Worldvolume Hybrid Monte Carlo algorithm for group manifolds

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Based on work with

Yusuke Namekawa (Hiroshima Univ)

also with

Naoya Umeda (PwC)
Nobuyuki Matsumoto (Boston Univ)
Issaku Kanamori (RIKEN R-CCS)

Introduction

Sign problem (1/2)

A large system with a complex action:

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

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

highly oscillatory

$$= \frac{\int_{\mathbb{R}^N} dx\, e^{-\mathrm{Re}\, S(x)} e^{-i\, \mathrm{Im}\, S(x)}\, \mathcal{O}(x) \Big/ \int_{\mathbb{R}^N} dx\, e^{-\mathrm{Re}\, S(x)}}{\int_{\mathbb{R}^N} dx\, e^{-\mathrm{Re}\, S(x)} e^{-i\, \mathrm{Im}\, S(x)} \Big/ \int_{\mathbb{R}^N} dx\, e^{-\mathrm{Re}\, S(x)}} = \frac{e^{-O(N)}}{e^{-O(N)}} \quad \big(= O(1)\big)$$

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

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

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

Sign problem (2/2)

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:

Extension of WV-HMC algorithm to group manifolds **[MF, in preparation]**

Plan

1. Introduction (done)
2. Basics of the WV-HMC method
3. WV-HMC for group manifolds
4. Examples : 1-site model
5. Conclusion and outlook

cf. Application to the Hubbard model

⇨ Namekawa's talk (NEXT)

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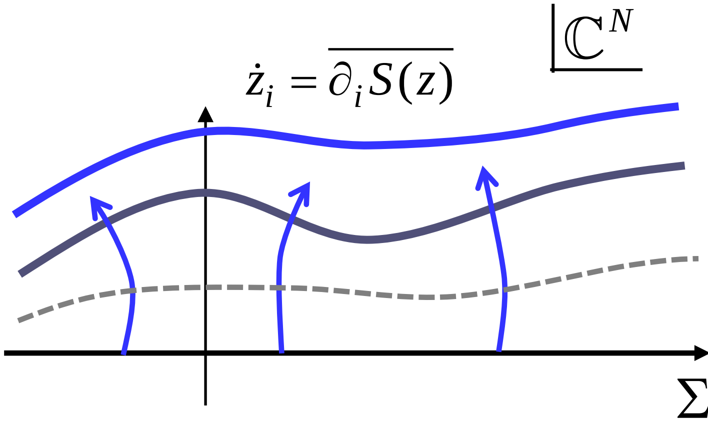
Lefschetz thimble method and ergodicity problem

To alleviate the highly oscillatory behavior,
deform the integration surface into $\mathbb{C}^N$: $\Sigma_0 = \mathbb{R}^N \to \Sigma \subset \mathbb{C}^N$



$\mathcal{J}$ (Lefschetz thimble) ⇦ $\mathrm{Im}\, S(z)$: const

Σ ⇦ $\mathrm{Im}\, S(z)$: almost const
(sign probem alleviated)

$\Sigma_0 = \mathbb{R}^N$ ⇦ $\mathrm{Im}\, S(x)$: changes rapidly
(severe sign problem)

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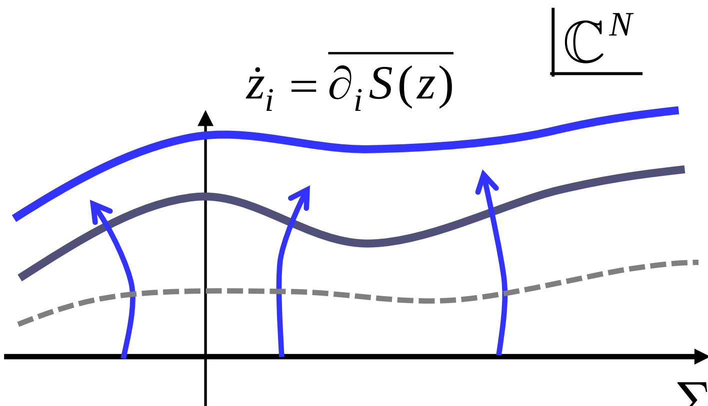

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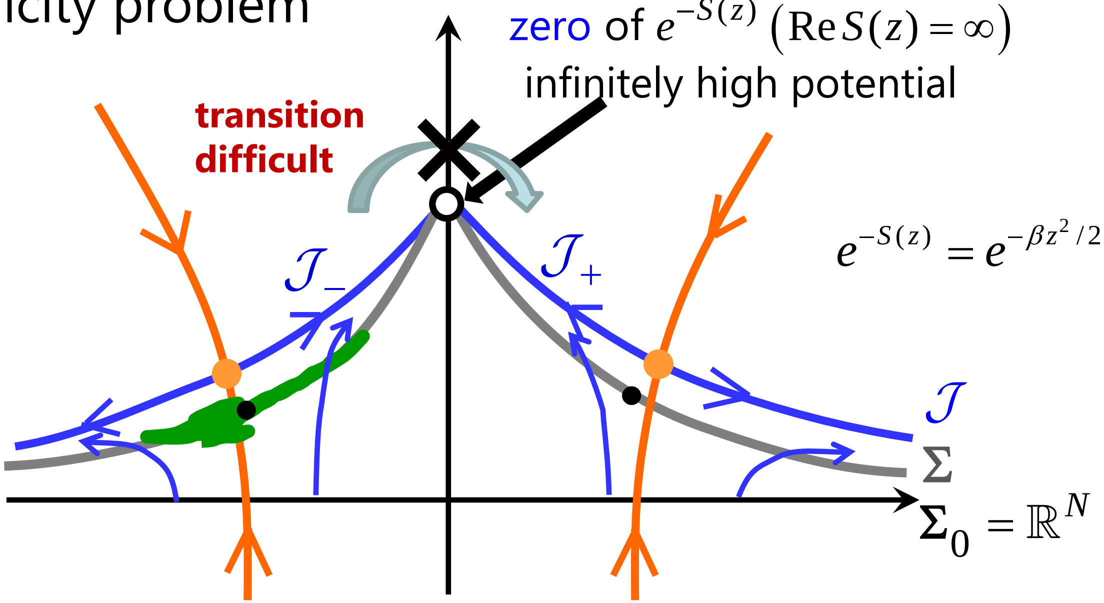
ergodicity problem



$$e^{-S(z)} = e^{-\beta z^2/2}(z-i)^{\gamma} \quad \left(\beta \gg 1,\ \gamma \in \mathbb{Z}_{>0}\right)$$

