The Worldvolume Hybrid Monte Carlo method : A versatile solution to the sign problem and its application to lattice gauge theories

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Based on work with

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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

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

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

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

Boltzmann weight

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

highly oscillatory

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

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

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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!**

Example : Gaussian

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

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

large β mimics large DOF

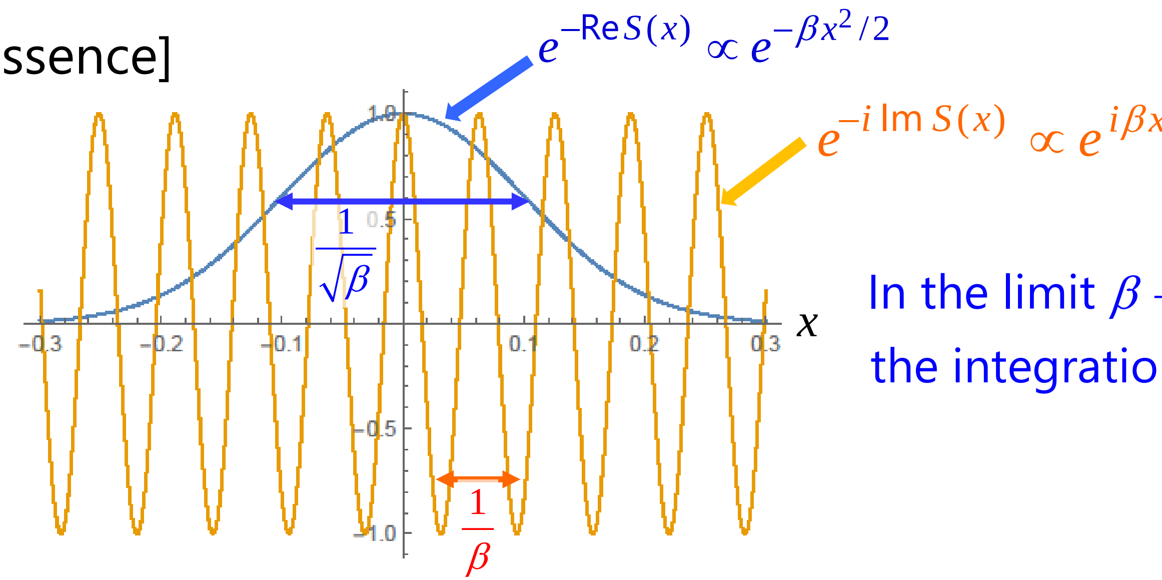
$$\Rightarrow \quad \langle x^2\rangle = \frac{\langle e^{-i\mathrm{Im}S(x)}\,x^2\rangle_{\text{rewt}}}{\langle e^{-i\mathrm{Im}S(x)}\rangle_{\text{rewt}}} = \frac{\left(\beta^{-1}-1\right)e^{-\beta/2}}{e^{-\beta/2}}$$

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

$\Rightarrow$ 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

Sign problem: 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] [Aarts et al. 2010, …] [Nagata-Nishimura-Shimasaki 2016]
- Lefschetz thimble method
  - Original **(LT)** [Witten 2010] [Cristoforetti et al. 2012, Fujii et al. 2013] (Komaba group)
  - 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:

- 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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   5-2. Chiral random matrix model [MF-Matsumoto 2020]
   5-3. **Hubbard model** [MF-Namekawa 2507.23748, 2508.02659, in prep]
   5-4. **Group manifolds** [MF 2506.12002]
   5-5. Real-time dynamics [MF+, ongoing]
6. Summary and outlook

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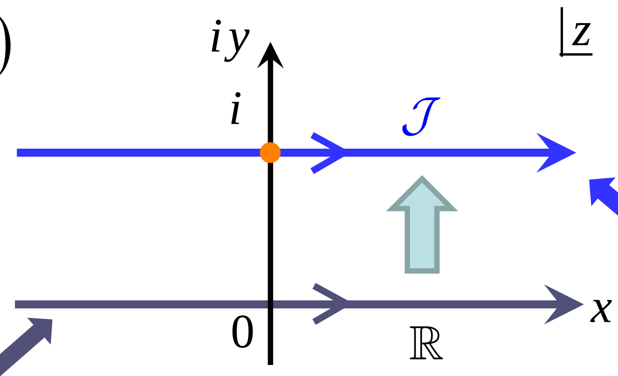
Warm-up: Gaussian (revisited)

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



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

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)

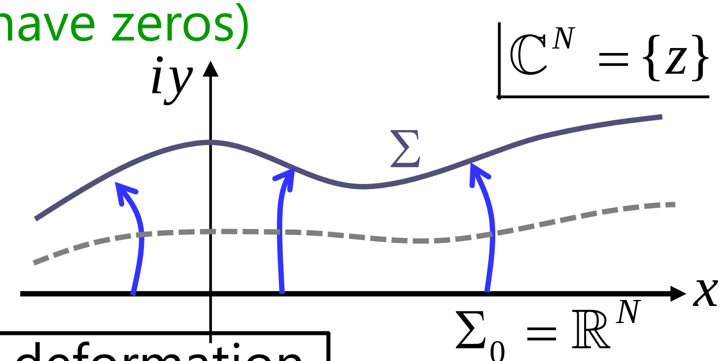
$\mathrm{Im}\, S(z)$: const $(=0)$ on $\mathcal{J}$

Basic idea of the thimble method (1/2)

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

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

(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

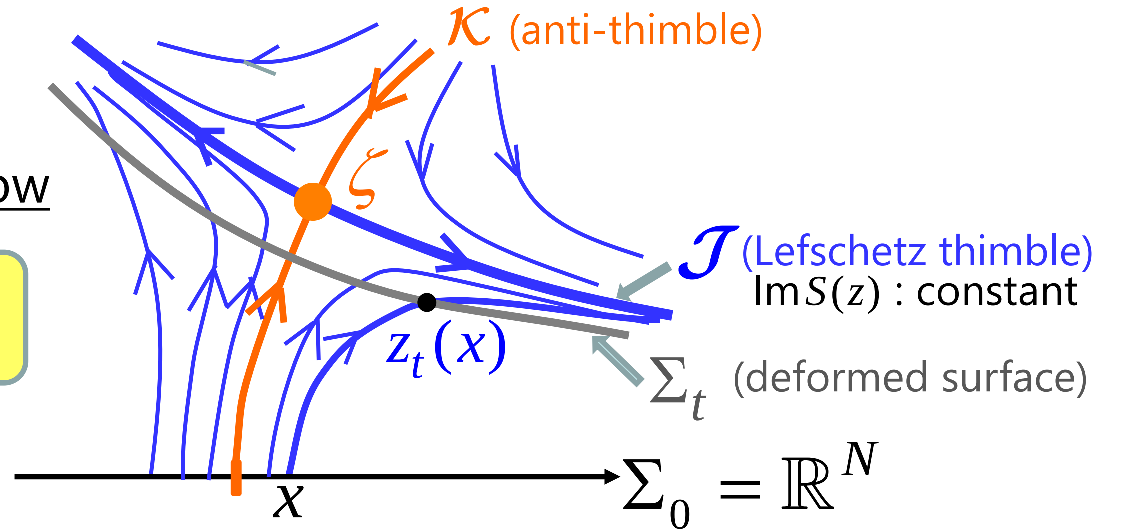
sign problem will be significantly reduced if $\mathrm{Im}\, S(z)$ is almost constant on Σ

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

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

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

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

Ergodicity problem in thimble-based methods

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

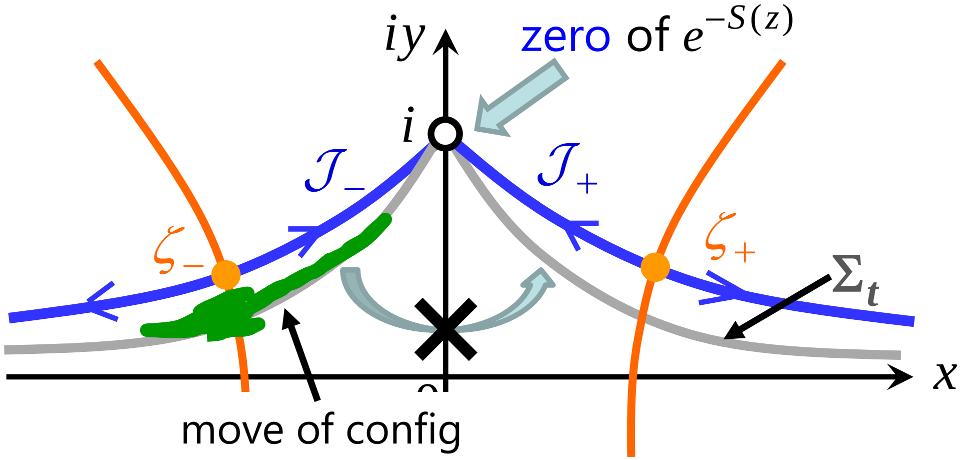
NO!

Ergodicity problem in thimble-based methods

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



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

$\oplus$

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

zero at $z_* = i$ ⇔ $\mathrm{Re}\, S(z) = +\infty$ at $z_* = i$
⇔ [∞ potential barrier on Σ_T] ⇔ configs cannot move

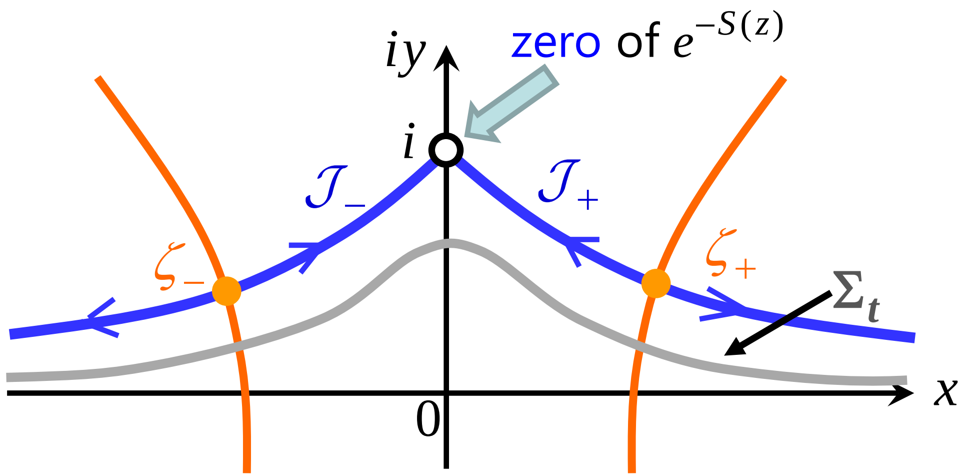
Generalized thimble method

[Alexandru et al. 1512.08764]

Idea

Take a flow time t,

which is $\begin{cases} \text{sufficiently large to mitigiate oscillatory behaviors} \\ \text{not too large so as to avoid ergodicity issues} \end{cases}$



However,

A closer investigation shows that the oscillatory behavior is reduced only after the deformed surface reaches a zero of $e^{-S(z)}$

[MF-Matsumoto-Umeda 2019]

solution : $\boxed{\textbf{Tempered Lefschetz thimble method}}$

[MF-Umeda 2017]

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Tempered Lefschetz thimble method

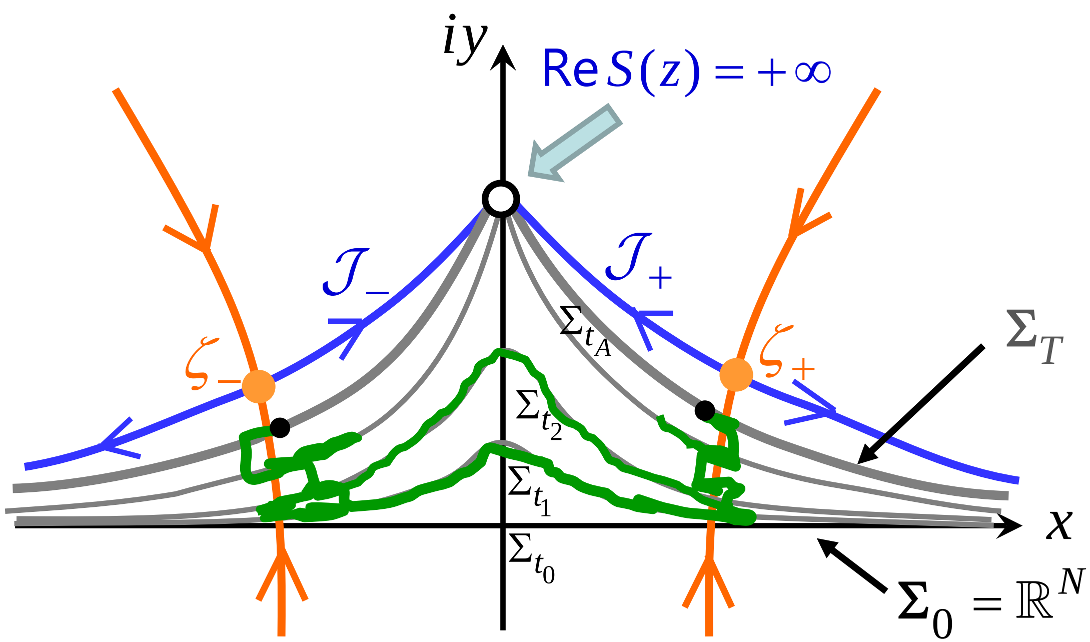
[Fukuma-Umeda 1703.00861]

