Sign problem and the Worldvolume HMC method II: various applications

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in collaboration with

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Introduction

Sign problem is an obstacle to 1st-principles calculations of important physics, such as finite density QCD

⇨ We utilize Wolrdvolume Hybrid Monte Carlo (WV-HMC) method

Fukuma,Matsumoto(2020),Fukuma,Matsumoto,YN(2021)

- Feature : WV-HMC solves the sign and the ergodicity problems simultaneously at low cost Talk by Masafumi Fukuma

[This talk] Fukuma and YN (in prep)

◇ No dynamical fermion case (Complex ϕ^4 theory at finite density)

◇ Dynamical fermion case (Hubbard model)

cf. full QCD = pure YM + dynamical fermions

WV-HMC algorithm (1 / 4)

Fukuma,Matsumoto(2020),Fukuma,Matsumoto,YN(2021)

WV-HMC = HMC on worldvolume $\mathcal{R}$, which is defined as follows

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

$x \in \mathbb{R}^N \to z(x,t) \in \mathbb{C}^N$

Cauchy's theorem

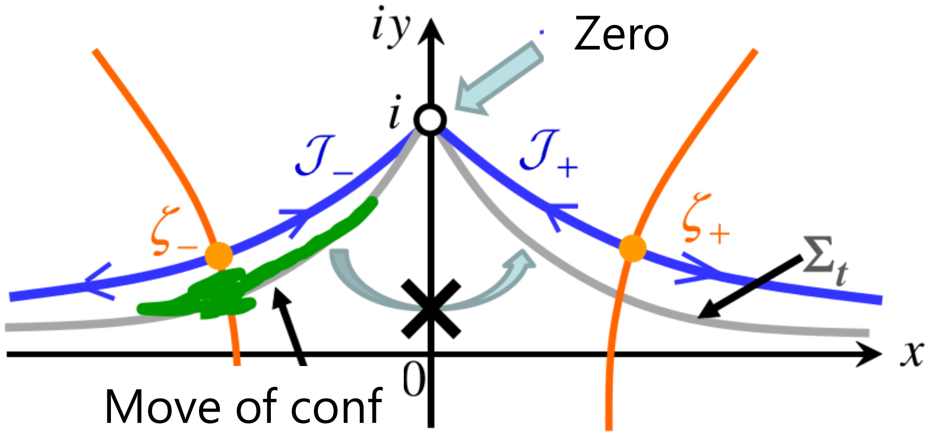
$$= \frac{\int_{\Sigma_t} dz\, \mathcal{O}\, e^{-S(z(x,t))}}{\int_{\Sigma_t} dz\, e^{-S(z(x,t))}}$$

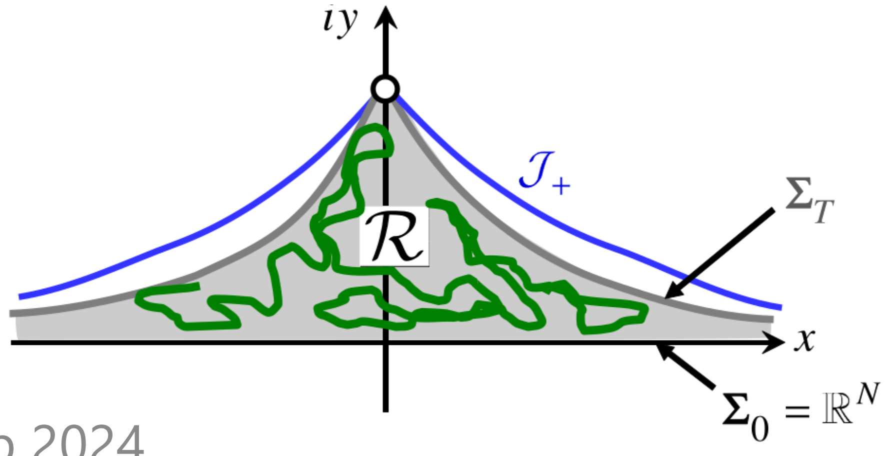
t-independent

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

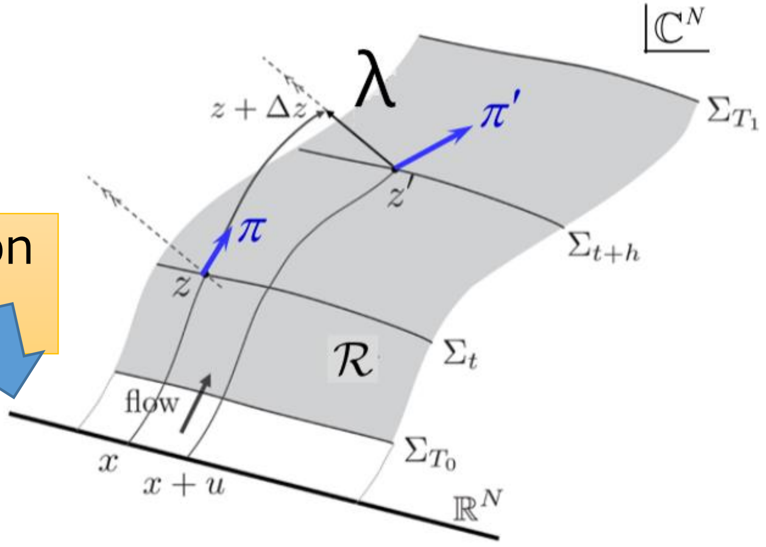
Arbitrary function

$$\mathcal{R} \equiv \bigcup_{0 \le t \le T} \Sigma_t$$





WV-HMC algorithm (2 / 4)



WV-HMC = HMC on worldvolume $\mathcal{R}$

(1) generate momentum π

Original integration path $(t = 0)$

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

Tangent space of $\mathcal{R}$ at z

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

(2) RATTLE (constrained MD) Andersen(1983), Leimkuhler, Skeel(1994)

$$\pi_{1/2} = \pi - \Delta s\, \overline{\partial V(z)} - \lambda, \quad V(z) \equiv \mathrm{Re}\, S(z) + W(t)$$

