Applying the Worldvolume Hybrid Monte Carlo method to the complex ϕ^4 theory at finite density

Yusuke Namekawa
(Hiroshima Univ)

in collaboration with

Masafumi Fukuma (Kyoto Univ)

Contents

1 Introduction

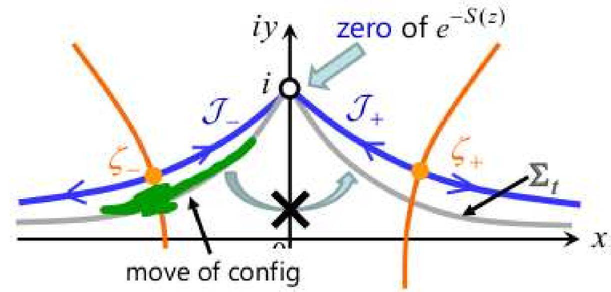
Several methods have been proposed to overcome the sign problem

- Complex Langevin (CL) method Parisi(1983),Klauder(1984),...
  [Low cost, works only in limited parameter regions
  Conditions for correct CL result have been clarified Aarts et al.(2009), Nishimura,Shimasaki(2015), Nagata et al.(2016)]
- Lefschetz thimble method Witten(2010),...
  - ◇ Original Lefschetz thimble method Cristoforetti et al.(2012),Fujii et al.(2013),Alexandru et al.(2015),...
    [Middle cost, hard to solve the sign and ergodicity problems simultaneously]
  - ◇ Tempered Lefschetz thimble method Fukuma,Umeda(2017),...
    [Middle cost, solves the sign and ergodicity problems simultaneously]
  - ◇ Worldvolume Hybrid Monte Carlo (WV-HMC) method Fukuma,Matsumoto(2020),...
    [Low cost, solves the sign and ergodicity problems simultaneously]
- Path Optimization Method Mori,Kashiwa,Ohnishi(2017),Alexandru et al.(2018),...
  [Middle cost, searches for the best path via machine learning,
  combined with parallel tempering for the ergodicity problem]
- Tensor Network method Levin,Nave(2007),...
  [High cost, non-MC approach]

[How is the sign problem resolved by Lefschetz thimble method?]

- Sign problem is reduced if Im $S(z_t)$ is almost constant

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



Cauchy's theorem ensures the equality

Flow eq. $\dot{z}_t = \overline{\partial S(z_t)}, \quad z_{t=0} = x$

Im$S(z_t)$ is const along the flow $\left[\begin{array}{l} [S(z_t)]^{\cdot} = \partial S(z_t)\, \dot{z}_t = |\partial S(z_t)|^2 \geq 0 \\ \therefore [\text{Re}S(z_t)]^{\cdot} \geq 0, \quad [\text{Im}S(z_t)]^{\cdot} = 0 \end{array} \right]$

On Lefschetz thimbles, Im$S(z_t) =$ const so that $\int dz_t \exp(-\text{Re}S(z_t) - i\,\text{Im}S(z_t))$ can be computed efficiently

$\rightarrow$ This is not the end of the story due to Ergodicity problem

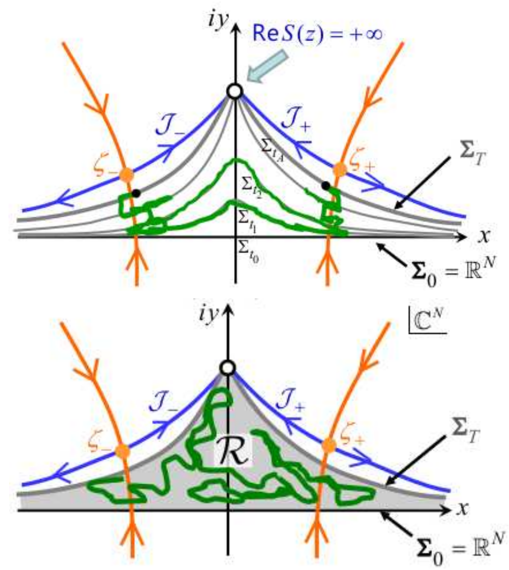
- Ergodicity problem :
  Zeros of $\exp(-S(z_t))$ produce infinitely high potential, which restricts movement of configurations

[Worldvolume Hybrid Monte Carlo (WV-HMC) method] Fukuma,Matsumoto(2020),...

