Applying the Worldvolume HMC (WV-HMC) method to lattice field theories

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Lattice 2022

Aug 8, 2022 @Univ of Bonn

Based on work with

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Yusuke Namekawa (Hiroshima Univ)
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1. Introduction

Overview

The **numerical sign problem** is one of the major obstacles
when performing first-principles calculations in various fields of physics

Typical examples:

① Finite density QCD
② Quantum Monte Carlo simulations of quantum statistical systems
③ θ vacuum with finite θ
④ Real-time dynamics of quantum fields

Various approaches:

▼ complex Langevin method **[Parisi 1983, Klauder 1983, Aarts et al. 2009, …]**

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

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

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

Worldvolume HMC method **[MF-Matsumoto 2020]**
(= Worldvolume TLTM)

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

▼ tensor network **[Levin-Nave 2007, Shimizu-Kuramshi 2014, Kadoh et al. 2020, …]**

Overview

The aim of my talk is

- to review the basics of the Worldvolume HMC (**WV-HMC**) method (**WV-TLTM**)
- to argue that
  when applied to local field theories,
  the computational cost for generating a configuration is $O(V)$

The argument will be made for scalar field theory at finite density
[MF-Matsumoto-Namekawa, work in progress]

The application to Yang-Mills theory is on-going
[MF-Kanamori-Namekawa, work in progress]
based on the WV-HMC for group manifolds **[MF, in preparation]**

Plan

1. Introduction (done)
2. Basics of WV-HMC method
3. Application to scalar field theory at finite density
4. Summary and outlook

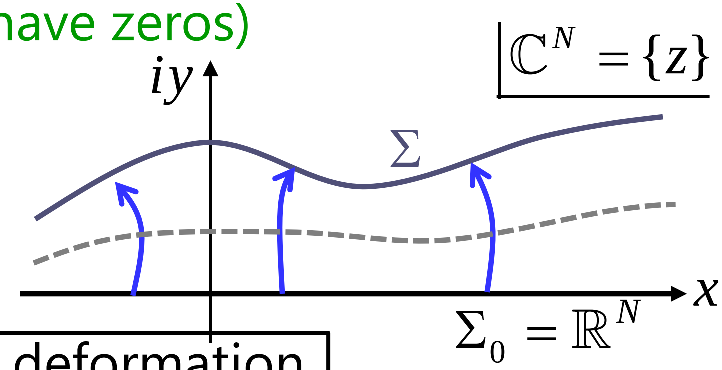
2. Basics of WV-HMC method

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)

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

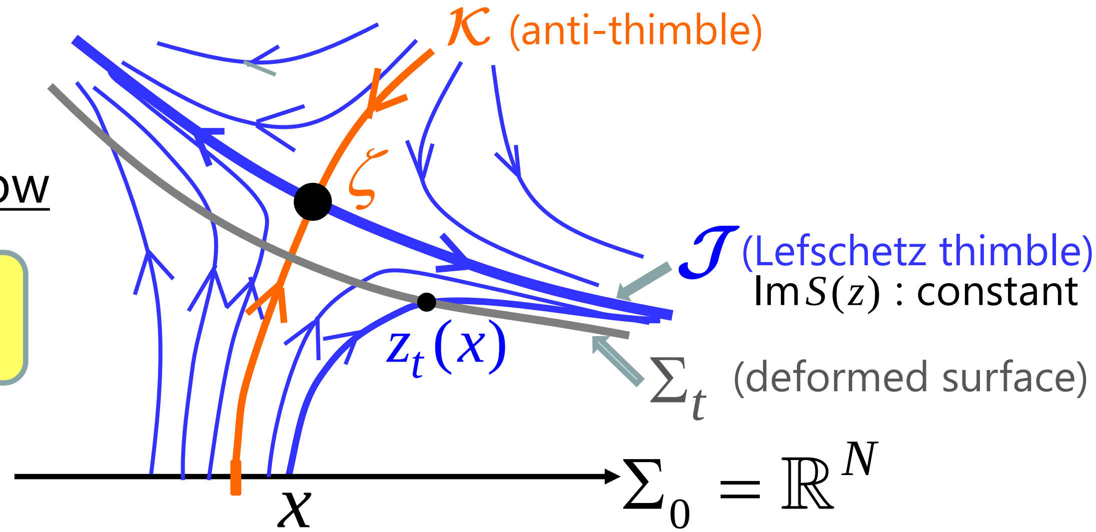
severe sign problem

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

■ prescription for deformation

anti-holomorphic gradient flow

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



property

$$[S(z_t)]^{\bullet} = \partial S(z_t) \cdot \dot{z}_t = \left|\partial S(z_t)\right|^2 \geq 0$$