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

$$\pi' = \pi_{1/2} - \Delta s\, \overline{\partial V(z')} - \lambda'$$

λ is determined easily with simplified Newton method s.t. z' on $\mathcal{R}$

Fukuma(2023); cf. Fujii et al.(2013) for original Lefschetz Thimble

(3) accept / reject test

λ' is determined s.t. $\pi' \in T_z\mathcal{R}$

WV-HMC algorithm (3 / 4)

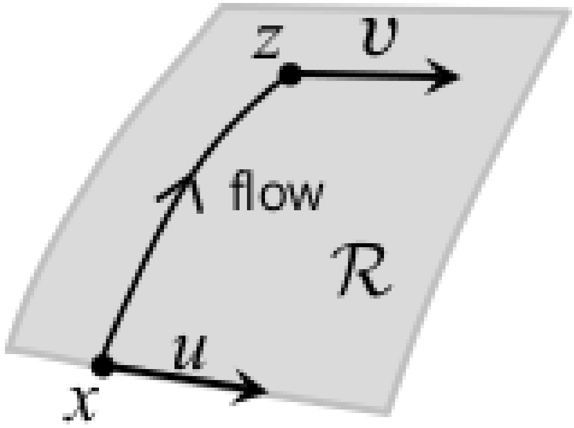
Projections are composed of flow equations

- config flow eq : map $x \in \mathbb{R}^N \to z(x,t) \in \mathbb{C}^N$

  $\dot{z} = \overline{\partial S(z)}$, $z(x, t = 0) = x$

- vector flow eq : map of vector $u \to v(x,t)$

  $\dot{v} = \overline{\left(\partial\partial S(z)\right) v}$, $v(x, t = 0) = u$



Computational cost:

- $O(N^1)$ for a local theory (ex. complex ϕ^4 theory)
- $O(N^{2-3})$ for dynamical fermion (ex. Hubbard model)

➡ See Next page

WV-HMC algorithm (4 / 4)

Flow equations in the presence of fermion

$$Z = \int dA \det D(A)\, e^{-S_0(A)} = \int dA\, e^{-S(A)}, \qquad S(A) = S_0(A) - \log\det D(A)$$

$$\dot{A} = \overline{\partial S(A)}, \qquad \partial S(A) = \partial S_0 - \mathrm{tr}(D^{-1}\,\partial D)$$

$$\dot{v} = \overline{(\partial\partial S(A))\, v}, \quad \partial\partial S(A) = \partial\partial S_0 - \mathrm{tr}(D^{-1}\,\partial\partial D) + \mathrm{tr}(D^{-1}(\partial D)D^{-1}(\partial D))$$

Computational cost

- $O(N^2)$ using CG-type solver
- $O(N^3)$ using direct solver

$N \equiv$ Degrees of Freedom

Complex ϕ^4 theory at finite density

- At finite density, action becomes complex and causes sign problem
- Several methods have been applied
  - Complex Langevin (CL) D=4 Aarts (2009)
  - Lefschetz thimble D=4 Cristoforetti et al. (2012), Fujii et al. (2013)
  - Path optimization D=2 Mori et al. (2017)
  - Tensor renormalization group (TRG) D=2 Kadoh et al. (2019), D=4 Akiyama et al. (2020)

$S_{\mathrm{lat}}^{\mathrm{Euclid}}[\phi = (z+iw)/\sqrt{2}]$ $\quad z, w \in \mathbb{R} \to \mathbb{C}$ $\quad$ Aarts (2009)

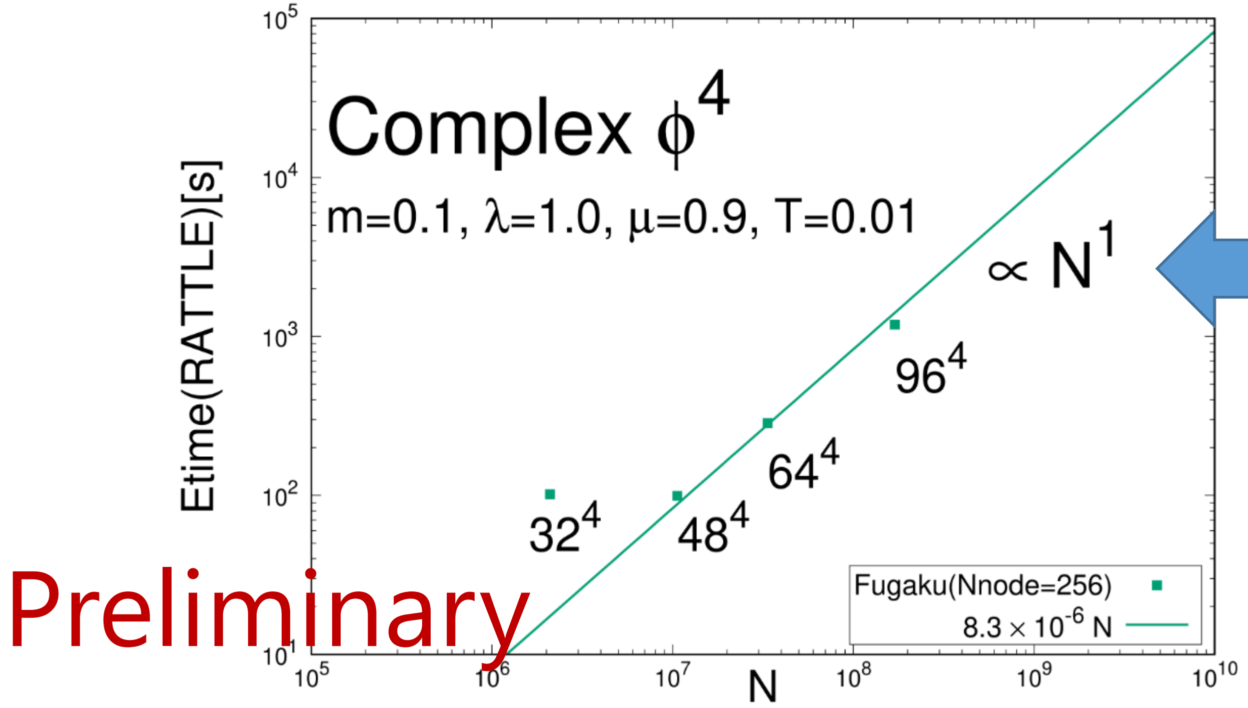
$$= \sum_n \left[-\sum_{\nu=1}^{D-1} (z_{n+\nu} z_n + w_{n+\nu} w_n) + \cosh(\mu)\,(z_{n+\hat{0}} z_n + w_{n+\hat{0}} w_n) + i \sinh(\mu)\,(z_{n+\hat{0}} w_n - w_{n+\hat{0}} z_n) \right.$$

$$\left. + \frac{2D+m^2}{2}(z_n^2 + w_n^2) + \frac{\lambda}{4}(z_n^2 + w_n^2)^2 \right]$$

