Applying the Worldvolume Hybrid Monte Carlo method to the (1+2)-dim Hubbard model

Yusuke Namekawa (Hiroshima Univ.)

in collaboration with

Masafumi Fukuma (Kyoto Univ.)

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

◇ Group manifolds ⇐ Talk by Masafumi Fukuma

◇ Dynamical fermion systems (Hubbard model as a testbed) ⇐ This talk Fukuma and YN (in prep)

cf. full QCD = pure Yang-Mills theory + dynamical quarks

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

WV-HMC needs no dominant thimble approx., because WV-HMC has already solved the ergodicity problem

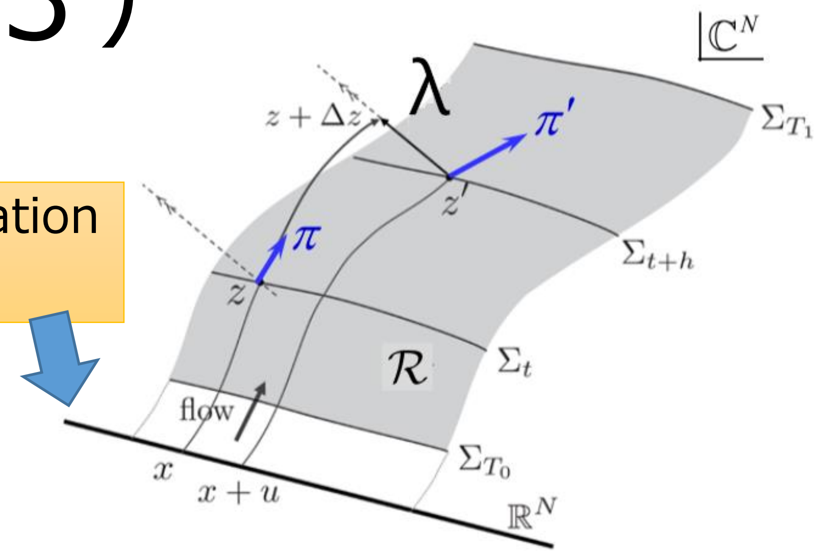
- Tempered Lefschetz thimble method Fukuma, Matsumoto, Umeda (2019)
  - Solved sign and ergodicity problems simultaneously
  - High cost limits the lattice size to $N_t \times N_s \times N_s = 5 \times 2 \times 2$

WV-HMC cost is significantly smaller than that of tempered Lefschetz thimble method

cf. non-Monte Carlo approach

- Tensor RG method D=1+1 Akiyama, Kuramashi (2021), D=2+1 Akiyama et al. (2021)

WV-HMC algorithm（1 / 3）



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

Original integration path $(t=0)$

(1) generate momentum π

$\tilde{\pi}$ 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)

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

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

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

(λ, h, u) is determined with Newton method s.t. $z_{t+h}(x+u) = z'$ on $\mathcal{R}$

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

(3) accept / reject test

WV-HMC algorithm（2 / 3）

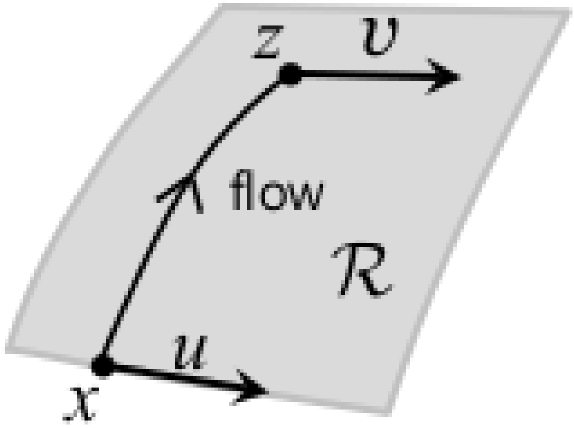
Projections and RATTLE are composed of flow equations

- config flow eq : map $x \in \mathbb{R}^N \to z = z_t \in \mathbb{C}^N$

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

- vector flow eq : map of vector $u \to v = v_t$

  $\dot{v}_t = \overline{\left(\partial\partial S(z_t)\right) v_t}$, $v_{t=0} = u$



See next page for computational cost of the flow eq.