■ 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 using the subsample on Σ_T

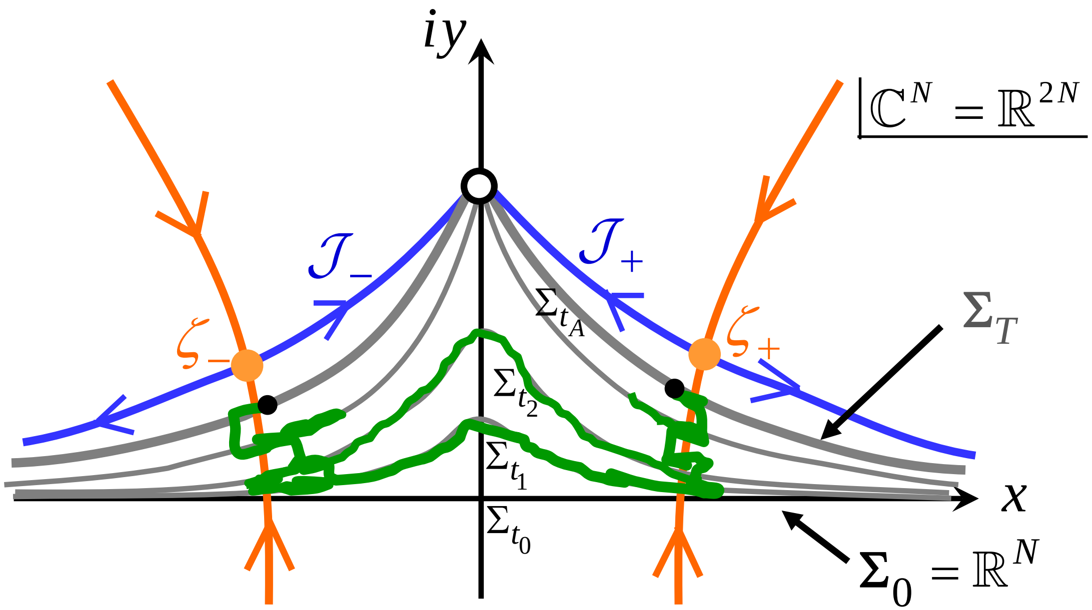


Sign and ergodicity problems are solved simultaneously !

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

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

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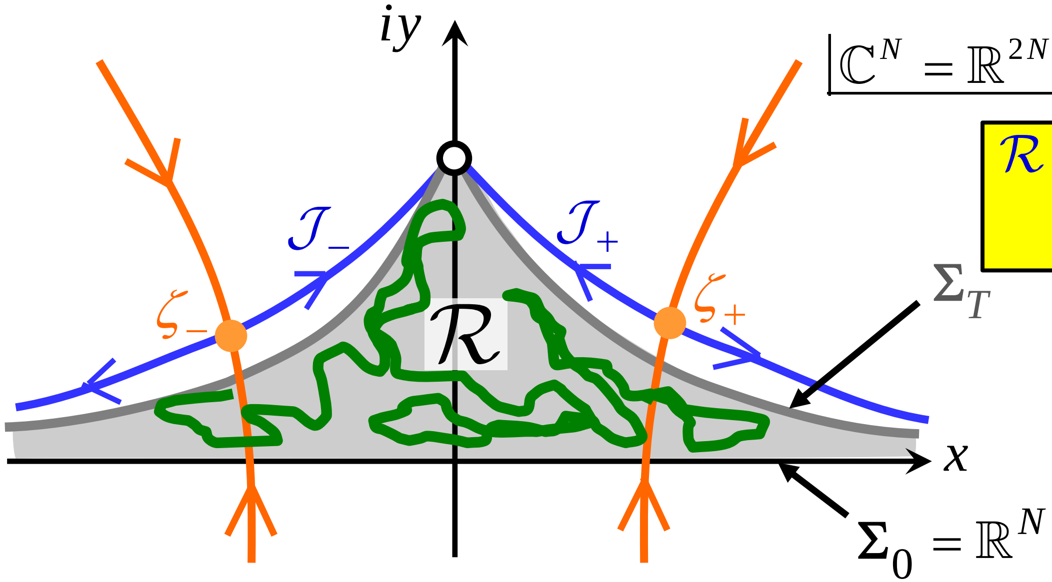
Worldvolume HMC (1/3)

[MF-Matsumoto 2012.08468]

■ Worldvolume Hybrid Monte Carlo (WV-HMC)

HMC on a continuous union of deformed 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 $\rightarrow$ worldline
orbit of string $\rightarrow$ worldsurface
orbit of surface (membrane) $\rightarrow$ worldvolume

Pros : 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 (2/3)

[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

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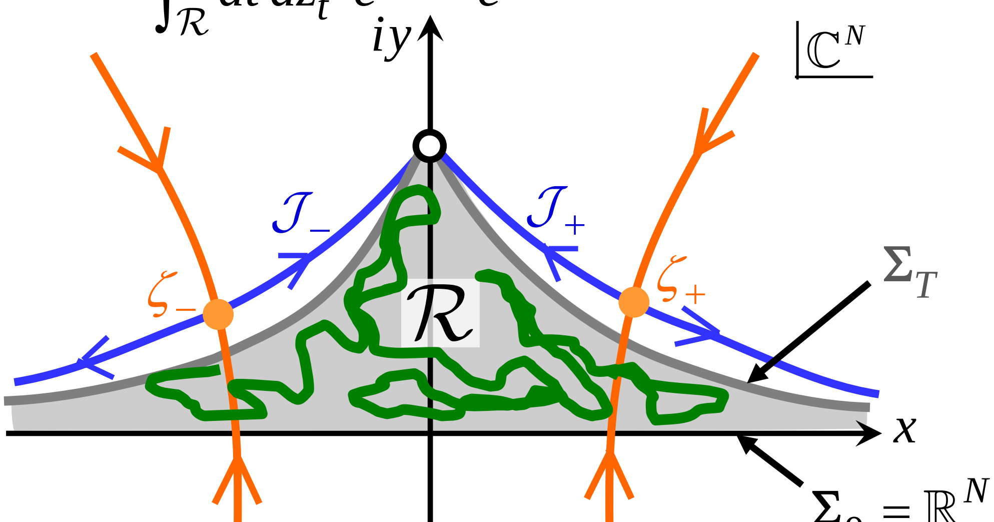
$$= \frac{\int_0^T dt\, e^{-W(t)} \int_{\Sigma_t} dz_t\, e^{-S(z_t)}\, \mathcal{O}(z_t)}{\int_0^T dt\, e^{-W(t)} \int_{\Sigma_t} dz_t\, e^{-S(z_t)}}$$

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

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

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

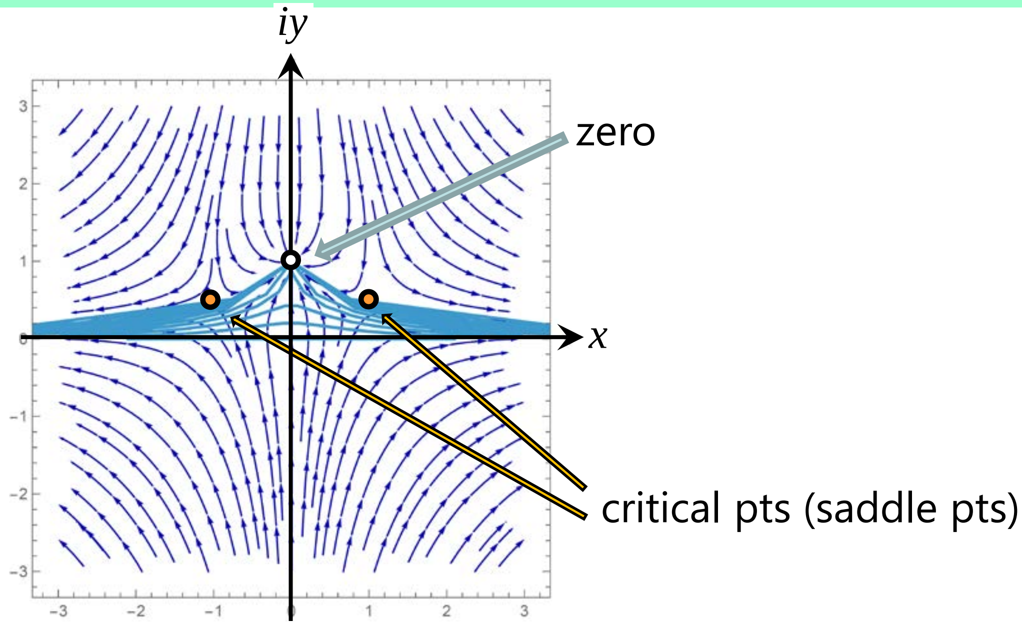
$\Leftarrow$ path integral over the worldvolume $\mathcal{R}$

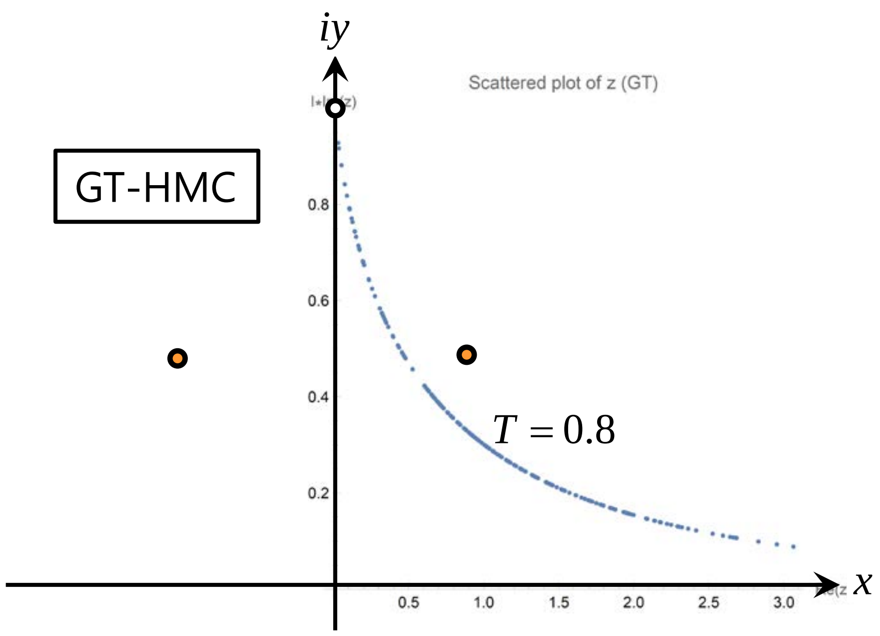


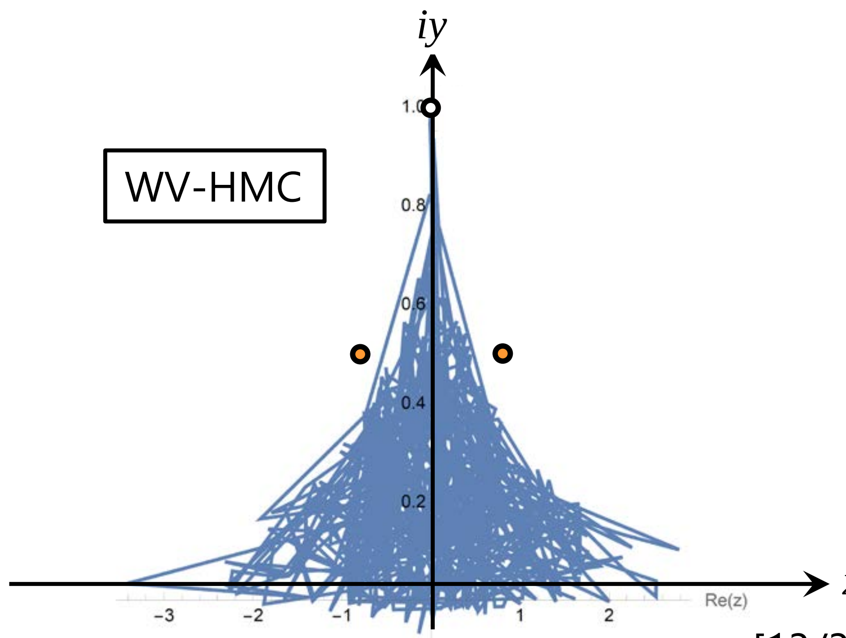
Statistical analysis method for the WV-HMC is established in **[MF-Matsumoto-Namekawa 2107.06858]**