⇨ $[\mathrm{Re}\,S(z_t)]^{\bullet} \geq 0$: always increases except at crit pt ζ (ζ : crit pt $\Leftrightarrow \partial S(\zeta) = 0$)

$[\mathrm{Im}\,S(z_t)]^{\bullet} = 0$: always constant

⇨ $\Sigma_t \xrightarrow{t \to \infty} \mathcal{J}$ (Lefschetz thimble) $\equiv$ set of orbits starting from ζ

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

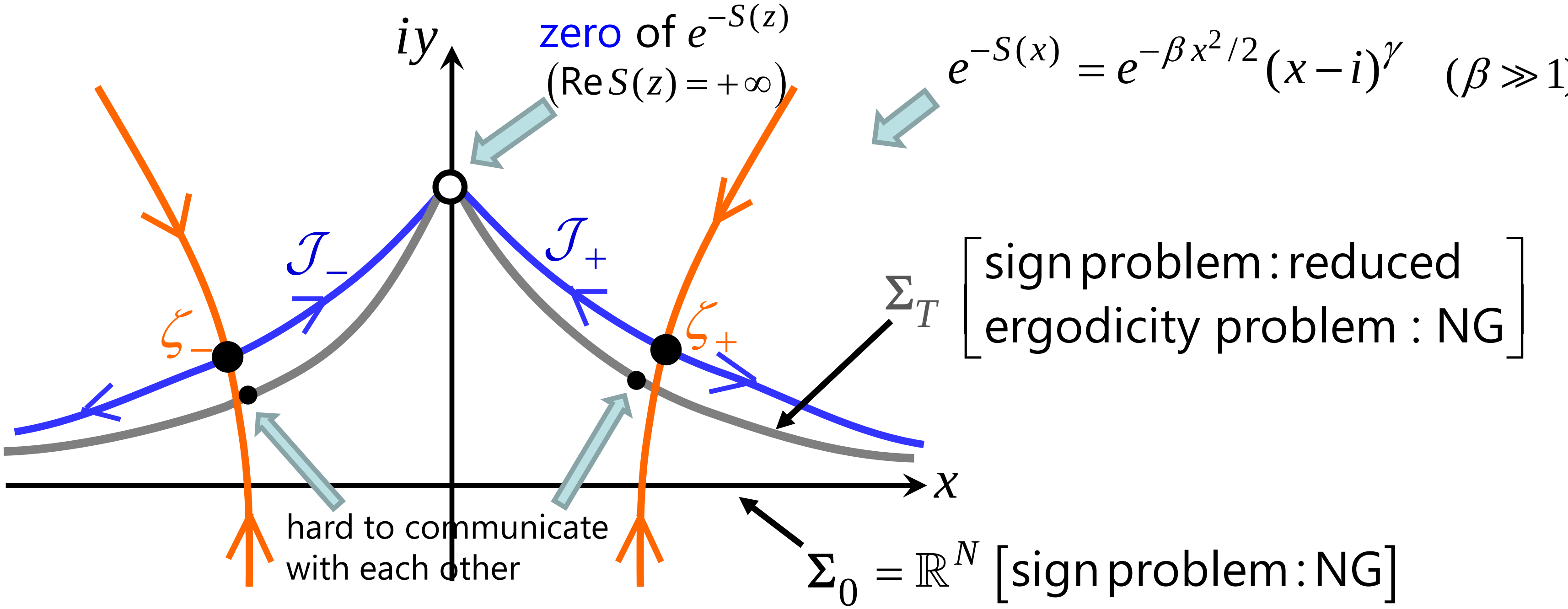
⇨ Oscillatory integral is expected to be tamed on Σ_t if we take a sufficiently large t

Ergodicity problem

[MF-Umeda 1703.00861]