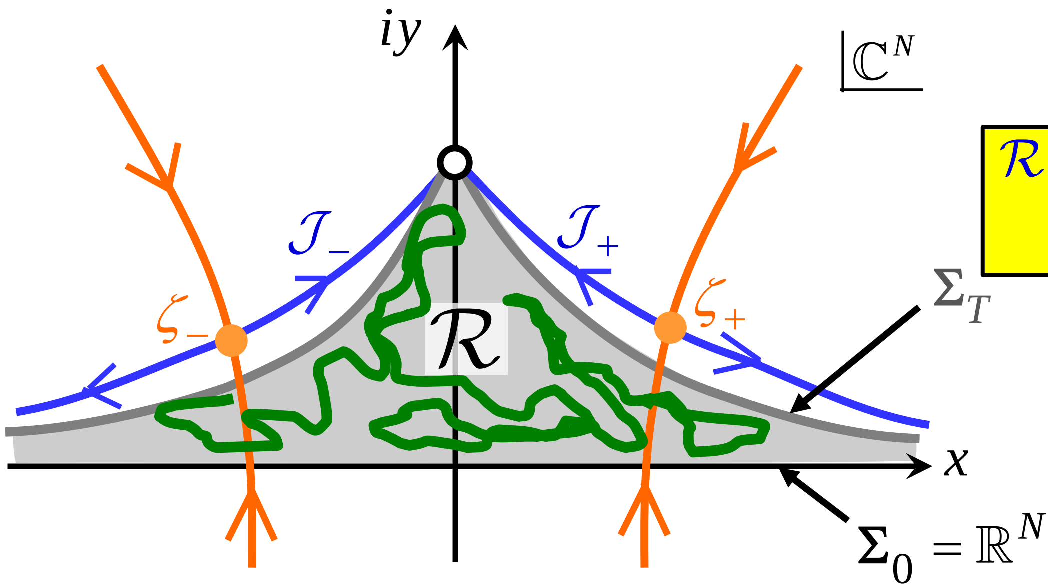
Worldvolume HMC method (1/2)

[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 compared with TLT

- No need to introduce replicas explicitly
- No need to calculate Jacobian $E_a^i(x) = \partial z^i(x) / \partial x^a$ in MD processes
- Autocorrelation is reduced due to the use of HMC

Worldvolume HMC method (2/2)

[MF-Matsumoto 2012.08468]

■ mechanism

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

$\Leftarrow$ t-independent

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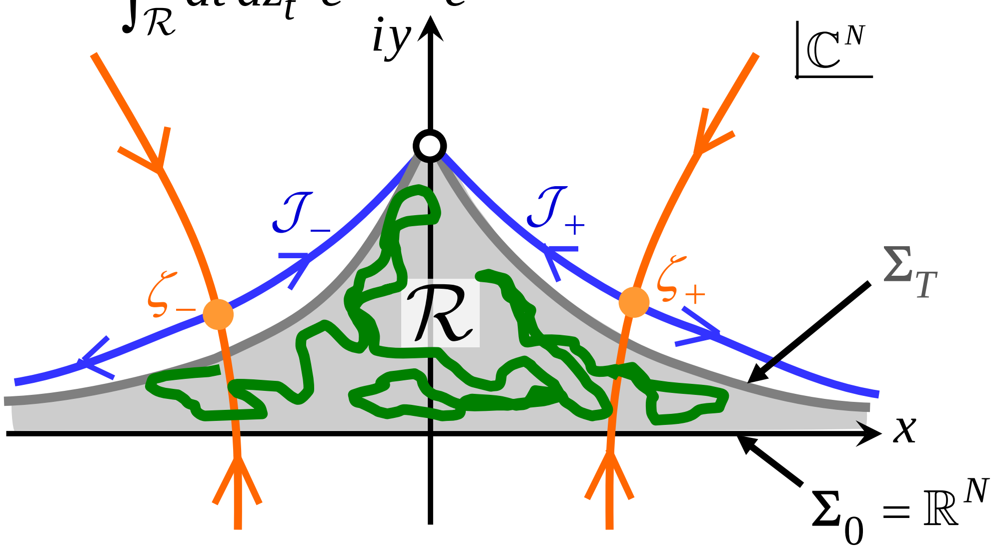
$$= \frac{\int_0^T dt\, e^{-W(t)} \int_{\Sigma_t} dz_t\ e^{-S(z_t)}\, \mathcal{O}(z_t)}{\int_0^T dt\, e^{-W(t)} \int_{\Sigma_t} dz_t\ e^{-S(z_t)}}$$

($W(t)$: arbitrary fcn)

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

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

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



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

Algorithm

[MF-Matsumoto 2012.08468]
[MF 2311.10663]