WV-HMC algorithm（3 / 3）

ex. config flow eq. in the presence of fermion

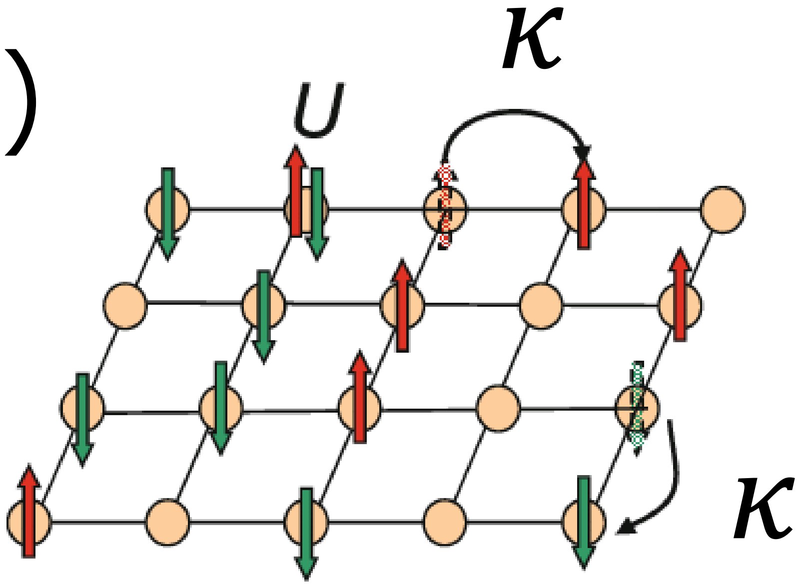
$$Z = \int dA \det D(A)\, e^{-S} = \int dA\, e^{-S_{eff}(A)}, \qquad S_{eff}(A) = \frac{1}{2}A^2 - \log\det D(A)$$

$$\dot{z}_t = \overline{\partial S_{eff}(z_t)}, \qquad \partial S_{eff}(A) = A - \mathrm{tr}\left(D^{-1}\frac{D(A)}{\partial A}\right)$$

Solver is needed for each flow eq.

- Direct solver costs $O(N^3)$ $\quad N \equiv$ Degrees of Freedom
- CG-type solver costs $O(N^2)$ Fukuma and YN (in prep)
- cf. BiCGStab-type solver costs $O(N)$, but suffers from non-convergence

Hubbard model（1 / 4）



Wikipedia(2024)

A model for electrons in a solid Hubbard (1963)

Hamiltonian in spatial d-dim

$$H = -\kappa \sum_{<\boldsymbol{x},\boldsymbol{y}>,s} c^{\dagger}_{\boldsymbol{x},s}\, c_{\boldsymbol{y},s} - \mu \sum_{\boldsymbol{x}} \left(n_{\boldsymbol{x},\uparrow} + n_{\boldsymbol{x},\downarrow}\right) + U \sum_{\boldsymbol{x},s} n_{\boldsymbol{x},\uparrow} n_{\boldsymbol{x},\downarrow} \;, n_{\boldsymbol{x},s} \coloneqq c^{\dagger}_{\boldsymbol{x},s} c_{\boldsymbol{x},s}$$

Nearest neighbor electron pairs

Sign problem occurs at $\mu \neq U/2$ (away from half filling)

Hubbard model（2 / 4）

Partition function in $(1+d)$-dim

$$Z = \mathrm{tr}\, e^{-\beta H} \qquad \beta = N_t \epsilon = \text{inverse temperature}$$

$$= \mathrm{tr}\, \hat{T}^{N_t} \qquad \hat{T} = \text{transfer matrix}$$

$$= \int d\bar{\psi}\, d\psi\, e^{-S(\bar{\psi},\psi)}$$

$$S(\bar{\psi},\psi) = \sum_x \left[\bar{\psi}_x \left(\psi_{x+\hat{0}} - \psi_x - \epsilon\kappa \sum_{i=1}^{d} (\psi_{x+\hat{\imath}} + \psi_{x-\hat{\imath}}) - \epsilon\mu\, \psi_x \right) + \frac{\epsilon U}{2} (\bar{\psi}_x \psi_x)^2 \right]$$

Apply Hubbard-Stratonovich transformation
→ Next page

Hubbard model（3 / 4）

Generalized Hubbard-Stratonovich transformation Beyl et al. (2018)

$$(\hat{n}_{\boldsymbol{x},\uparrow}-\hat{n}_{\boldsymbol{x},\downarrow})^2 = \alpha\,(\hat{n}_{\boldsymbol{x},\uparrow}-\hat{n}_{\boldsymbol{x},\downarrow})^2 - (1-\alpha)(\hat{n}_{\boldsymbol{x},\uparrow}+\hat{n}_{\boldsymbol{x},\downarrow}-1)^2 + (1-\alpha)$$

