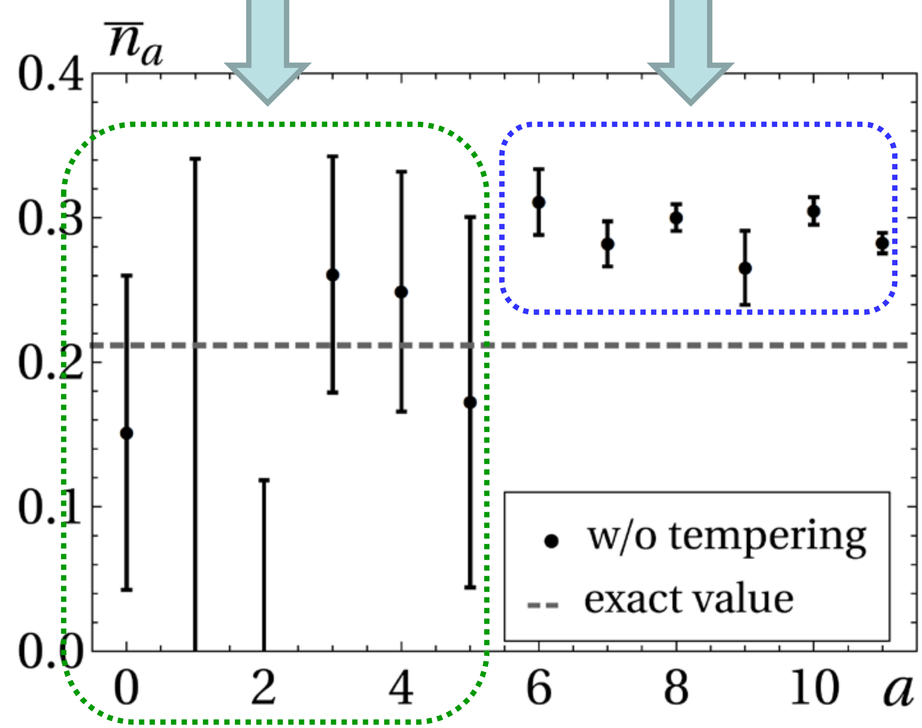
Example: $\beta\mu = 5$

GT



large stat errors (due to sign problem)

wrong value (due to multimodality)



It is a hard task to find an intermediate flow time that solves both sign problem and multimodality

Generalized Thimble method vs TLT method (2/2)

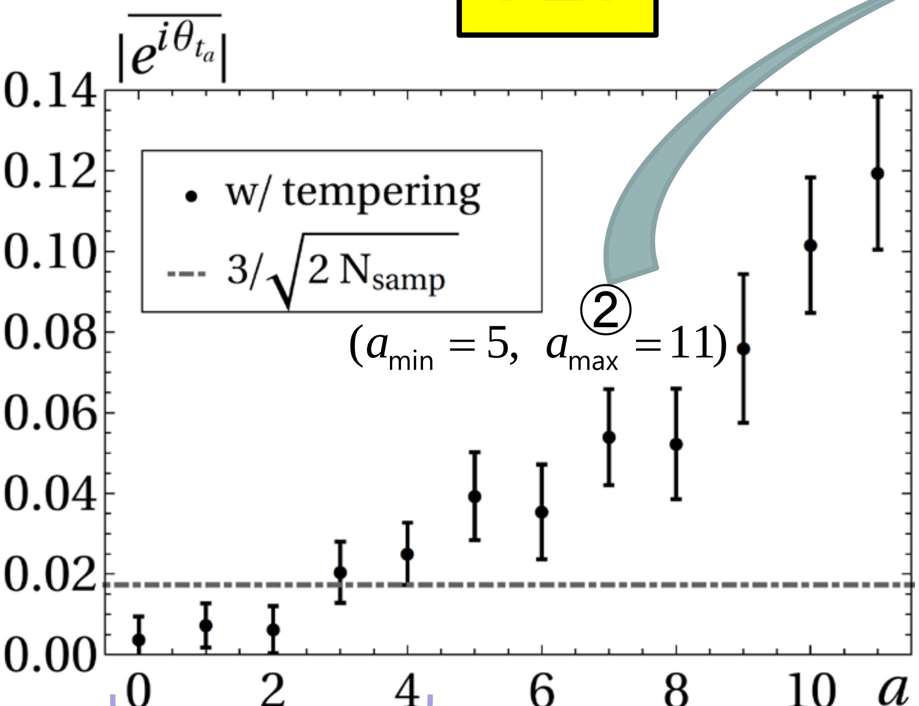
[MF-Matsumoto-Umeda 1906.04243]

imaginary time : 5 steps ($N_\tau = 5$)
spatial lattice: 2D periodic lattice with $N_s = 2 \times 2$
$\beta\kappa = 3,\ \ \beta U = 13,$ max flow time $T = 0.5$
sample size: 5,000~25,000 depending on $\beta\mu$

$$\left(\langle n \rangle = \frac{\langle e^{i\theta(z)} n(z) \rangle_{\Sigma_{t_a}}}{\langle e^{i\theta(z)} \rangle_{\Sigma_{t_a}}} \approx \overline{n}_a \right)$$

Example: $\beta\mu = 5$

TLT



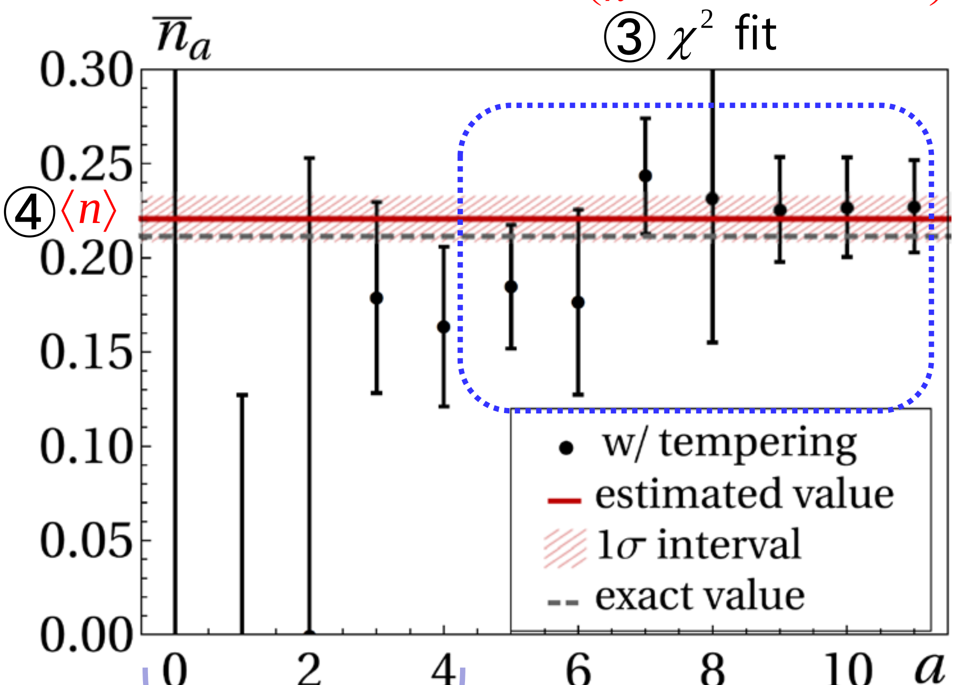
① discarded

② ($a_{\min} = 5,\ \ a_{\max} = 11$)

$\left(\begin{array}{l} \langle n \rangle \approx 0.221 \pm 0.012 \\ \chi^2 / \mathrm{DOF} = 0.45 \end{array} \right)$

③ χ^2 fit

④ $\langle n \rangle$



discarded

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6. Group manifolds **[MF, in preparation]**
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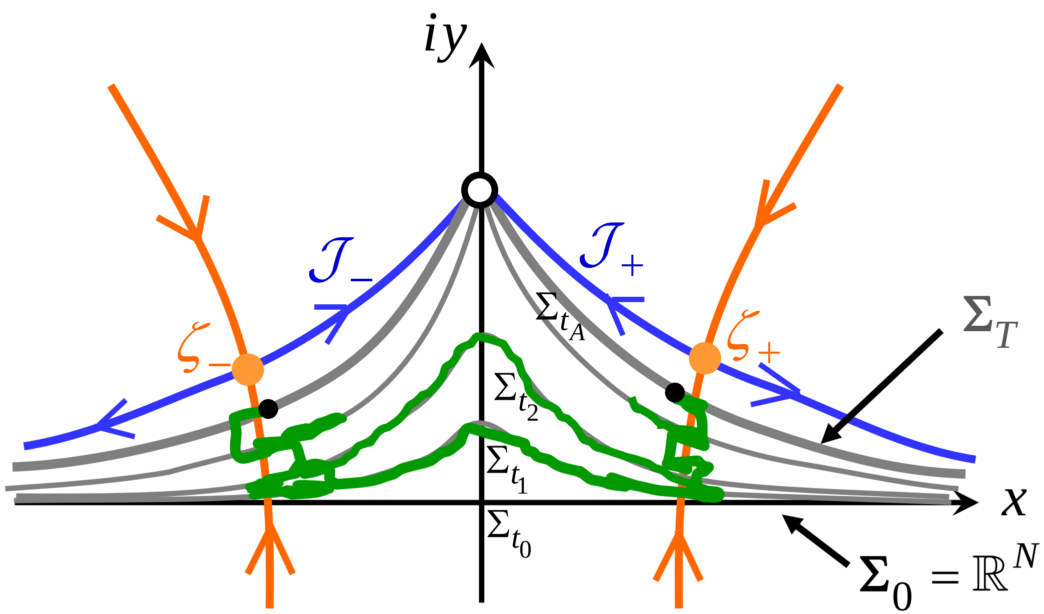
Pros and cons of the original TLT method

■ TLT method **[MF-Umeda 2017]**

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



Pros : solves the sign and ergodicity problems simultaneously
applicable to any systems once formulated by PI with cont variables