Algorithm

(i) generation of an initial momentum

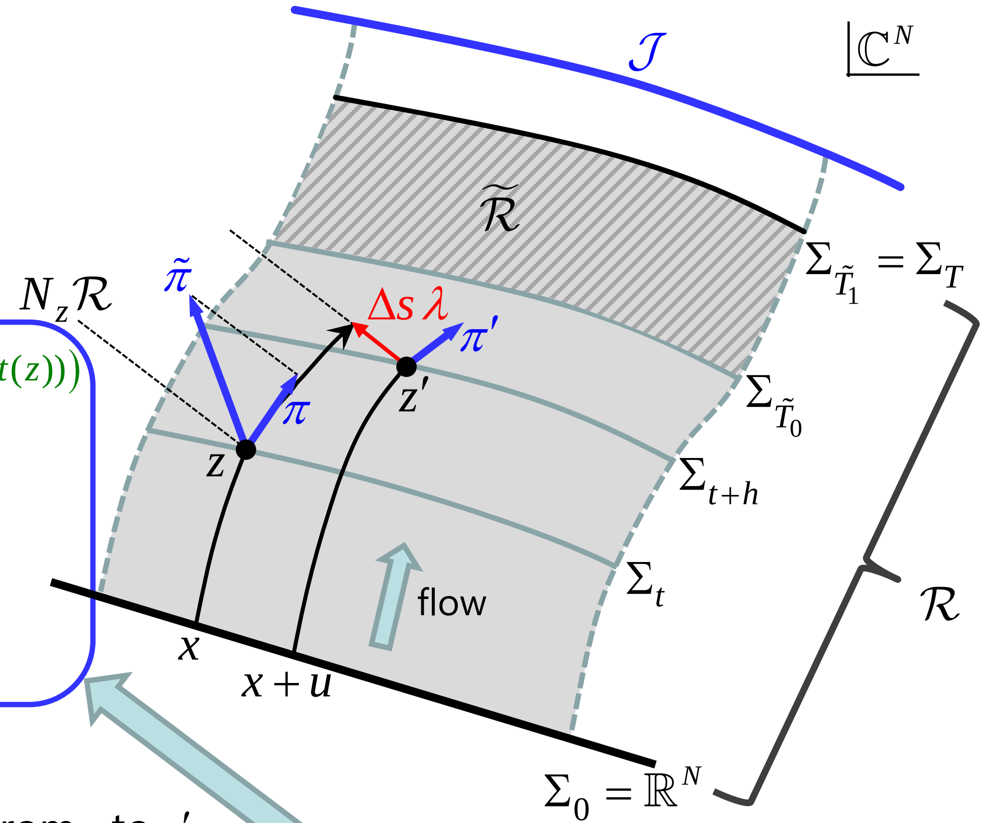
① $\tilde{\pi} = (\tilde{\pi}^i) \in \mathbb{C}^N \leftarrow e^{-\tilde{\pi}^\dagger \tilde{\pi}/2}$

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

(ii) constrained MD (RATTLE)

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

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

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]**

(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]

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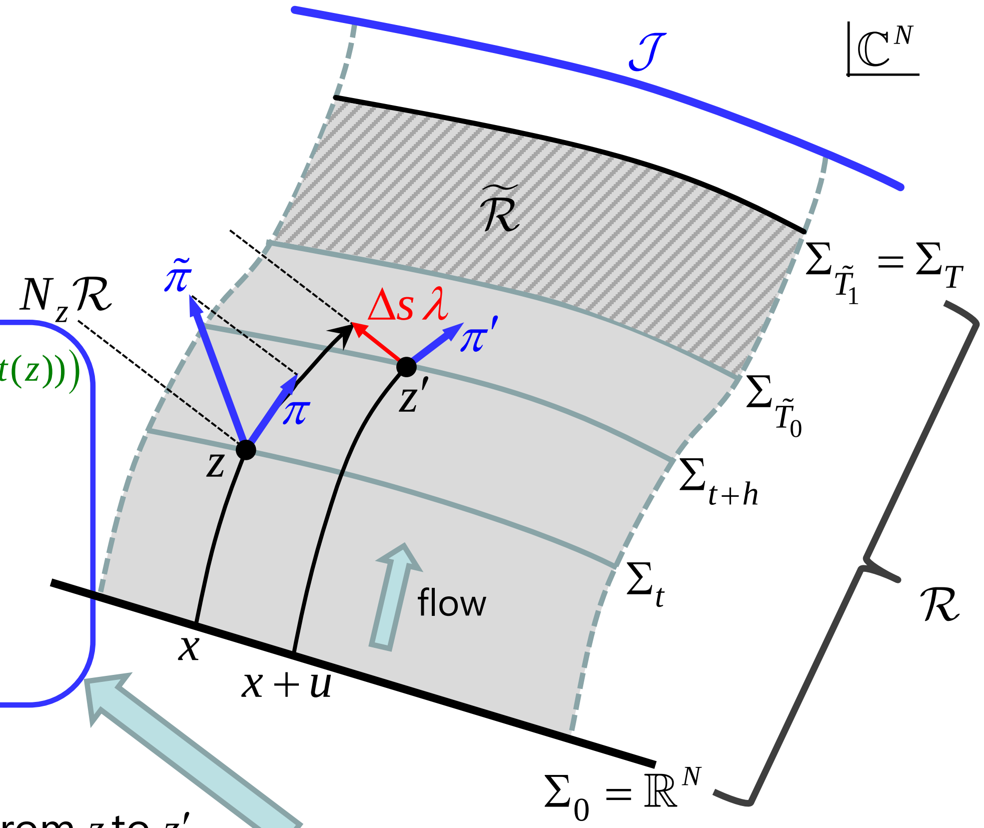

λ, λ' can be found easily by using the simplified Newton $\left[\#\text{itr}=O\left((\ln N)^{1-2}\right)\right]$
[MF 2311.10663]

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[MF-Matsumoto-Namekawa 2107.06858]

Comput. cost for local bosonic actions (1/2)