Sign problem resolved? **NO!**

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



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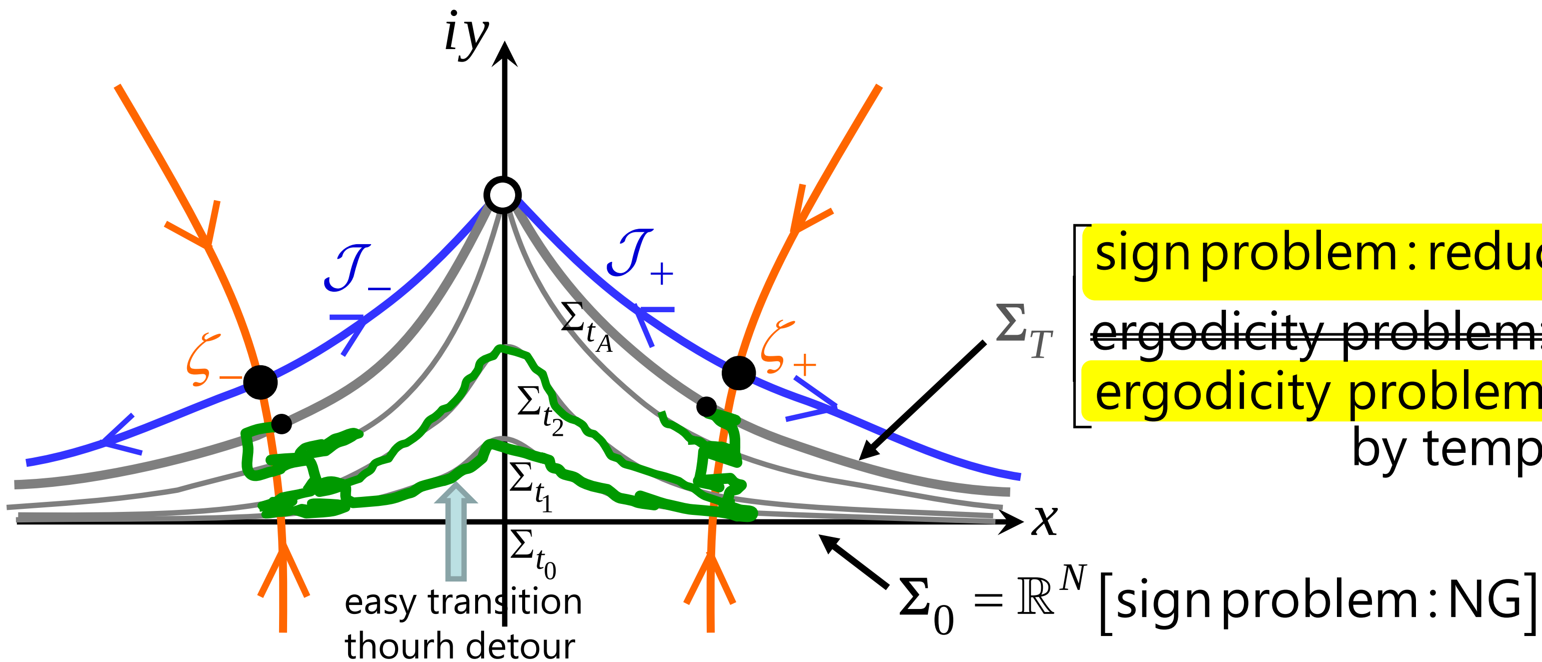

Solution

➡ **Tempered Lefschetz thimble method (TLTM)** [MF-Umeda 2017] [Alexandru et al. 2017]

tempering the system with the flow time

➡ prompts the equilibration on Σ_T

This solves the sign and ergodicity problems simultaneously

Numerical cost : $O(N^3)$ (computation of Jacobian $J = (\partial z^i / \partial x^a)$)

Ergodicity problem

[MF-Umeda 1703.00861]