Cons : 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

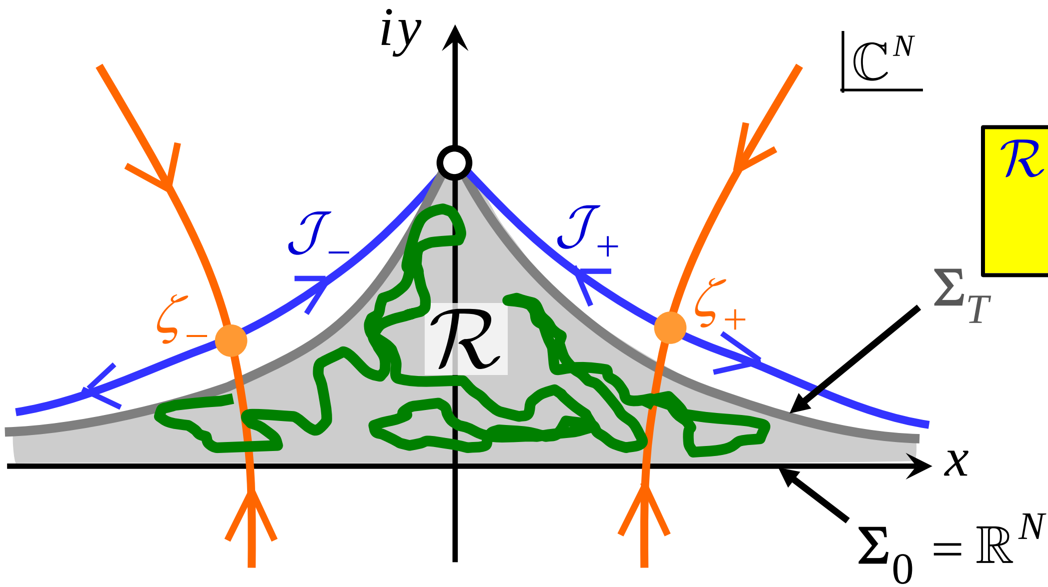
Worldvolume HMC (1/2)

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

orbit of particle → worldline
orbit of string → worldsurface
orbit of surface (membrane) → worldvolume

<u>Pros</u> : solves the sign and ergodicity problems simultaneously
applicable to any systems once formulated by PI with cont variables

⊕ 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
- Autocorrelation is reduced 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

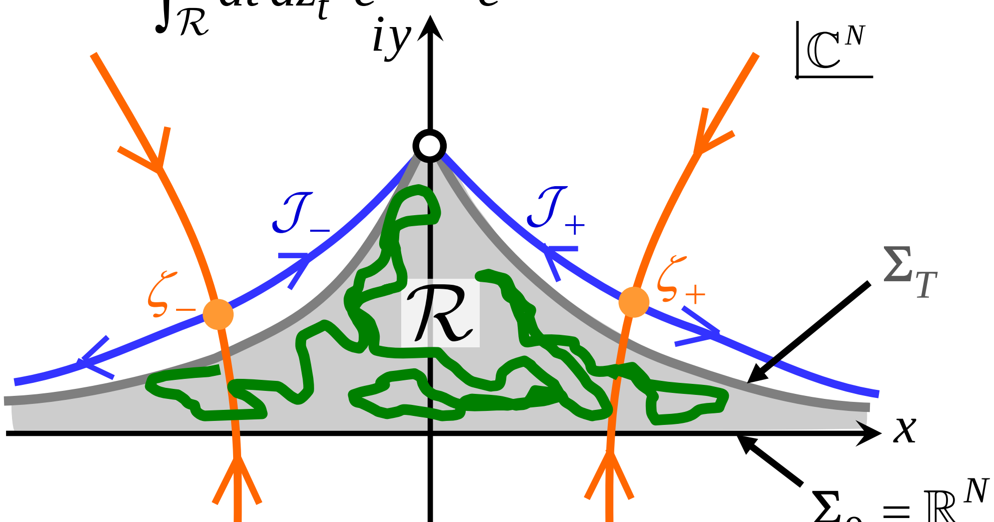
$$= \frac{\int_0^T dt\, e^{-W(t)} \int_{\Sigma_t} dz_t\; e^{-S(z_t)}\,\mathcal{O}(z_t)}{\int_0^T dt\, e^{-W(t)} \int_{\Sigma_t} dz_t\; e^{-S(z_t)}}$$

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

(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]

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⇒WV-HMC)**

- 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 2024, 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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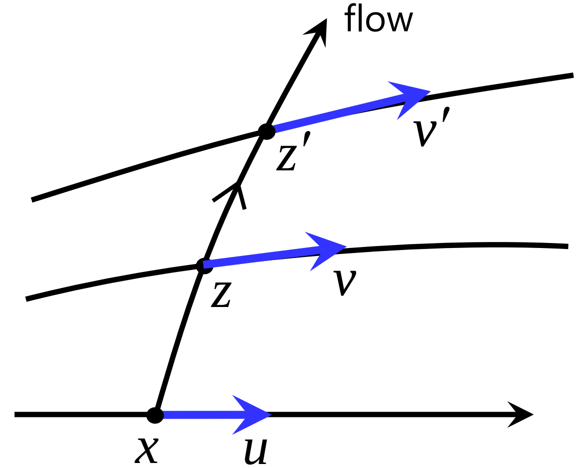
Two ways to deal with det$D(z)$ in WV-HMC

[MF-Namekawa, ongoing]

$$Z = \int dx d\bar{\psi} d\psi e^{-S_0(x) - \bar{\psi} D(x) \psi} \quad \left(x = (x^i) \ \Leftrightarrow \ U = (U_{x,\mu}) \right)$$
$$= \int dx\, e^{-S_0(x)} \det D(x)$$
$$\equiv \int dx\, e^{-S(x)} \qquad \left(S(x) = S_0(x) - \log\det D(x) \right)$$



method 1 : directly treating $-\log\det D(x)$

$$\begin{cases} \text{config} : \dot{z} = \overline{\partial S(z)} & \left(\dot{z}^i = \overline{\partial_i S(z)} \right) \\ \text{tangent} : \dot{v} = \overline{\partial^2 S(z)\, v} & \left(\dot{v}^i = \overline{\partial_i \partial_j S(z)\, v^j} \right) \end{cases}$$

$$\text{with} \begin{cases} \partial_i S = \partial_i S_0 - \mathrm{tr} D^{-1} \partial_i D \\ \partial_i \partial_j S = \partial_i \partial_j S_0 - \mathrm{tr} D^{-1} \partial_i \partial_j D + \mathrm{tr} \underline{D^{-1}} \partial_i D \underline{D^{-1}} \partial_j D \end{cases}$$

local direct direct

⇨ cost : $O(N^3)$

method 2 : use of "Majorana" pseudofermions

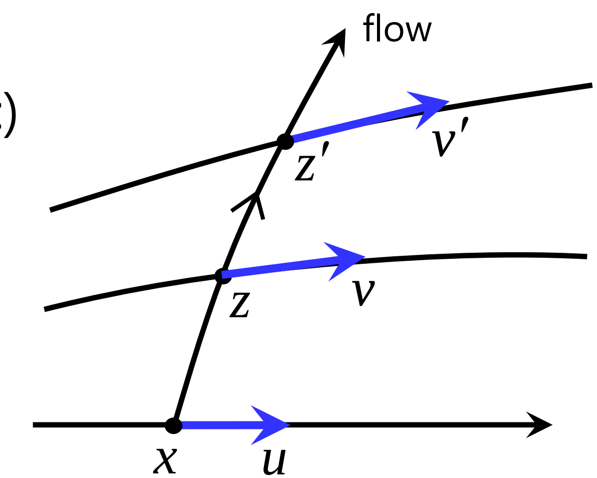
⇨ cost : $O(N^2)$

Use of "Majorana" pseudofermions

[MF-Namekawa, ongoing]

$$Z=\int dx d\bar{\psi} d\psi e^{-S_0(x)-\bar{\psi}D(x)\psi}=\int dx\, e^{-S_0(x)}\det D(x)$$

Introduce $\boxed{M(x)\equiv D(x)\,D^T(x)}$ (complex symmetric)



If $\begin{cases} \text{1) Re}\det M(x)>0 \\ \text{2) Re}\,M^{-1}(x)>0 \end{cases}$

then

$$\boxed{\det D(x)=\left(\det M(x)\right)^{1/2}=\int d\varphi\, e^{-(1/2)\varphi^T M^{-1}(x)\varphi}}$$

φ : real pseudofermion ("Majorana" pseudofermion)

$$Z=\int dx d\varphi\, e^{-S_0(x)-(1/2)\varphi^T M^{-1}(x)\varphi}=\int dx d\varphi\, e^{-S(x,\varphi)}$$

$$\boxed{S(x,\varphi)\equiv S_0(x)+\frac{1}{2}\varphi^T M^{-1}(x)\varphi}$$

Use of iterative solvers for $M^{-1}(z)$ ⇨ cost : $O(N^2)$ ⇨ **Namekawa-san's talk**

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Path integral over a compact group

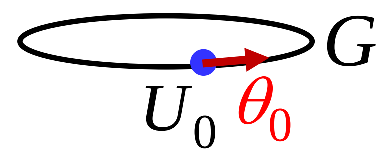
[MF, in preparation]

G : compact group ($N \equiv \dim G$: #DOF)

Lie G : Lie alg of G with basis $T_a\,(a=1,\ldots,N)$ $\left(T_a^\dagger = -T_a \text{ and } \mathrm{tr}\,T_a T_b = -\delta_{ab}\right)$

$\theta_0 \equiv dU_0\,U_0^{-1} = \sum_a T_a\,\theta_0^a$ $\left(\theta_0^a : \text{real 1-form}\right)$: Maurer-Cartan 1-form

$ds^2 = \mathrm{tr}\,\theta_0^\dagger \theta_0 = \sum_a (\theta_0^a)^2 \Rightarrow \theta_0^a\ (a=1,2,\ldots,N)$: vielbein