■ Example: 1DOF

$$e^{-S(z)} = e^{-z^2/2}(z-i)$$







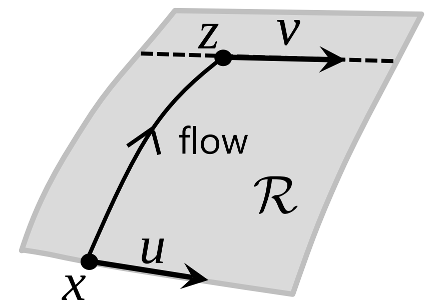
Expected computational cost of WV-HMC

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

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 $\dot{z}_i = \overline{\partial_i S(z)} \Rightarrow O(N)$ [when $\partial_i S(z)$ is known (local field case)]
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)]



expected computational cost :

no fermion determinants : $O(N)$

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

Plan

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   5-1. Complex scalar at finite density **[MF-Namekawa Lattice2024]**
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   5-5. Real-time dynamics **[MF+, ongoing]**
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)**
[MF-Namekawa, 2507.23748, 2508.02659] **(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 prep]** **(WV-HMC)**

— **group manifolds** **[MF 2506.12002]** **(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

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

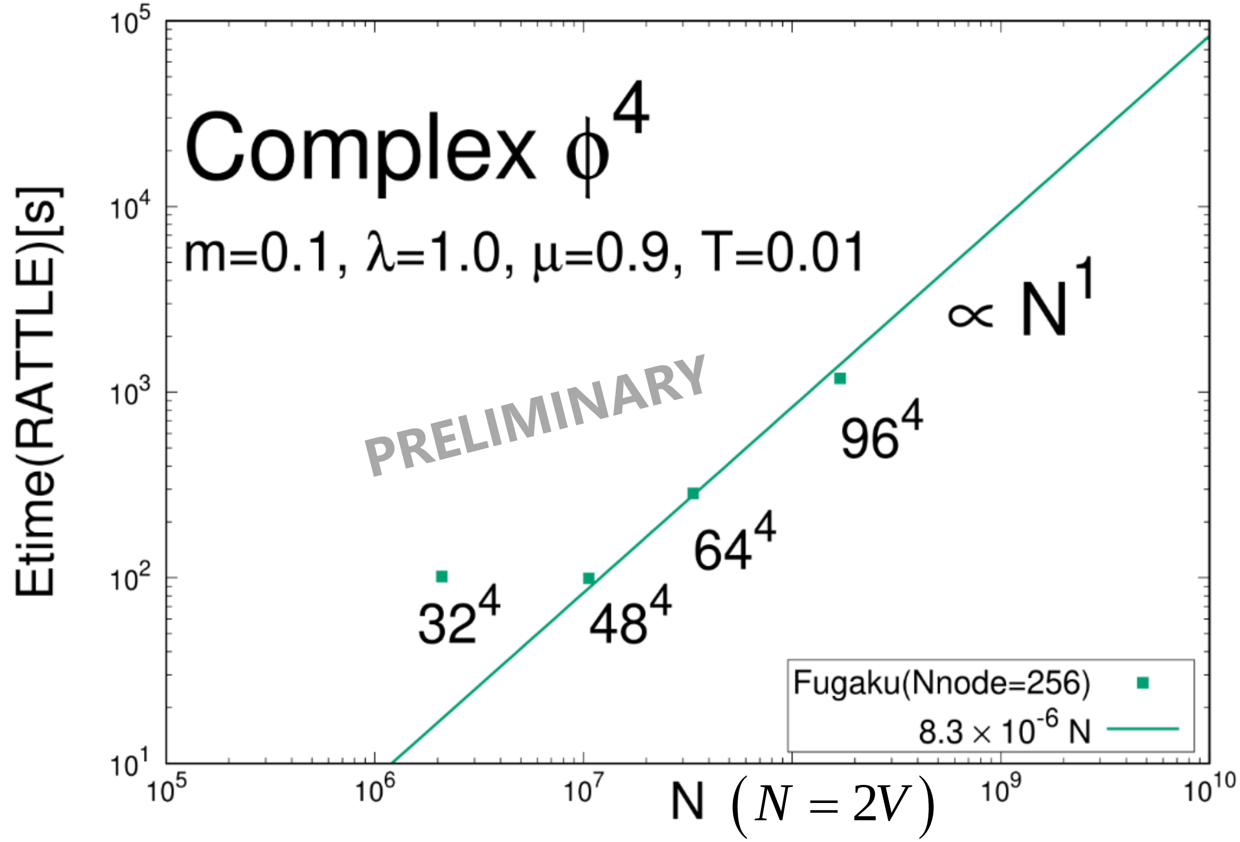
We complexify $(\xi, \eta) \in \mathbb{R}^{2V}$ to $(z, w) \in \mathbb{C}^{2V}$ with the flow equation

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

Finite-density complex scalar (2/3)

[MF-Namekawa Lattice2024]

■ 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

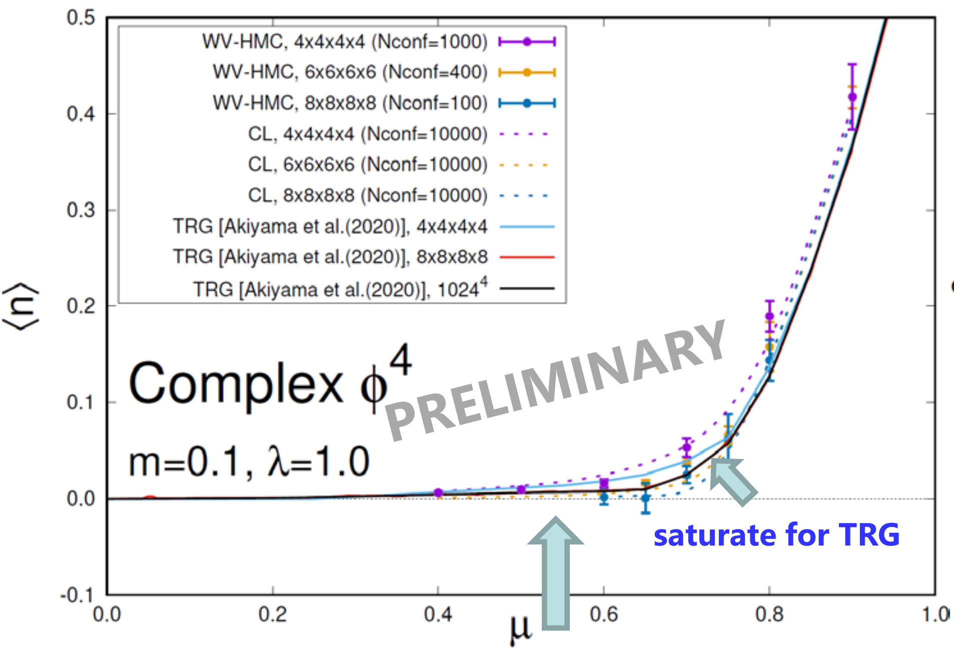
Finite-density complex scalar (3/3)

[MF-Namekawa Lattice2024]

■ 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)

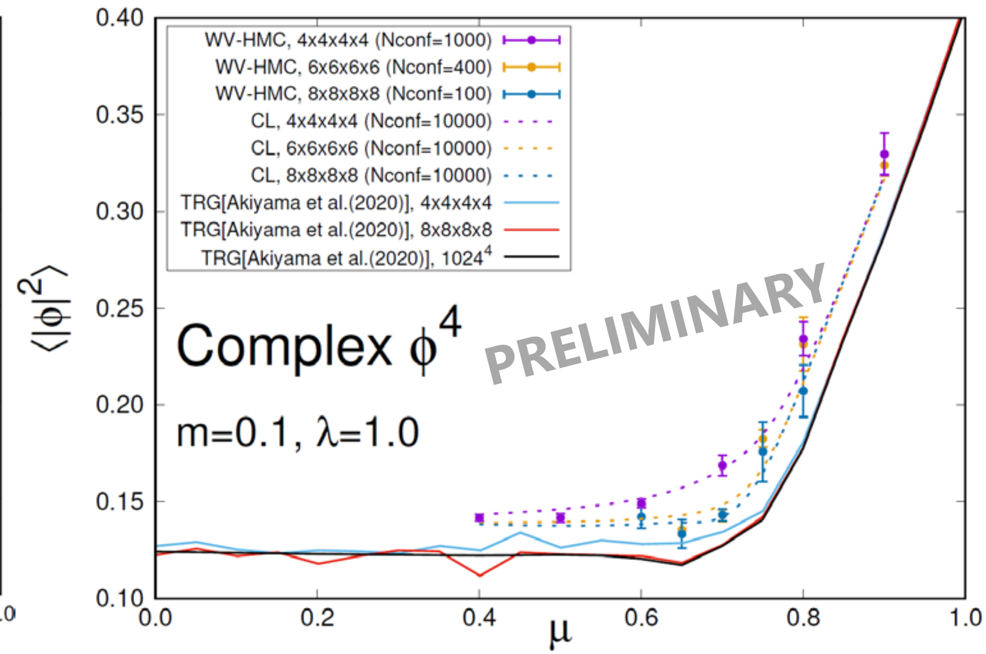
4D



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]

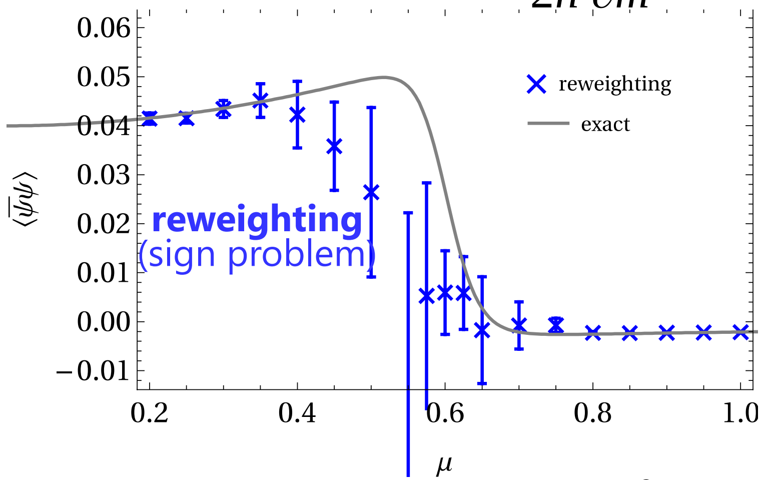
Chiral random matrix model (2/2)

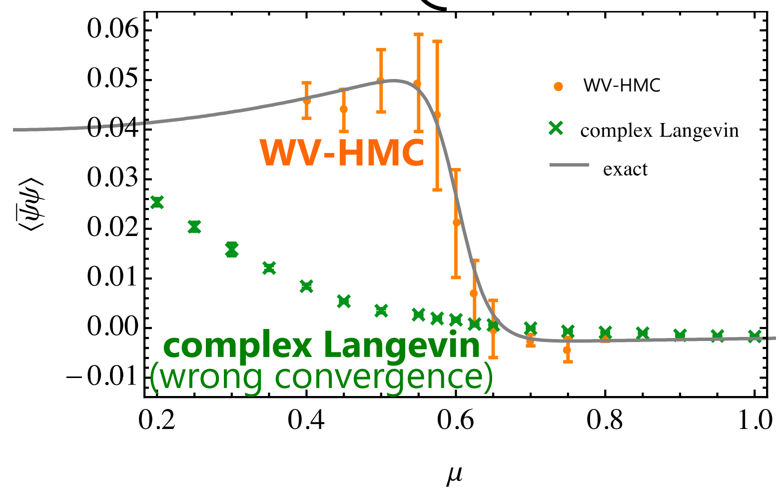
[MF-Matsumoto 2012.08468]