- solves the sign problem and ergodicity problem simultaneously
- significantly reduces the computational cost compared with other Lefschetz thimble methods

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

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



- Cauchy's theorem ensures the equalities
- Enlarge integration surface of the original $\Sigma_0 = \mathbb{R}^N$ [N : degrees of freedom] to worldvolume (orbit of integration surface) $\mathcal{R} := \bigcup_{0 \le t \le T} \Sigma_t$

  $\rightarrow$ Perform HMC on the worldvolume $\mathcal{R}$

[WV-HMC algorithm $1/2$: overview]

(1) Generate random momentum π in tangent space of the worldvolume $T_z\mathcal{R}$

$\tilde{\pi}$ with $P(\tilde{\pi}) = \exp(-\tilde{\pi}^\dagger\tilde{\pi}/2)$

$\pi = \Pi_{T_z\mathcal{R}}\,\tilde{\pi}, \quad \Pi_{T_z\mathcal{R}}$: projection onto $T_z\mathcal{R}$

(2) RATTLE (constrained molecular dynamics)

$$\pi_{1/2} = \pi - \frac{\Delta s}{2}\partial(\mathrm{Re}S(z) - W(t(z))) - \lambda$$

$$z' = z + \Delta s\,\pi_{1/2}$$

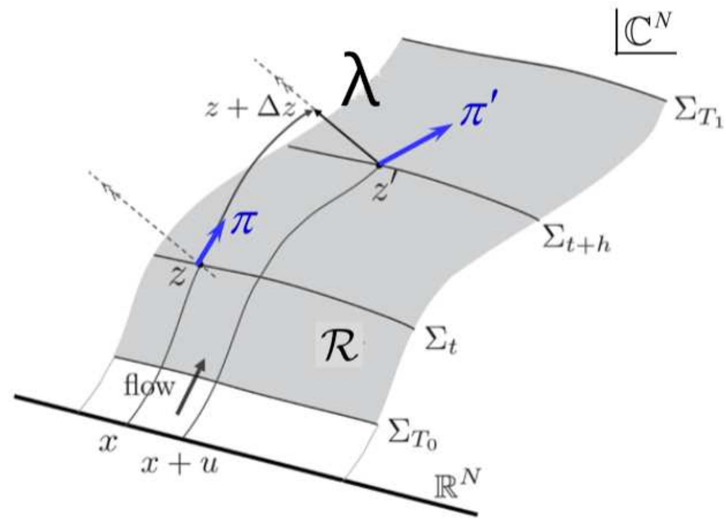
$$\pi' = \Pi_{\mathcal{R}}\left(\pi_{1/2} - \frac{\Delta s}{2}\partial(\mathrm{Re}S(z') - W(t(z')))\right)$$

$\Pi_{\mathcal{R}}$: projection onto $\mathcal{R}$

λ is determined s.t. z' comes on $\mathcal{R}$

i.e., $z_{t+h}(x+u) = z'$ is realized by choice of (h, u, λ)

$(h, u, \lambda) \to (h, u, \lambda) + \Delta(h, u, \lambda)$: Newton method



(3) Metropolis accept/reject

[WV-HMC algorithm $2/2$: flow equations]

Projections and RATTLE consist of the following flow equations

- Configuration flow eq. maps $x = (x^i) \in \mathbb{R}^N \to z_t(x) \in \mathbb{C}^N$

$$\dot{z}_t = \overline{\partial S(z_t)}, \quad z_{t=0} = x \quad O(N^1) \text{ cost}$$