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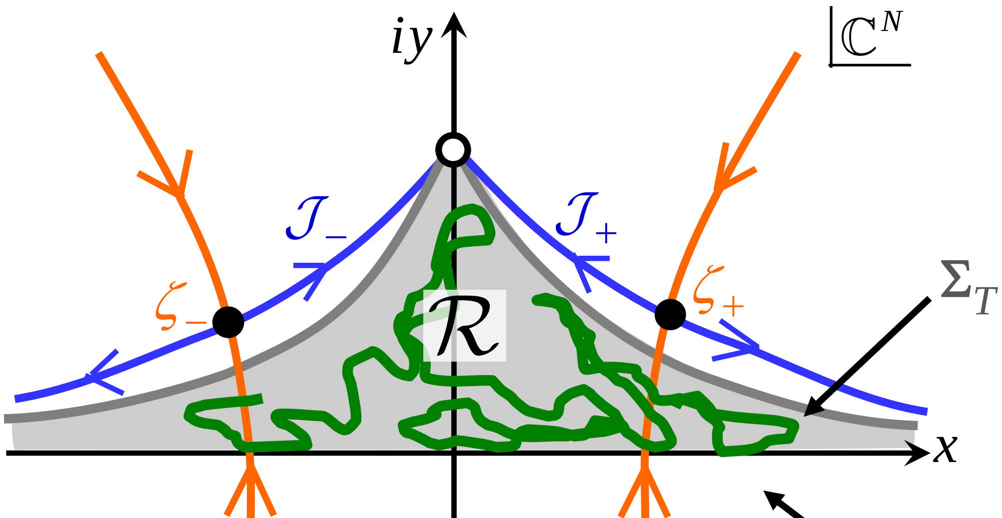


[sign problem : reduced
~~ergodicity problem: NG~~
ergodicity problem : OK]
by tempering

$\Sigma_0 = \mathbb{R}^N$ [sign problem : NG]

Solution

Tempered Lefschetz thimble method (TLTM) [MF-Umeda 2017] [Alexandru et al. 2017]

tempering the system with the flow time

Worldvolume-TLTM (or WV-HMC) [MF-Matsumoto 2019]

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

No need to compute the Jacobian

Worldvolume TLTM (WV-HMC)

[MF-Matsumoto 2012.08468]

■ Basic Idea

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

⇐ t-independent (Cauchy's theorem)

⇐ t-independent

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

($W(t)$: arbitrary function)

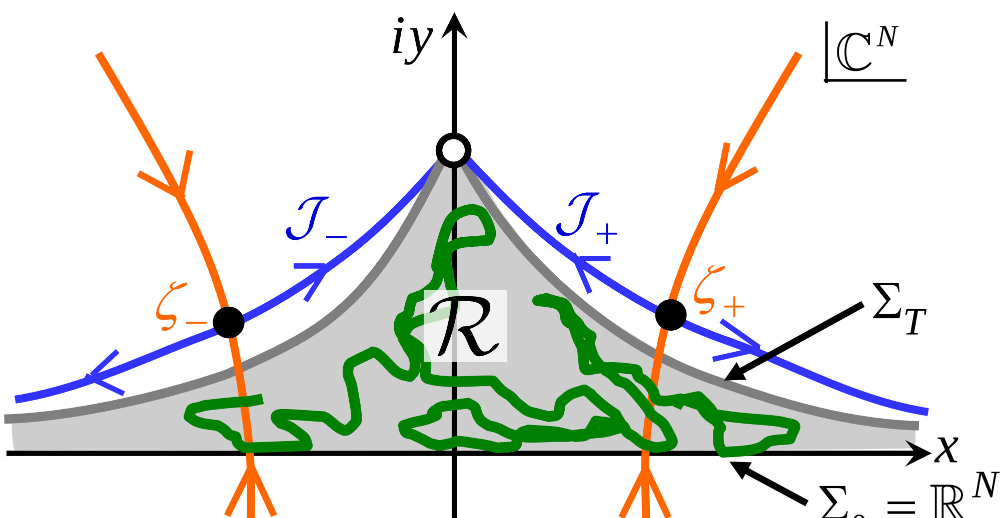
(chosen s.t. the appearance prob at different t are almost the same)

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

⇐ Path integrals over the **worldvolume** $\mathcal{R}$

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

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



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

Two pictures in WV-HMC (1/2)

[MF-Matsumoto 2012.08468]