Result 1-1 : cost scaling

Fukuma and YN (in prep)

We evaluate the computational cost of RATTLE using GT-HMC (fixed flow time version of WV-HMC) Alexandru@Lattice2019,Fukuma et al. (2019)



$O(N^1)$ is confirmed

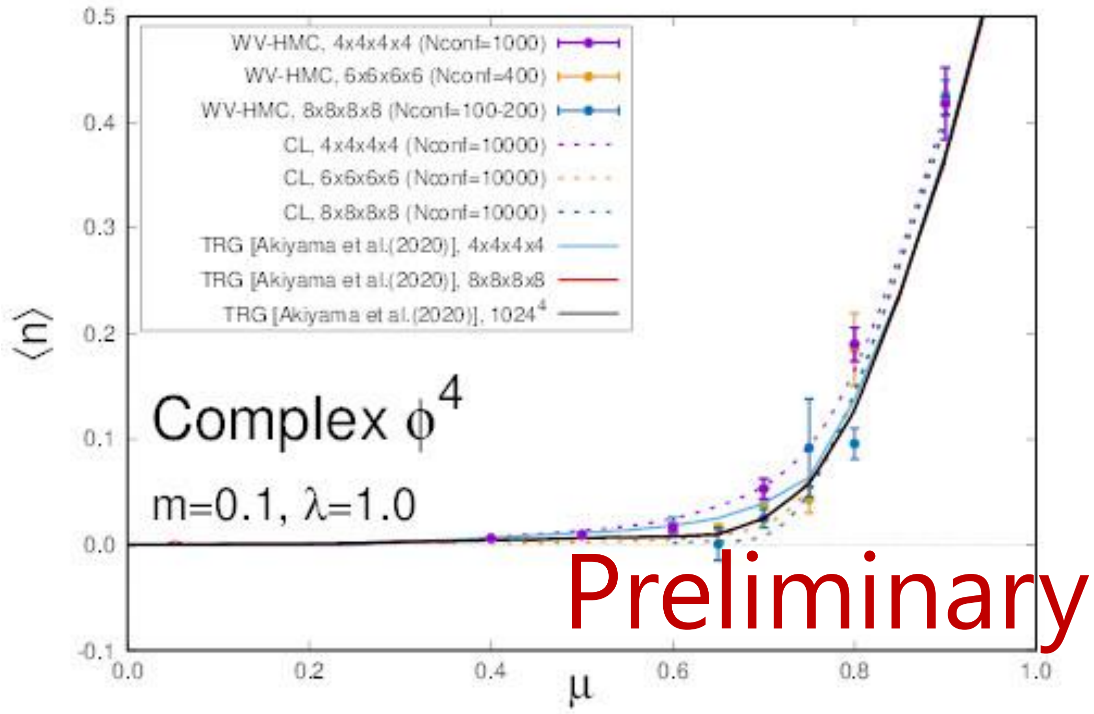
Result 1-2 : number density

WV-HMC is compared with CL and TRG

CL is confirmed to satisfy validity condition
Aarts et al.(2011), Nagata et al.(2016)

- All results agree

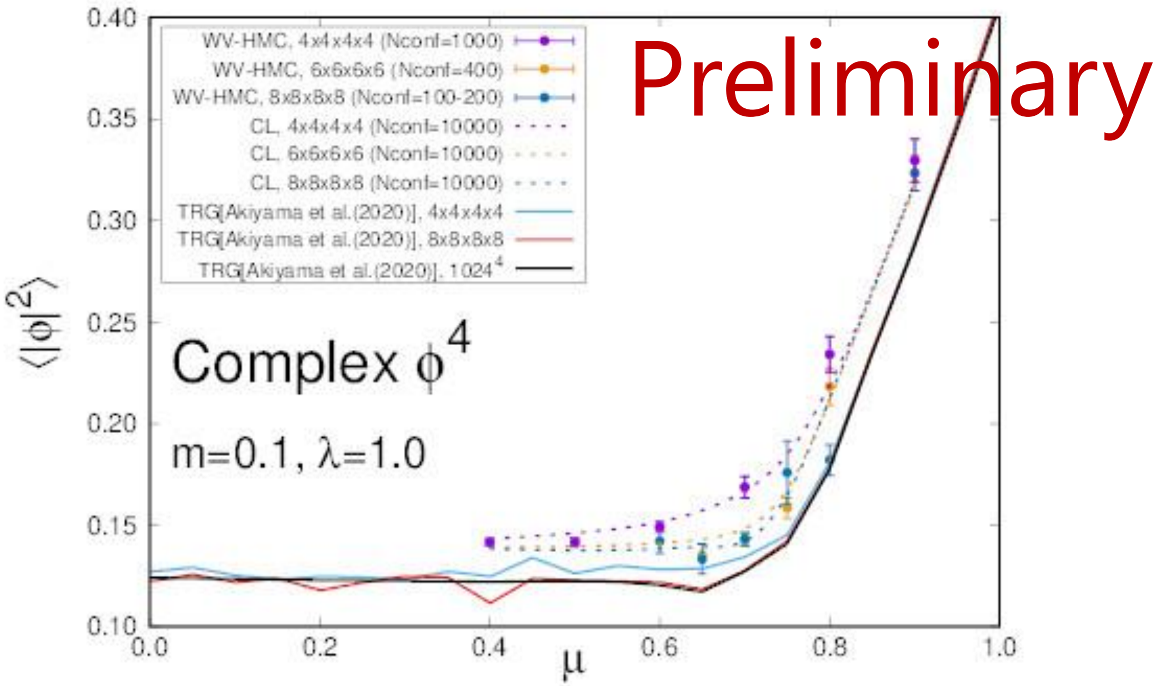
$$n = \frac{1}{V}\partial_\mu S$$
$$= \frac{1}{V}\sum_n \sum_{\nu=1}^{D-1} [\sinh(\mu)\,(z_{n+\hat{0}} z_n + w_{n+\hat{0}} w_n)$$
$$+ i\cosh(\mu)\,(z_{n+\hat{0}} w_n - w_{n+\hat{0}} z_n)]$$