α is a redundant parameter, but affects sign problem

$$Z = \int d\bar{\psi}\, d\psi\, e^{-S(\bar{\psi},\psi)}$$

$$= \int dA\, d\bar{\psi}\, d\psi\, e^{-\frac{1}{2}\sum_{x,a=1,2} A_{x,a}^2 - \sum_{x,y,f} (\bar{\psi}_f)_x (D_f)_{xy} (\psi_f)_y}$$

$$= \int dA\, e^{-\frac{1}{2}\sum_{x,a=1,2} A_{x,a}^2}\ \mathrm{det}D_a\, \mathrm{det}D_b$$

$$\left(D_{a/b}\right)_{xy} \equiv \delta_{x+\hat{0},y} - \delta_{xy} + \epsilon\kappa \sum_{i=1}^{d} \left(\delta_{x+\hat{\imath},y} + \delta_{x-\hat{\imath},y}\right) \pm \left(\epsilon\mu + i\sqrt{\alpha\epsilon U} A_1(x)\right)\delta_{xy} + \left(\sqrt{(1-\alpha)\epsilon U} A_2(x) - (1-\alpha)\right)\delta_{xy} + O(\epsilon^2)$$

Hubbard model（4 / 4）

We can further introduce pseudofermions:

Fukuma and YN (in prep)

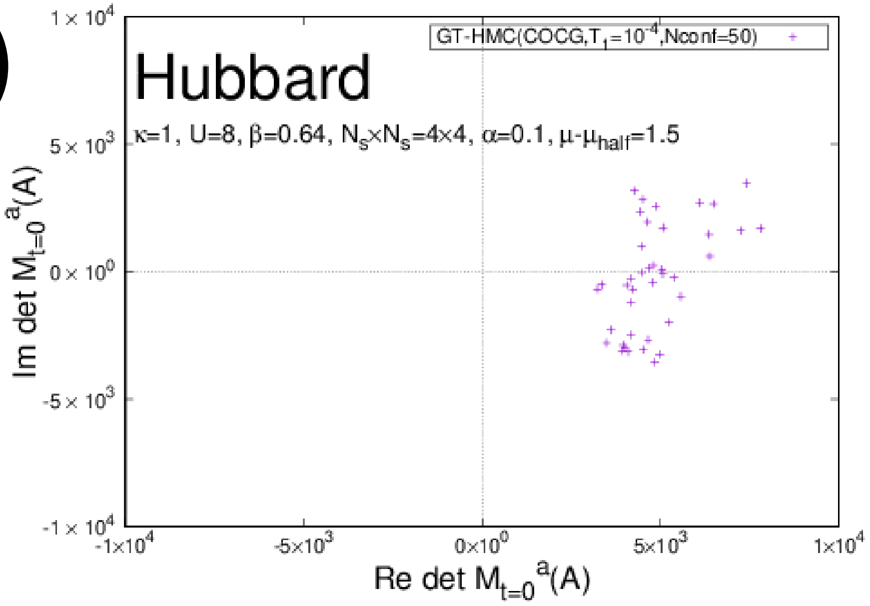
$$Z = \int dA\, e^{-\frac{1}{2}\sum_{x,a=1,2} A_{x,a}^2}\ \mathrm{det}D_a\ \mathrm{det}D_b$$

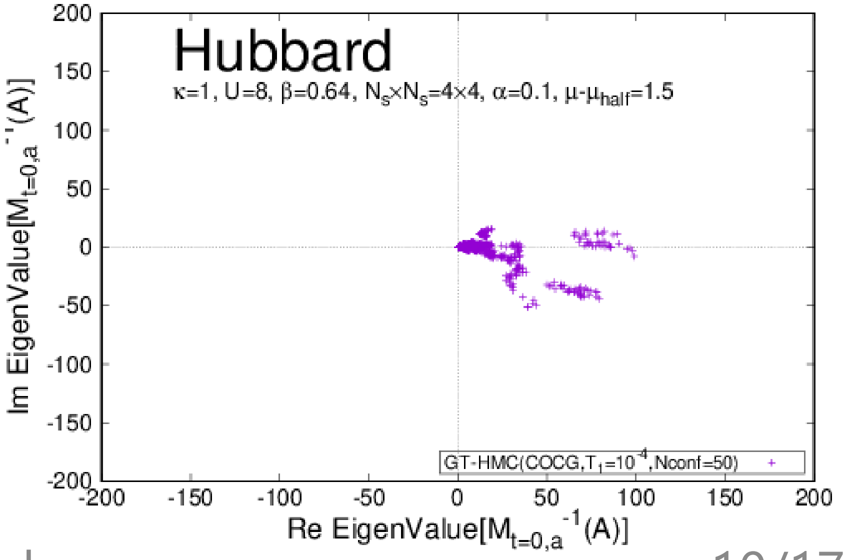
$$= \int dA\, d\varphi\, e^{-S(A,\varphi)}$$

