Application of the Worldvolume HMC method to lattice field theories

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Based on work with

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also with

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

Introduction

Sign problem

A large system with a complex action:

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

e.g. scalar field

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

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

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

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

highly oscillatory

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

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

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

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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

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

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

large β mimics large DOF

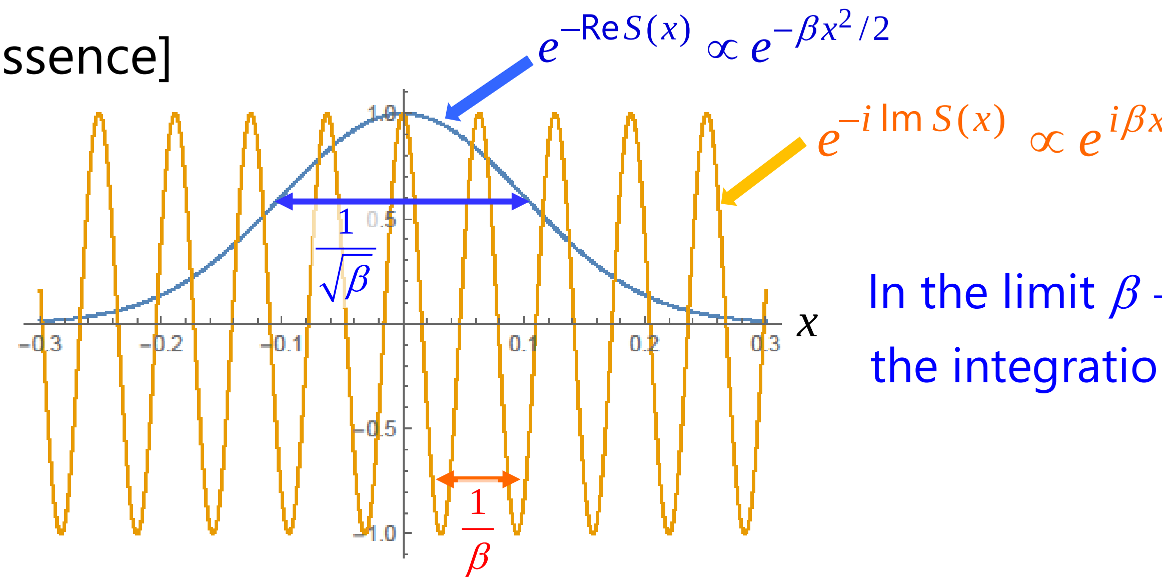
$$\Rightarrow \quad \langle x^2 \rangle = \frac{\langle e^{-i\,\mathrm{Im}\,S(x)}\, x^2 \rangle_{\text{rewt}}}{\langle e^{-i\,\mathrm{Im}\,S(x)} \rangle_{\text{rewt}}} = \frac{\left(\beta^{-1}-1\right)e^{-\beta/2}}{e^{-\beta/2}}$$

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

$\Rightarrow$ 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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<u>Today's talk</u>:

- Basics of the TLT and WV-HMC methods

- Application to various lattice field theories

Plan

1. Introduction (done)
2. Lefschetz thimble (LT) method [Witten 2010, Cristoforetti et al. 2012, Fujii et al. 2013]
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5. Application to various models
   - 5-1. Complex scalar at finite density [MF-Namekawa, in preparation]
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   - 5-5. Real-time dynamics [MF+, ongoing]
6. Summary and outlook

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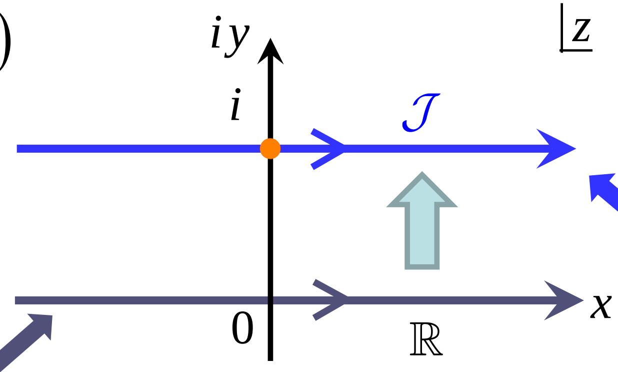
Warm-up: Gaussian (revisited)

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



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

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)

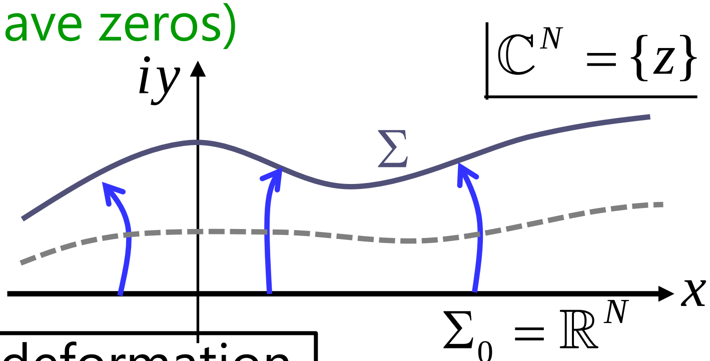
$\mathrm{Im}\, S(z)$: const $(=0)$ on $\mathcal{J}$

Basic idea of the thimble method (1/2)

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

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)

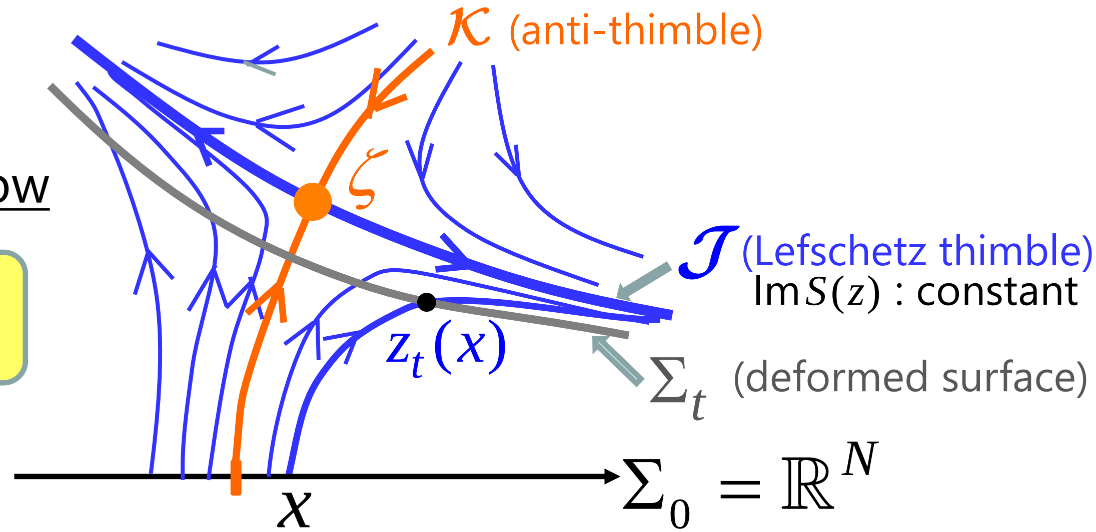
$$\langle\mathcal{O}(x)\rangle \equiv \frac{\int_{\Sigma_0} dx\, e^{-S(x)}\,\mathcal{O}(x)}{\int_{\Sigma_0} dx\, e^{-S(x)}} = \frac{\int_{\Sigma} dz\, e^{-S(z)}\,\mathcal{O}(z)}{\int_{\Sigma} dz\, e^{-S(z)}}$$

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

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

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

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 $t=0$)

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

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

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

flow

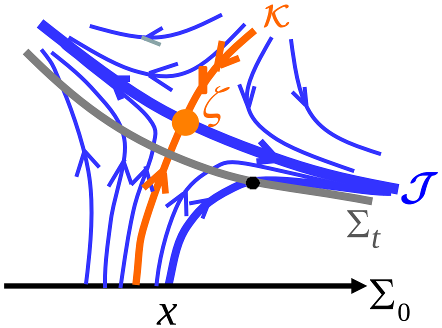
- Integration on a deformed surface Σ_t (flow time t)

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

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

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

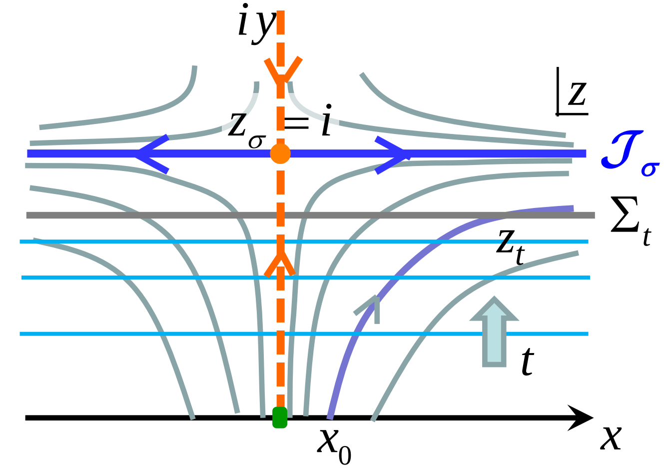
$$= \frac{O(1) \pm O(1/\sqrt{N_{\text{conf}}})}{O(1) \pm O(1/\sqrt{N_{\text{conf}}})}$$



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

NO!