$\Rightarrow$ Haar measure : $|dU_0| = \theta_0^1 \wedge \cdots \wedge \theta_0^N$

$$\boxed{\langle \mathcal{O} \rangle \equiv \frac{\int_G |dU_0|\, e^{-S(U_0)}\, \mathcal{O}(U_0)}{\int_G |dU_0|\, e^{-S(U_0)}}}$$

$\begin{pmatrix} U_0 \in G : \text{dynamical variable} \\ S(U_0) \in \mathbb{C} : \text{complex action} \end{pmatrix}$

E.g. lattice gauge theory

$$G = \prod_{x,\mu} SU(n) \quad \text{(product group)}$$

dynamical variable $U_0 = \left((U_0)_{x,\mu}\right)$ $\left((U_0)_{x,\mu} \in SU(n)\right)$

action : $S(U_0) = -\dfrac{\beta}{2n} \sum_x \sum_{\mu<\nu} \mathrm{tr}\left[(U_0)_{x,\mu,\nu} + (U_0)_{x,\nu,\mu}\right] - i\,\theta \sum_x q_x(U_0)$

Cauchy's theorem for group manifolds

[MF, in preparation]

G : compact group

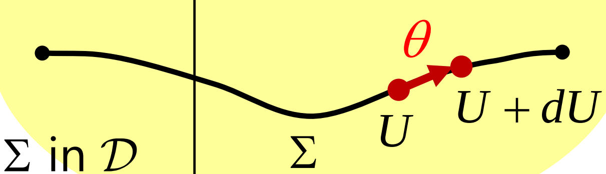
$\mathrm{Lie}\,G = \bigoplus_a \mathbb{R}T_a$: Lie alg of G

$\Downarrow$

$(\mathrm{Lie}\,G)^{\mathbb{C}} \equiv \bigoplus_a \mathbb{C}T_a$: complexification of Lie$G$

$G^{\mathbb{C}} \equiv e^{T_a z^a} e^{T_a z'^a} \cdots e^{T_a z''^a} \quad (z^a, z'^a, \ldots z''^a \in \mathbb{C})$: complexification of G

$\mathcal{D}\,(\subset G^{\mathbb{C}})$



Thm

Let $\begin{cases} \mathcal{D} \text{ : region in } G^{\mathbb{C}}, \\ f(U) \text{ : holomorphic function in } \mathcal{D}. \end{cases}$

Then, the integral of $f(U)$ over a real N-dim submfd Σ in $\mathcal{D}$

$$I_\Sigma = \int_\Sigma (dU)_\Sigma \, f(U)$$

depends only on the boundary of Σ. Here, for $U, U + dU \in \Sigma$,

$$\theta \equiv dU\,U^{-1} = T_a\,\theta^a$$

$$(dU)_\Sigma \equiv \theta^1 \wedge \cdots \wedge \theta^N$$

proof

Maurer-Cartan eq. $d\theta = \theta \wedge \theta \Rightarrow d\theta^a = \frac{1}{2}\sum_{b,c} C_{bc}{}^a\,\theta^b \wedge \theta^c \Rightarrow \boxed{d(dU)_\Sigma = 0}$

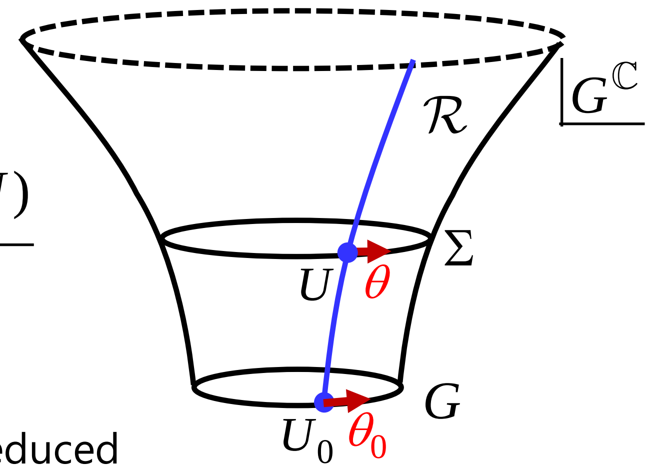
$\left([T_b, T_c] = \sum_{b,c} C_{bc}{}^a T_a \right)$

The rest is the same as in the flat case.

Path integral over the worldvolume (1/2)

[MF, in preparation]

Deformation of the integration surface:



Cauchy's thm

$$\langle \mathcal{O} \rangle = \frac{\int_G |dU_0|\, e^{-S(U_0)}\, \mathcal{O}(U_0)}{\int_G |dU_0|\, e^{-S(U_0)}} = \frac{\int_\Sigma (dU)_\Sigma\, e^{-S(U)}\, \mathcal{O}(U)}{\int_\Sigma (dU)_\Sigma\, e^{-S(U)}}$$

severe sign problem   sign problem significantly reduced

Define $DS(U)$ by

$$\delta S(U) = -\mathrm{tr}(\delta U U^{-1}) DS(U)$$

$$\boxed{\dot{U} = -[DS(U)]^\dagger U}$$

$$\left(\begin{aligned} [S(U)]^{\cdot} &= -\mathrm{tr}\, \dot{U} U^{-1} DS(U) \\ &= +\mathrm{tr}[DS(U)]^\dagger DS(U) \geq 0 \end{aligned} \right)$$

NB

$$\begin{cases} \theta_0 \equiv dU_0 U_0^{-1} = \sum_a T_a\, \theta_0^a \\ \theta \equiv dU\, U^{-1} = \sum_a T_a\, \theta^a \end{cases}$$

θ^a is linear in θ_0^a : $\theta^i = \sum_a E_a^i \theta_0^a$

$$(dU)_\Sigma = \theta^1 \wedge \cdots \wedge \theta^N = \theta_0^1 \wedge \cdots \wedge \theta_0^N \det E$$

$$= |dU_0| \det E$$

Path integral over the worldvolume (2/2)

[MF, in preparation]

$$\langle \mathcal{O} \rangle = \frac{\int_{\Sigma_t} (dU)_{\Sigma_t}\ e^{-S(U)}\,\mathcal{O}(U)}{\int_{\Sigma_t} (dU)_{\Sigma_t}\ e^{-S(U)}}$$

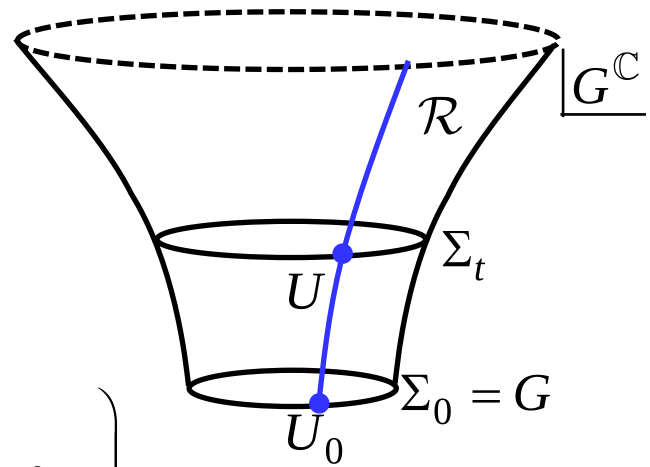
t-independent

t-independent

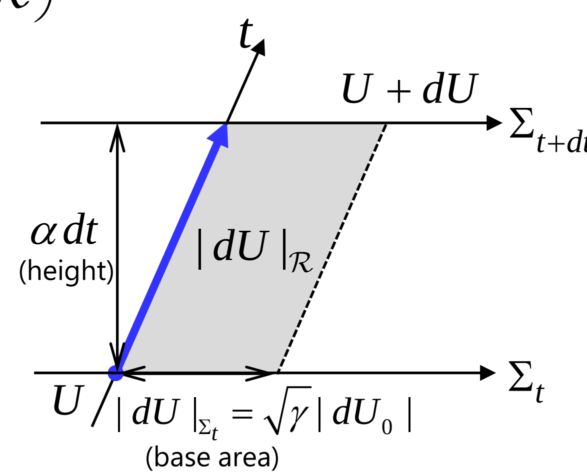
$$= \frac{\int dt\, e^{-W(t)} \int_{\Sigma_t} (dU)_{\Sigma_t}\ e^{-S(U)}\,\mathcal{O}(U)}{\int dt\, e^{-W(t)} \int_{\Sigma_t} (dU)_{\Sigma_t}\ e^{-S(U)}}$$

$$= \frac{\int_{\mathcal{R}} |dU|_{\mathcal{R}}\ e^{-V(U)}\,\mathcal{F}(U)\,\mathcal{O}(U)}{\int_{\mathcal{R}} |dU|_{\mathcal{R}}\ e^{-V(U)}\,\mathcal{F}(U)}$$

($|dU|_{\mathcal{R}}$: inv vol element of $\mathcal{R}$)



$$\left(\begin{array}{l} V(U) = \mathrm{Re}\, S(U) + W(t(U)) \\ \mathcal{F}(U) = \dfrac{dt\,(dU)_{\Sigma_t}}{|dU|_{\mathcal{R}}}\, e^{-i\,\mathrm{Im}\,S(U)} = \alpha^{-1}\dfrac{\det E}{\sqrt{\gamma}}\, e^{-i\,\mathrm{Im}\,S(U)} \end{array} \right)$$



$$\left(ds_\Sigma^2 = \mathrm{Re}\,\mathrm{tr}\,\theta^\dagger\theta = \gamma_{ab}\theta_0^a\theta_0^b \right)$$

Constrained molecular dynamics (RATTLE) on $\mathcal{R}$ can be defined in a similar way to the flat case