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

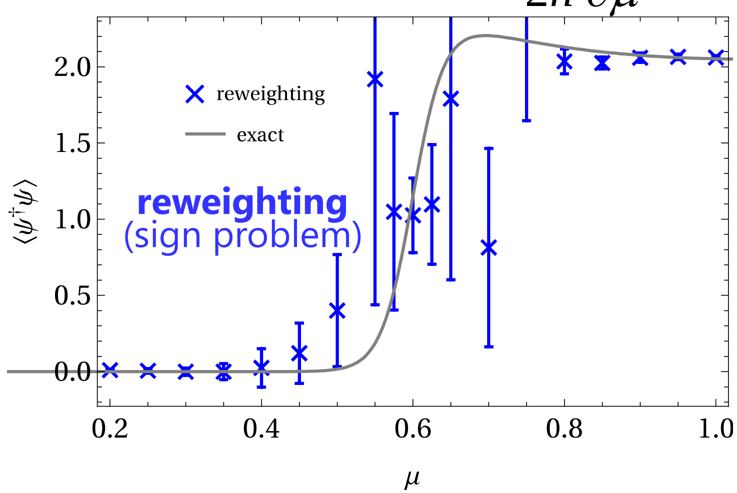
sample size
- reweighting : 10k
- complex Langevin :10k
- WV-HMC : 4k-17k

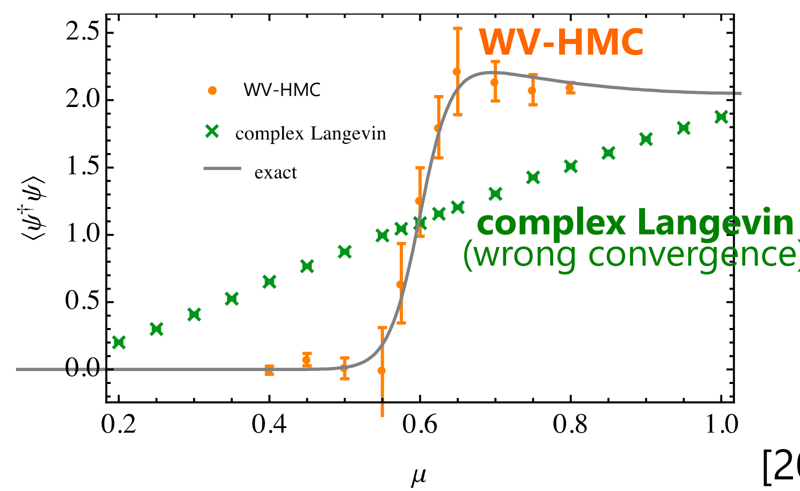
chiral condensate $\langle \bar{\psi}\psi \rangle \equiv \dfrac{1}{2n}\dfrac{\partial}{\partial m}\ln Z_{\text{Steph}}$ $[m = 0.004,\ T = 0]$





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





Plan

Hubbard model

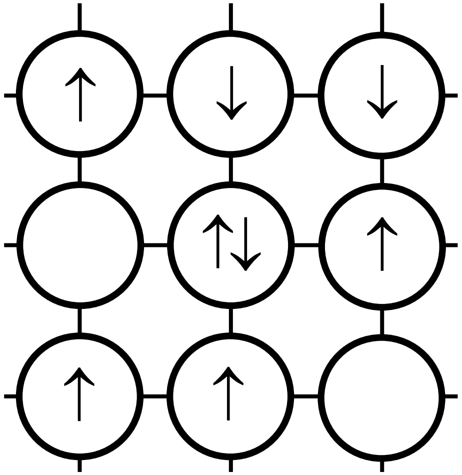
■ Hubbard model toy model of electrons in a solid **[Hubbard 1963]**

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

- Hamiltonian

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

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



$\left(N_s = L_s^d \text{ : \# of sites} \right)$

- particle-hole transformation :

$$a_{\mathbf{x}} \equiv c_{\mathbf{x},\uparrow},\quad b_{\mathbf{x}} \equiv (-1)^{\mathbf{x}} c^\dagger_{\mathbf{x},\downarrow}$$

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

- half filling :

$$\tilde{\mu} = 0 \iff \frac{1}{N_s} \sum_{\mathbf{x}} \langle n^a_{\mathbf{x}} - n^b_{\mathbf{x}} \rangle = 0 \iff \frac{1}{N_s} \sum_{\mathbf{x}} \langle n_{\mathbf{x},\uparrow} + n_{\mathbf{x},\downarrow} \rangle = 1$$

Quantum Monte Carlo computations

[MF-Namekawa 2507.23748, 2508.02659]

- discretize the imaginary time direction : $\beta = N_t \epsilon$

⇨ Trotter decomposition + bosonization (HS transformation)

- 【trick】introduce a nonphysical redundant parameter α : [Beyl et al. 2018]

$$\left(n_{\mathbf{x}}^a - n_{\mathbf{x}}^b\right)^2 = \alpha \underbrace{\left(n_{\mathbf{x}}^a - n_{\mathbf{x}}^b\right)^2}_{\text{HS field } A} - (1-\alpha) \underbrace{\left(n_{\mathbf{x}}^a + n_{\mathbf{x}}^b - 1\right)^2}_{\text{HS field } B} + 1 - \alpha \quad \left(\text{NB}: \ (n_{\mathbf{x}})^2 = n_{\mathbf{x}}\right)$$

⇨

$$\boxed{\begin{aligned} Z &= \mathrm{tr}\,(e^{-\epsilon H})^{N_t} = \mathrm{tr} \prod_{\ell=1}^{N_t} e^{-\epsilon H} \\ &= \int dA\, dB\, e^{-\sum_x (1/2)(A_x^2 + B_x^2)} \det D_a(A,B) \det D_b(A,B) \\ \left(D_{a/b}\psi\right)_x &= e^{\pm(\epsilon\tilde{\mu} + i c_0) A_x + c_1 B_x - c_1^2} \psi_x - \psi_{x-0} + \epsilon\kappa \sum_{i=1}^{d} \left(\psi_{x+i} + \psi_{x-i}\right) \end{aligned}}$$

$$x = (\ell, \mathbf{x}) \ \left(\ell = 1, \ldots, N_t\right), \quad c_0 = \sqrt{\alpha\epsilon U}, \quad c_1 = \sqrt{(1-\alpha)\epsilon U}$$

- choice of α :

$\exists$zeros of $\det D_{a/b}(A,B)$ on $\mathbb{R}^N$

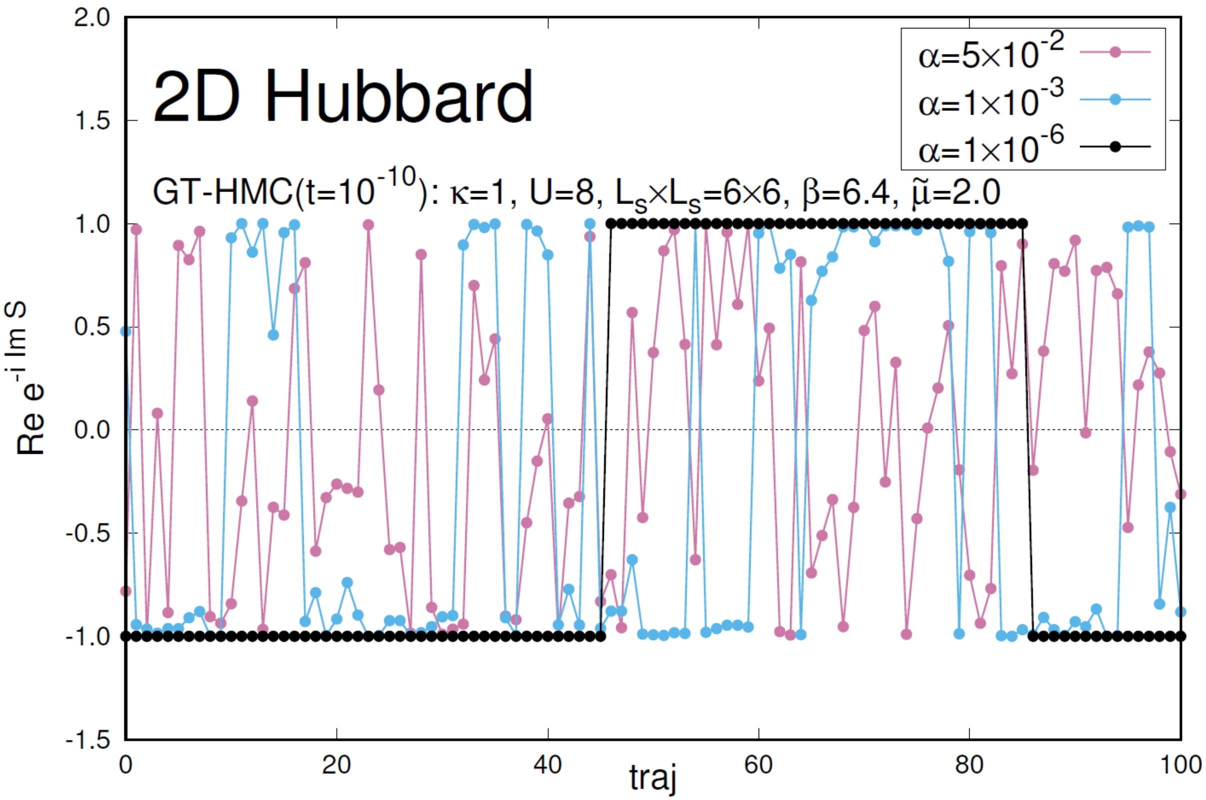
phase $\Rightarrow$ sign(± 1)

$$\begin{cases} \alpha = 0 \ (c_0 = 0) : \text{sign problem } \triangle, \ \text{ergodicity problem } \times \\ \alpha = 1 \ (c_1 = 0) : \text{sign problem } \times, \ \text{ergodicity problem } \bigcirc \end{cases}$$

⇨ optimal α

Tuning of α

[MF-Namekawa 2507.23748, 2508.02659]



[2507.23748] $\alpha = 1.0\times10^{-2}$ with $T_1 = 1.0\times10^{-1}$

[2508.02659] $\alpha = 5.0\times10^{-3}$ with $T_1 = 4.0\times10^{-3}$

⇨ worldvolume: very thin layer (confs can be trapped at corners)

⇨ ergodicity enhancement via embedding GT-HMC (以毒制毒)

How to deal with det$D$ in WV-HMC

[MF-Namekawa 2507.23748, 2508.02659, in prep]
[MF-Namekawa Lattice2024]

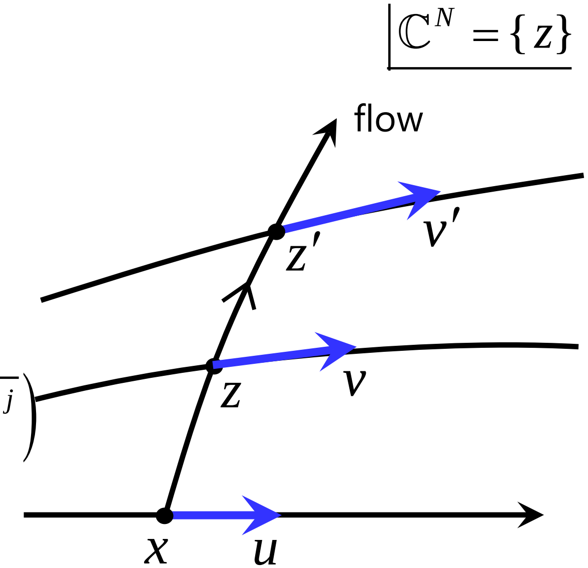
$$Z = \int dx d\bar{\psi} d\psi e^{-S_0(x) - \bar{\psi} D(x) \psi}$$
$$= \int dx\, e^{-S_0(x)} \det D(x) \qquad \left(x = (x_i) \;\Leftrightarrow\; \begin{Bmatrix} A = (A_x) \\ B = (B_x) \end{Bmatrix} \right)$$
$$\equiv \int dx\, e^{-S(x)} \quad \big(S(x) = S_0(x) - \log \det D(x) \big)$$

method 1 : treat x as the only dyn variable,
compute $D^{-1}(x)$ with direct solvers
[MF-Namekawa 2507.23748, 2508.02659]

main part
= integration of flow eqs : $\begin{cases} \dot{z} = \overline{\partial S(z)} & \left(\dot{z}^i = \overline{\partial_i S(z)} \right) \\ \dot{v} = \overline{\partial^2 S(z)\, v} & \left(\dot{v}^i = \overline{\partial_i \partial_j S(z)\, v^j} \right) \end{cases}$

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

sparse ⇧ ; direct method ⇧ ; direct method ⇧ ⇧



⇨ comput cost : $O(N^3)$

method 2 : use of real pseudofermions **[MF-Namekawa, in prep]**

⇨ comput cost : $O(N^2)$ $[O(N^1)?]$

Real pseudofermion

[MF-Namekawa Lattice2024]
[MF-Namekawa, in prep]

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

① $\boxed{M(x) \equiv D(x)\, D^T(x)}$ (complex symmetric matrix)

② If $\boxed{\begin{cases} 1)\ A > 0 \\ 2)\ \mathrm{Re}\left[\det{}^{1/2}(1 + iA^{-1}B)\right] > 0 \end{cases}}$ for $M^{-1} = A + iB$,

can be realilzed by tuning the redundant parameter α

then $\det D(x)$ can be rewritten to the form

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

(φ : <u>real</u> pseudofermion ("Majorana" pseudofermion))