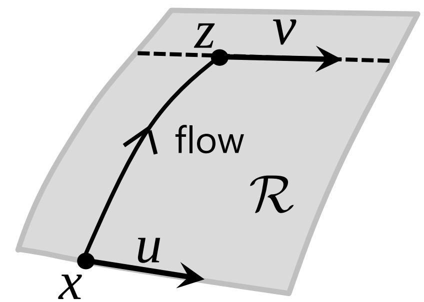
$z=(z^i)\in\mathbb{C}^N$ ($N\propto V$: #DOF)

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

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

2. **Vector flow** $\dot{v}_i=\overline{\partial_i\partial_j S(z)\,v_j}$ $\Rightarrow O(N)$ [when $\partial_i\partial_j S(z)$ is sparse (local field case)]

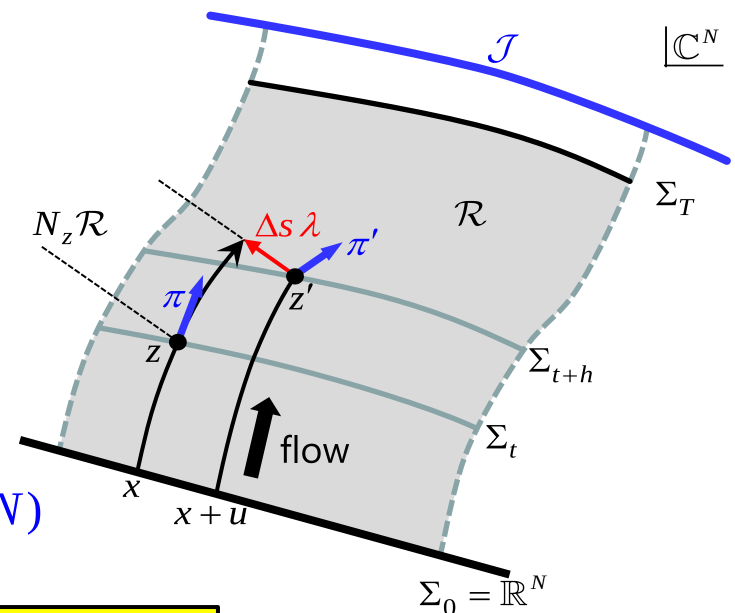
3. **RATTLE**
$$\begin{cases}\pi_{1/2}=\pi-\Delta s\,\overline{\partial V(z)}-\lambda\\ z'=z+\Delta s\,\pi_{1/2}\\ \pi'=\pi_{1/2}-\Delta s\,\overline{V(z')}-\lambda'\end{cases}\qquad (V(z)=\mathrm{Re}S(z)+W(t(z)))$$



$\lambda\in N_z\mathcal{R}$ 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 using simplified Newton with BiCGStab for linear inversion (which requires only config/vector flows) $\Rightarrow O(N)$

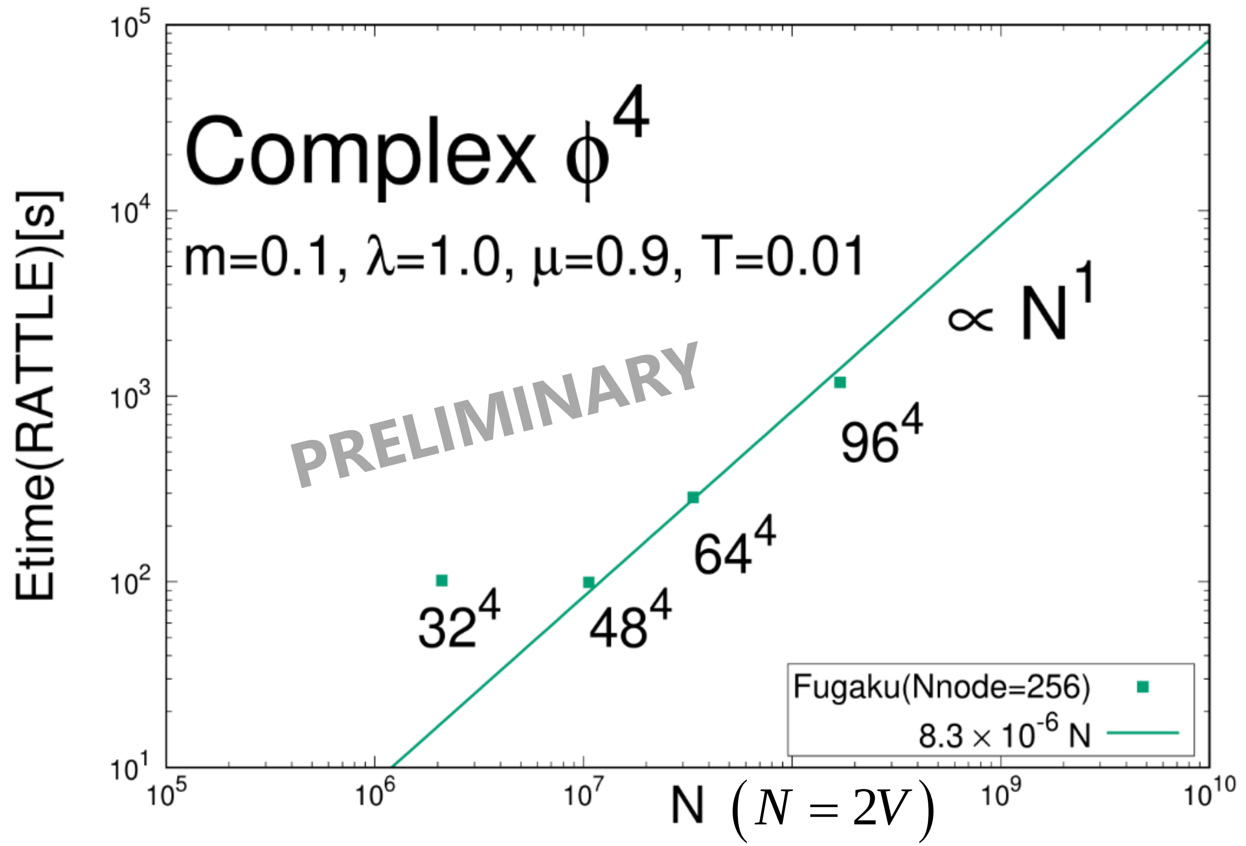


Comput cost at each MD step is expected to be $O(N)$ for local field theories (with no fermion determinants)