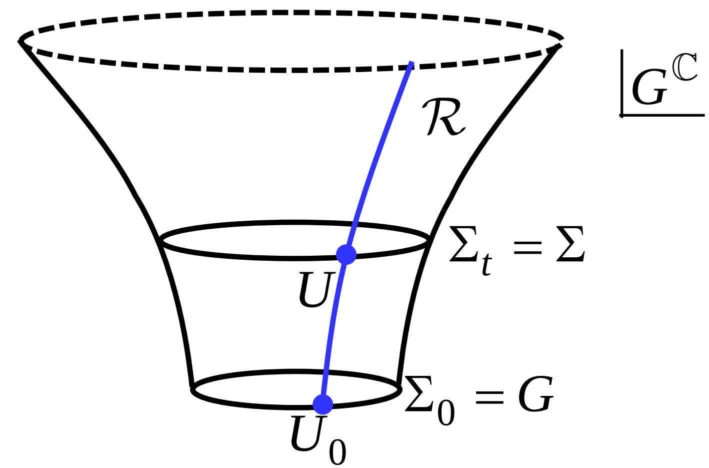
- exact reversibility
- exact volume preservation
- approximate energy conservation to $O(\Delta s^2)$ at one MD step

E.g. 1-site with a pure imaginary coupling

[MF, in preparation]

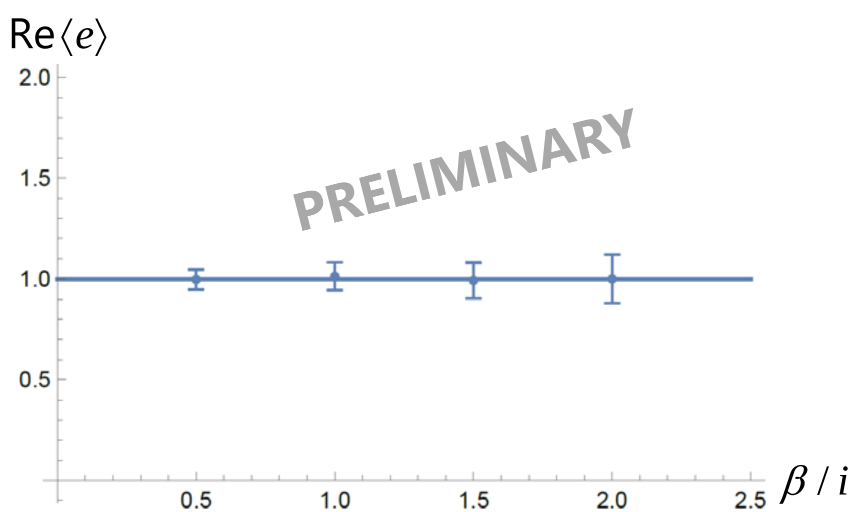
$G = SU(2)$

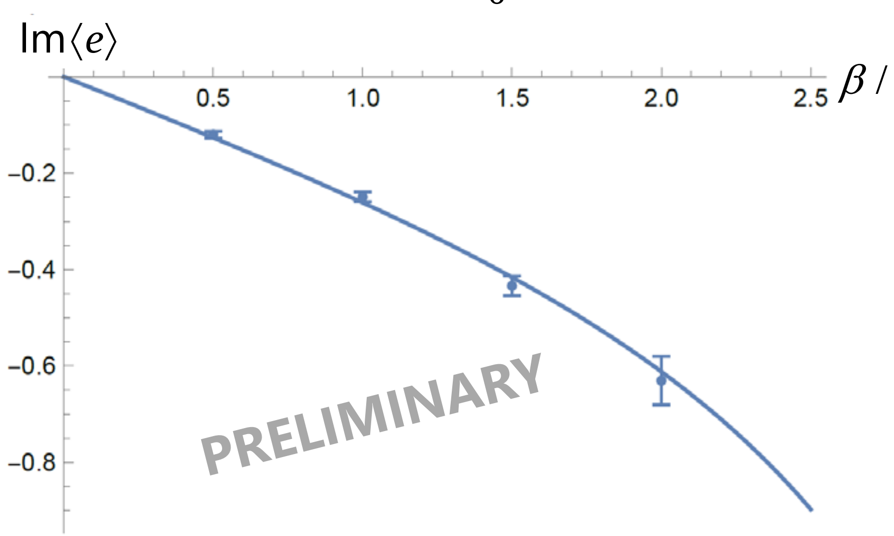
$$S(U) \equiv \beta\, e(U) \equiv \frac{\beta}{4}\,\mathrm{tr}\left(2 - U - U^{-1}\right) \quad (\beta \in i\,\mathbb{R})$$



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

numerical result (WV-HMC):



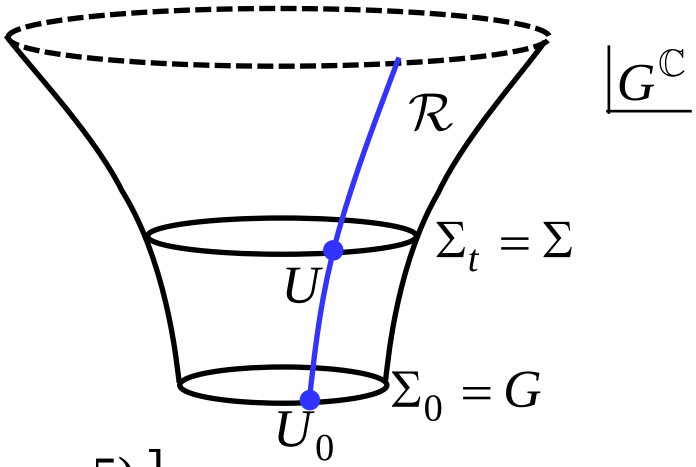


E.g. 1-site with a topological term

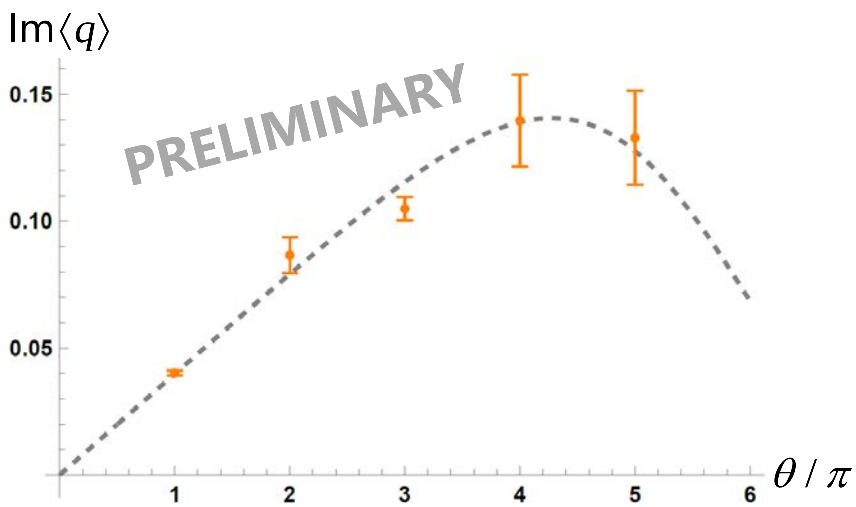
[MF, in preparation]

$\underline{G = U(2)}$ $\left(\underline{\text{NB}} : U(2) = SU(2) \times U(1) / Z_2 \neq SU(2) \times U(1)\right)$

$$S(U) \equiv \beta\, e(U) - i\theta q(U)$$
$$\equiv -\frac{\beta}{4} \operatorname{tr}\left(U + U^{-1}\right) - \frac{\theta}{4\pi} \operatorname{tr}\left(U - U^{-1}\right)$$
$$\left(\beta, \theta \in \mathbb{R}\right)$$



result (WV-HMC): $\left[\ \beta = 0.5,\quad \theta = n\pi\ (n = 1, \ldots, 5)\ \right]$

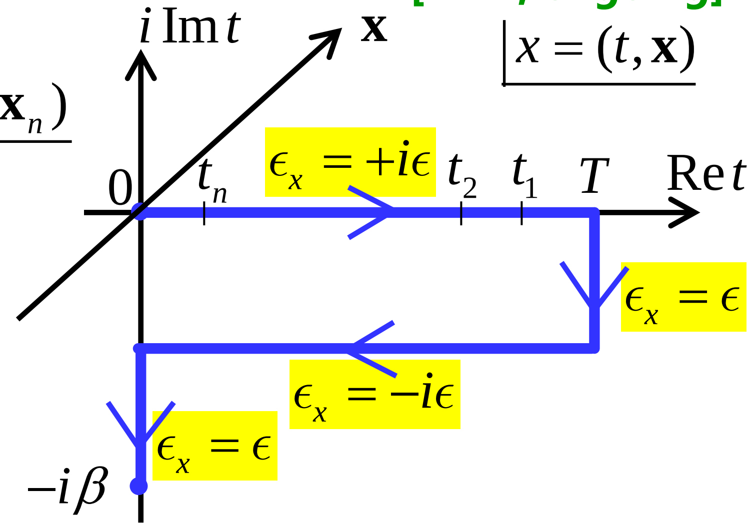


Plan

1. Introduction
2. Lefschetz thimble (LT) method **[Witten 2010, Cristoforetti et al. 2012, Fujii et al. 2013]**
   / Generalized thimble (GT) method **[Alexandru et al 2017]**
3. Tempered Lefschetz thimble (TLT) method **[MF-Umeda 2017]**
4. Worldvolume Hybrid Monte Carlo (WV-HMC) method **[MF-Matsumoto 2020]**
5. Dynamical fermions **[MF-Namekawa, ongoing]**
6. Group manifolds **[MF, in preparation]**
7. Real-time dynamics **[MF+, ongoing]** **cf) Nishimura-san's talk**
8. Summary and outlook

Case 1: Thermal equilibrium

[MF+, ongoing]



Target

$e^{i\hat{H}T}$ $e^{-i\hat{H}T}$

$$\langle \mathcal{O}(t_1,\mathbf{x}_1)\cdots\mathcal{O}(t_n,\mathbf{x}_n)\rangle_\beta \equiv \frac{\mathrm{tr}\, e^{-\beta H}\mathcal{O}(t_1,\mathbf{x}_1)\cdots\mathcal{O}(t_n,\mathbf{x}_n)}{\mathrm{tr}\, e^{-\beta H}}$$