- Vector flow eq. maps $u \to v$

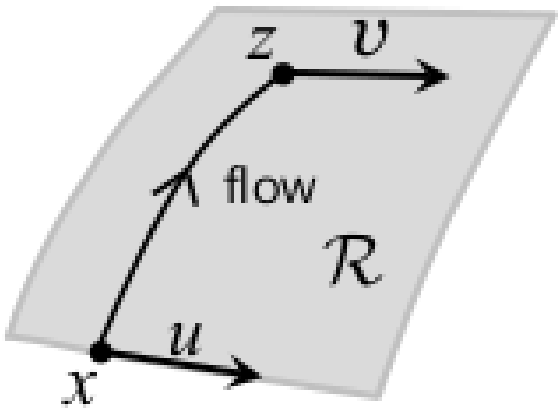
$H(z_t) := \partial\partial S(z_t)$: Hessian

$$\dot{v}_t = \overline{H(z_t) v_t}, \quad v_{t=0} = u$$

$O(N^1)$ cost if H is a sparse matrix,

such as that of complex ϕ^4 at finite density

($O(N^2)$ cost if H is a dense matrix)



◊ Total computational cost is $O(N)$ for complex ϕ^4 at finite density

2 Application of WV-HMC to complex ϕ^4 at finite density

[Complex ϕ^4 at finite density]

- $\mu \neq 0$ makes the action complex $\rightarrow$ sign problem
- Good testbed for several methods

Complex Langevin method D=4 : Aarts(2005)

Lefschetz thimble method D=4 : Cristoforetti et al.(2013), Fujii et al.(2013)

Path optimization method D=2 : Mori et al.(2017)

Tensor renormalization group method D=2 : Kadoh et al.(2019), D=4 : Akiyama et al.(2020)

$$S_{\rm lat}^{\rm Euclid}[\phi = (z+iw)/\sqrt{2}] \qquad z, w \in \mathbb{R} \rightarrow \mathbb{C}$$

$$= \sum_n \Bigg[-\sum_{\nu=1}^{D-1} (z_{n+\nu} z_n + w_{n+\nu} w_n) + \cosh(\mu)(z_{n+\hat{0}} z_n + w_{n+\hat{0}} w_n) + i \sinh(\mu)(z_{n+\hat{0}} w_n - w_{n+\hat{0}} z_n) + \frac{2D+m^2}{2}(z_n^2 + w_n^2) + \frac{\lambda}{4}(z_n^2 + w_n^2)^2 \Bigg], \quad D = 2, 4$$

[Flow equations]

- Configuration flow eq.

$$\begin{pmatrix} \dot{z}_m \\ \dot{w}_m \end{pmatrix} = \overline{\begin{pmatrix} (\partial S_{\text{lat}}(z,w)/\partial z_n) \\ (\partial S_{\text{lat}}(z,w)/\partial w_n) \end{pmatrix}}$$

$$\frac{\partial S_{\text{lat}}(z,w)}{\partial z_n} = -\cosh(\mu)(z_{n+\hat{0}} + z_{n-\hat{0}}) + i\sinh(\mu)(w_{n-\hat{0}} - w_{n+\hat{0}}) - \sum_{\nu=1}^{3}\left\{(z_{n+\nu} + z_{n-\nu})\right\}$$
$$+ (8+m^2)z_n + \lambda(z_n^2 + w_n^2)z_n$$

- Vector flow eq.