③ path integral representation with dyn variable (x, φ) :

$$\boxed{\begin{aligned} & Z = \int dx d\varphi\, e^{-S_0(x) - (1/2)\varphi^T M^{-1}(x)\varphi} = \int dx d\varphi\, e^{-S(x,\varphi)} \\ & \text{with } S(x,\varphi) \equiv S_0(x) + \frac{1}{2}\varphi^T M^{-1}(x)\varphi \end{aligned}}$$

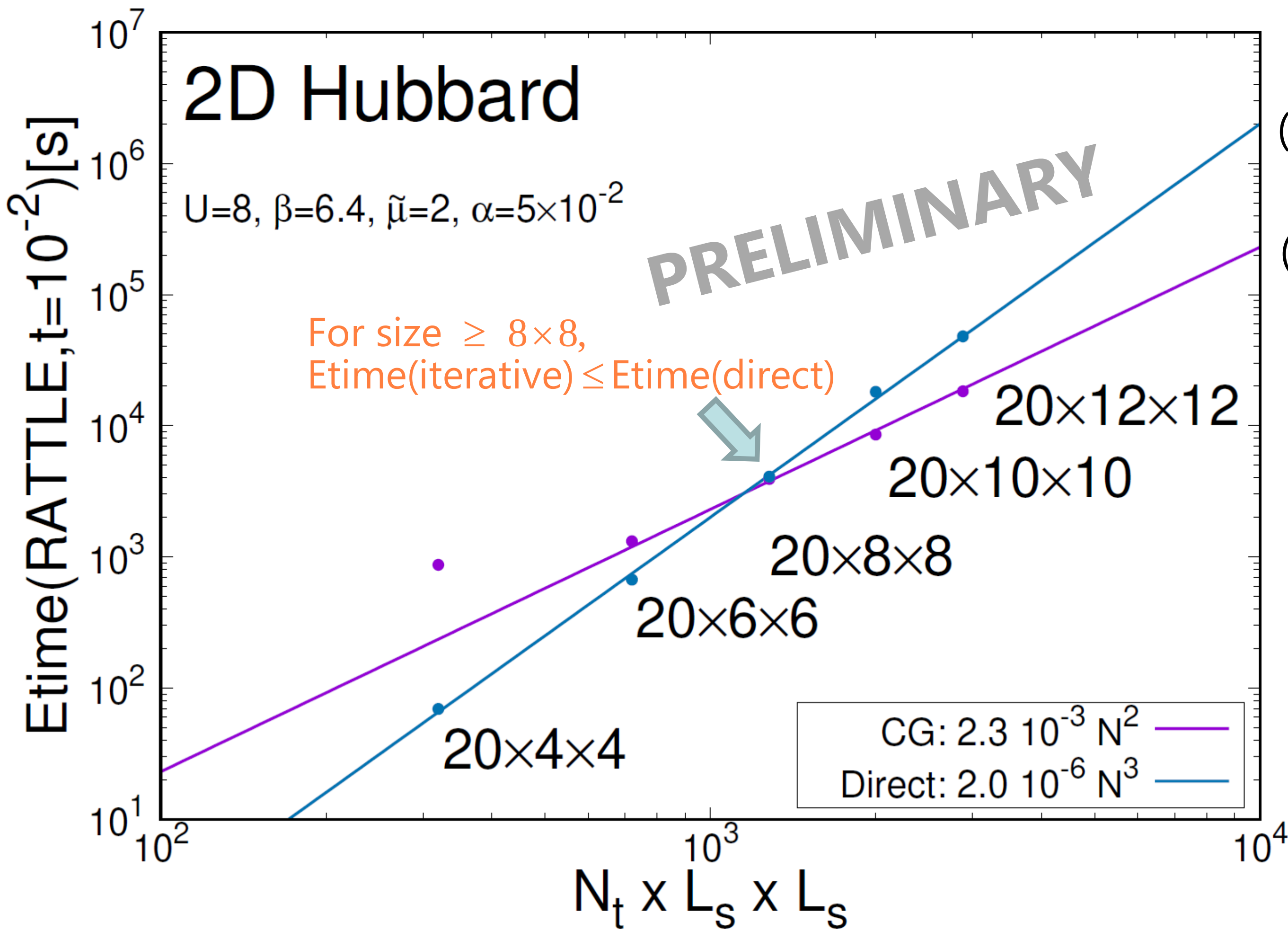
⇒ Monte Carlo

④ compute $M^{-1}(z)\varphi$ with iterative solvers ⇒ comput cost : $O(N^2)$ $[O(N^1)?]$

Computational cost scaling

[MF-Namekawa Lattice2024]

elapsed time for 1 MD trajectory with a single core (flow time : fixed)

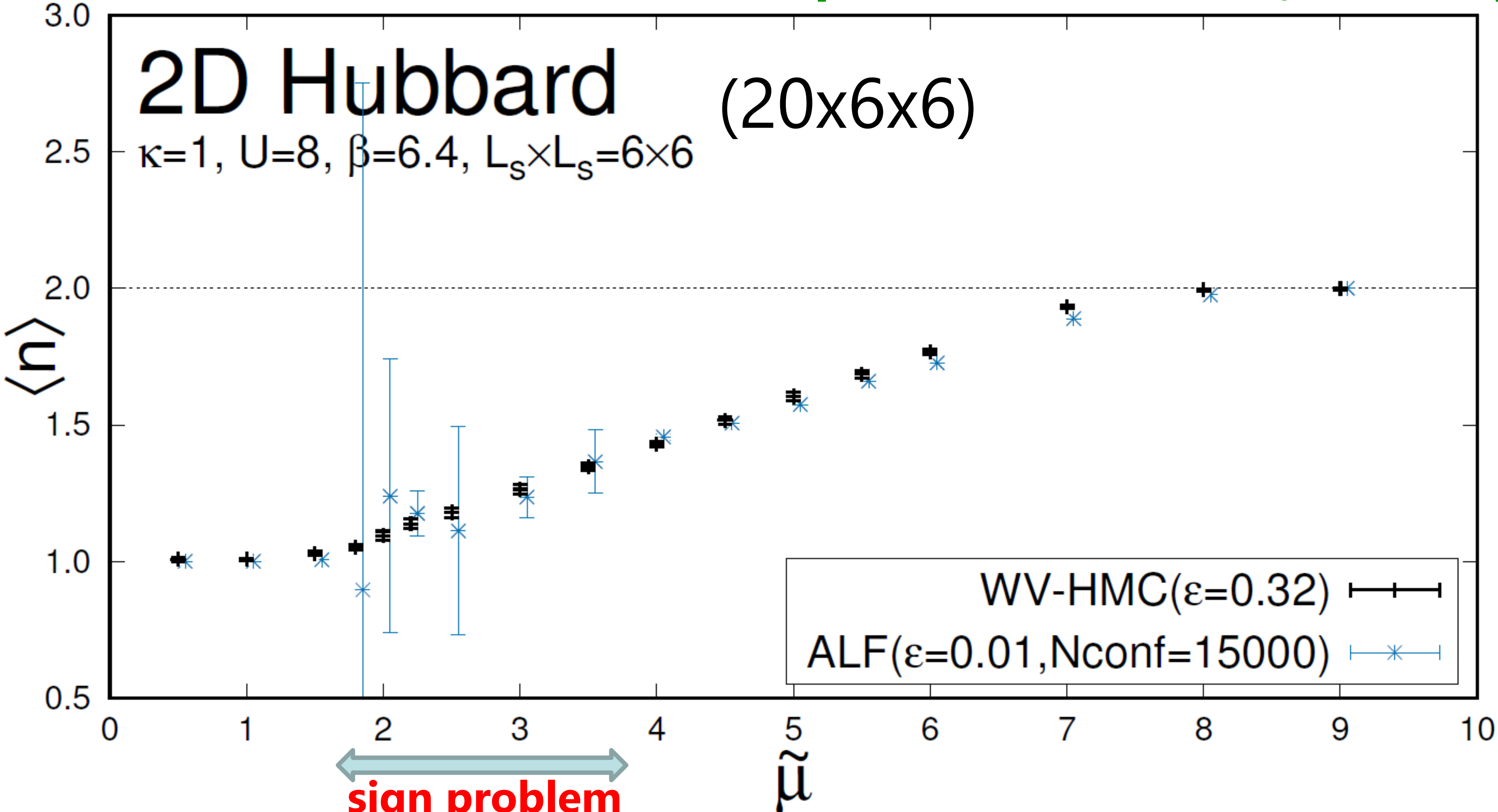


(1) direct solvers $\propto N^3$

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

N^3 algorithm: observables (2D : 6x6, near *T*=0)

[MF-Namekawa 2507.23748, 2508.02659]

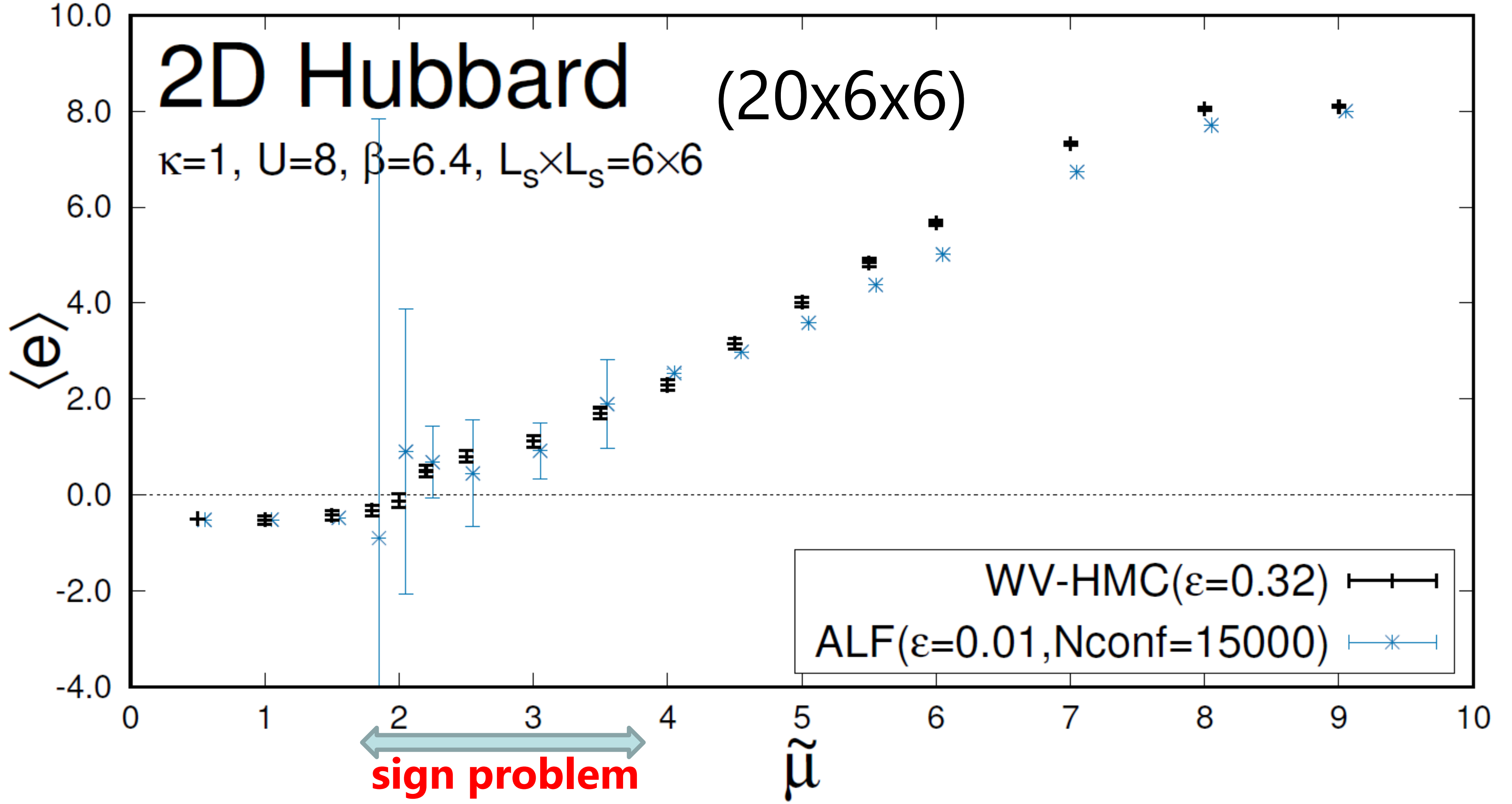


- ALF (well established MC code in cond - mat) **[Assaad et al.]**

- For such parameters where ALF does not work, WV - HMC does work with small statistical errors