$e^{i\hat{H}T}$ $e^{-i\hat{H}T}$

where

$$\mathcal{O}(x) = e^{i\hat{P}\cdot x}\mathcal{O}(0)\,e^{i\hat{P}\cdot x} \quad \big(x=(t,\mathbf{x})\big)$$

Path-integral representation

lattice Schwinger-Keldysh path

⇔ parameter-dependent temporal lattice spacing **[Alexandru et al. 2017]**

$$S(\varphi) = \sum_x \epsilon_x a^{d-1}\left[\begin{array}{l}\frac{1}{2}\left[V(\varphi_x)+V(\varphi_{x+0})\right]+\frac{(\varphi_x-\varphi_{x+0})^2}{2\epsilon_x^2}\\ +\frac{1}{4a^2}\sum_{i=1}^{d-1}\left[(\varphi_x-\varphi_{x+i})^2+(\varphi_{x+0}-\varphi_{x+0+i})^2\right]\end{array}\right] \quad \big(x=(t,\mathbf{x})\big)$$

$$\langle \varphi(t_1,\mathbf{x}_1)\cdots\varphi(t_n,\mathbf{x}_n)\rangle_\beta \equiv \int (d\varphi)\,e^{-S(\varphi)}\varphi(t_1,\mathbf{x}_1)\cdots\varphi(t_n,\mathbf{x}_n) \Big/ \int (d\varphi)\,e^{-S(\varphi)}$$

Large time separations $(\Delta t) \gtrsim 4\beta$ encounters the ergodicity problem ⇨ WV-HMC
[Alexandru et al. 2017]

First target : Transport coefficients **[MF+, ongoing]**

directly calculate from real-time correlators (w/o using Kubo relation)

Case 2: Nonequilibrium processes

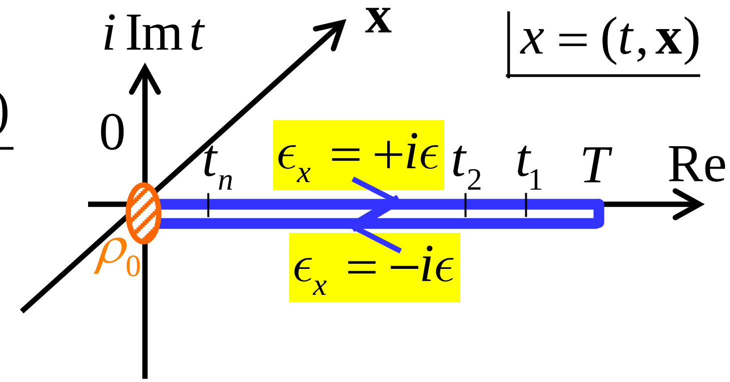
[MF+, ongoing]

<u>Initial density matrix</u> ρ_0

$$e^{i\hat{H}T}e^{-i\hat{H}T}$$

$$\langle \mathcal{O}(t_1,\mathbf{x}_1)\cdots\mathcal{O}(t_n,\mathbf{x}_n)\rangle \equiv \frac{\mathrm{tr}\,\rho_0 \, \mathcal{O}(t_1,\mathbf{x}_1)\cdots\mathcal{O}(t_n,\mathbf{x}_n)}{\mathrm{tr}\,\rho_0}$$

$$e^{i\hat{H}T}e^{-i\hat{H}T}$$



⇩

$$\langle \varphi(t_1,\mathbf{x}_1)\cdots\varphi(t_n,\mathbf{x}_n)\rangle_\beta \equiv \int (d\varphi)\, e^{-S(\varphi)}\varphi(t_1,\mathbf{x}_1)\cdots\varphi(t_n,\mathbf{x}_n) \Big/ \int (d\varphi)\, e^{-S(\varphi)}$$

The computation is essentially the same as before.

Plan

1. Introduction
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Summary and outlook

■ **Summary** : WV-HMC algorithm has been extended to various cases successfully

- exact reversibility
- exact volume preservation
- approximate energy conservation to $O(\Delta s^2)$ at one MD step

■ **Outlook**

▼ Roadmap to **finite-density QCD** with WV-HMC :

local fields
(e.g. complex scalars)

group manifolds
(e.g. 1-site model)

→ pure YM
(e.g. w/ finite θ)
[MF, MF-Kuwahara-
-Namekawa-..., ongoing]

fermions
(e.g. Thirring, Stephanov, Hubbard)

→ finite-density QCD
(w/ or w/o θ)
[MF-Kanamori-Kuwahara-
-Namekawa-..., ongoing]

▼ Developing the algorithm itself **[MF, ongoing]**

- incorporation of machine learning technique
- incorporation of other algorithm(s)

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

▼ Important in the near future : MC for real-time dyn of quant many-body systems **[MF+, ongoing]**

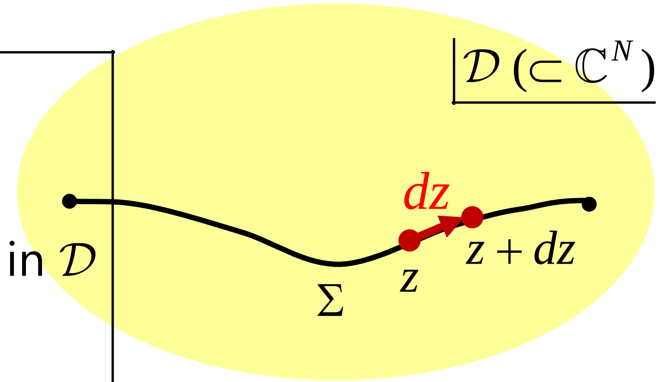
⇨ first-principles calculations of nonequilibrium processes
(such as the early universe, heavy-ion collision experiments, new devices, ...)

Thank you.

Appendix

Cauchy's theorem in a flat space

Thm



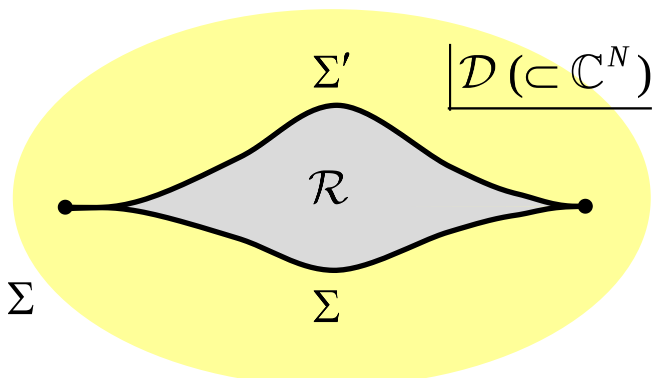
Let $\begin{cases} \mathcal{D} : \text{region in a complex } N\text{-dim space } \mathbb{C}^N = \mathbb{R}^{2N}, \\ f(z) : \text{holomorphic function in } \mathcal{D}. \end{cases}$

Then, the integral of $f(z)$ over a real N-dim submfd Σ in $\mathcal{D}$

$$I_\Sigma = \int_\Sigma dz\, f(z) \quad (dz = dz^1 \wedge \cdots \wedge dz^N)$$

depends only on the boundary of Σ

proof



We set

$\begin{cases} \Sigma, \Sigma' : \text{(oriented) real } N\text{-dim submfd in } \mathcal{D} \\ \qquad\quad \text{sharing common boundaries} \\ \mathcal{R} : \text{region surrounded by } \Sigma \text{ and } \Sigma' \end{cases}$ $\quad \therefore\ \partial\mathcal{R} = \Sigma' - \Sigma$

Then, due to Stokes' thm, we have $\boxed{d(dz) = 0}$

$$I_{\Sigma'} - I_\Sigma = \int_{\partial\mathcal{R}} dz\, f(z) = \int_{\mathcal{R}} d\,[dz\, f(z)] = (-1)^N \int_{\mathcal{R}} dz \wedge df(z)$$

Here, since $df(z) = dz^i \dfrac{\partial f(z)}{\partial z^i} + d\bar{z}^i \underbrace{\dfrac{\partial f(z)}{\partial \bar{z}^i}}_{0} = dz^i \dfrac{\partial f(z)}{\partial z^i}$, we have

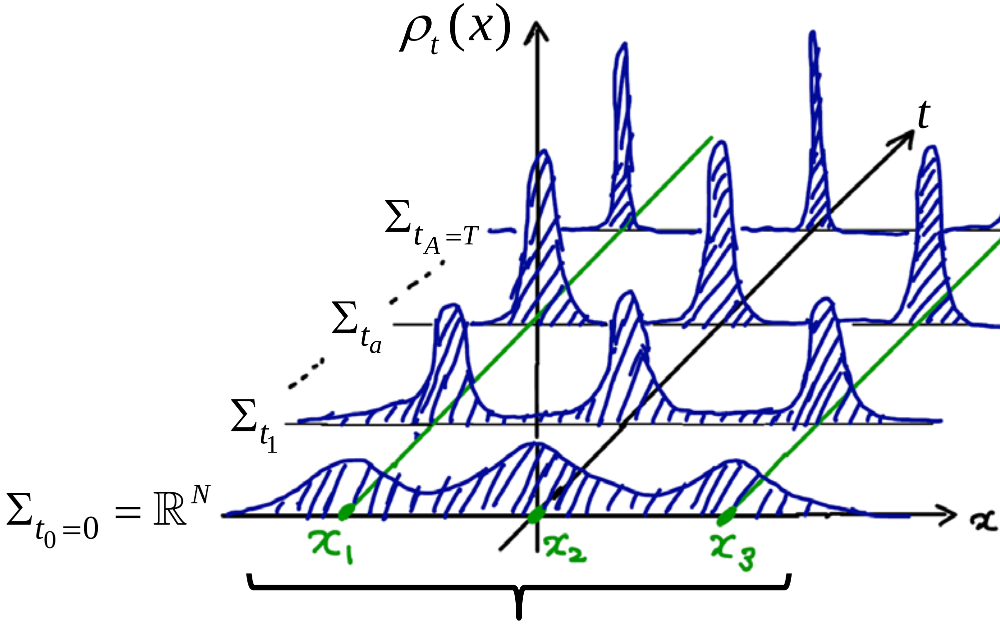
$$dz \wedge df(z) = \underbrace{(dz^1 \wedge \cdots \wedge dz^N) \wedge dz^i}_{0} \frac{\partial f(z)}{\partial z^i} = 0 \quad \therefore\ I_{\Sigma'} - I_\Sigma = 0 \quad \text{(QED)}$$

No overlap problem for TLT method

[MF-Umeda 1703.00861, MF-Matsumoto-Umeda 1906.04243]

Important point in TLTM:

large overlaps in the temporal direction



$$\rho_t(x) \propto e^{-\mathrm{Re}\, S(z_t(x))} \left| \det \frac{\partial z_t(x)}{\partial x} \right|$$

Distribution functions have peaks at the same positions x_σ
for varying tempering parameter (which is t in our case)

⇨ We can expect significant overlap between adjacent replicas!