Result 1-3 : $|\phi|^2$

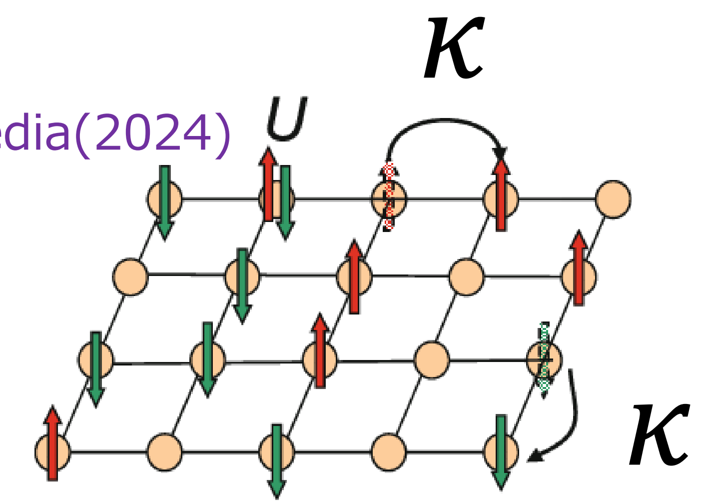
WV-HMC is compared with CL and TRG

- WV-HMC and CL results agree
- TRG deviates from WV-HMC and CL, due to systematic error from $D_{\mathrm{cut}} = 45$ Akiyama et al. (private communication)



Hubbard model (1 / 2)

Wikipedia(2024)



d-dim Hamiltonian after particle-hole trans.

$$H = -\kappa \sum_{<\mathbf{x},\mathbf{y}>} \left(a^\dagger_{\mathbf{x}} a_{\mathbf{y}} + b^\dagger_{\mathbf{x}} b_{\mathbf{y}}\right) - \mu \sum_{\mathbf{x}} \left(n^a_{\mathbf{x}} - n^b_{\mathbf{x}}\right) + \frac{U}{2} \sum_{\mathbf{x}} \left(n^a_{\mathbf{x}} - n^b_{\mathbf{x}}\right)^2, \; n^a \equiv a^\dagger a$$

Nearest neighbor pairs

$\mu \neq 0$ causes sign problem

Beyl et al. (2018)

Generalized Hubbard-Stratonovich trans.

$$\left(n^a - n^b\right)^2 = \alpha \left(n^a - n^b\right)^2 - (1-\alpha)\left(n^a + n^b - 1\right)^2 + (1-\alpha)$$

HS field "A" HS field "B"

$\beta = N_t \epsilon =$ inverse temperature

$$Z = \mathrm{tr}\, e^{-\beta H} = \mathrm{tr}\, \left(e^{-\epsilon H}\right)^{N_t}$$

$x \equiv (x_0, \mathbf{x})$

$$= \int dA\, dB\, e^{-\frac{1}{2}\sum_x \left(A_x^2 + B_x^2\right)} \det D_a(A,B) \det D_b(A,B)$$

$$\left(D_{a/b}\right)_{xy} \equiv e^{\pm\left(\epsilon\mu + i\sqrt{\alpha\epsilon U}\right)A_x + \sqrt{(1-\alpha)\epsilon U} B_x - (1-\alpha)\epsilon U}\, \delta_{xy} - \delta_{x-\hat{0},y} + \epsilon\kappa \sum_{i=1}^{d} \left(\delta_{x+\hat{\imath},y} + \delta_{x-\hat{\imath},y}\right)$$

Hubbard model (2 / 2)

We can introduce Majorana pseudofermion φ

Fukuma and YN (in prep)

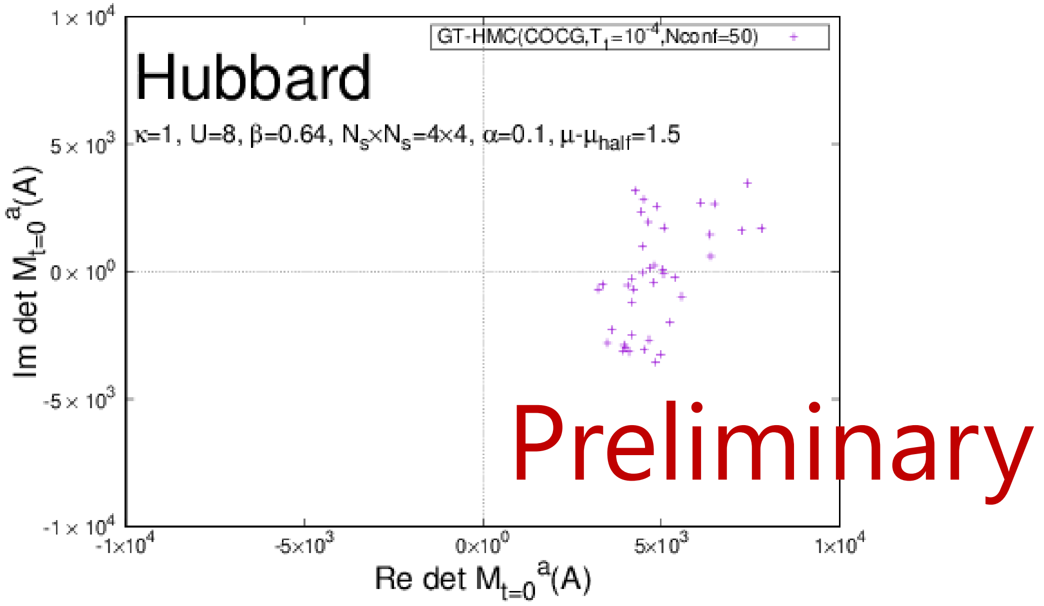
$$Z = \int dA\, dB\, e^{-\frac{1}{2}\sum_x (A_x^2+B_x^2)}\, \mathrm{det}D_a\, \mathrm{det}D_b$$