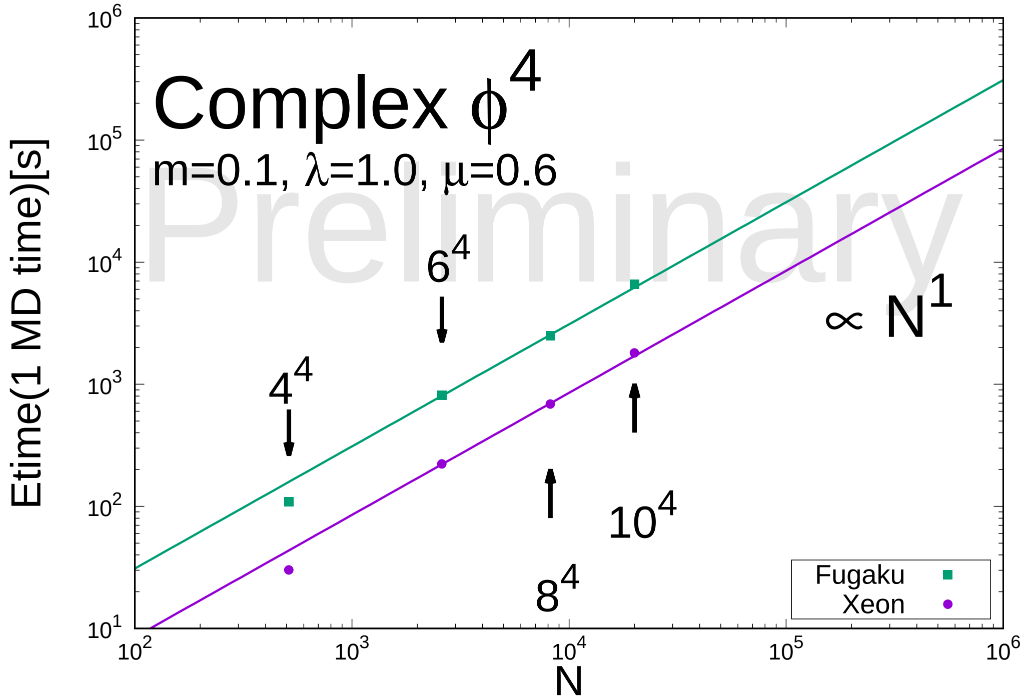
$$\begin{pmatrix} \dot{u}_m \\ \dot{v}_m \end{pmatrix} = \overline{H_{mn}(z,w)\begin{pmatrix} u_n \\ v_n \end{pmatrix}} = \begin{pmatrix} \overline{(Hu)}_m \\ \overline{(Hv)}_m \end{pmatrix}$$

$$\begin{aligned}(Hu)_m &= \frac{\partial^2 S_{\text{lat}}(z,w)}{\partial z_m \partial z_n} u_n + \frac{\partial^2 S_{\text{lat}}(z,w)}{\partial z_m \partial w_n} v_n \\ &= -\cosh(\mu)(u_{m-\hat{0}} + u_{m+\hat{0}}) - i\sinh(\mu)(v_{m-\hat{0}} - v_{m+\hat{0}}) \\ &\quad - \sum_{\nu=1}^{3}(u_{m-\nu} + u_{m+\nu}) + \left((8+m^2) + \lambda(3z_m^2 + w_m^2)\right)u_m + 2\lambda z_m w_m v_m\end{aligned}$$

◇ Hessian H is a sparse matrix, which has non-zero values only at diagonal and semi-diagonal parts. → The cost is $O(N^1)$.

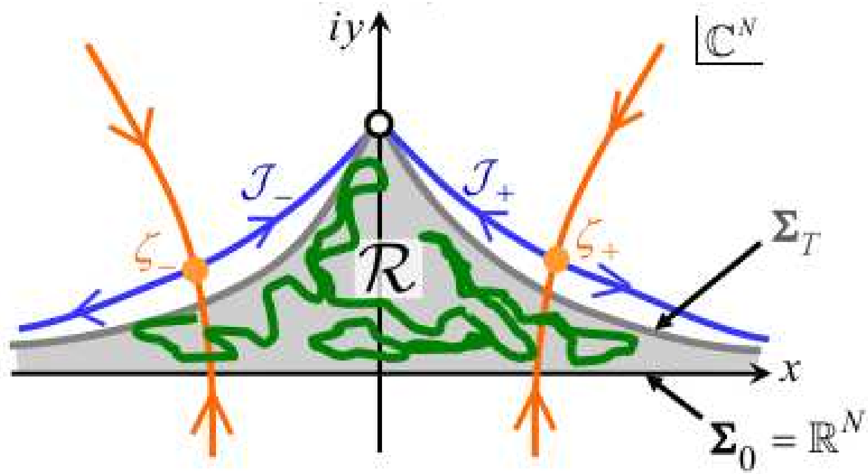
[Result: numerical cost of configuration generation]

We confirmed the cost of WV-HMC is $O(N^1)$ for complex ϕ^4 at finite density



[Simulation parameters]