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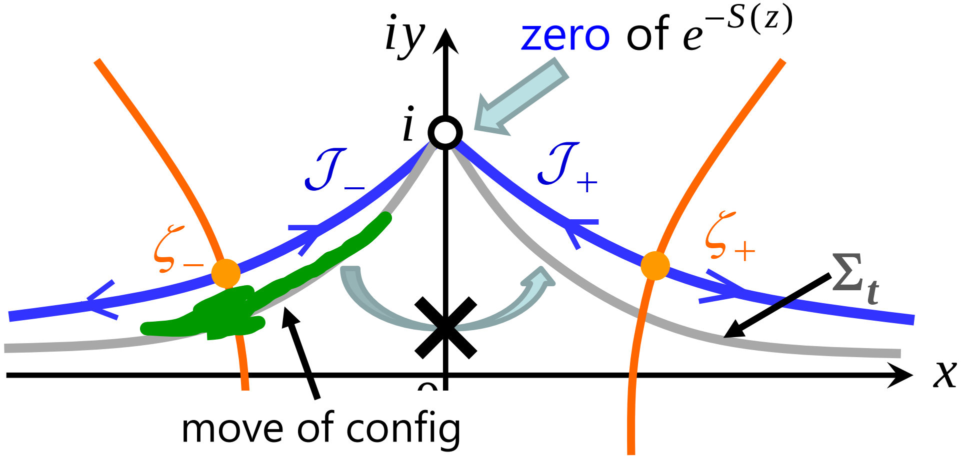
large flow time t ⇨ relaxation of oscillatory integral ⇨ **Sign problem** resolved? **NO!**

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

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



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

$\oplus$

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

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

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

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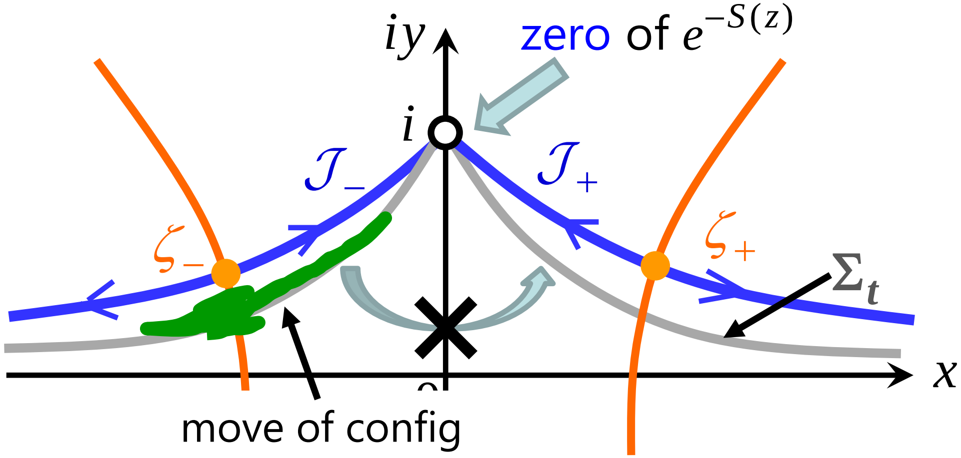

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(parallelly) tempering w.r.t. flow time

⇨ **solution : Tempered Lefschetz thimble method**

[MF-Umeda 2017]

Tempered Lefschetz thimble method

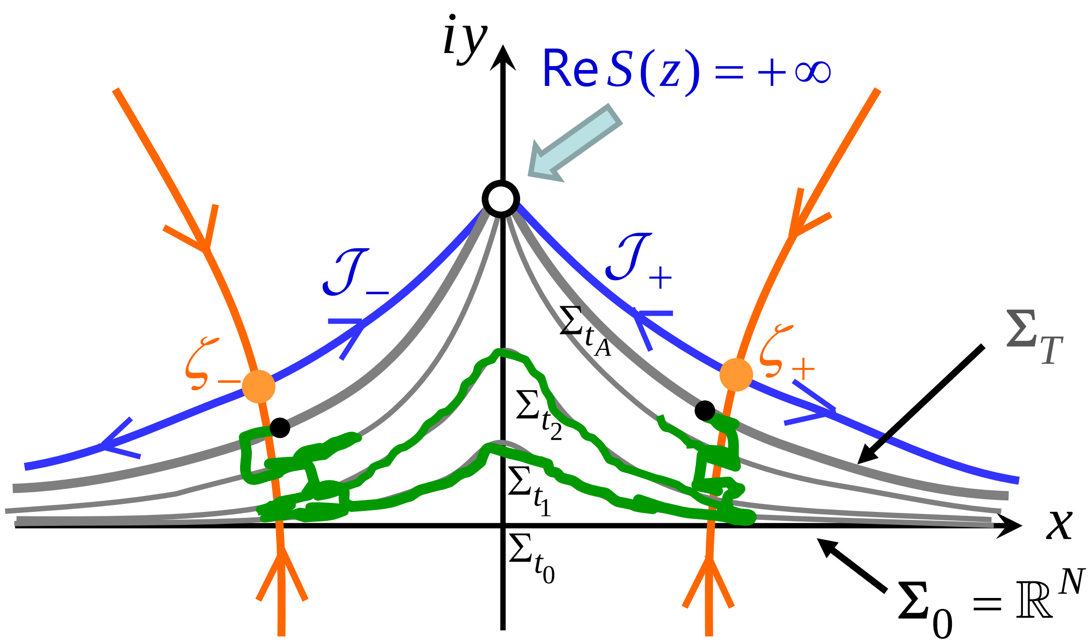
[Fukuma-Umeda 1703.00861]

■ 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 thermalization, estimate observables with a subsample on Σ_T



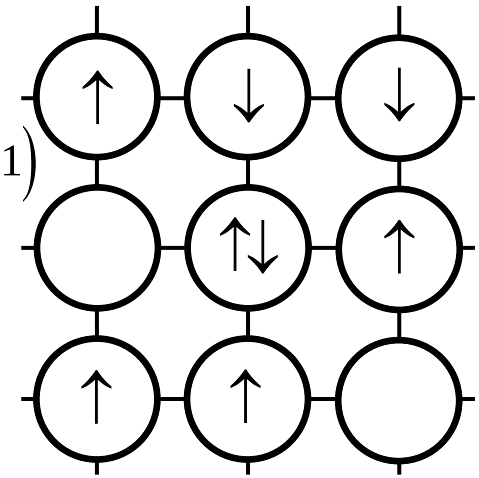
Sign and ergodicity problems are solved simultaneously !

■ 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)

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

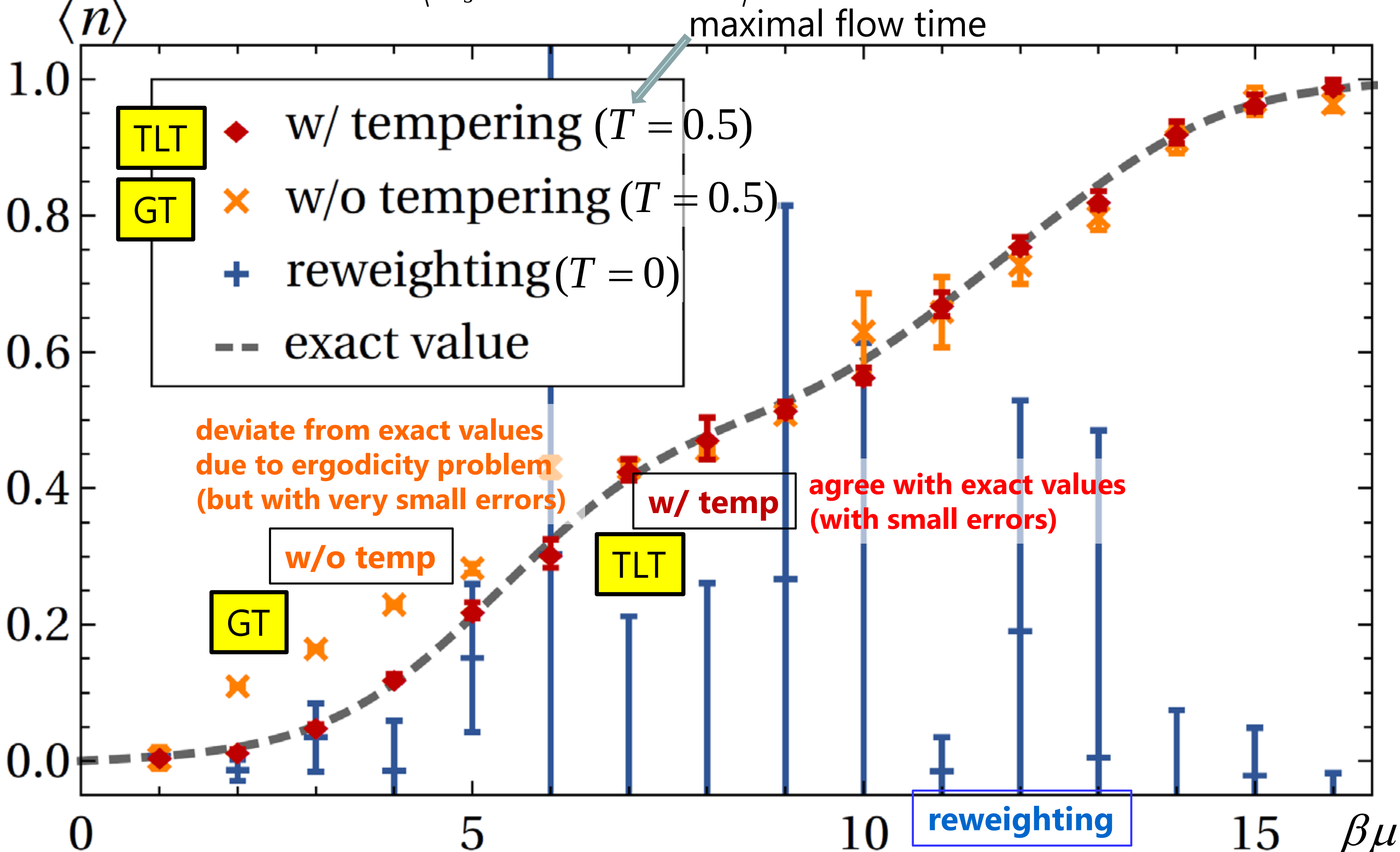
$$\approx \int [d\phi] e^{-S[\phi_{\ell,\mathbf{x}}]} \equiv \int \prod_{\ell=1}^{N_t} \prod_{\mathbf{x}} d\phi_{\ell,\mathbf{x}}\ e^{-(1/2)\sum_{\ell,\mathbf{x}} \phi_{\ell,\mathbf{x}}{}^2} \det M_a[\phi] \det M_b[\phi]$$