Details of GT/WV-HMC algorithm (1/5)

■ RATTLE

HMC on a submanifold $\mathcal{M}$ in $\mathbb{C}^N = \mathbb{R}^{2N}$

$\mathcal{M} = \mathcal{J}$: Lefschetz thimble ⇨ original (**LT-HMC**) [Fujii et al. 2013]

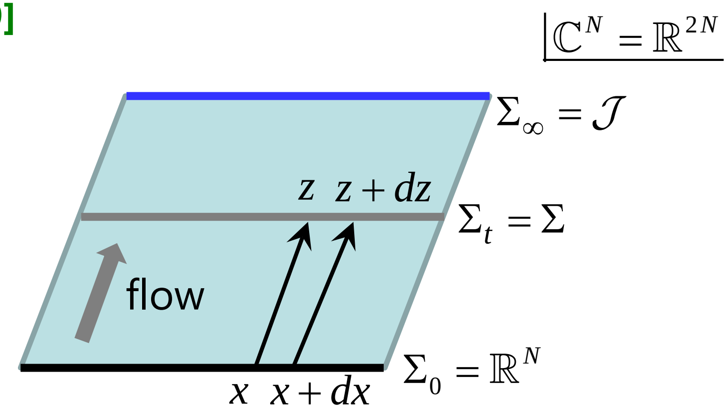
$\mathcal{M} = \Sigma$: deformed surface ⇨ Generalized thimble HMC (**GT-HMC**) [Alexandru@Lattice2019, MF-Matsumoto-Umeda 2019]

$\mathcal{M} = \mathcal{R}$: worldvolume ⇨ Worldvolume HMC (**WV-HMC**) [MF-Matsumoto 2020]

■ LT-HMC / GT-HMC

[Alexandru@Lattice2019, MF-Matsumoto-Umeda 2019]

$$\langle \mathcal{O} \rangle = \frac{\int_\Sigma dz\, e^{-S(z)} \mathcal{O}(z)}{\int_\Sigma dz\, e^{-S(z)}} = \frac{Z_\mathcal{O}}{Z}$$



parametrization of Σ

$$z = (z^i(x)) \text{ with } x = (x^a) \quad \begin{pmatrix} i = 1,\ldots,N \\ a = 1,\ldots,N \end{pmatrix}$$

basis of $T_z\Sigma$: $\boxed{E_a = (E_a^i) \text{ with } E_a^i \equiv \partial z^i / \partial x^a}$

⇨ $dz = dz^1 \wedge \cdots \wedge dz^N = \det E\, dx$

induced metric

$$ds_\Sigma^2 \equiv |dz^i(x)|^2 = \gamma_{ab} dx^a dx^b \quad (\gamma_{ab} \equiv \mathrm{Re}\, \overline{E_a^i} E_b^i = \overline{E_a^i} E_b^i)$$

invariant volume element $\boxed{|dz| = |\det E|\, dx = \sqrt{\gamma}\, dx}$

Details of GT/ WV-HMC algorithm (2/5)

[Alexandru@Lattice2019, MF-Matsumoto-Umeda 2019] [MF 2311.10663]

Here, for $\boxed{|dz| = |\det E|\, dx = \sqrt{\gamma}\, dx}$, we have

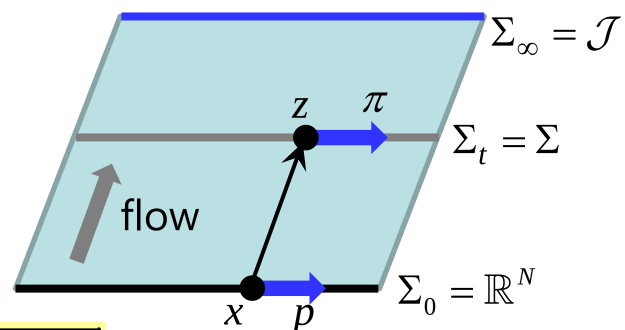
$$\begin{cases} |dz| = \sqrt{\gamma}\, dx = dx\, dp\, e^{-(1/2)\gamma^{ab} p_a p_b} = \dfrac{\omega^N}{N!} e^{-(1/2)\gamma^{ab} p_a p_b} & \left[(\gamma^{ab}) \equiv (\gamma_{ab})^{-1}\right] \\ \omega \equiv dp_a \wedge dx^a \text{ (symplectic 2-form)} \end{cases}$$

Substitute this to $Z = \int_\Sigma dz\, e^{-S(z)} = \int_\Sigma |dz|\, e^{-\operatorname{Re} S(z)} \times \dfrac{dz}{|dz|} e^{-i \operatorname{Im} S(z)}$:

$$\boxed{Z = \int_{T\Sigma} \frac{\omega^N}{N!} e^{-H(x,p)} \mathcal{F}(x) \text{ with } \begin{cases} H(x,p) = \dfrac{1}{2}\gamma^{ab} p_a p_b + \operatorname{Re} S(z(x)) \\ \mathcal{F}(x) = \dfrac{dz}{|dz|} e^{-i \operatorname{Im} S(z)} \text{ (reweighting factor)} \end{cases}}$$

"parameter-space representation"

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



Furthermore, we introduce $\pi^i \equiv p^a E_a^i \in T_z\Sigma$, which gives

$$\begin{cases} (\omega =)\ dp_a \wedge dx^a = \operatorname{Re} d\overline{\pi^i} \wedge dz^i \\ \gamma^{ab} p_a p_b = \pi^\dagger \pi \end{cases}$$

$$\Rightarrow \boxed{Z = \int_{T\Sigma} \frac{\omega^N}{N!} e^{-H(z,\pi)} \mathcal{F}(z) \text{ with } \begin{cases} H(z,\pi) = \dfrac{1}{2}\pi^\dagger \pi + \operatorname{Re} S(z) \\ \mathcal{F}(z) = \dfrac{dz}{|dz|} e^{-i \operatorname{Im} S(z)} \end{cases}}$$

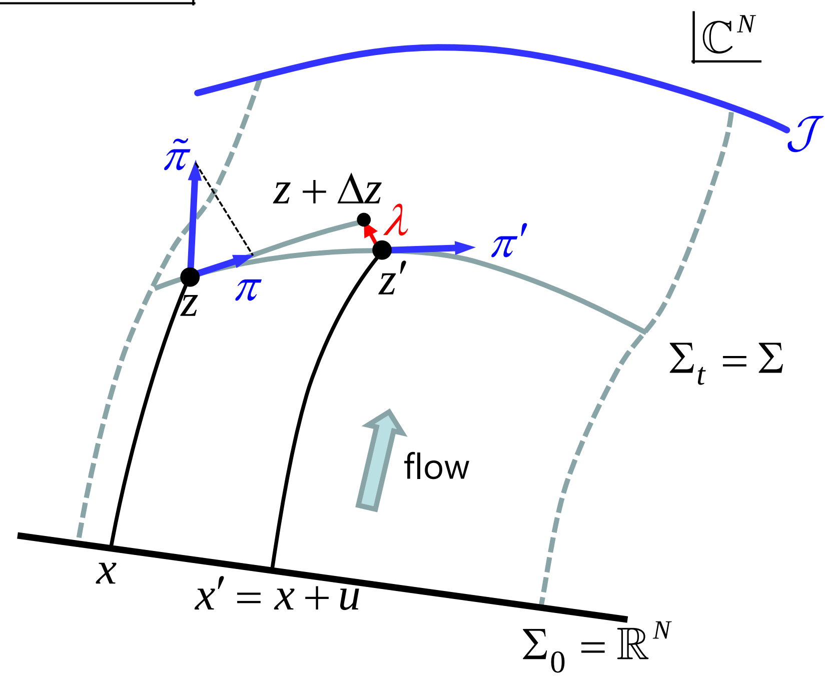
"target-space representation"

no need to calculate the Jacobian $\det E = \sqrt{\gamma}$

Details of GT/ WV-HMC algorithm (3/5)

$$Z = \int_{T\Sigma} \frac{\omega^N}{N!} e^{-H(z,\pi)} \mathcal{F}(z) \quad \text{with} \quad \begin{cases} H(z,\pi) = \frac{1}{2}\pi^\dagger \pi + \mathrm{Re}\, S(z) \\ \mathcal{F}(z) = \frac{dz}{|dz|} e^{-i\,\mathrm{Im} S(z)} \end{cases}$$

[Alexandru@Lattice2019, MF-Matsumoto-Umeda 2019]
[MF 2311.10663]



Algorithm of GT-HMC

(i) generation of an initial momentum

① $\tilde{\pi} = (\tilde{\pi}^i) \in \mathbb{C}^N \leftarrow e^{-\tilde{\pi}^\dagger \tilde{\pi}/2}$

② $\tilde{\pi} \to \pi \in T_z \Sigma$

(ii) constrained MD (RATTLE)

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

where $\begin{cases} \lambda \in N_z \Sigma \ \text{ s.t. } \ z' \in \Sigma \\ \lambda' \in N_{z'} \Sigma \ \text{ s.t. } \ \pi' \in T_{z'} \Sigma \end{cases}$