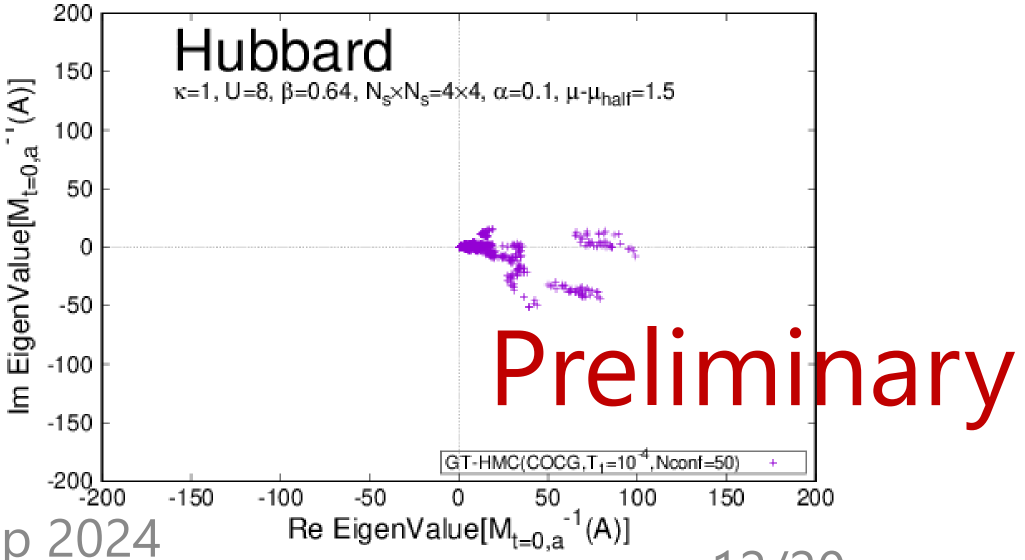
$$= \int dA\, dB\, d\varphi\, e^{-S(A,B,\varphi)}$$

$$M_f \equiv D_f(A) D_f^T(A)$$

$$S(A,B,\varphi) = \frac{1}{2}\sum_x (A_x^2+B_x^2) + \frac{1}{2}\sum_{x,y,f=a,b} (\varphi_f)_x^T \left(M_f\right)_{xy}^{-1} (\varphi_f)_y$$

- This rewrite can be justified,
  if (Re det M)>0、(Re M^{-1})>0
- CG-type solver is available





Previous works on Hubbard model with thimble approach

- (Generalized) thimble method with dominant thimble approx.
  Mukherjee and Cristoforetti (2014), Ulybyshev et al. (2020, 2023), Ulybyshev and Assaad (2024)
  - Calculated only dominant thimbles, avoiding ergodicity problem
- Tempered Lefschetz thimble method Fukuma, Matsumoto, Umeda (2019)
  - Solved sign and ergodicity problems simultaneously
  - High cost limits the lattice size to small extent

cf. other approaches
- Auxiliary Field MC, ex. ALF code ALF collab. (2017, 2020)
- Variational MC, ex. mVMC code Misama et al. (2019)
- Tensor RG method D=1+1 Akiyama, Kuramashi (2021), D=2+1 Akiyama et al. (2021)

Choice of α (1 / 2)

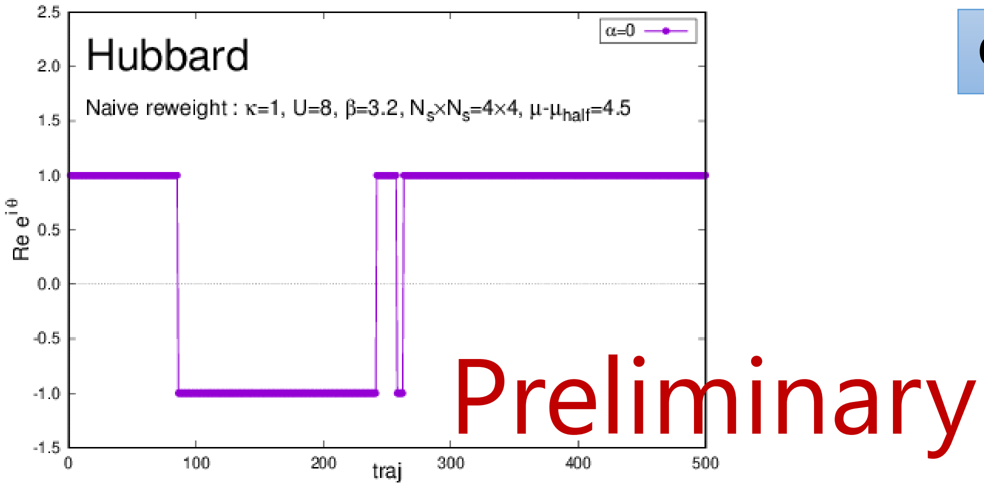
Fukuma and YN (in prep)

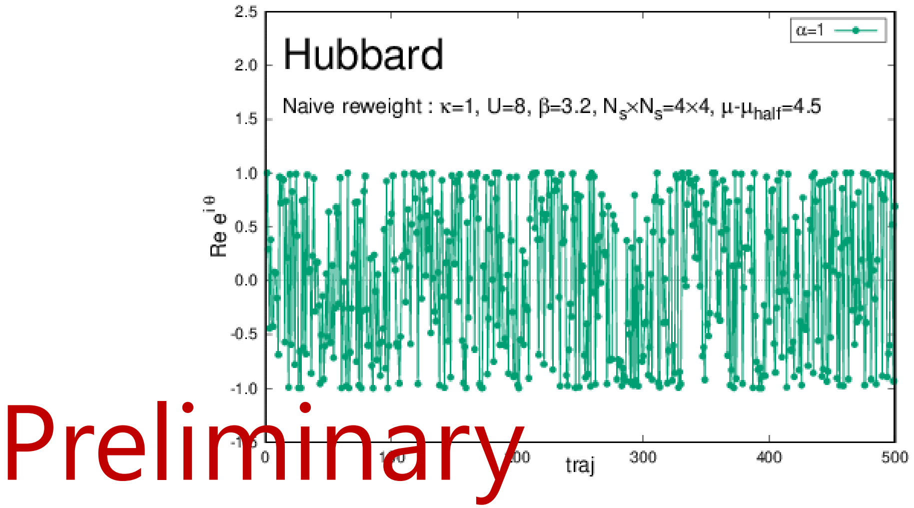
Redundant parameter α affects the sign and the ergodicity problems