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

Hubbard model (2/4)

[MF-Matsumoto-Umeda 1906.04243]

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



large errors
due to sign problem

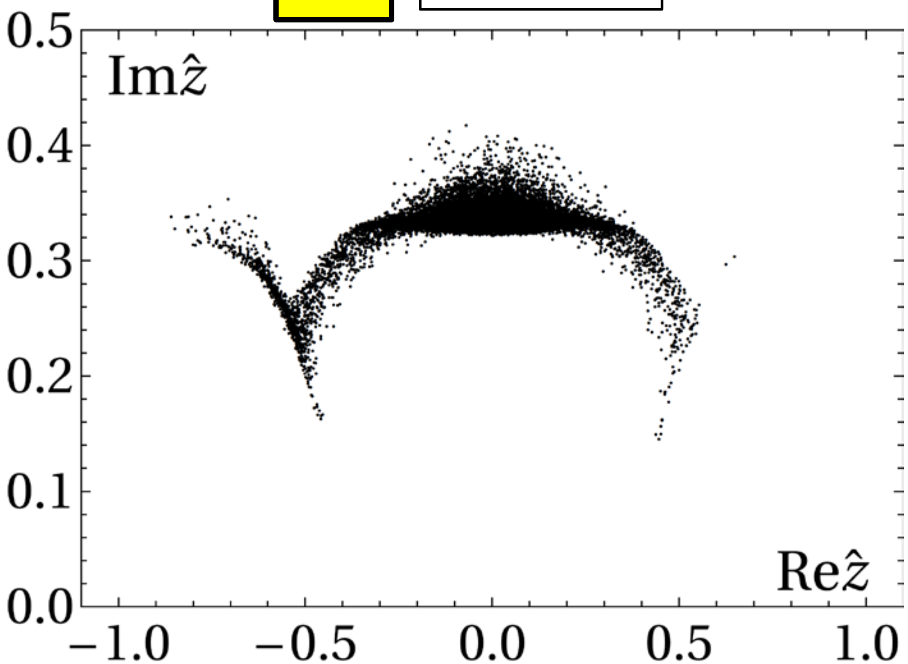
Hubbard model (3/4)

[MF-Matsumoto-Umeda 1906.04243]

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

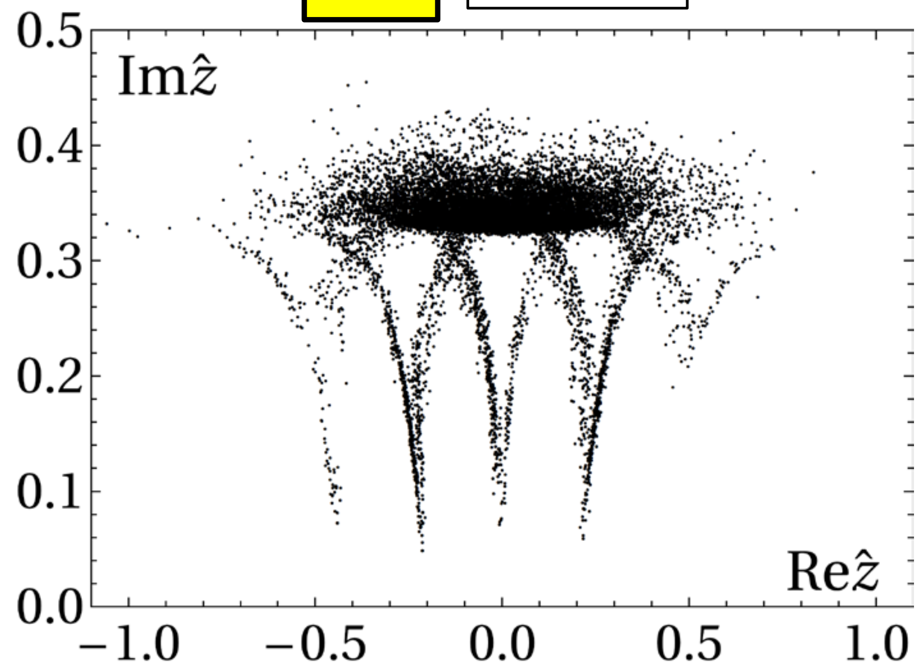
(projected on a plane $\hat{z} = (1/N)\sum_i z^i$)

GT **w/o temp**



stuck to a small # of thimbles

TLT **w/ temp**



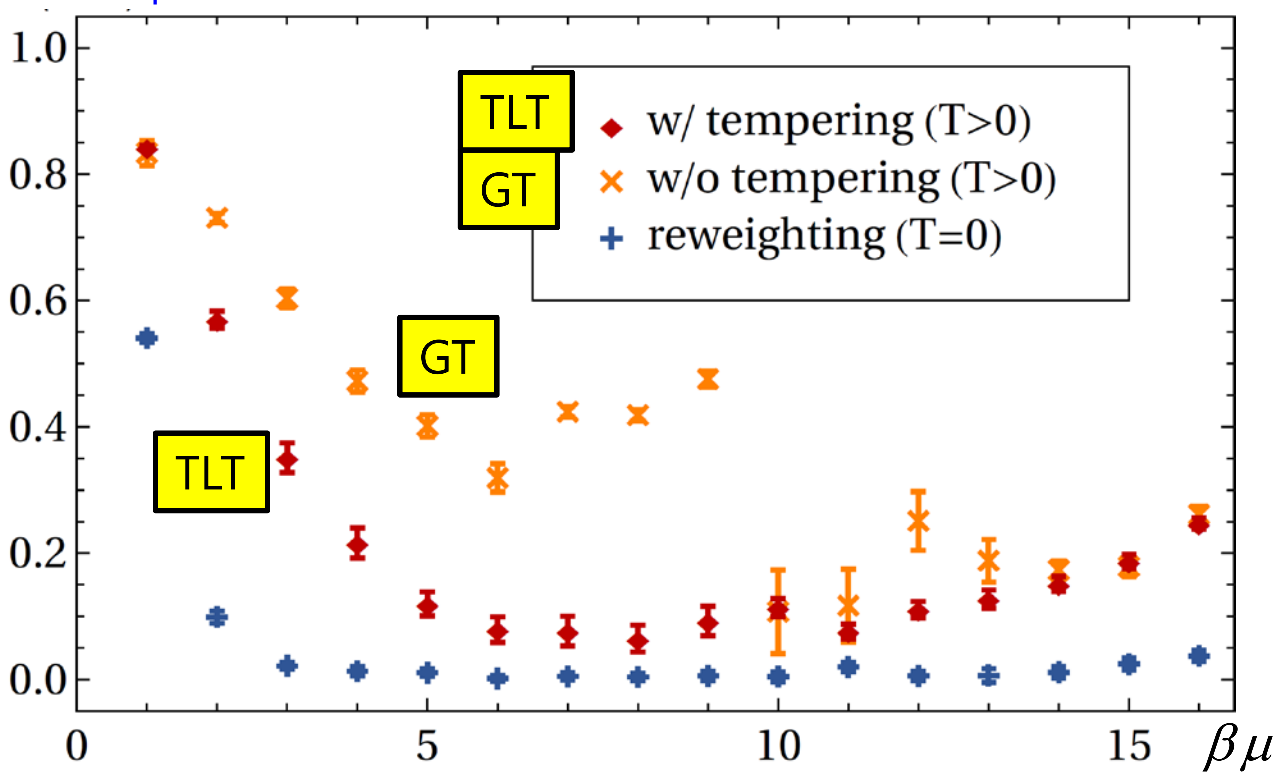
distributed widely
over many thimbles

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

[MF-Matsumoto-Umeda 1906.04243]