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

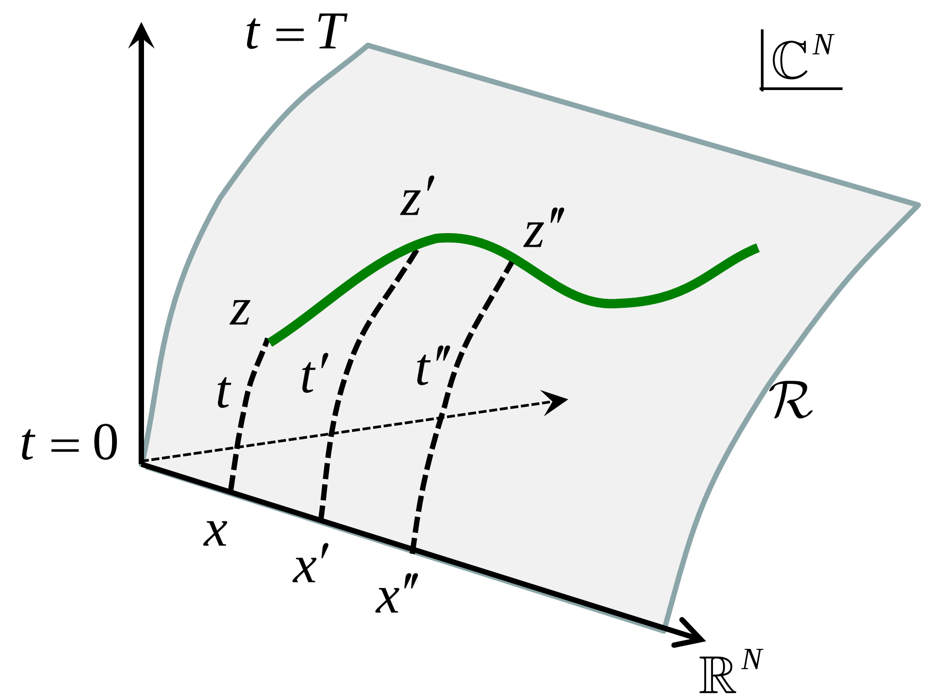
[MF-Matsumoto 2012.08468]

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

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

[MF-Matsumoto 2012.08468]
[Fujisawa et al. 2112.10519]

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



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

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

Computational cost for WV-HMC

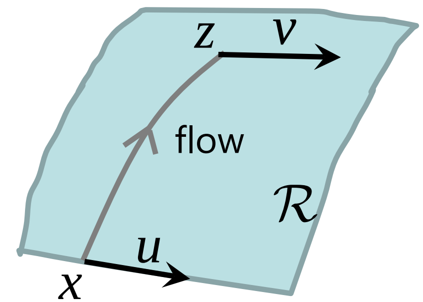
[MF-Matsumoto 2012.08468]
[MF-Matsumoto-Namekawa, on-going]

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

Configuration flow $\quad \dot{z}_i = (\partial_i S(z))^* \;\Rightarrow O(N)$

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

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



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

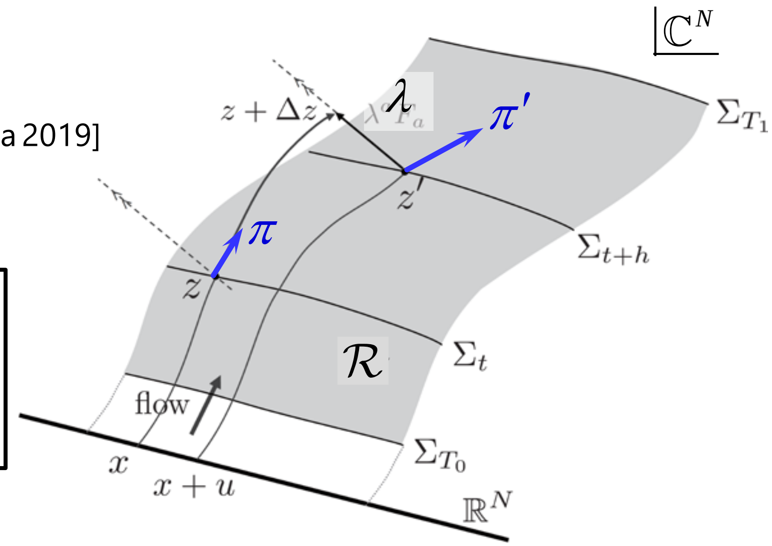
$\left(V(z) = \mathrm{Re}S(z) + W(t(z))\right)$

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

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

⇔

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



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

Comput cost at each MD step is expected to be $O(N)$

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

[MF-Matsumoto 2012.08468]