$\alpha = 0$: no sign problem, severe ergodicity problem

$\alpha = 1$: severe sign problem, no ergodicity problem

optimal α



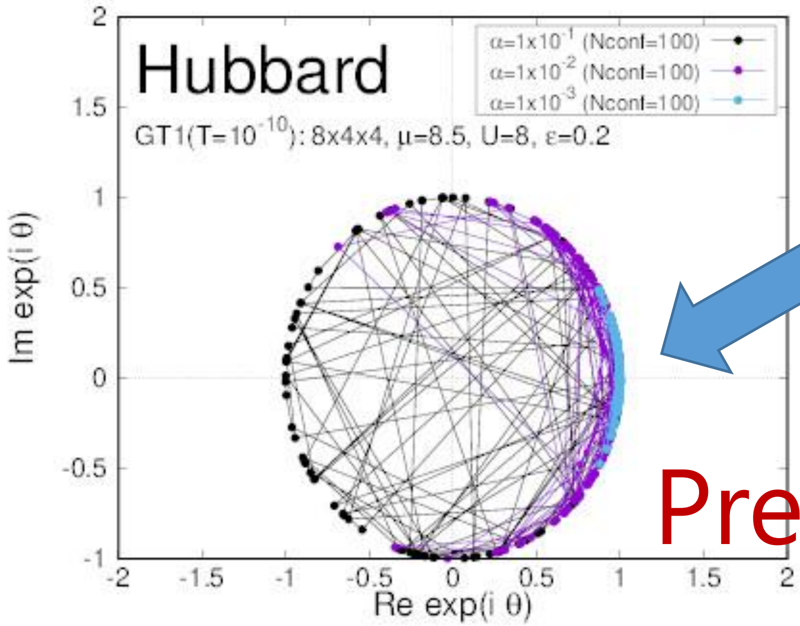


Choice of α (2 / 2)

Fukuma and YN (in prep)

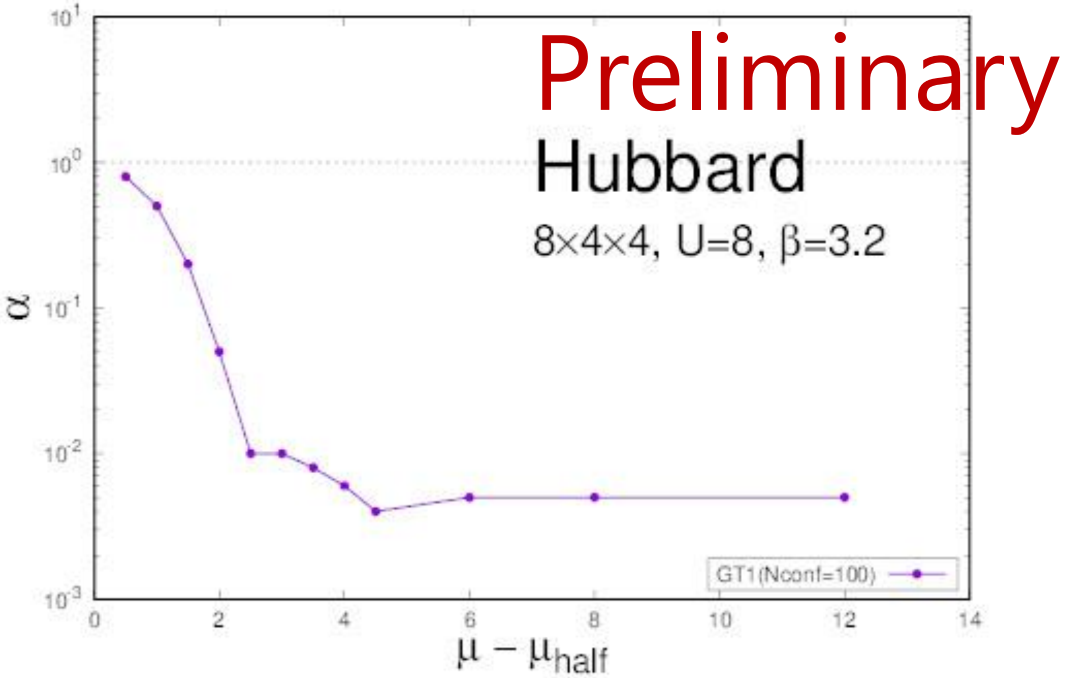
We choose α at min value which avoids the ergodicity problem.

- Sign problem is reduced at $t_{\mathrm{flow}} = 0$ by choice of α
- Optimal value of α depends on μ