average phase factor

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



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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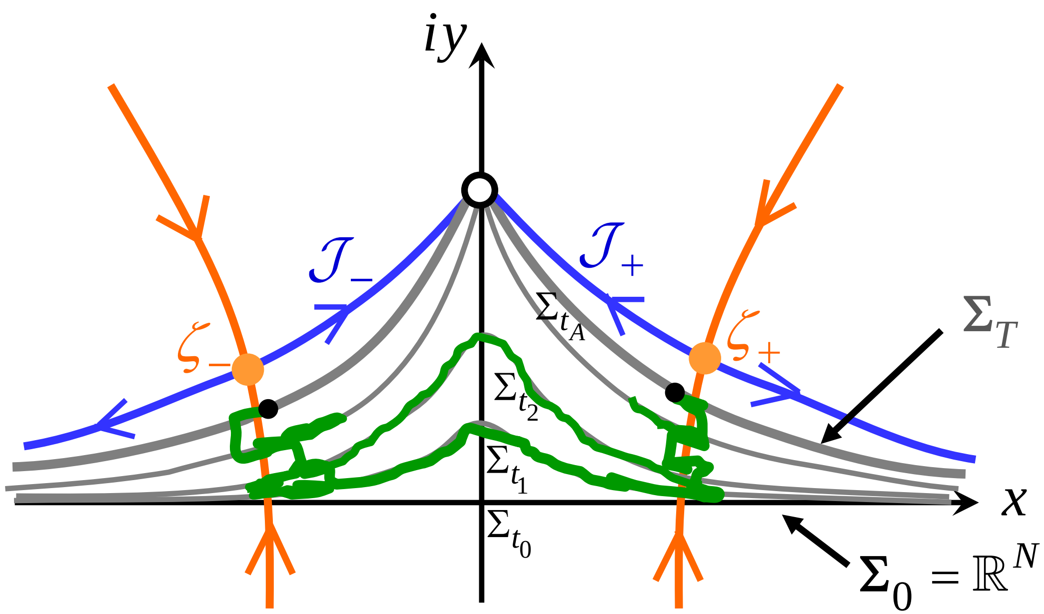
Pros and cons of the original TLT method

■ 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 computational cost at large DOF

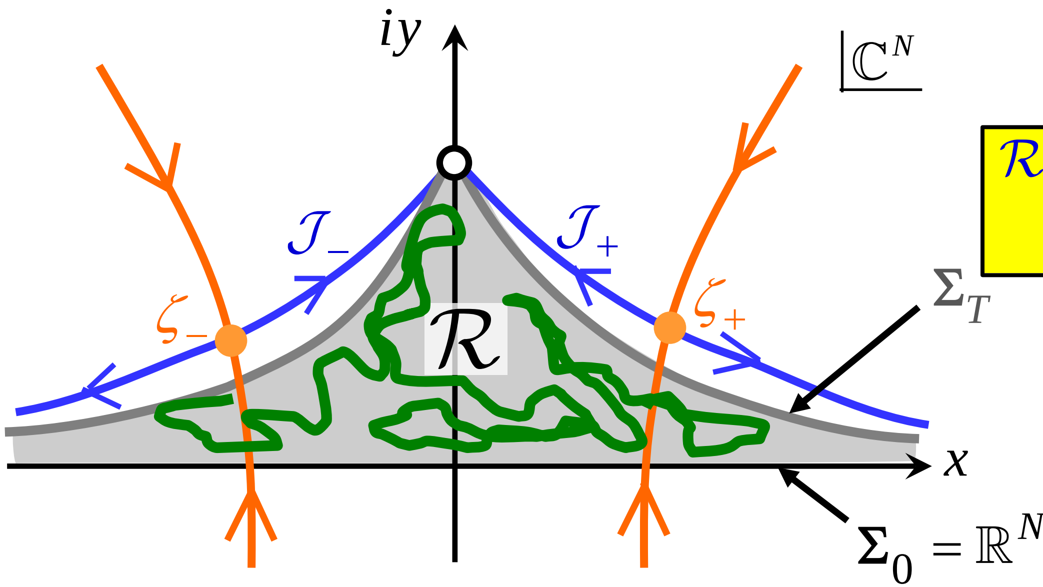
- necessary # of replicas $\propto O(N^{0-1})$
- need to calculate Jacobian $E_t(x) = \partial z_t(x) / \partial x \propto O(N^3)$ everytime we exchange configs between adjacent replicas

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 $\to$ worldline
orbit of string $\to$ worldsurface
orbit of surface (membrane) $\to$ worldvolume

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

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

- No need to introduce replicas explicitly
- No need to calculate Jacobian $E_t(x) = \partial z_t(x) / \partial x$ 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

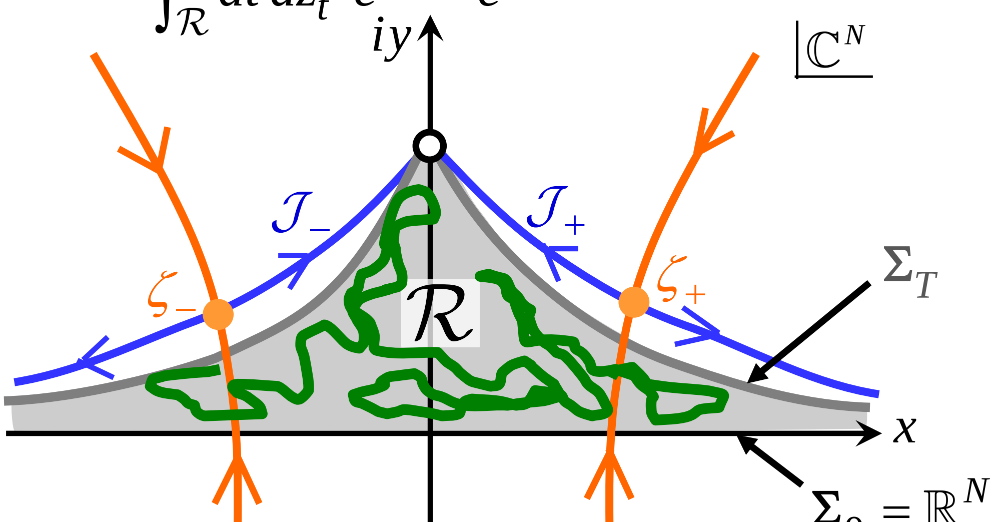
$$= \frac{\int_0^T dt\, e^{-W(t)} \int_{\Sigma_t} dz_t\; e^{-S(z_t)}\mathcal{O}(z_t)}{\int_0^T dt\, e^{-W(t)} \int_{\Sigma_t} dz_t\; e^{-S(z_t)}}$$

$\big(W(t)$: 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]**

Expected computational cost of WV-HMC

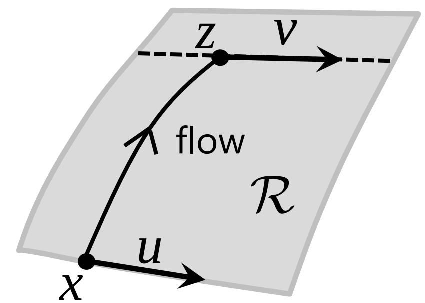
[MF-Matsumoto 2012.08468]
[MF-Matsumoto-Namekawa, Lattice2022]
[MF 2311.10663]

The whole problem comes down to integrating the flow eqs:

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

1. Configuration flow $\dot{z}_i = \overline{\partial_i S(z)} \quad \Rightarrow O(N)$ $\left[\begin{array}{c}\text{when } \partial_i S(z) \text{ is known} \\ (\text{local field case})\end{array}\right]$

2. Vector flow $\dot{v}_i = \overline{\partial_i \partial_j S(z)\, v_j} \quad \Rightarrow O(N)$ $\left[\begin{array}{c}\text{when } \partial_i \partial_j S(z) \text{ is sparse} \\ (\text{local field case})\end{array}\right]$



expected computational cost :

no fermion determinants : $O(N)$

$\exists$fermion determinants : $O(N^{2-3})$

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6. Summary and outlook

TLT/WV-HMC have been 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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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