- Lattice size : $4^4, 6^4$ $(D = 4)$
- $m = 0.1$, $\lambda = 1.0$
- $T = 0.08$
- $N_{\rm conf} = 1000 - 2000$ for 4^4, 200 for 6^4



[Observables]

$$\langle n \rangle := \frac{1}{V} \partial_\mu \log Z$$

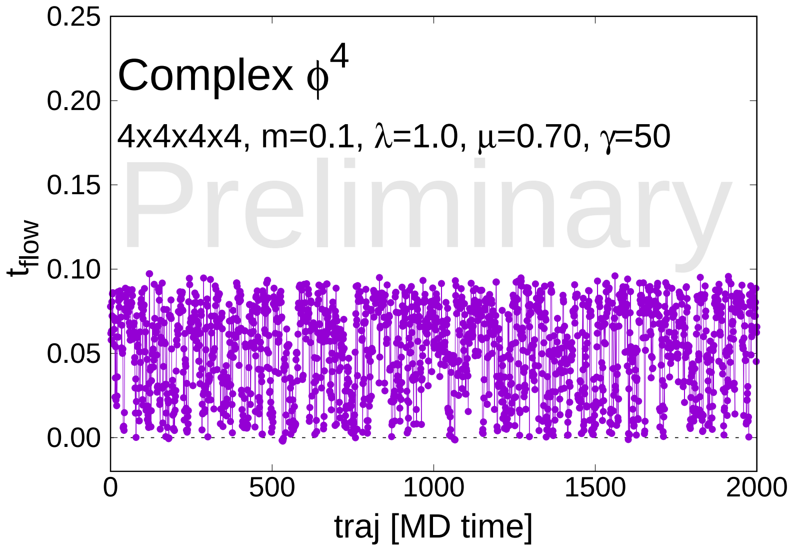
$$= \frac{1}{V} \left\langle \sum_n (\sinh(\mu)(z_{n+0} z_n + w_{n+0} w_n) + i \cosh(\mu)(z_{n+0} w_n - w_{n+0} z_n)) \right\rangle$$

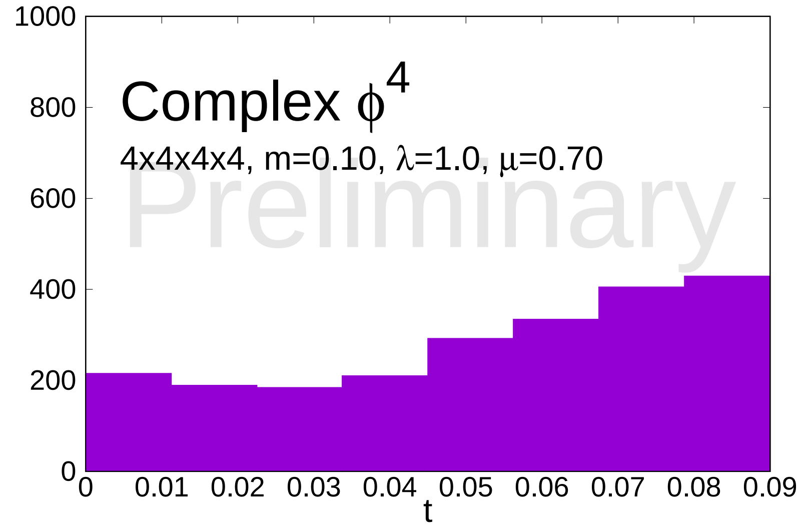
$$\left\langle |\phi|^2 \right\rangle := \frac{1}{V} \left\langle \sum_n \left(\frac{z_n - i w_n}{\sqrt{2}} \right) \left(\frac{z_n + i w_n}{\sqrt{2}} \right) \right\rangle = \frac{1}{V} \left\langle \frac{1}{2} \sum_n (z_n^2 + w_n^2) \right\rangle$$

[Tuning of $W(t)$]

- With $W(t) = 0$, configurations come to small t region
  $\rightarrow W(t)$ is tuned s.t. configurations move around small and large t regions
- We employed a simple ansatz $W(t) = -\gamma t$, $\gamma =$ const with reflection or slopes at boundaries of t