Comput. cost for local bosonic actions (2/2)

[MF-Namekawa, in preparation]

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



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

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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Cauchy's theorem for group manifolds

[MF, in preparation]

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

We want to calculate the following path integral:

$$\boxed{\langle \mathcal{O} \rangle \equiv \frac{\int_G |dU_0|\, e^{-S(U_0)}\, \mathcal{O}(U_0)}{\int_G |dU_0|\, e^{-S(U_0)}}} \qquad \begin{pmatrix} U_0 \in G : \text{dynamical variable} \\ S(U_0) \in \mathbb{C} : \text{complex action} \end{pmatrix}$$

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

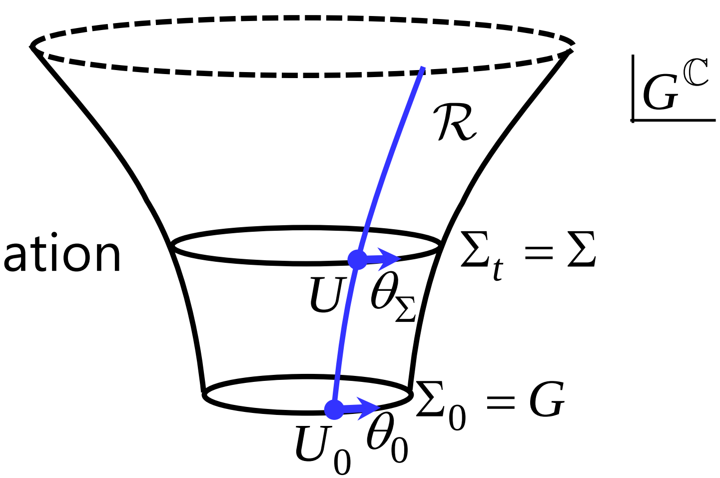
$\theta_0 \equiv dU_0\, U_0^{-1} = T_a\, \theta_0^a$: Maurer-Cartan 1-form

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

The path integral does not change under continuous deformations $\Sigma_0 = G \to \Sigma \subset G^{\mathbb{C}}$:

complexification

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



Here, for $U, U + dU \in \Sigma$

$$\theta_\Sigma \equiv dU\,U^{-1} = T_i\, \theta_\Sigma^i \equiv T_i\,(E_a^i\, \theta_0^a) \quad (a, i = 1, \ldots, N)$$

$$(dU)_\Sigma \equiv \theta_\Sigma^1 \wedge \cdots \wedge \theta_\Sigma^N = \det E\, |dU_0|$$

Path integral over the worldvolume

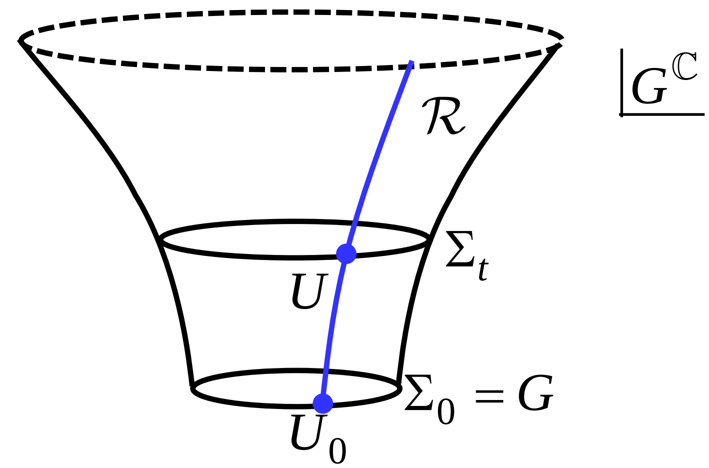
[MF, in preparation]

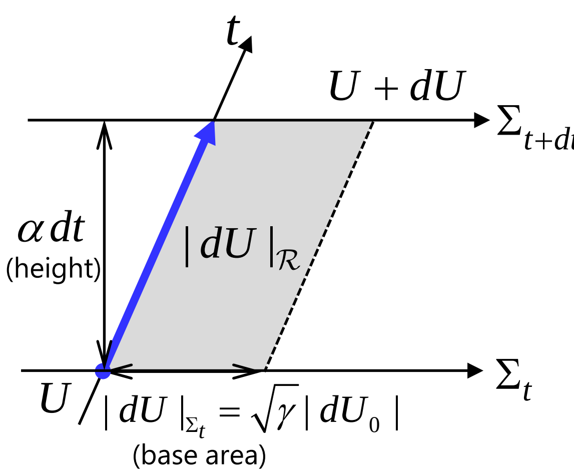
$$\langle \mathcal{O} \rangle = \frac{\int_{\Sigma_t} (dU)_{\Sigma_t}\; e^{-S(U)}\,\mathcal{O}(U)}{\int_{\Sigma_t} (dU)_{\Sigma_t}\; e^{-S(U)}}$$

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

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

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





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

⇩

Constrained molecular dynamics (RATTLE) on $\mathcal{R}$ can be introduced 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