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

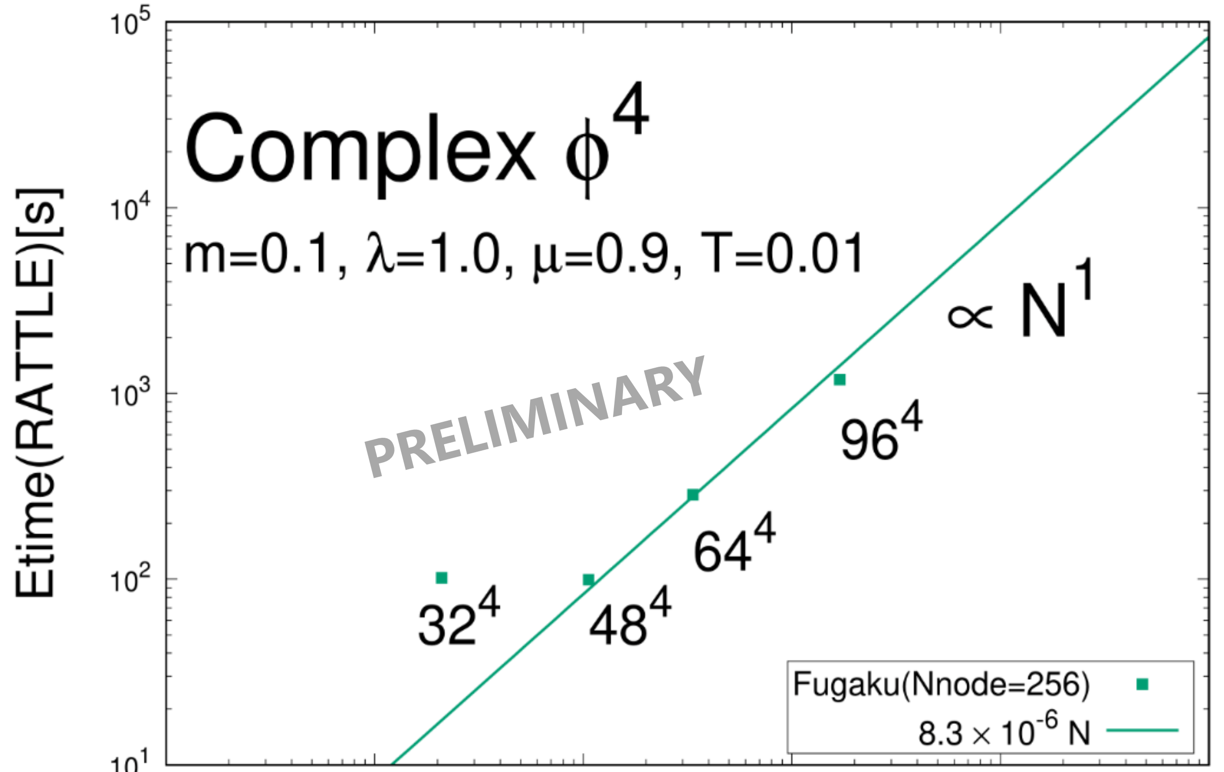
We complexify $(\xi,\eta)\in\mathbb{R}^{2V}$ to $(z,w)\in\mathbb{C}^{2V}$ with the flow equation

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

Finite-density complex scalar (2/3)

[MF-Namekawa, in preparation]

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



$N \; (N = 2V)$

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)

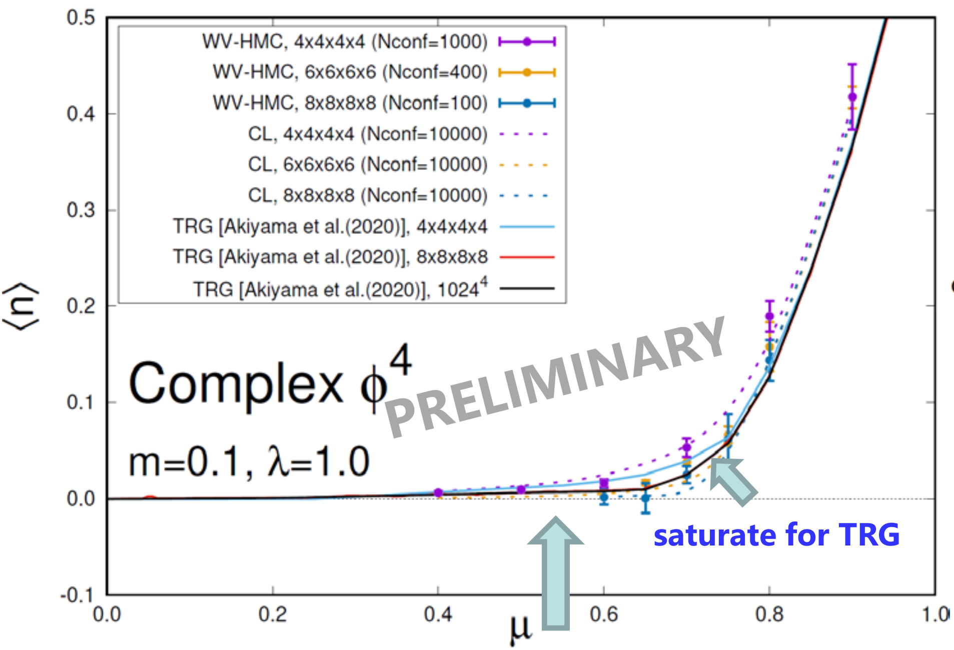
Finite-density complex scalar (3/3)

[MF-Namekawa, in preparation]

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

NB: CL works without suffering from wrong convergence problem
(satisfies a reliability condition)

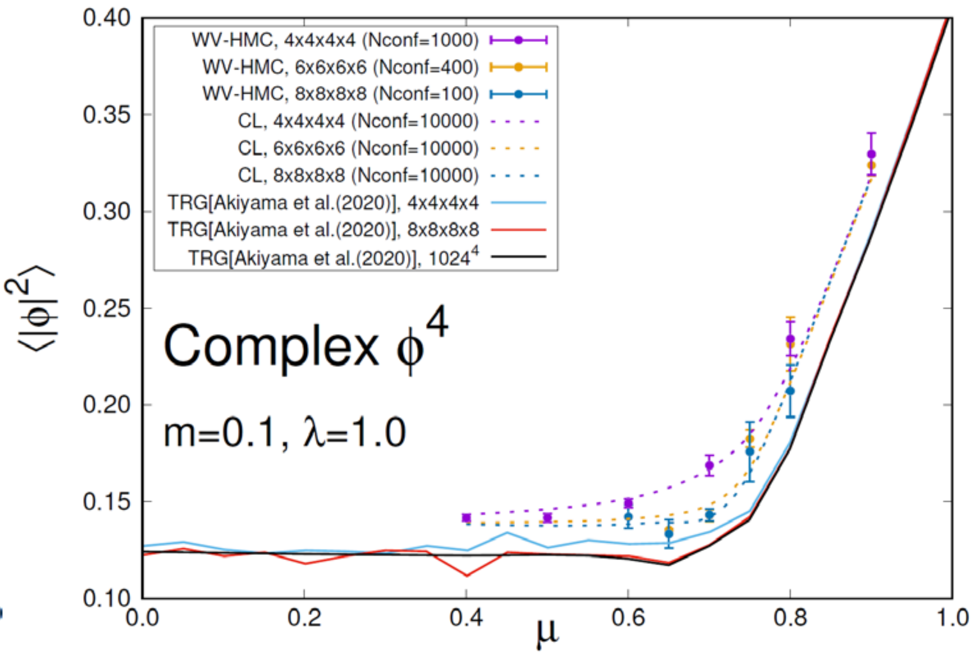
4D



Silver Blaze

WV-HMC = CL

4D



WV-HMC = CL

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Chiral random matrix model (1/2)

[MF-Matsumoto 2012.08468]

■ finite density QCD

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

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

⇩ toy model

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

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

(quantum field replaced by a matrix incl spacetime DOF)

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

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

(DOF : $N=2n^2 \ \Leftrightarrow\ 4L^4(N_c^2-1)$)

■ role of an important benchmark model

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

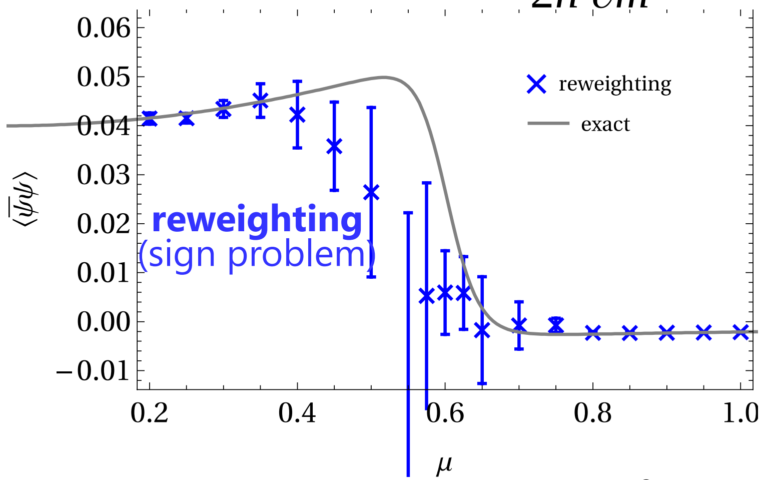
Chiral random matrix model (2/2)