N^3 algorithm: observables (2D : 6x6, near T=0)

[MF-Namekawa 2507.23748, 2508.02659]



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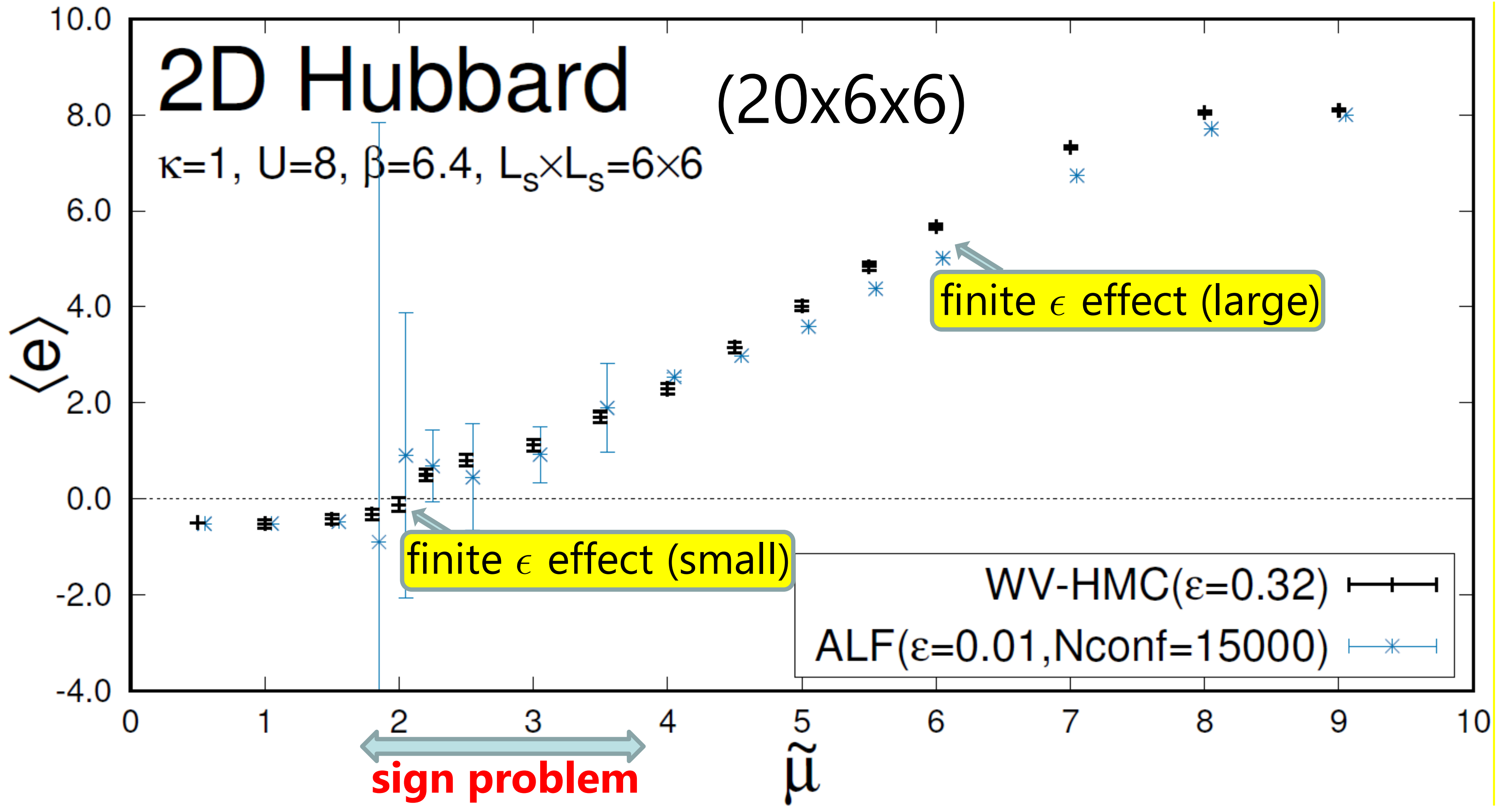

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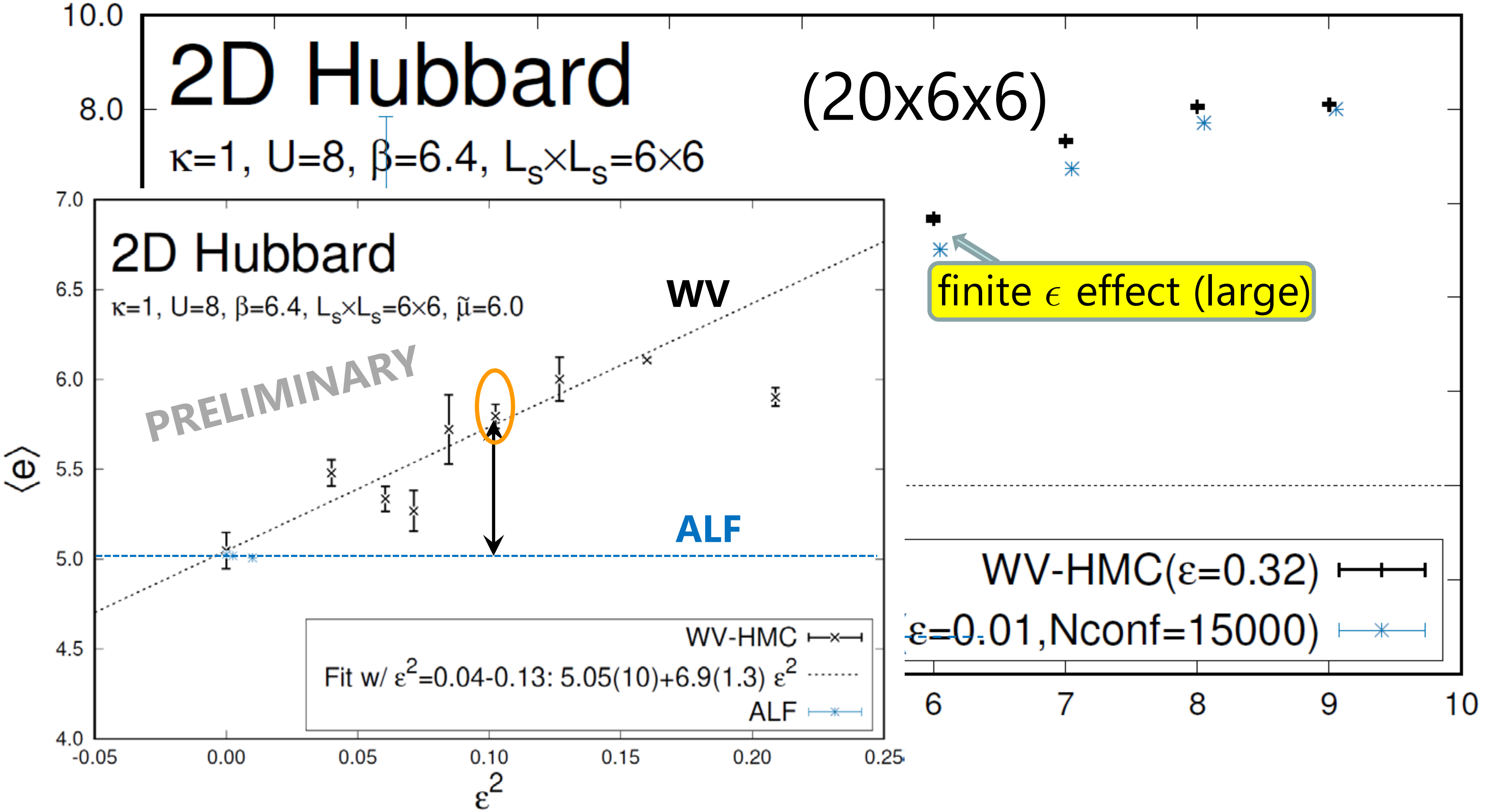

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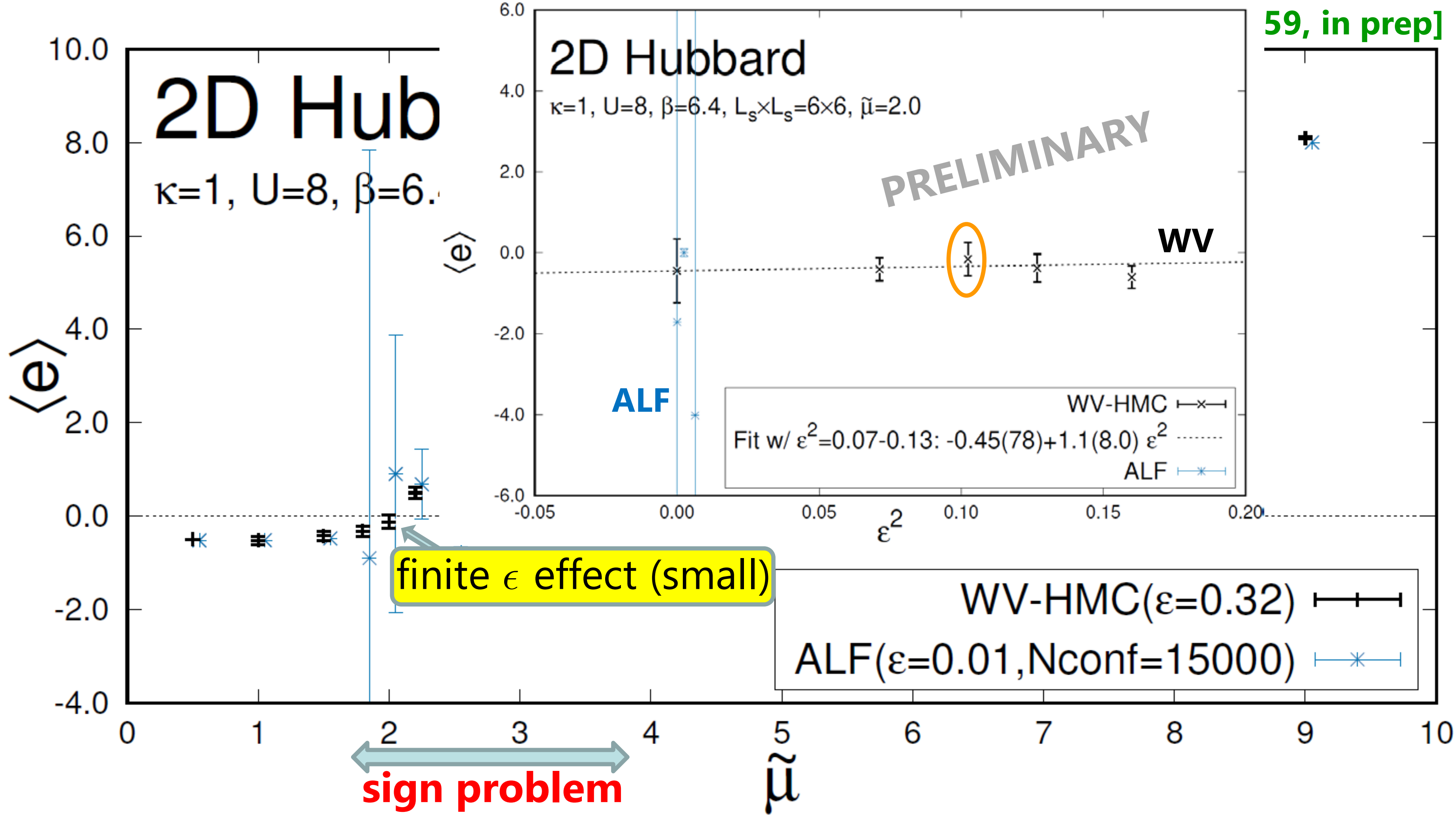