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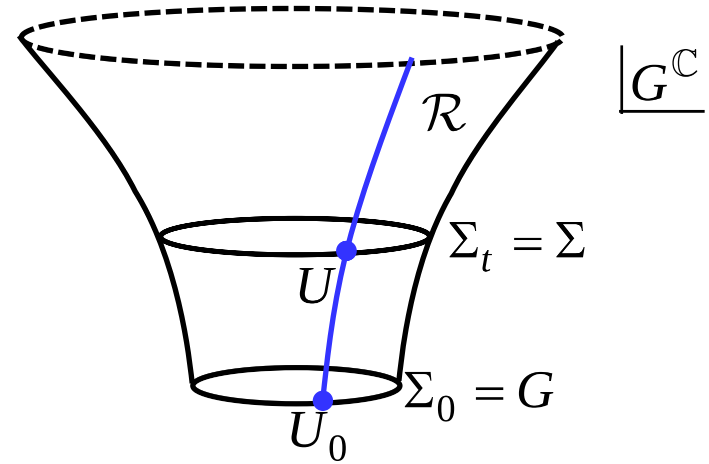
SU(2) with a pure imaginary coupling

[MF, in preparation]

$G = SU(2)$

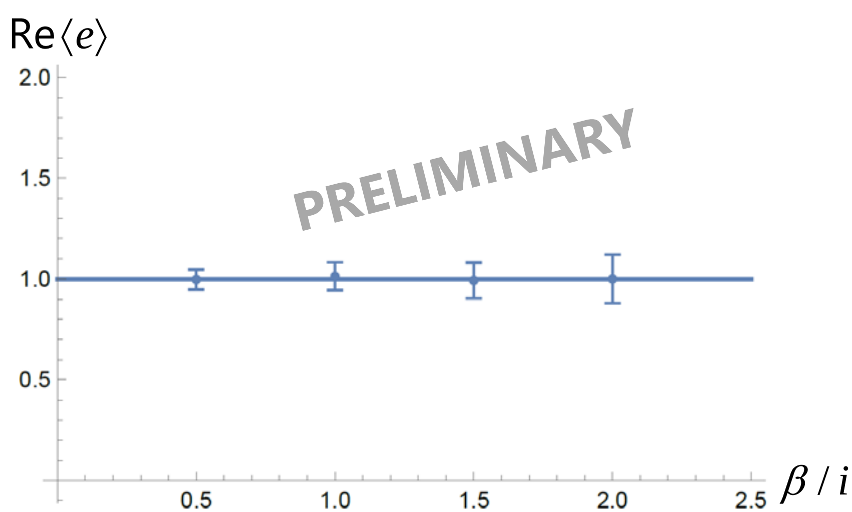
$$S(U) \equiv \beta\, e(U) \equiv \frac{\beta}{4}\,\mathrm{tr}\left(2 - U - U^{-1}\right) \quad (\beta \in i\,\mathbb{R})$$

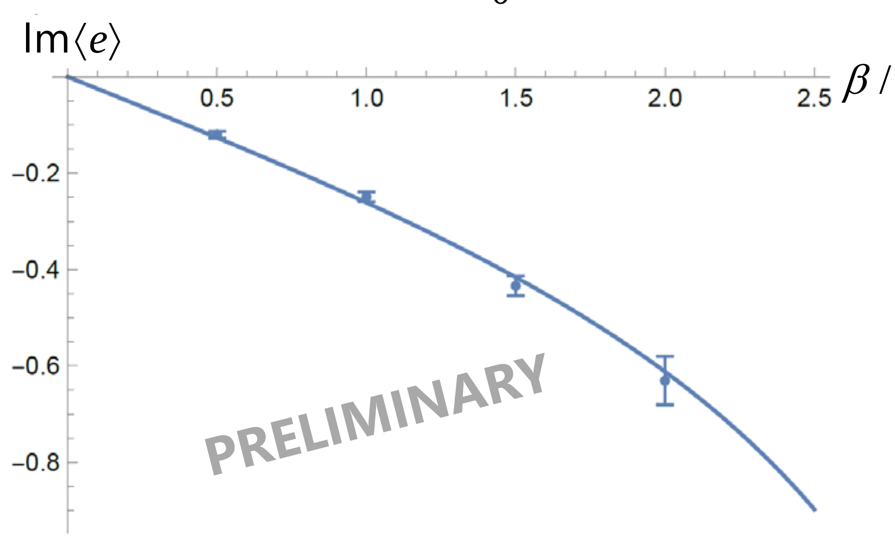


analytic result: $\langle e\rangle = 1 - I_2(\beta)/I_1(\beta)$

numerical result (WV-HMC):

$T = 0.2$



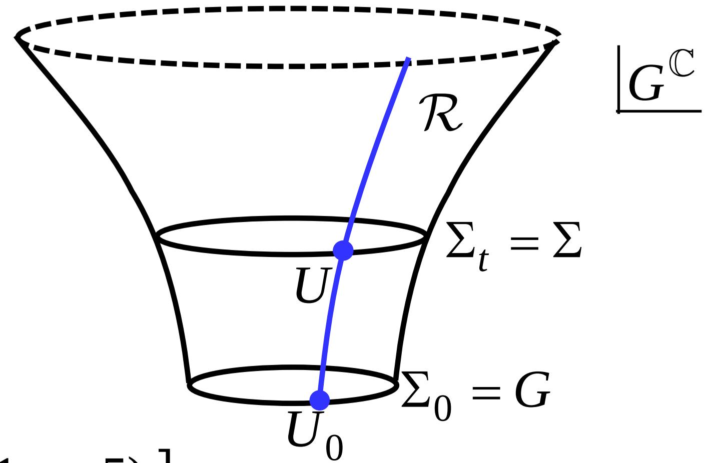


U(2) with a topological term

[MF, in preparation]