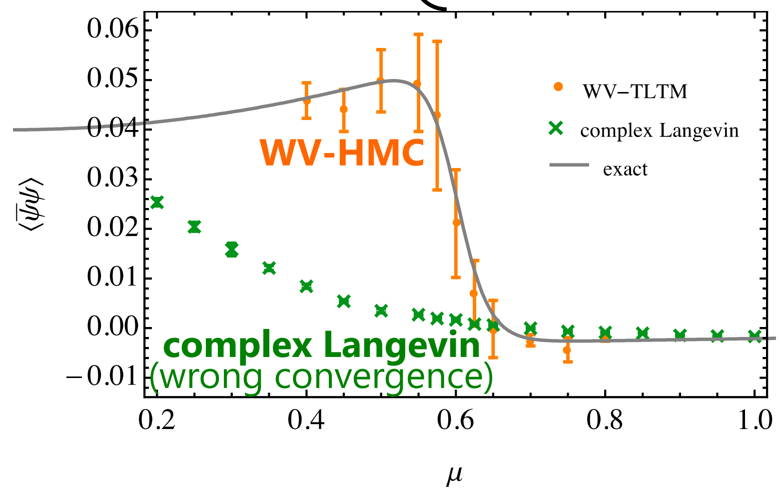
[MF-Matsumoto 2012.08468]

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

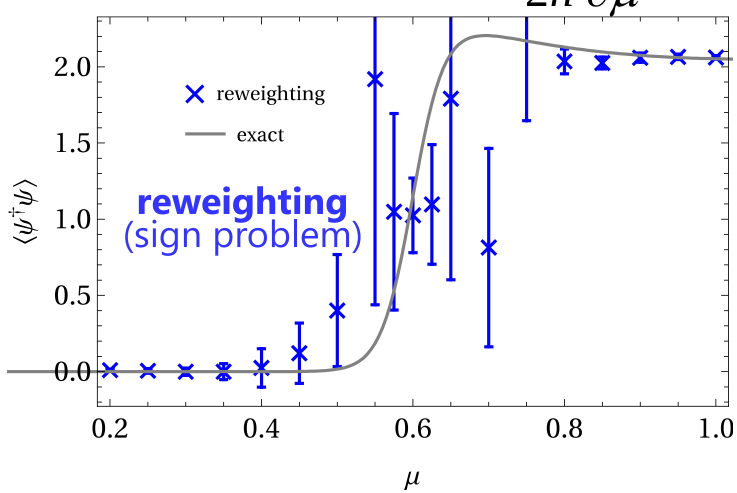
sample size
reweighting : 10k
complex Langevin :10k
WV-TLTM : 4k-17k

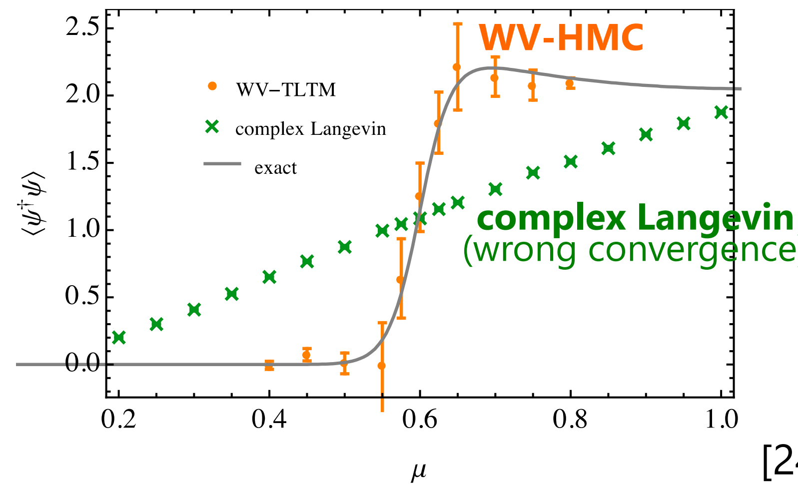
chiral condensate $\langle \bar{\psi}\psi \rangle \equiv \frac{1}{2n}\frac{\partial}{\partial m}\ln Z_{\text{Steph}}$ $[m = 0.004,\ T = 0]$





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





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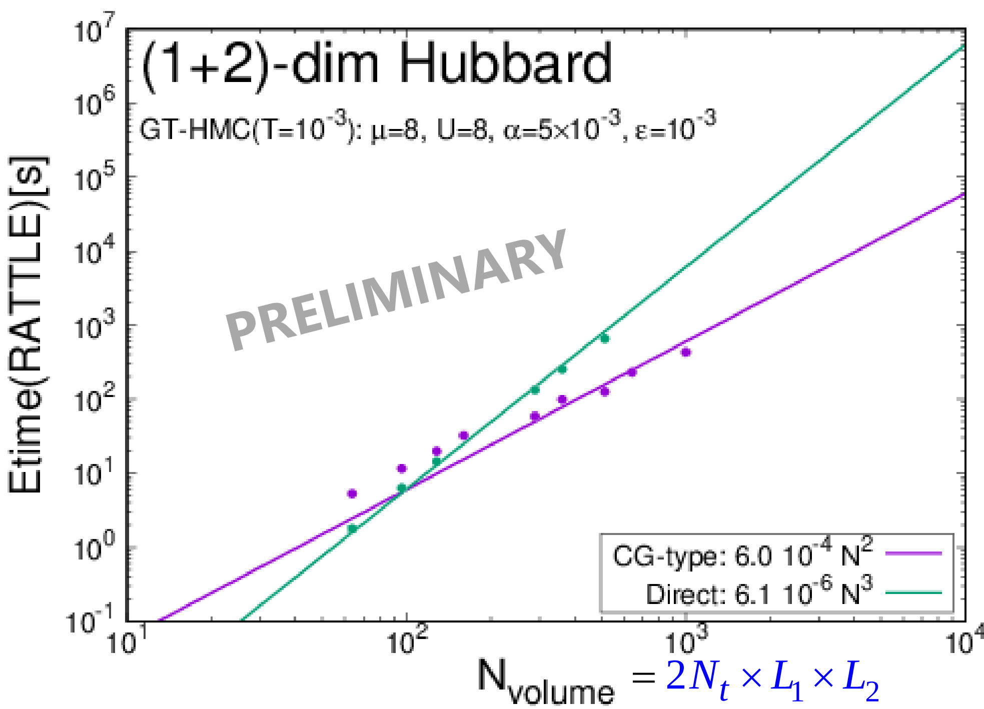
Hubbard model revisited (1/2)

[MF-Namekawa, ongoing]

- particle-hole transformation : $a_{\mathbf{x}} \equiv c_{\mathbf{x},\uparrow},\ b_{\mathbf{x}} \equiv (-1)^{\mathbf{x}} c^{\dagger}_{\mathbf{x},\downarrow}$

$$\Rightarrow H = -\kappa \sum_{\langle \mathbf{x},\mathbf{y}\rangle} \left(a^{\dagger}_{\mathbf{x}} a_{\mathbf{y}} + b^{\dagger}_{\mathbf{x}} b_{\mathbf{y}} \right) + \frac{U}{2} \sum_{\mathbf{x}} \left(n^a_{\mathbf{x}} - n^b_{\mathbf{x}} \right)^2 - \mu \sum_{\mathbf{x}} \left(n^a_{\mathbf{x}} - n^b_{\mathbf{x}} \right)$$

elapsed time for 1 MD trajectory with a single core (GT-HMC)



$N_{\mathrm{volume}} = 2N_t \times L_1 \times L_2$

(1) direct method $\propto N^3$

(2) real pseudofermions w/ iterative solvers $\propto N^2$

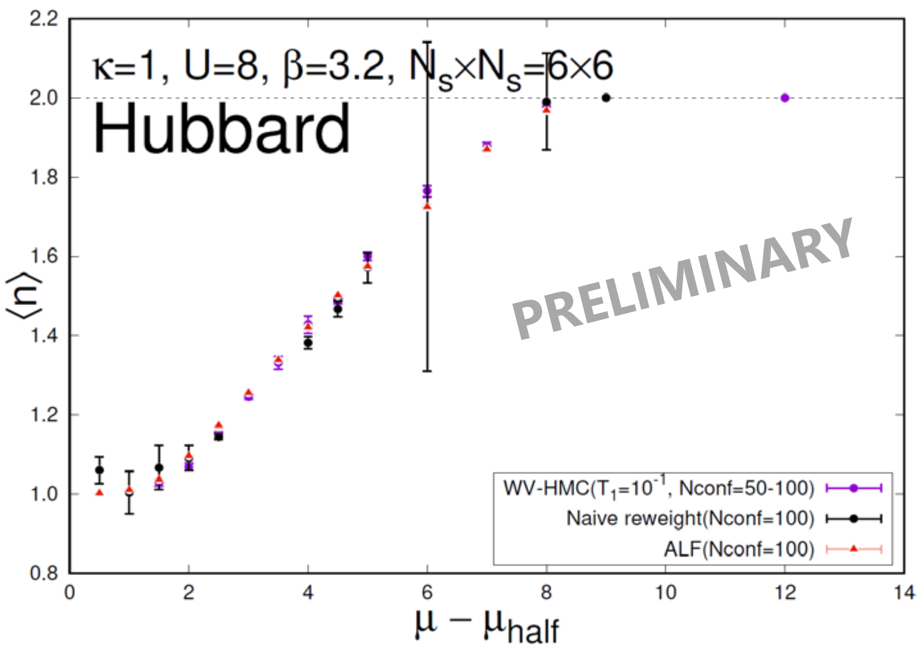
Hubbard model revisited (2/2)