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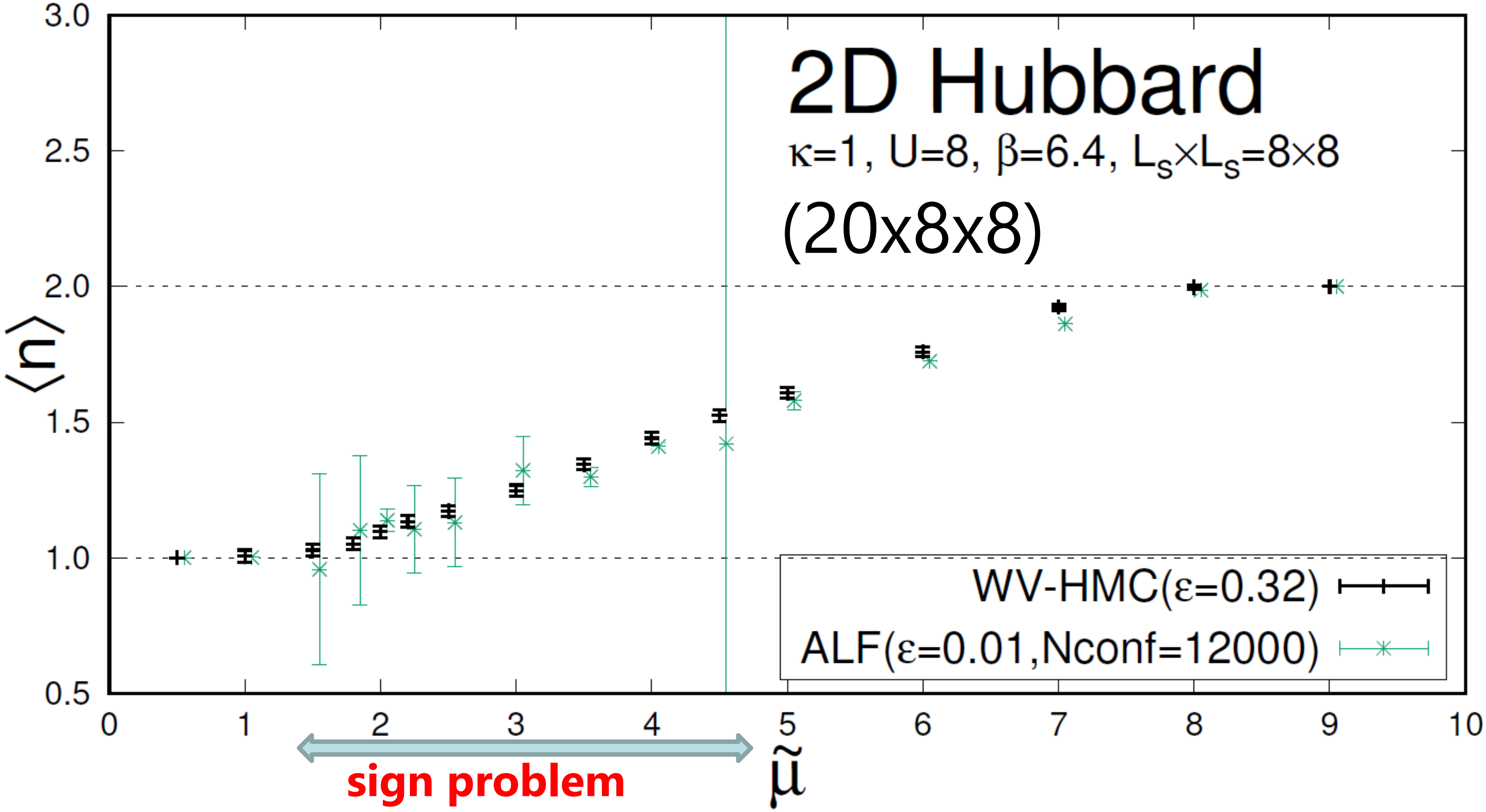
- For such parameters where ALF does not work, WV - HMC does work with small statistical errors

N^3 algorithm: observables (2D : 8x8, near *T*=0)

[MF-Namekawa 2507.23748, 2508.02659]



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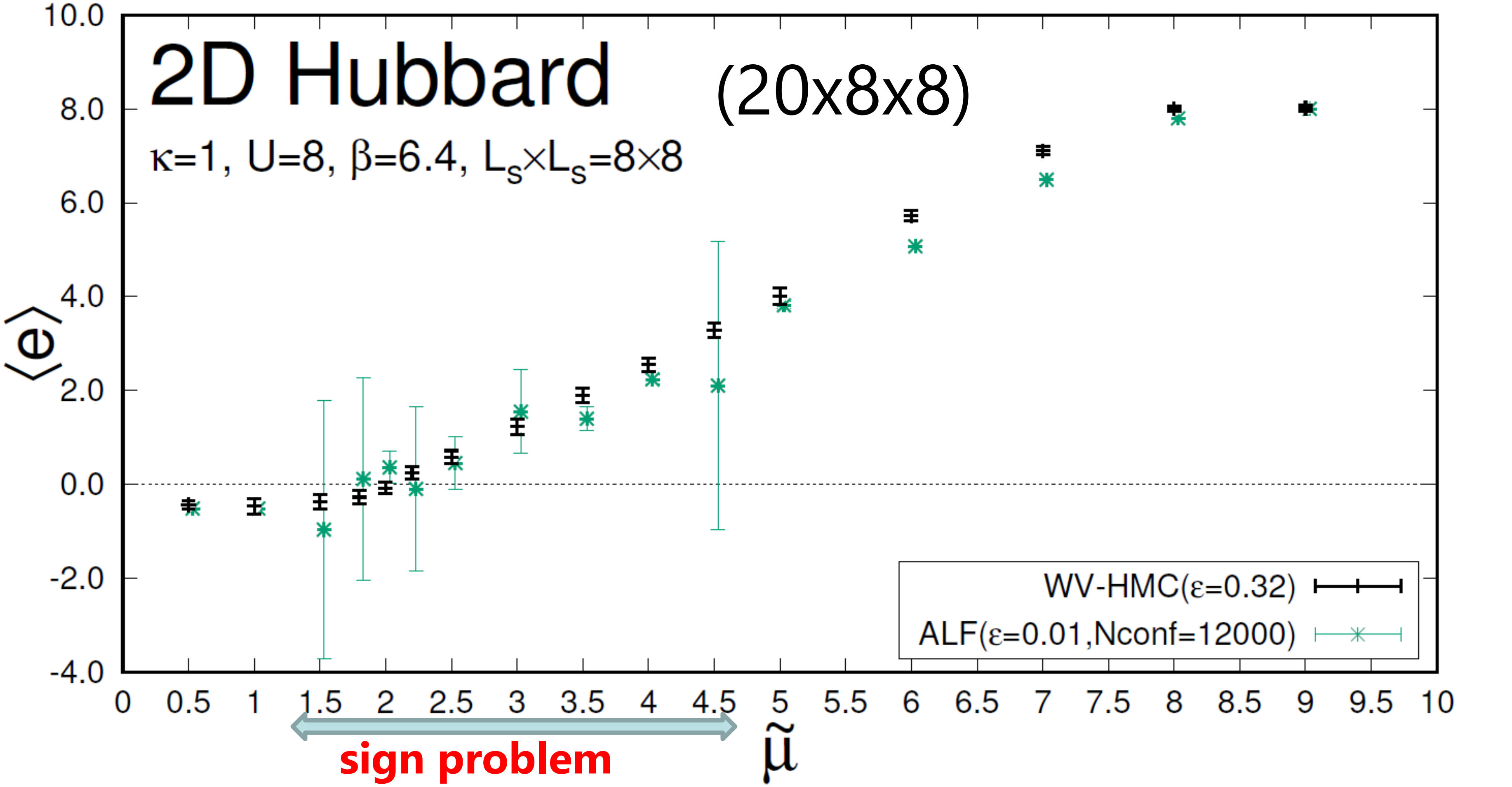
N^3 algorithm: observables (2D : 8x8, near *T*=0)

[MF-Namekawa 2507.23748, 2508.02659]



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Cauchy's theorem for group manifolds (1/2)

[MF 2506.12002]

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

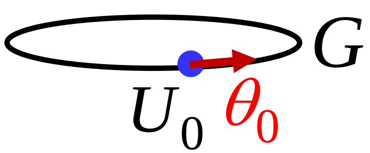
We want to evaluate the following path integral:

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

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



bi-invariant metric : $ds^2 = \mathrm{tr}\, \theta_0^\dagger \theta_0 = (\theta_0^a)^2$

⇨ θ_0^a : vielbein

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

Cauchy's theorem for group manifolds (2/2)

[MF 2506.12002]

$G^{\mathbb{C}}$: complexification of G

$$\left(\begin{array}{l} \text{Lie}G = \bigoplus_a \mathbb{R}\, T_a \quad \Rightarrow \quad (\text{Lie}G)^{\mathbb{C}} = \bigoplus_a \mathbb{C}\, T_a \\ G^{\mathbb{C}} \equiv \{ e^{Z} e^{Z'} \cdots e^{Z''} \mid Z, Z', \ldots, Z'' \in (\text{Lie}G)^{\mathbb{C}} \} \end{array} \right)$$

Cauchy's them for $G^{\mathbb{C}}$

The integral of a holomorphic function on a real N-dim submanifold Σ in $G^{\mathbb{C}}$

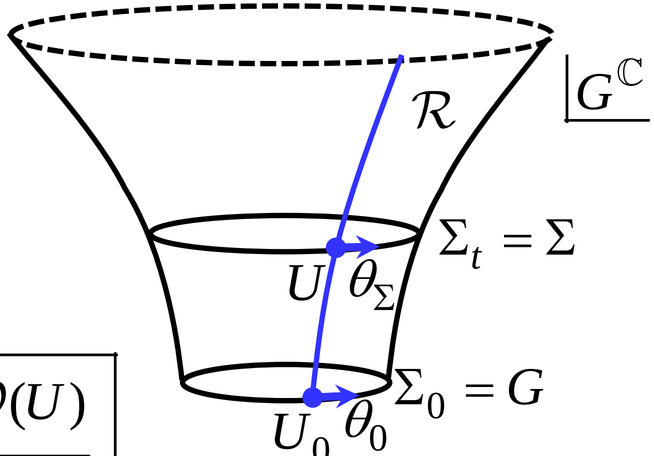
$$\int_\Sigma (dU)_\Sigma \, f(U)$$

does not change under continuous deformations of Σ

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

$$\theta_\Sigma \equiv dU\, U^{-1} = T_a\, \theta_\Sigma^a \quad \equiv T_a\, (E_b^a\, \theta_0^b) \quad (a, b = 1, \ldots, N)$$

$$(dU)_\Sigma \equiv \theta_\Sigma^1 \wedge \cdots \wedge \theta_\Sigma^N = \det E\, (dU_0) \quad \left(E = (E_b^a) \right)$$



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

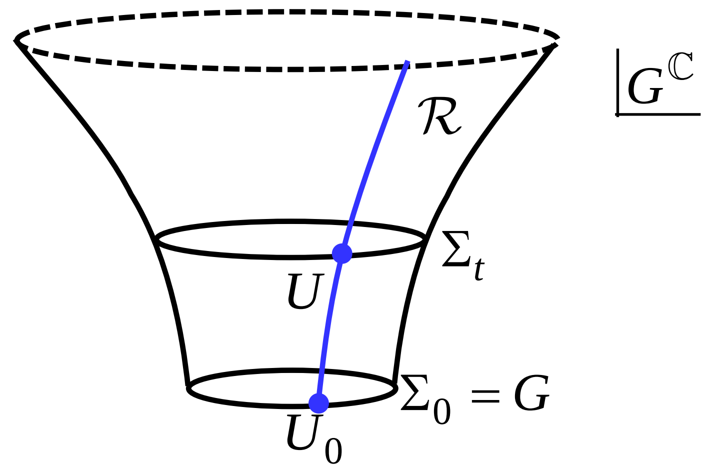
Path integral over the worldvolume

[MF 2506.12002]

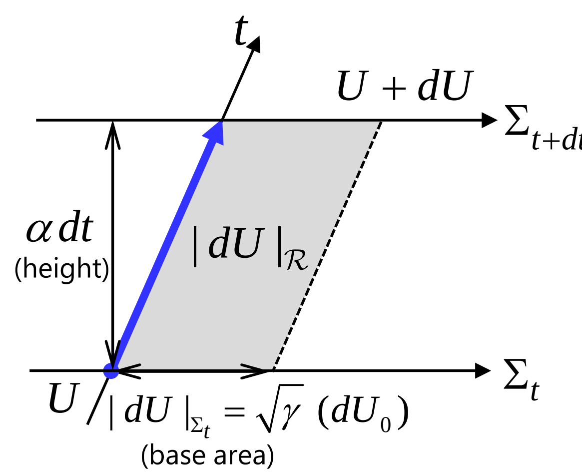
$$\langle \mathcal{O} \rangle = \frac{\int_{\Sigma_t} (dU)_{\Sigma_t}\; e^{-S(U)}\,\mathcal{O}(U)}{\int_{\Sigma_t} (dU)_{\Sigma_t}\; e^{-S(U)}}$$