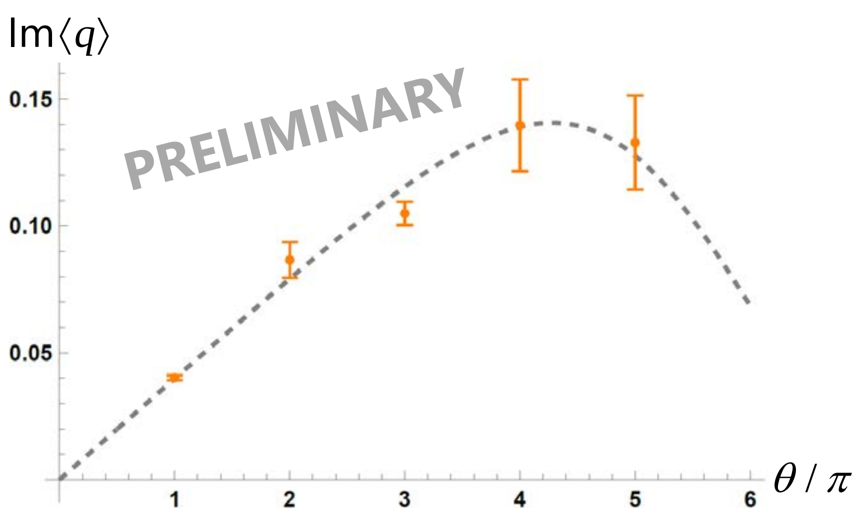
$\underline{G = U(2)}$ $\left(\underline{\text{NB}} : U(2) = SU(2)\times U(1)/Z_2 \neq SU(2)\times U(1)\right)$

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



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

$T = 0.2$



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   ⇨ Namekawa’s talk (NEXT)

Summary and outlook

■ **Summary** : WV-HMC algorithm has been extended to group manifolds 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 field
(e.g. complex scalars)

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

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

fermions
(e.g. Thirring, Stephanov, Hubbard) ⇦ **Namekawa's talk (NEXT)**

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

▼ Important in the near future : MC for real-time dyn of quant many-body systems

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

Thank you.

Appendix

NB: Details of WV-HMC algorithm (1/5)

■ RATTLE

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

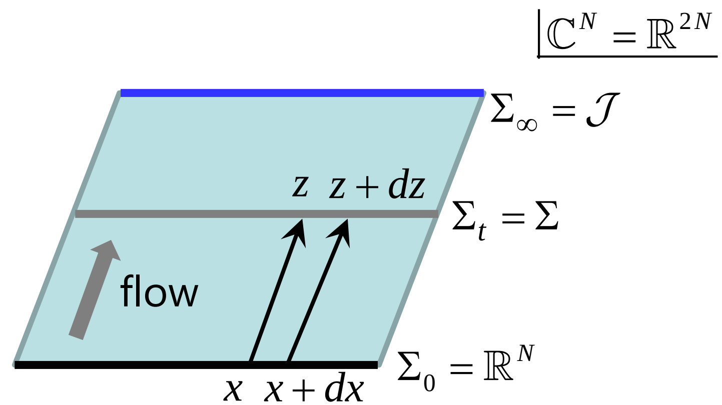
$\mathcal{M} = \mathcal{J}$: Lefschetz thimble ⇨ original (**LT-HMC**) [Fujii et al. 2013]

$\mathcal{M} = \Sigma$: 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

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



parametrization of Σ

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

Jacobian $\boxed{E^i_a \equiv \partial z^i / \partial x^a}$

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

induced metric

$$ds^2_\Sigma \equiv |dz^i(x)|^2 = \gamma_{ab} dx^a dx^b \quad (\gamma_{ab} \equiv \mathrm{Re}\, \overline{E^i_a} E^i_b = \overline{E^i_a} E^i_b)$$

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

NB: Details of WV-HMC algorithm(2/5)

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

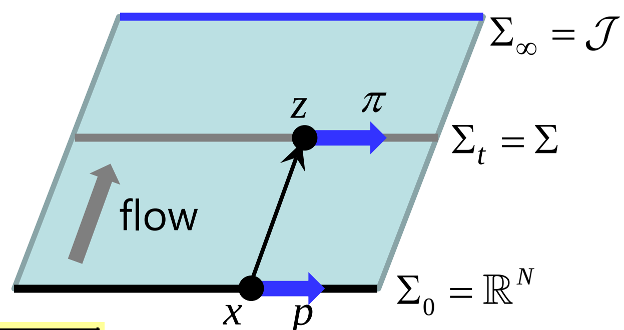
$$\boxed{Z = \int_{T\Sigma} \frac{\omega^N}{N!} e^{-H(x,p)} \mathcal{F}(x) \ \text{ with } \begin{cases} H(x,p) = \dfrac{1}{2} \gamma^{ab} p_a p_b + \operatorname{Re} S(z(x)) \\ \mathcal{F}(x) = \dfrac{dz}{|dz|} e^{-i \operatorname{Im} S(z)} \ \text{(reweighting factor)} \end{cases}}$$

"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 $\det E = \sqrt{\gamma}$

NB: Details of WV-HMC algorithm(3/5)