[MF-Namekawa, ongoing]

<u>reference method</u> : **ALF package** (Algorithms for Lattice Fermions) **[Assaad et al.]**

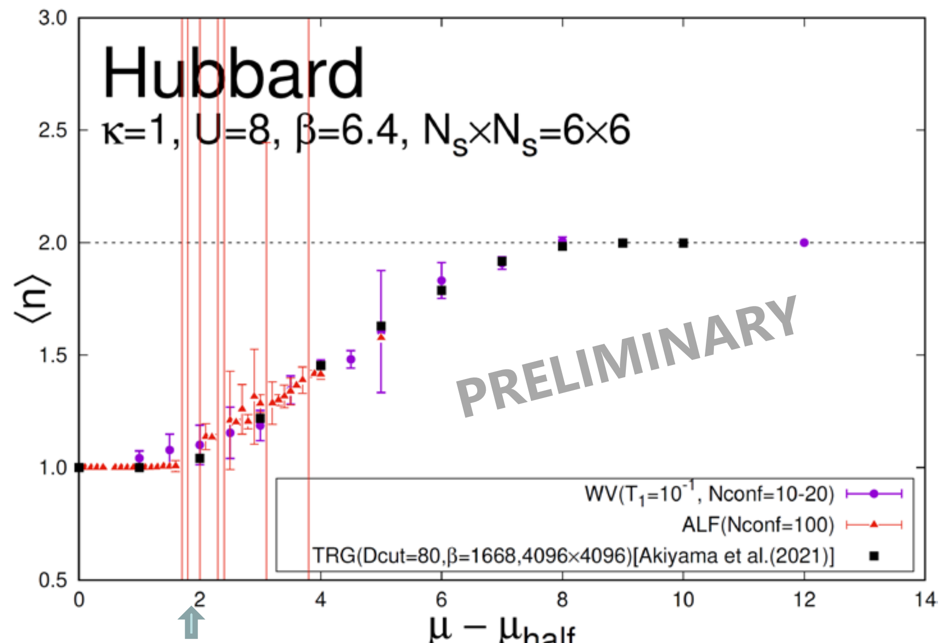
- established algorithm in cond-mat (Fortran/Python)
- using discrete HS variables
- polynomial cost (and fast) when sign problem is NOT severe
- exponential cost when sign problem is severe

6×6 spatial lattice with $\beta = 3.2$ $(N_t = 10)$



ALF works
WV agrees with ALF

6×6 spatial lattice with $\beta = 6.4$ $(N_t = 20)$



ALF fails
WV gives a prediction?

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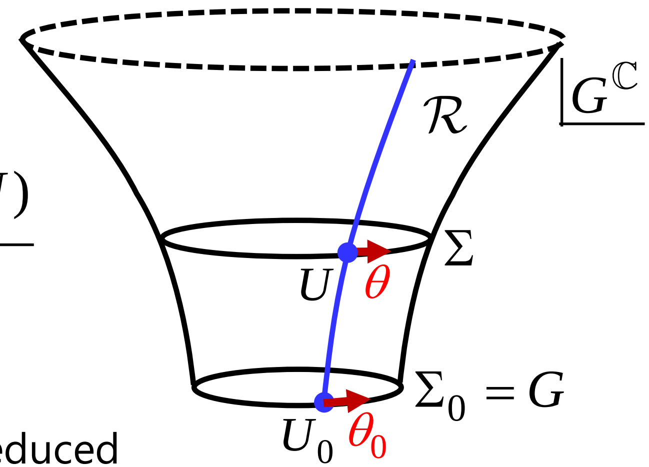
Path integral over group manifold (1/2)

[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

Maurer Cartan forms

$$\begin{cases} \theta_0 \equiv dU_0\, U_0^{-1} = \sum_a T_a\, \theta_0^a \text{ on } \Sigma_0 = G \\ \theta \equiv dU\, U^{-1} = \sum_a T_a\, \theta^a \text{ on } \Sigma \end{cases}$$

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

$$(dU)_\Sigma = \theta^1 \wedge \cdots \wedge \theta^N = \theta_0^1 \wedge \cdots \wedge \theta_0^N \det E$$
$$= |dU_0| \det E$$

Define $DS(U)$ by

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

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

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

Path integral over group manifold (2/2)

[MF, in preparation]

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

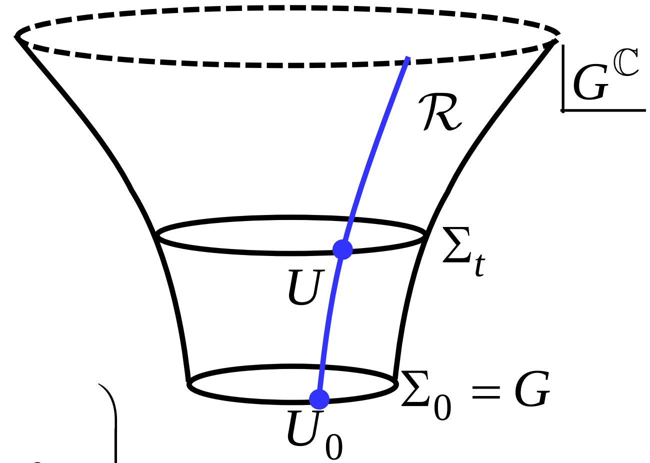
⇐ t-independent

⇐ 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 $\mathcal{R}$)

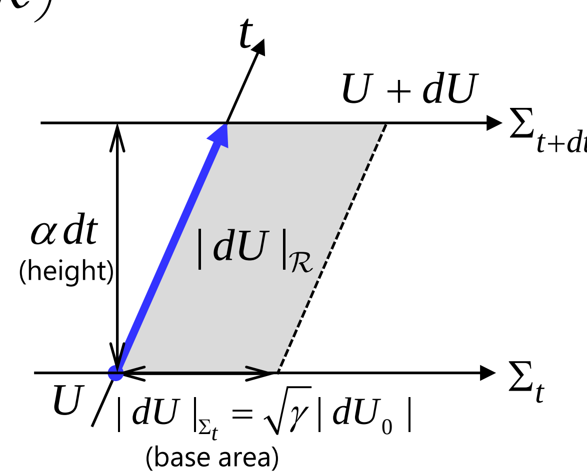


$$\left(\begin{aligned} & V(U) = \mathrm{Re}\, S(U) + W(t(U)) \\ & \mathcal{F}(U) = \frac{dt\,(dU)_{\Sigma_t}}{|\, dU\,|_{\mathcal{R}}}\, e^{-i\,\mathrm{Im}\, S(U)} = \alpha^{-1} \frac{\det E}{\sqrt{\gamma}}\, e^{-i\,\mathrm{Im}\, S(U)} \end{aligned} \right)$$

⇓

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



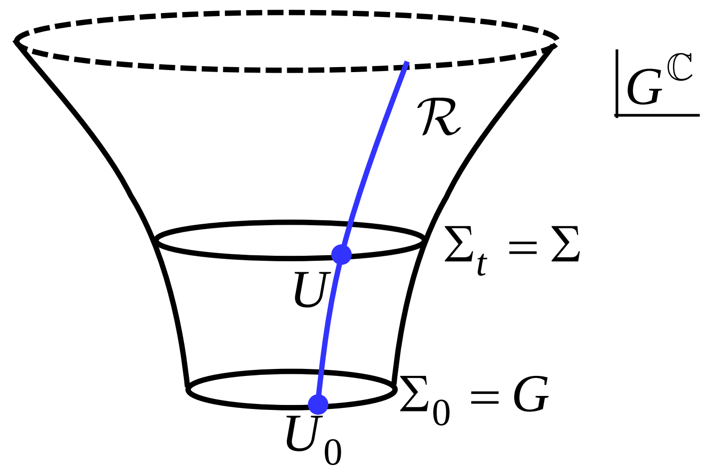
$$\left(ds_{\Sigma}^2 = \mathrm{Re}\, \mathrm{tr}\, \theta^\dagger \theta = \gamma_{ab} \theta_0^a \theta_0^b \right)$$

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

[MF, in preparation]