Too small α suffers from ergodicity problem

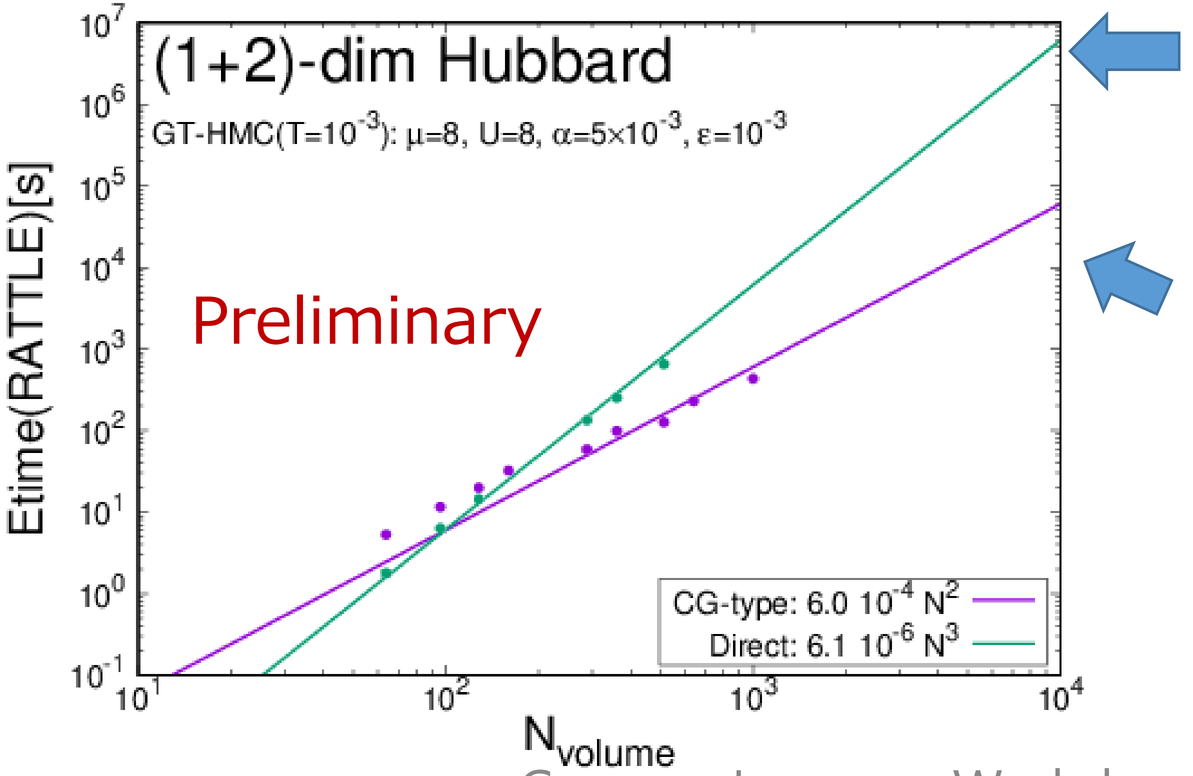
Preliminary



Result 2-1 : computational cost scaling

Fukuma and YN (in prep)

We evaluate the computational cost of RATTLE using GT-HMC with tuned α



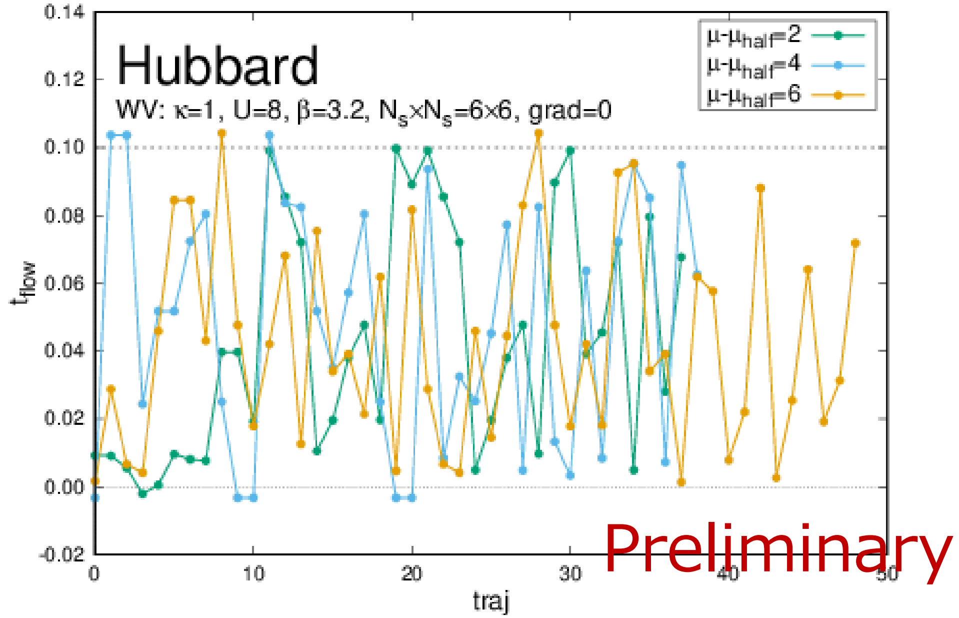
- Direct solver : $O(N^3)$
  Faster at small volumes
- CG-type solver : $O(N^2)$
  Faster at large volumes

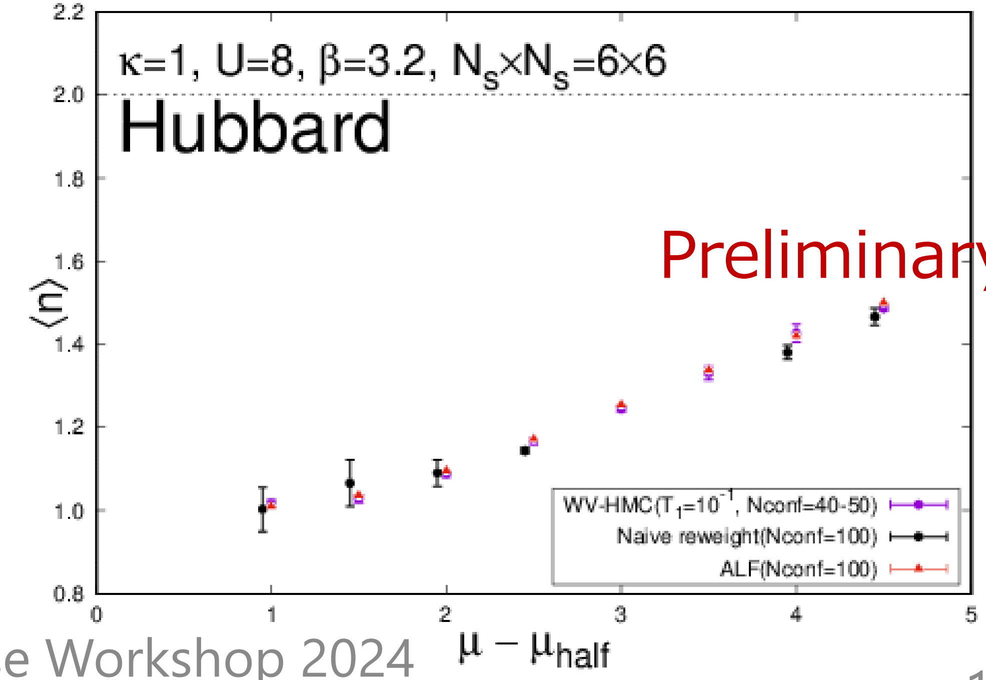
Result 2-2 : number density（$\beta = 3.2$）