■ Preparation

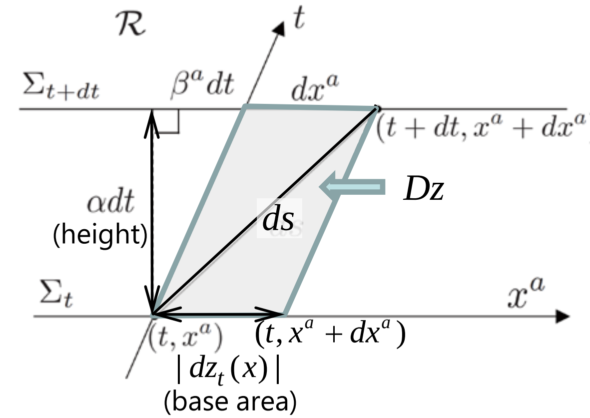
$$\langle \mathcal{O}(x) \rangle = \frac{\int_{\mathcal{R}} dt\, dz_t\; e^{-W(t)} e^{-S(z_t)} \mathcal{O}(z_t)}{\int_{\mathcal{R}} dt\, dz_t\; e^{-W(t)} e^{-S(z_t)}}$$

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

= vol element Dz of the induced metric

ADM decomposition

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



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

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

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

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

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

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

[MF-Matsumoto 2012.08468]

■ Algorithm

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

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

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

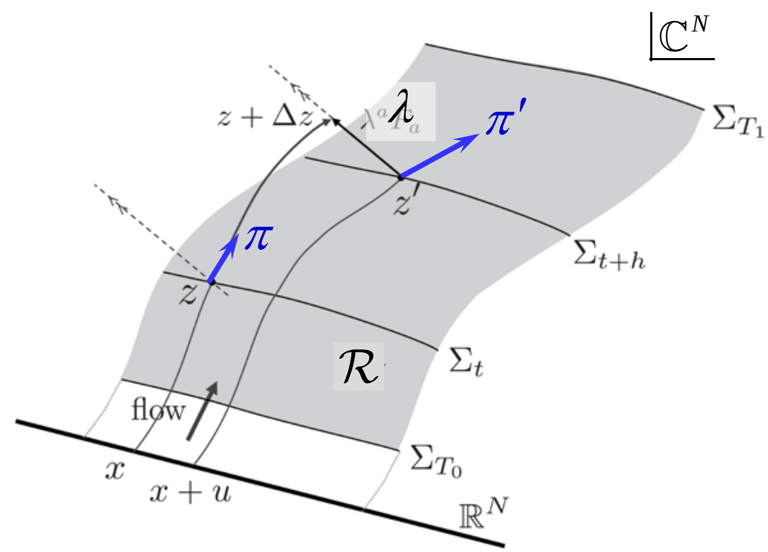
HMC on a constrained space **[Andersen 1983, Leimkuhler-Skeel 1994]**

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

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

λ and λ' are determined s.t.

$$\begin{cases} z' \in \mathcal{R} \ \text{ and } \ \langle E_0(z), \lambda \rangle = 0 \\ \pi' \in T_{z'}\mathcal{R} \ \text{ and } \ \langle E_0(z'), \lambda' \rangle = 0 \end{cases}$$



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

3. Application of WV-HMC method to scalar field theory at finite density

Model

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

Continuum action

(x_0 : Euclidean time)