λ, λ' can be found easily by using the simplified Newton $\left[\#\text{itr} = O\left((\ln N)^{1-2}\right)\right]$
[MF 2311.10663]

(iii) Metropolis test

after repeating MD steps, we update config from z to z' with prob $\min\left(1, e^{-H(z',\pi') + H(z,\pi)}\right)$

cf) "fixed-point method" for LT-HMC **[Fujii et al. 1309.4371]**)

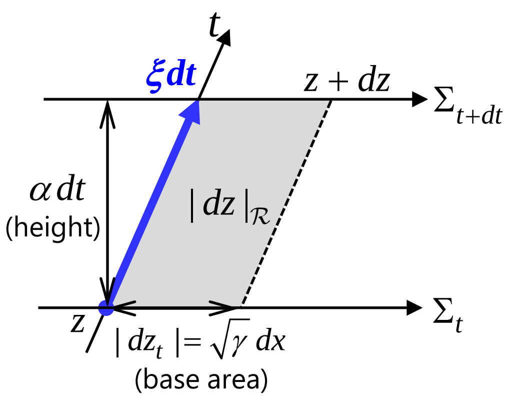
[MF-Matsumoto 2012.08468]
[MF 2311.10663]

■ WV-HMC

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

parametrization of $\mathcal{R}$

$$z = (z^i(\hat{x})) \text{ with } \hat{x} = (\hat{x}^\mu) = (\hat{x}^0 = t, \hat{x}^i = x^i) \quad \begin{pmatrix} i = 1,\ldots,N \\ \mu = 0,1,\ldots,N \\ a = 1,\ldots,N \end{pmatrix}$$



basis of $T_z\mathcal{R}$: $\boxed{\hat{E}_\mu = (\hat{E}^i_\mu) \text{ with } \hat{E}^i_\mu \equiv \partial z^i / \partial \hat{x}^\mu}$

induced metric

$$ds^2_{\mathcal{R}} \equiv |dz^i(x)|^2 = \hat{\gamma}_{\mu\nu} d\hat{x}^\mu d\hat{x}^\nu \quad (\hat{\gamma}_{\mu\nu} \equiv \overline{\hat{E}^i_a} \hat{E}^i_b)$$
$$= \alpha^2 dt^2 + \gamma_{ab}(dx^a + \beta^a dt)(dx^b + \beta^b dt)$$

invariant volume element $\quad |dz|_{\mathcal{R}} = \sqrt{\hat{\gamma}}\, d\hat{x} = \alpha\sqrt{\gamma}\, dt\, dx = \alpha dt\, |dz_t|$

Also, $\pi^i \equiv \hat{p}^\mu \hat{E}^i_\mu \;\Rightarrow\; \hat{\omega} \equiv d\hat{p}_\mu \wedge d\hat{x}^\mu = \mathrm{Re}\, d\overline{\pi^i} \wedge dz^i$

$$\sqrt{\hat{\gamma}}\, d\hat{x} = d\hat{x}\, d\hat{p}\, e^{-(1/2)\,\hat{\gamma}^{\mu\nu}\hat{p}_\mu \hat{p}_\nu} = \frac{\hat{\omega}^{N+1}}{(N+1)!} e^{-(1/2)\,\pi^\dagger \pi}$$

$$\boxed{dt\,|dz_t| = \frac{\hat{\omega}^{N+1}}{(N+1)!} e^{-(1/2)\,\pi^\dagger\pi} \alpha^{-1}}$$

$$\Rightarrow \boxed{Z = \int_{T\mathcal{R}} \frac{\hat{\omega}^{N+1}}{(N+1)!} e^{-H(z,\pi)} \mathcal{F}(z) \text{ with } \begin{cases} H(z,\pi) = \frac{1}{2}\pi^\dagger \pi + \mathrm{Re}\, S(z) + W(t(z)) \\ \mathcal{F}(z) = \alpha^{-1}(z) \frac{dz_t}{|dz_t|} e^{-i\,\mathrm{Im}\, S(z)} \end{cases}}$$

Details of GT/ WV-HMC algorithm (5/5)

[MF-Matsumoto 2012.08468]
[MF 2311.10663]

Algorithm

(i) generation of an initial momentum

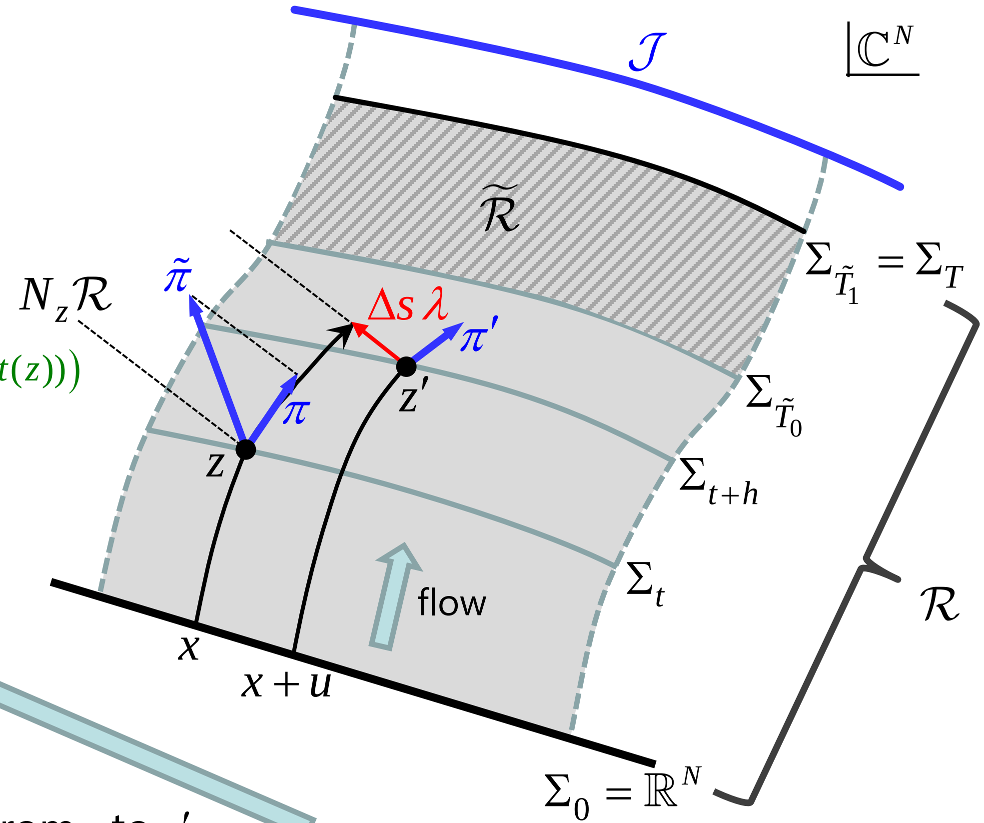
① $\tilde{\pi} = (\tilde{\pi}^i) \in \mathbb{C}^N \leftarrow e^{-\tilde{\pi}^\dagger \tilde{\pi}/2}$

② $\tilde{\pi} \to \pi \in T_z\mathcal{R}$

(ii) constrained MD (RATTLE)

$$\begin{cases} \pi_{1/2} = \pi - \Delta s\, \overline{\partial V(z)} - \lambda & (V(z) \equiv \mathrm{Re}\, S(z) + W(t(z))) \\ z' = z + \Delta s\, \pi_{1/2} \\ \pi' = \pi_{1/2} - \Delta s\, \overline{\partial V(z')} - \lambda' \end{cases}$$

where $\begin{cases} \lambda \in N_z\mathcal{R} \ \text{ s.t. } \ z' \in \mathcal{R} \\ \lambda' \in N_{z'}\mathcal{R} \ \text{ s.t. } \ \pi' \in T_{z'}\mathcal{R} \end{cases}$



(iii) Metropolis test

after repeating MD, we update config from z to z'

with prob $\min\left(1, e^{-H(z',\pi')+H(z,\pi)}\right)$

λ, λ' can be found easily by using the simplified Newton $\left[\#\text{itr}=O\left((\ln N)^{1-2}\right)\right]$ **[MF 2311.10663]**

(iv) measurement

we estimate observables from the subsample

in a subregion $\widetilde{\mathcal{R}} = \left\{ z \in \mathcal{R} \,\middle|\, \tilde{T}_0 \le t(z) \le \tilde{T}_1 \right\}$

[Ref] statistical analysis method for WV-HMC: **[MF-Matsumoto-Namekawa 2107.06858]**

Computational cost of GT/WV-HMC

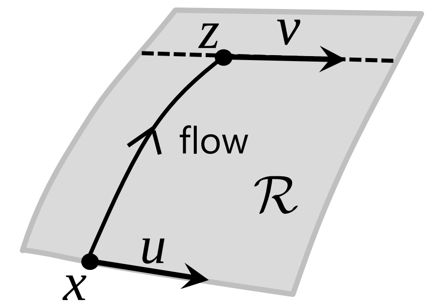
$z = (z^i) \in \mathbb{C}^N \quad (N \propto V$: DOF)

[MF-Matsumoto 2012.08468]
[MF-Matsumoto-Namekawa, Lattice2022]
[MF 2311.10663]

1. Configuration flow $\quad \dot{z}_i = \overline{\partial_i S(z)} \quad \Rightarrow O(N)$

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

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



3. RATTLE
$$\begin{cases} \pi_{1/2} = \pi - \Delta s\, \overline{\partial V(z)} - \lambda \\ z' = z + \Delta s\, \pi_{1/2} \\ \pi' = \pi_{1/2} - \Delta s\, \overline{V(z')} - \lambda' \end{cases} \qquad \big(V(z) = \mathrm{Re}\, S(z) + W(t(z))\big)$$