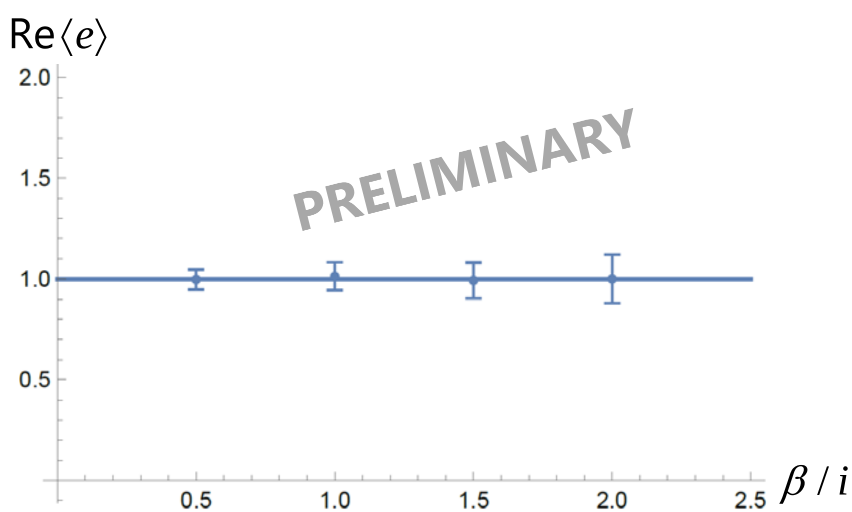
$G = SU(2)$

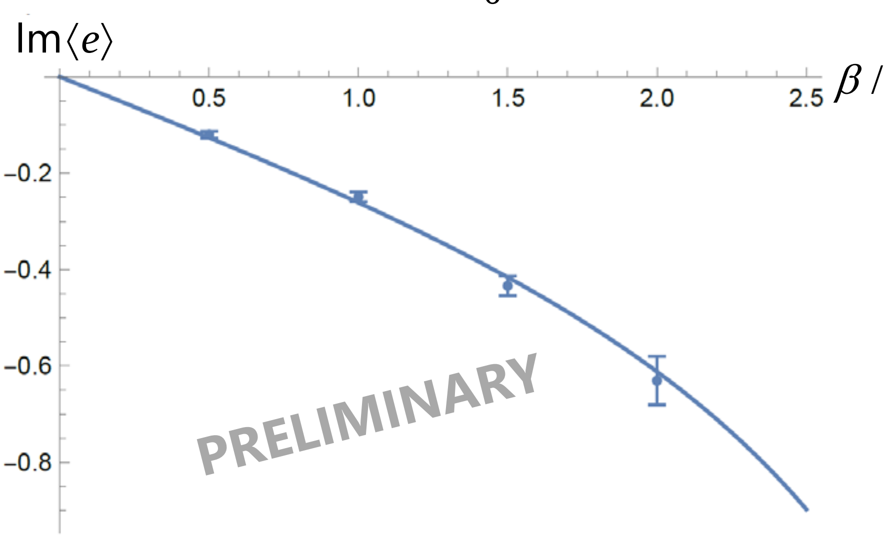
$$S(U) \equiv \beta\, e(U) \equiv \frac{\beta}{4}\,\mathrm{tr}\left(2 - U - U^{-1}\right) \quad (\beta \in i\,\mathbb{R})$$



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

numerical result (WV-HMC):



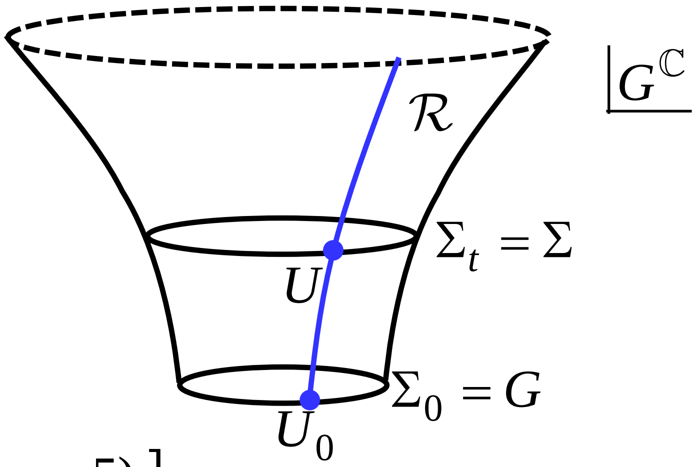


E.g. 1-site with a topological term

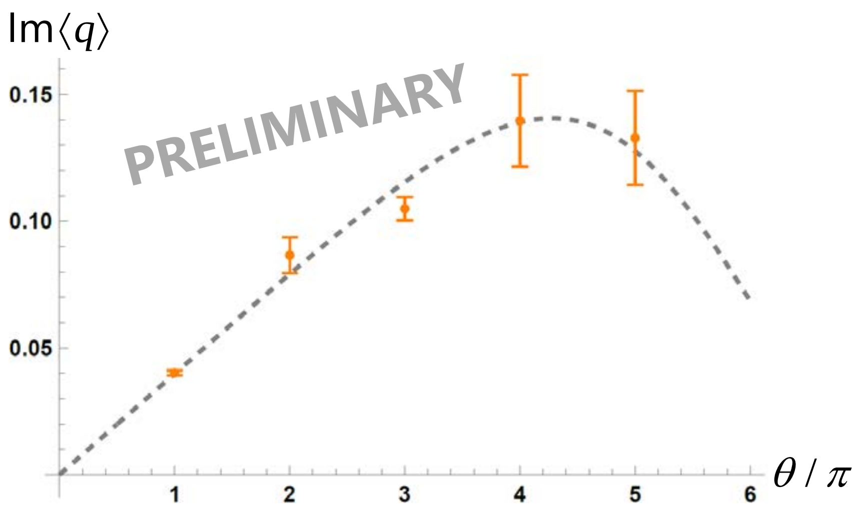
[MF, in preparation]

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

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



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



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]

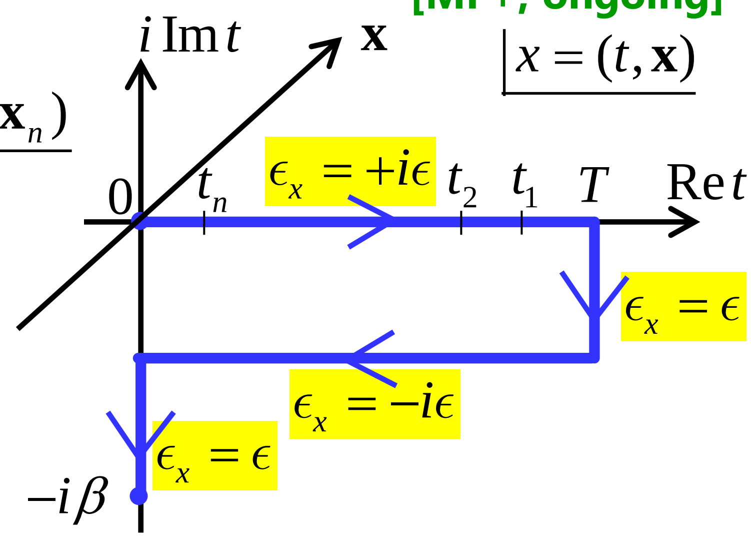
5. Application to various models

   5-1. Complex scalar at finite density [MF-Namekawa, in preparation]
   5-2. Chiral random matrix model [MF-Matsumoto 2020]
   5-3. Hubbard model [MF-Namekawa, in preparation]
   5-4. Group manifolds [MF, in preparation]
   5-5. Real-time dynamics [MF+, ongoing]

6. 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]**

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

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

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

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

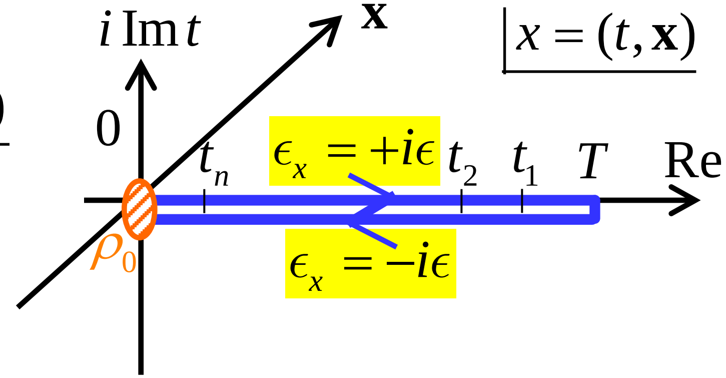
directly calculate from real-time correlators (w/o using Kubo relation)

Case 2: Nonequilibrium processes

[MF+, ongoing]

Initial density matrix ρ_0

$$\langle \mathcal{O}(t_1,\mathbf{x}_1)\cdots\mathcal{O}(t_n,\mathbf{x}_n)\rangle \equiv \frac{\mathrm{tr}\,\rho_0 \overset{e^{i\hat{H}T}e^{-i\hat{H}T}}{\vee} \mathcal{O}(t_1,\mathbf{x}_1)\cdots\mathcal{O}(t_n,\mathbf{x}_n)}{\mathrm{tr}\,\rho_0 \underset{e^{i\hat{H}T}e^{-i\hat{H}T}}{\wedge}}$$



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

The computation is essentially the same as before.

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6. Summary and outlook

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 techniques
- 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.