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

Lattice action

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

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

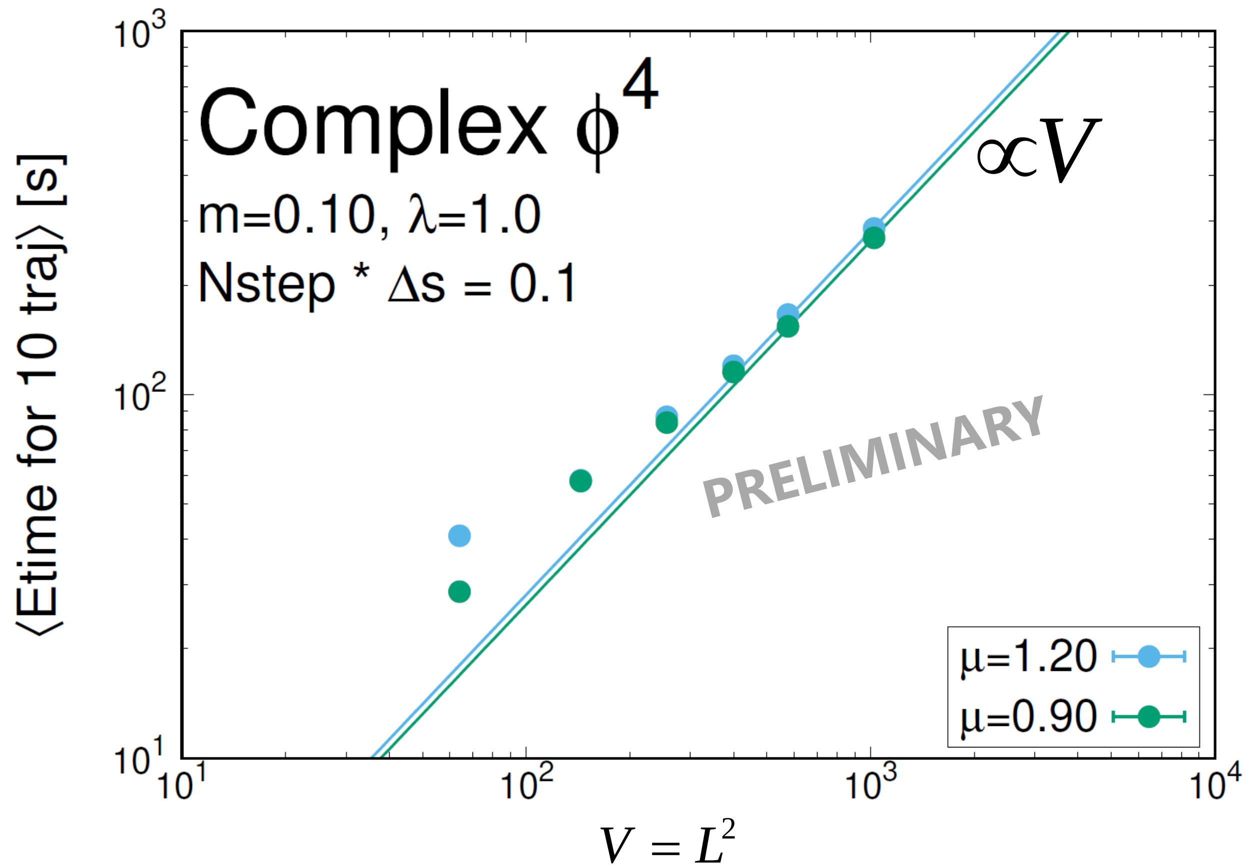
$$S(\xi,\eta) = \sum_n \left[\begin{array}{l} \frac{2d + m^2}{2}(\xi_n^2 + \eta_n^2) + \frac{\lambda}{4}(\xi_n^2 + \eta_n^2)^2 - \sum_{i=1}^{d-1} (\xi_{n+i}\xi_n + \eta_{n+i}\eta_n) \\ -\cosh\mu (\xi_{n+0}\xi_n + \eta_{n+0}\eta_n) - i \sinh\mu (\xi_{n+0}\eta_n - \eta_{n+0}\xi_n) \end{array} \right]$$

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

$\dot{z}_n = [\partial S(z,w) / \partial z_n]^*, \quad \dot{w}_n = [\partial S(z,w) / \partial w_n]^*$ (V : lattice volume)

Computational cost scaling in 2D

[MF-Matsumoto-Namekawa, on-going]



computed on Yukawa21 (@YITP, Kyoto Univ)

⇨ to be run on Fugaku

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

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

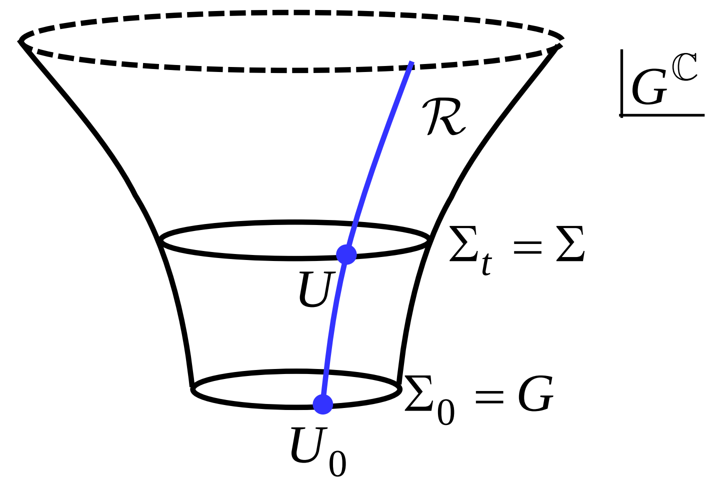
Towards Yang-Mills theories

WV-HMC also works for group manifolds

[MF, in preparation]