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

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



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



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

⇓

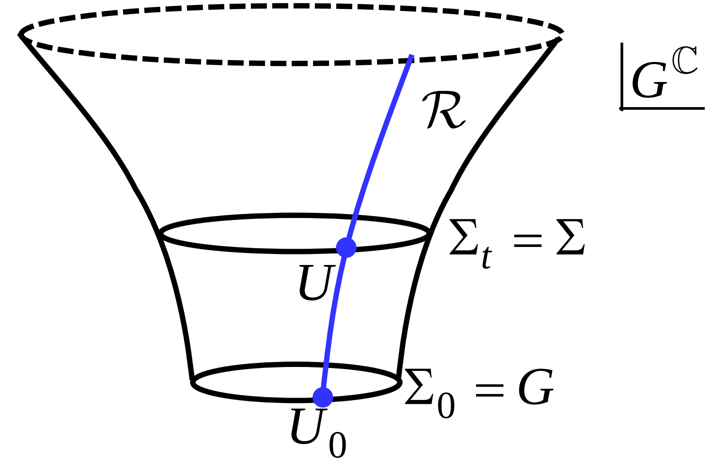
constrained molecular dynamics (RATTLE) on $\mathcal{R}$
can be introduced in a similar way to the flat case

one-site : SU(2) with a purely imag coupling

[MF 2506.12002]

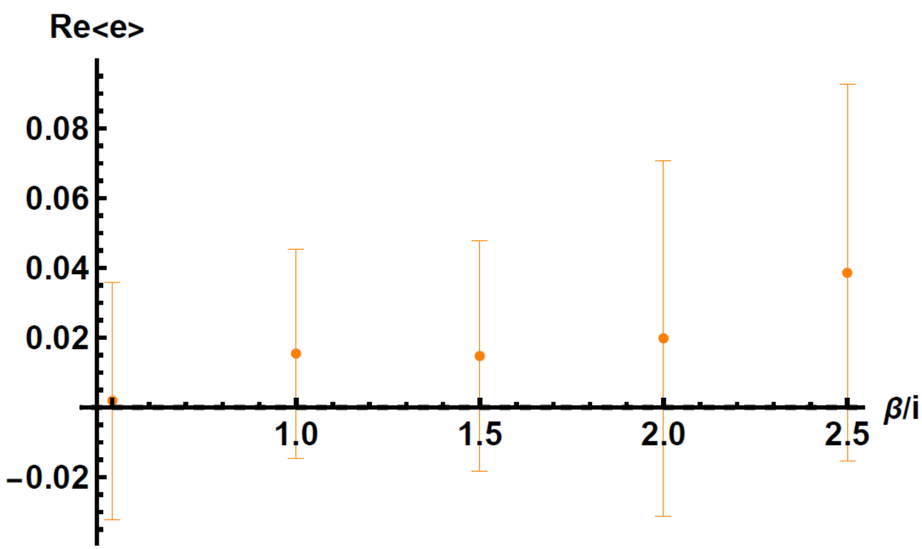
$\underline{G = SU(2)}$

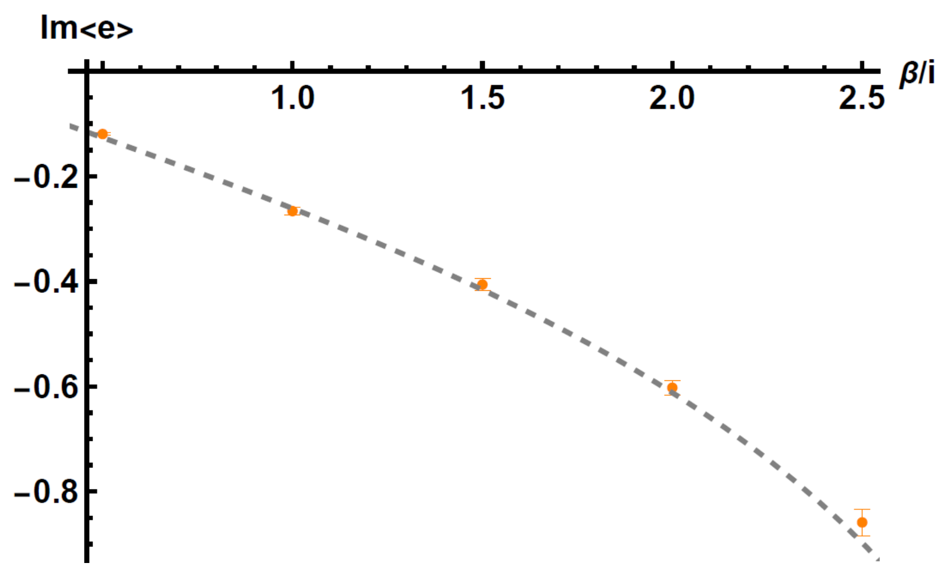
$$S(U) \equiv \beta\, e(U) \equiv -\frac{\beta}{4}\,\mathrm{tr}\left(U + U^{-1}\right) \quad (\beta \in i\,\mathbb{R})$$



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

numerical result (WV-HMC):



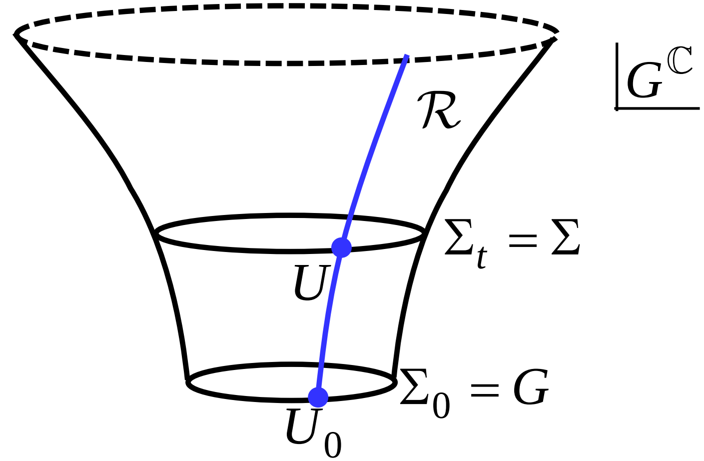


one-site : SU(3) with a purely imag coupling

[MF 2506.12002]

$G = SU(3)$

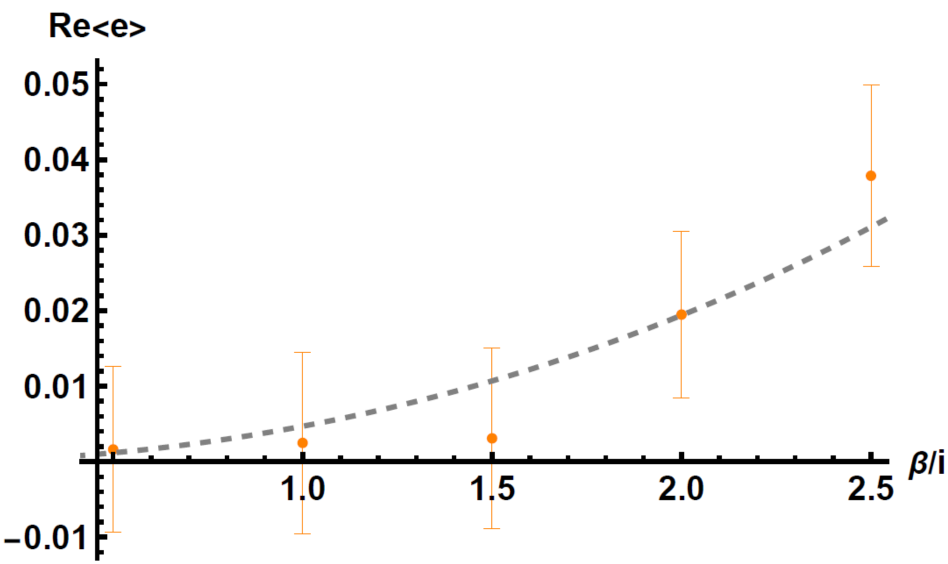
$$S(U) \equiv \beta\, e(U) \equiv -\frac{\beta}{4}\,\mathrm{tr}\left(U + U^{-1}\right) \quad \left(\beta \in i\,\mathbb{R}\right)$$

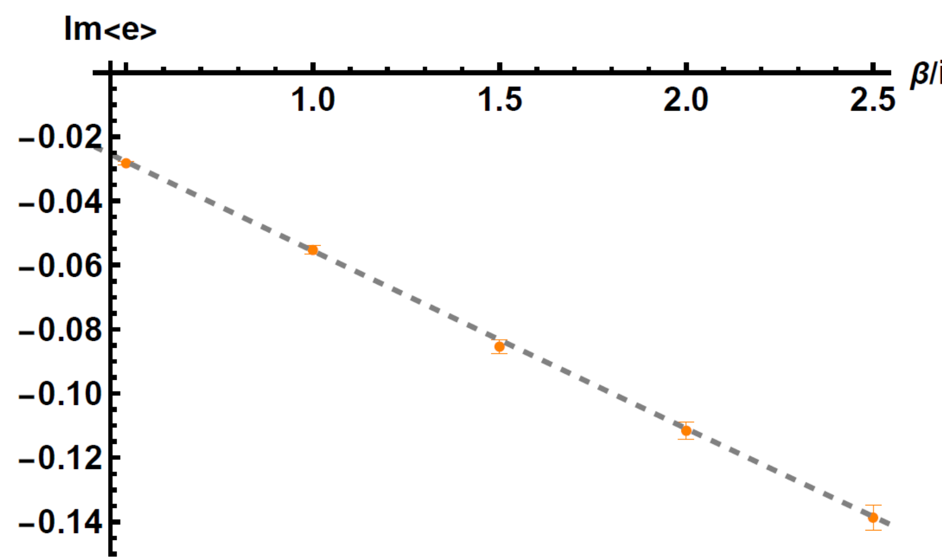


analytic result: $$Z(\beta) = \sum_{q \in Z} \det\left[I_{q+j-i}(\beta/3) \right]$$

$$\langle e \rangle = -\frac{\partial}{\partial \beta} \ln Z(\beta)$$

numerical result (WV-HMC):



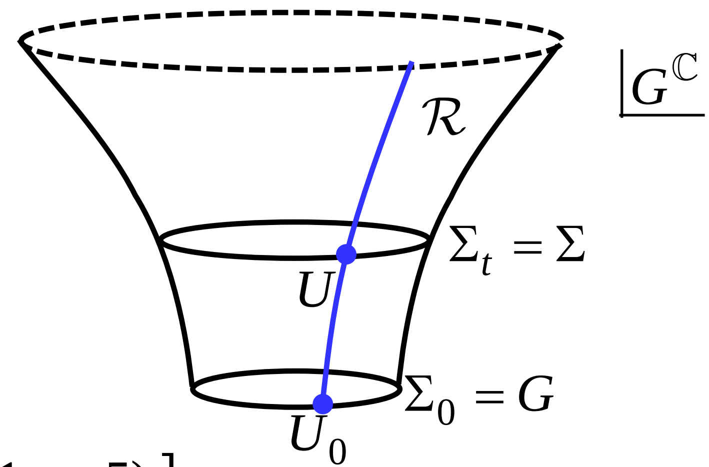


one-site : U(2) with a topological term

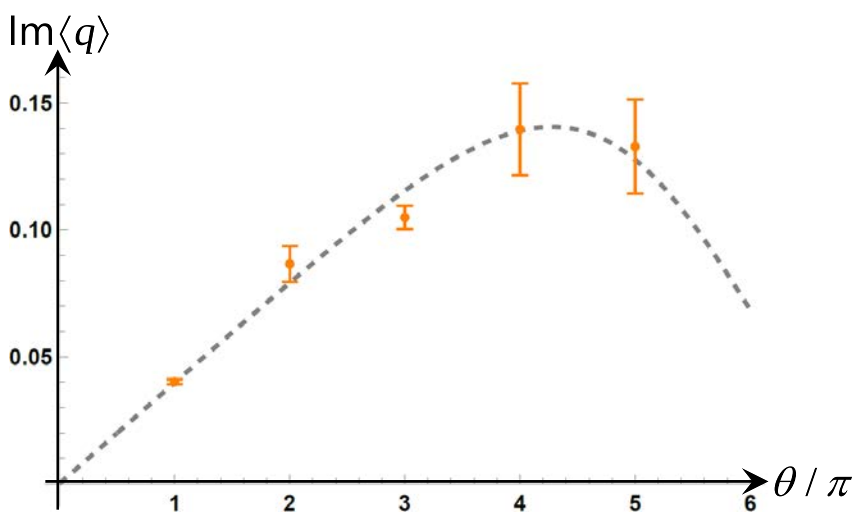
[MF, Lattice2024]

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

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



<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 Lattice2024]**
   5-2. Chiral random matrix model **[MF-Matsumoto 2020]**
   5-3. **Hubbard model** **[MF-Namekawa 2507.23748, 2508.02659, in prep]**
   5-4. **Group manifolds** **[MF 2506.12002]**
   5-5. Real-time dynamics **[MF+, ongoing]**
6. Summary and outlook

Summary and outlook

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

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

$$H' = H + O(\Delta s^3)$$

■ **Outlook**

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

local fields
(e.g. complex scalars)

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

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

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

→ finite-density QCD
(w/ or w/o θ)
[MF, MF+, 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.