Fukuma and YN (in prep)

WV-HMC is compared with naïve reweighting and ALF code on $N_s \times N_s = 6 \times 6$ at inverse temperature $\beta = 3.2$

- Results of WV-HMC agree with those of well-established ALF code developed in the condensed matter ALF collab. (2017, 2020)

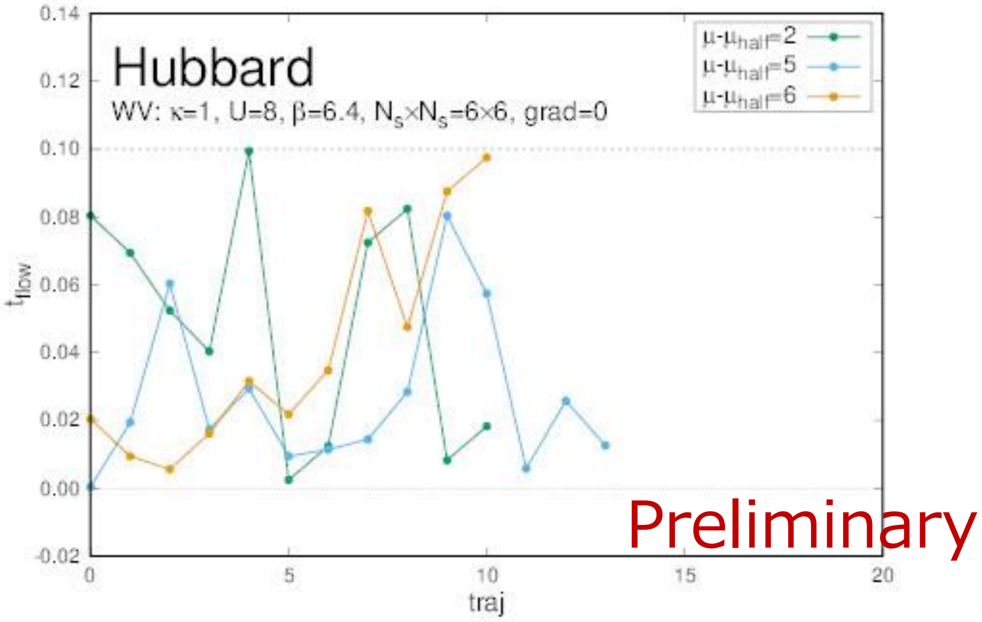


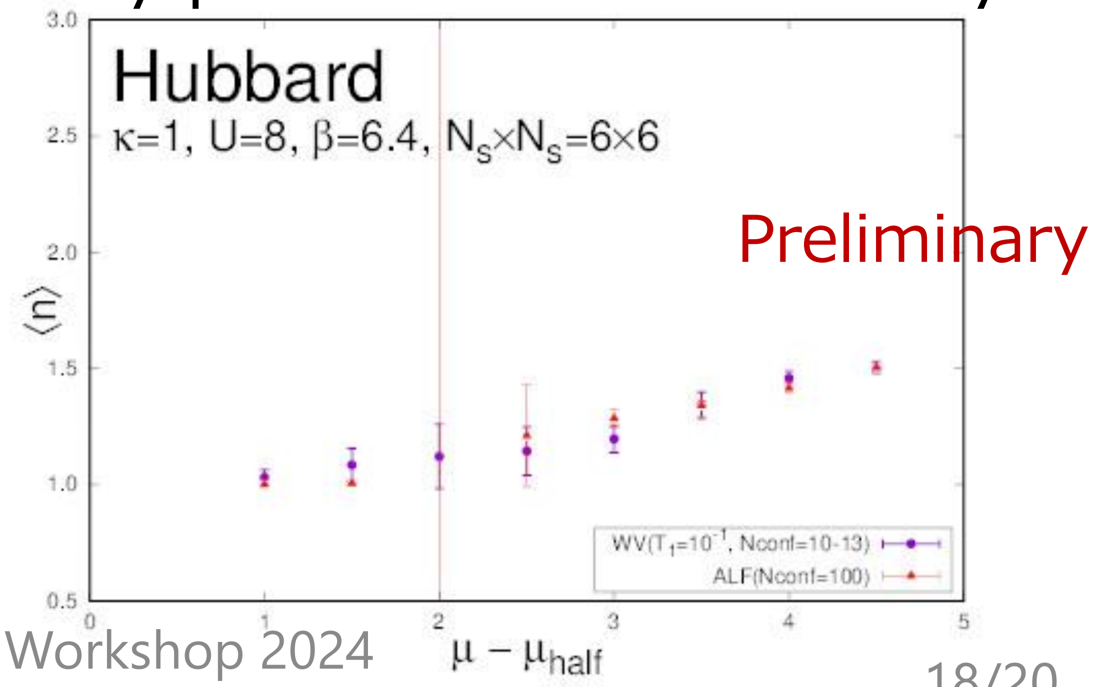


Result 2-3 : number density $(\beta = 6.4)$

Fukuma and YN (in prep)

- ALF code : uncontrolled huge errors near $\mu - \mu_{\text{half}} = 2$, where $e^{O(N)}$ cost is needed.
- WV-HMC : (though N_{conf} is still small) the error seems to be under control. WV-HMC successfully predicts number density!?





Summary

We applied WV-HMC to the sign problems in complex ϕ^4 theory at finite density and Hubbard model Fukuma and YN (in prep)

- Computational cost scaling N ≡Degrees of Freedom
  - A local theory with no dynamical fermion case : $O(N^1)$
  - Dynamical fermion case : $O(N^{2-3})$
- Estimates of observables
  - WV-HMC gives consistent results with those of established methods (CL for complex ϕ^4 and ALF code for Hubbard) and seems to work in severe sign problem region

[Future works]

- Toward thermodynamic limit ($N_s \times N_s = 8 \times 8, \ldots$ in Hubbard model)
- Apply WV-HMC to complicated case, such as finite density QCD

Memory of Yusuke Taniguchi (-2022)

- I learned lattice QCD from Yusuke Taniguchi, when I was a graduated student.

- I have 36 papers with him.

From left, (Namekawa's hand), T.Aoyama, H.Matsufuru, and Y.Taniguchi ; photo by K.Kanaya