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

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

- This rewriting is justified when (Re det M)>0 and (Re M^{-1})>0
- CG-type solver is then applicable





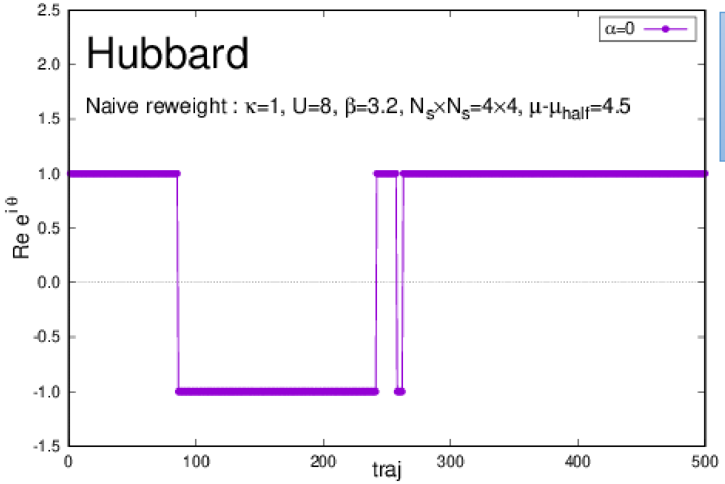
Setup 1 : choice of α Fukuma and YN (in prep)

Redundant parameter α affects the sign and the ergodicity problems

- We choose α at an intermediate value which avoids the ergodicity problem and a less sign problem than that at $\alpha = 1$.
- Remaining sign problem is solved by WV-HMC.

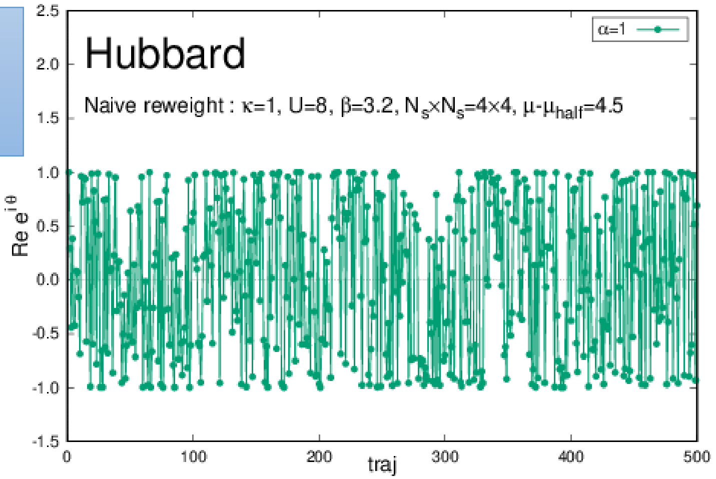
$\alpha = 0$: less sign problem, severe ergodicity problem