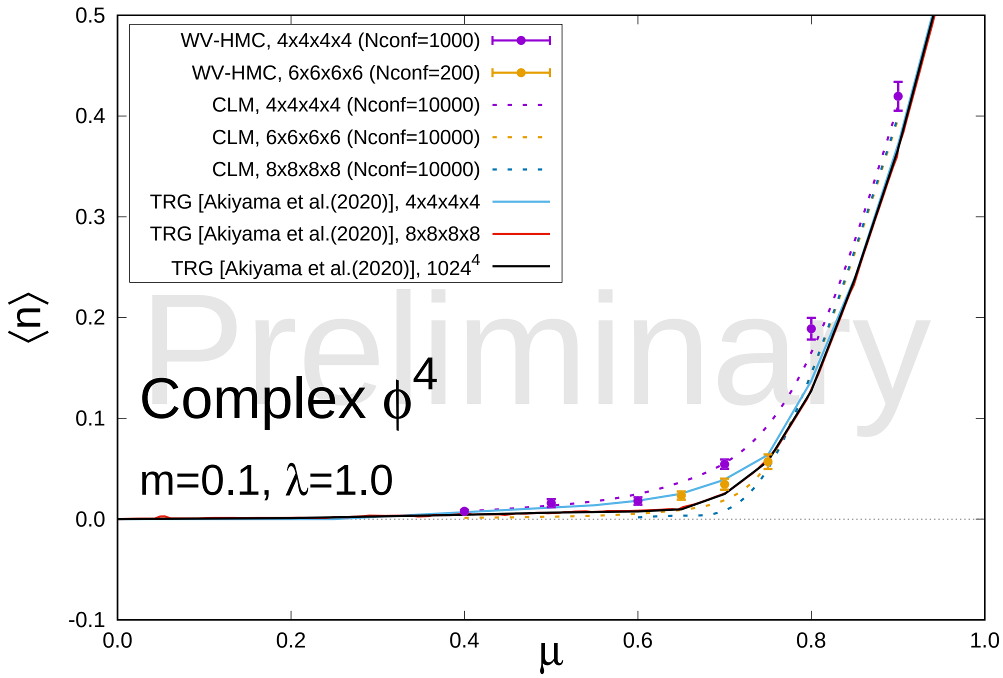
$$\langle \mathcal{O} \rangle = \frac{\int_{\mathcal{R}} dt dz_t \, e^{-W(t)} e^{-S(z_t)} \mathcal{O}(z_t)}{\int_{\mathcal{R}} dt dz_t \, e^{-W(t)} e^{-S(z_t)}}, \quad W(t) = \text{arbitrary function}$$





[Result: number density by WV-HMC]

- WV-HMC results agree with Complex Langevin ← done by ourselves (satisfying the convergence condition in the parameter region we consider)
- TRG ($D_{\rm cut} = 45$) deviates from WV-HMC and CL results Akiyama et al. (2020) (probably due to too small $D_{\rm cut} = 45$)



→ We plan to check the difference on larger lattice volumes

3 Summary

- We confirmed WV-HMC actually reduces the cost $O(N^3) \to O(N^1)$ for complex ϕ^4 at finite density
- We measured observables ($\langle n \rangle$, $\langle |\phi|^2 \rangle$) for comparison with other methods
  - ◇ WV-HMC results agree with Complex Langevin.
  - ◇ TRG ($D_{\rm cut} = 45$) Akiyama et al.(2020) deviate from WV-HMC and CL (probably due to too small $D_{\rm cut} = 45$)
    $\to$ Check the deviation with larger lattice volumes

[Future applications]

- Ongoing: apply WV-HMC to system with dynamical fermions Fukuma,YN,...
  $\to$ See the next talk by Masafumi Fukuma
- Ongoing: apply WV-HMC to gauge theory (1-site model Fukuma(in preparation), pure YM + θ-term Fukuma,Kanamori,YN,..., finite density QCD)
- Apply WV-HMC to real-time system
  $\leftarrow$ Real-time system has a sign problem due to $\exp(iS) \in \mathbb{C}$.

Appendix