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

Algorithm of GT-HMC

(i) generation of an initial momentum

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

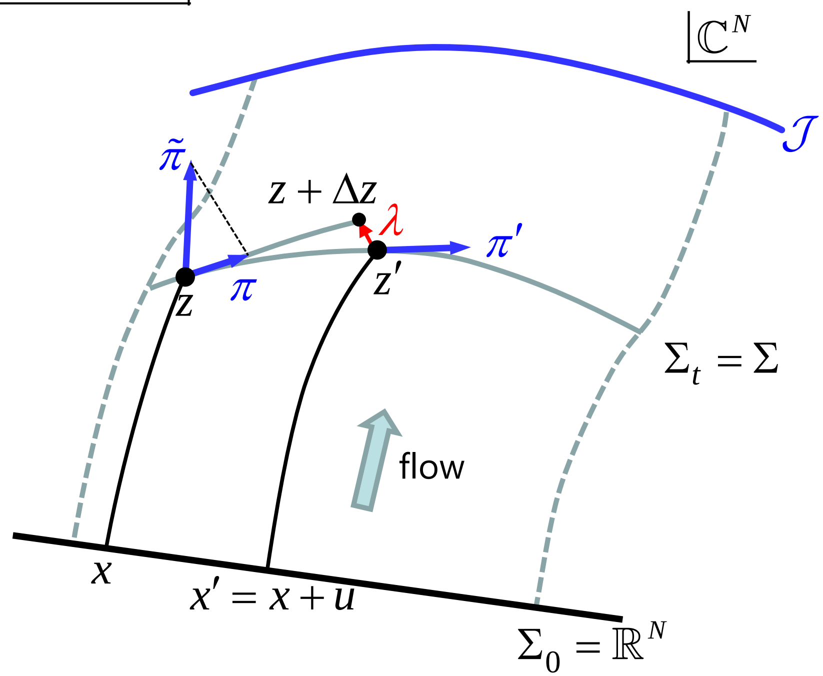
② $\tilde{\pi} \to \pi \in T_z \Sigma$

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

can be easily found with the simplified Newton **[MF 2311.10663]**
(corresponds to the "fixed-point method"
for LT-HMC **[Fujii et al. 1309.4371]**)



(iii) Metropolis test

after repeating MD steps, we update config

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

NB: Details of WV-HMC algorithm(4/5)

[MF-Matsumoto 2012.08468]

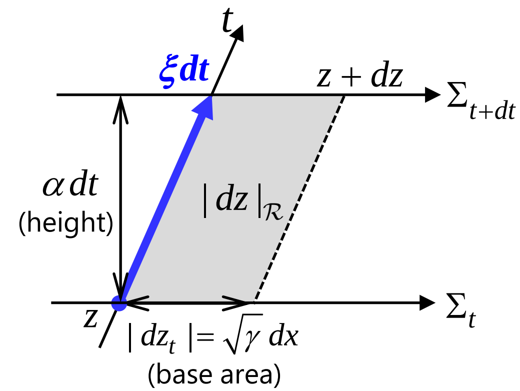
■ WV-HMC

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

parametrization of $\mathcal{R}$

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

"Jacobian" $\boxed{\hat{E}^i_\mu\equiv\partial z^i/\partial\hat{x}^\mu}$



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

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

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

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

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

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

NB: Details of WV-HMC algorithm(5/5)

[MF-Matsumoto 2012.08468]
[MF 2311.10663]

Algorithm

(i) generation of an initial momentum

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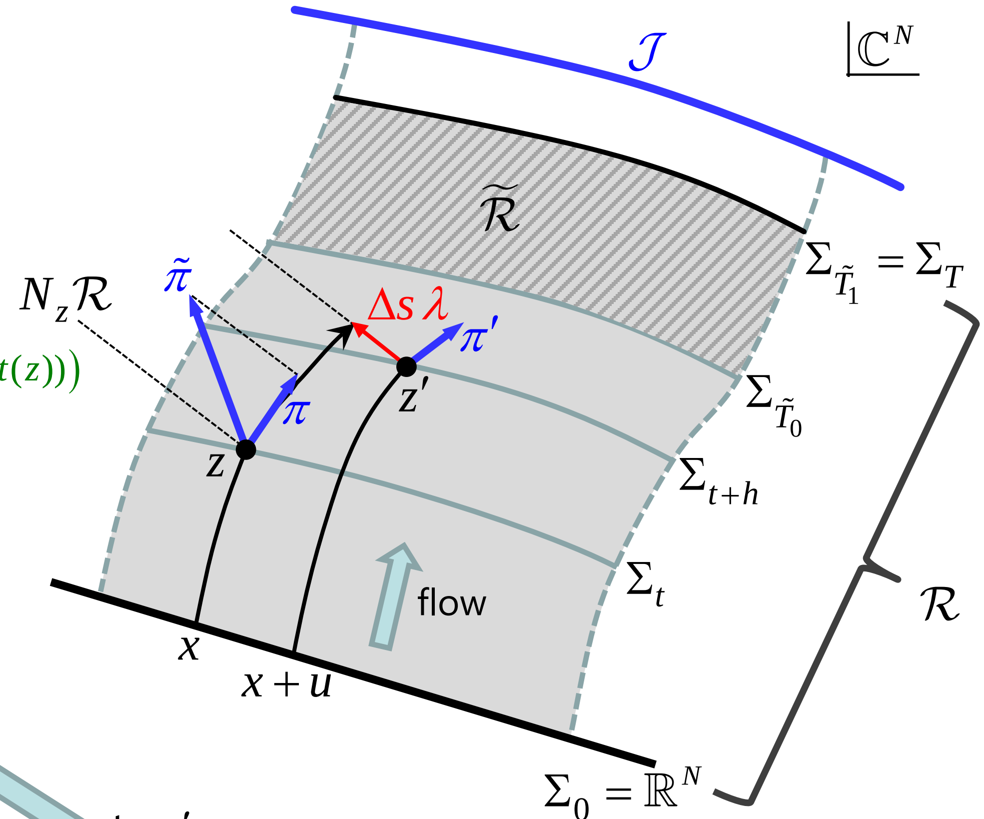
② $\tilde{\pi} \to \pi \in T_z\mathcal{R}$

(ii) constrained MD (RATTLE)

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

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



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(iii) Metropolis test

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

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

(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]**