[MF, in preparation]

[MF-Kanamori-Namekawa, on-going]



[Example]

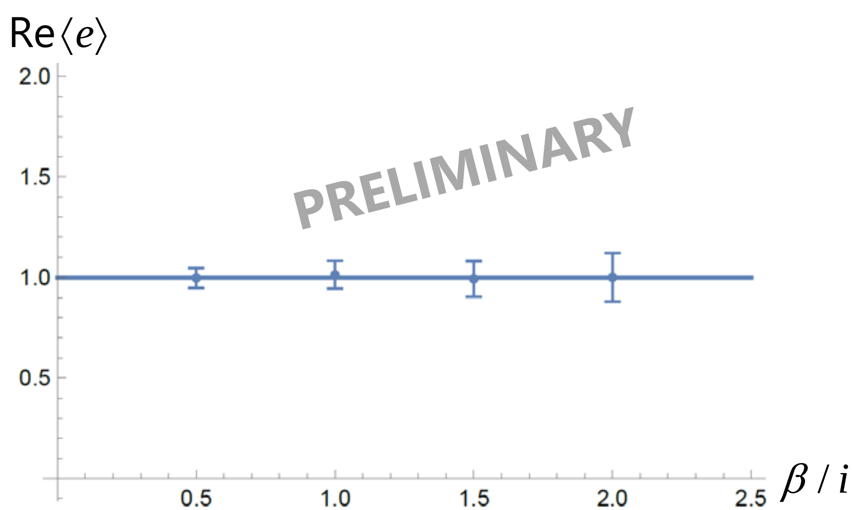
1-site model with a pure imaginary coupling:

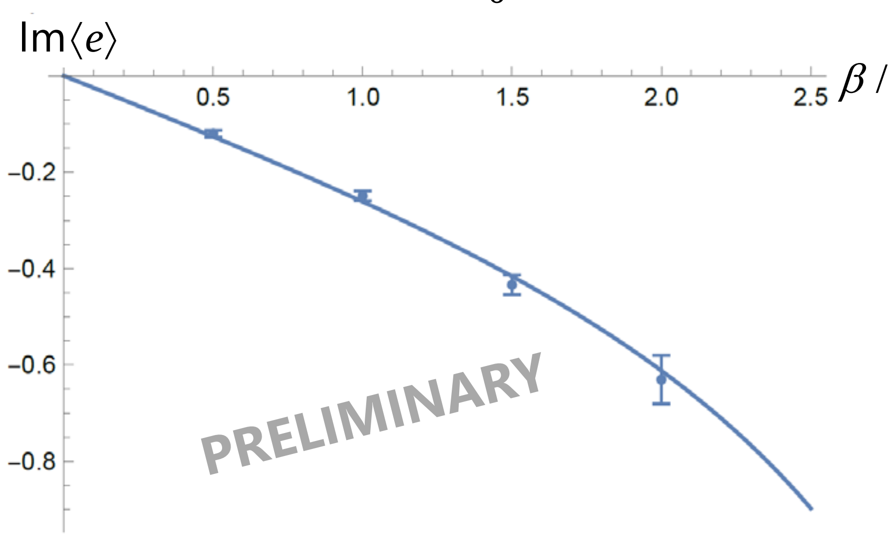
$$S(U) \equiv \beta\, e(U) \equiv \frac{\beta}{2N}\,\mathrm{tr}\left(2 - U - U^{-1}\right)$$

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

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

numerical result (WV-HMC):





The algorithm can be directly applied to Yang-Mills case

[MF-Kanamori-Namekawa, on-going]

5. Summary and outlook

Summary and outlook

■ Summary

▼ WV-HMC seems to be a powerful tool for local field theories

- Comutational cost is expected to scale as $O(V)$
- No wrong convergence problem (such as those for complex Langevin)
- Can give more accurate values by increasing the sample size (no need to introduce D_{cut} as in TRG) **"Power of Monte Carlo"**

■ Outlook

▼ Application to QCD

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

▼ Further improvements of algorithm **[MF-Matsumoto-Namekawa-..., on-going]**

▼ Combining various algorithms

(e.g.) TRG (non-MC) : good at calculating free energy **cf) TRG for 2D YM: [MF-Kadoh-Matsumoto 2107.14149]**

▼ Particularly important: MC calc for time-dependent systems

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

Thank you.