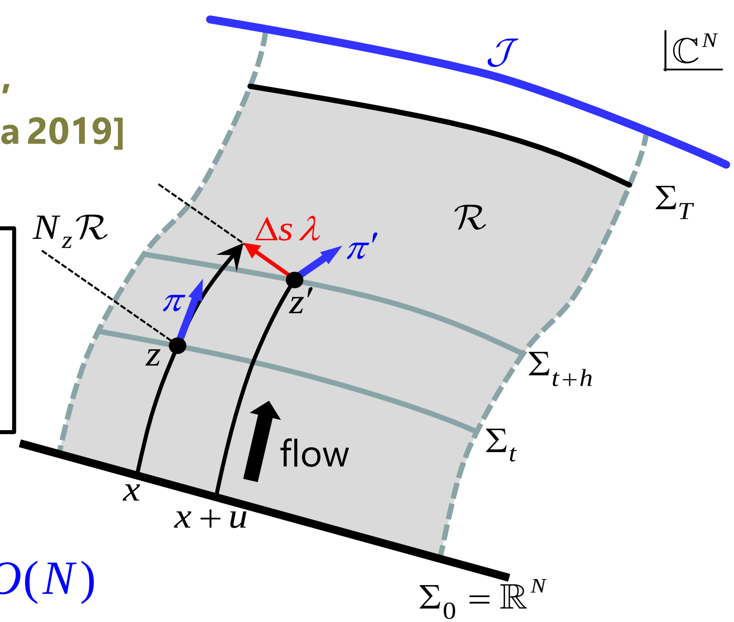
cf) RATTLE on a single thimble $\mathcal{J} = \Sigma_\infty$ **[Fujii et al. 2013]**
RATTLE on Σ_t **(GT-HMC)** **[Alexandru@Lattice2019, MF-Matsumoto-Umeda 2019]**

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

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 theories (with no fermion determinants)

Finite-density complex scalar (1/3)

$\varphi(x) = \frac{1}{\sqrt{2}}[\xi(x) + i\eta(x)]$: d-dim 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

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

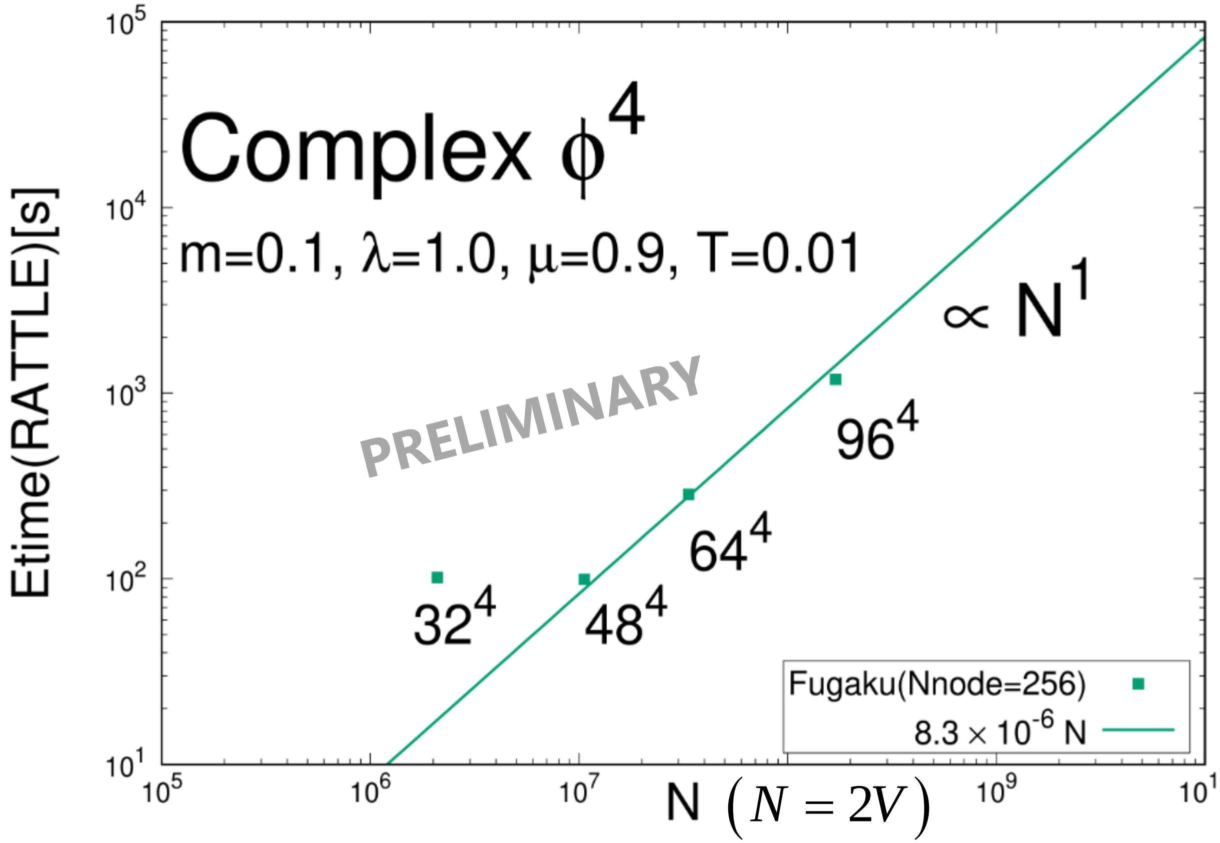
We complexify $(\xi,\eta) \in \mathbb{R}^{2V}$ to $(z,w) \in \mathbb{C}^{2V}$ with the flow equation

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

Finite-density complex scalar (2/3)

[MF-Namekawa, in preparation]

■ Computational cost scaling for d=4 (GT-HMC)



scaling: $O(N) = O(V)$ (as expected)

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

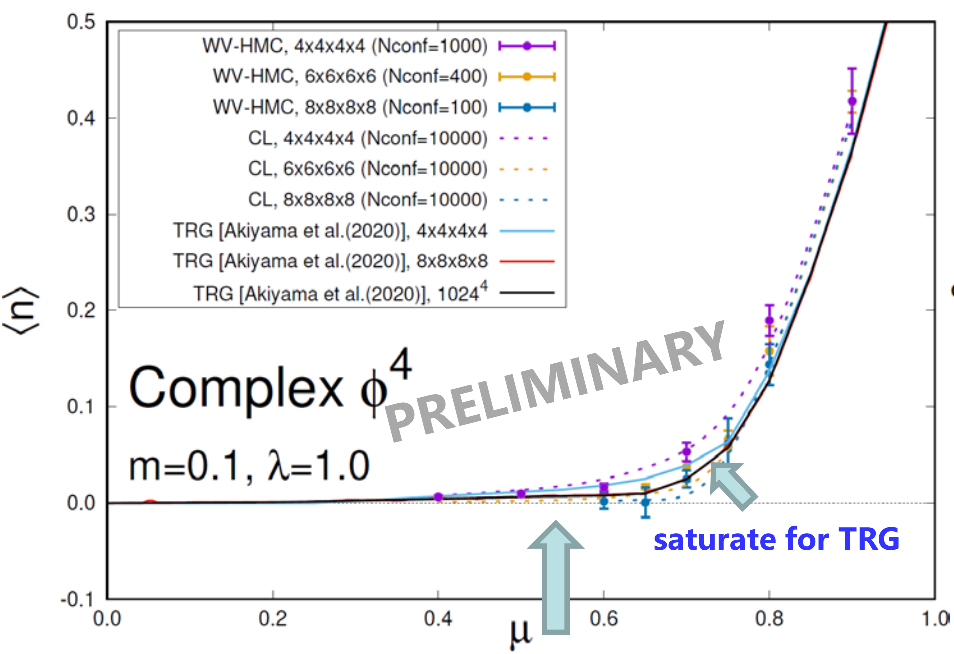
Finite-density complex scalar (3/3)

[MF-Namekawa, in preparation]

■ Comparison with TRG and CL [TRG (4D): Akiyama et al. 2005.04645 (Dcut=45)]

NB: CL does not suffer from wrong convergence problem
(satisfies a reliability condition)

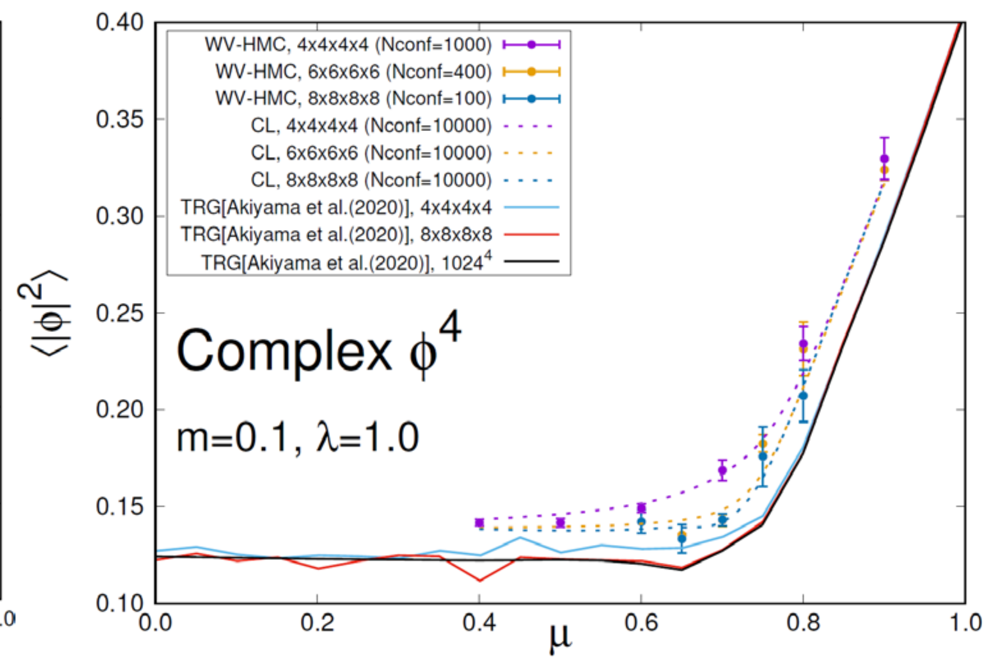
4D



Silver Blaze

WV-HMC = CL (= TRG)

4D



WV-HMC = CL