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



$0 < \alpha < 1$: less sign problem, less ergodicity problem

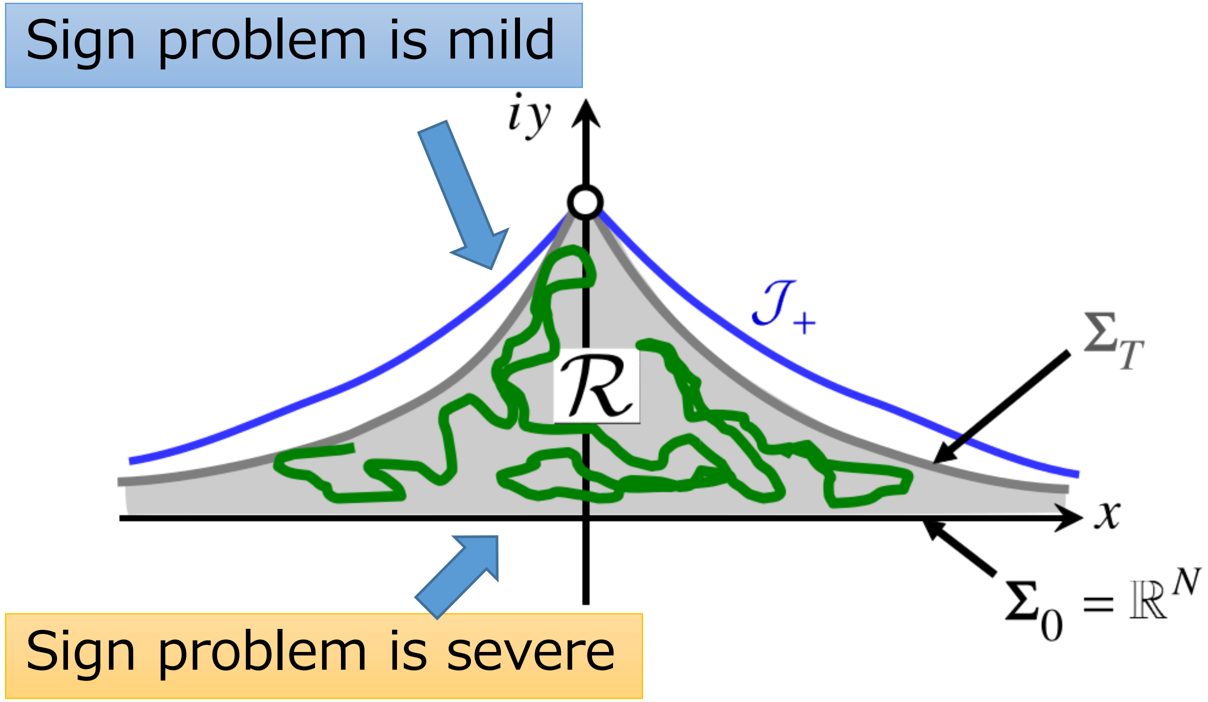
N.B. non-vanishing α can improve ergodicity Beyl et al. (2018)

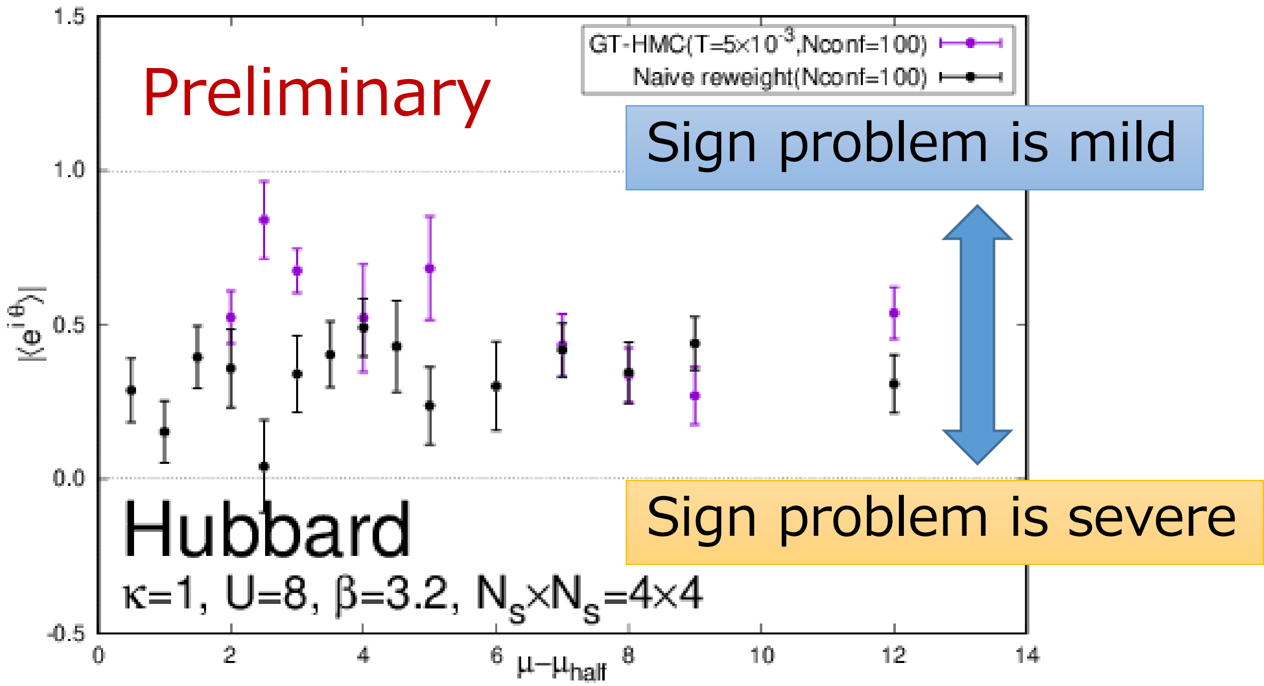


Setup 2 : choice of flow time

Fukuma and YN (in prep)

We set the target flow time T to the minimum value among those flow times that solve the remaining sign problem.



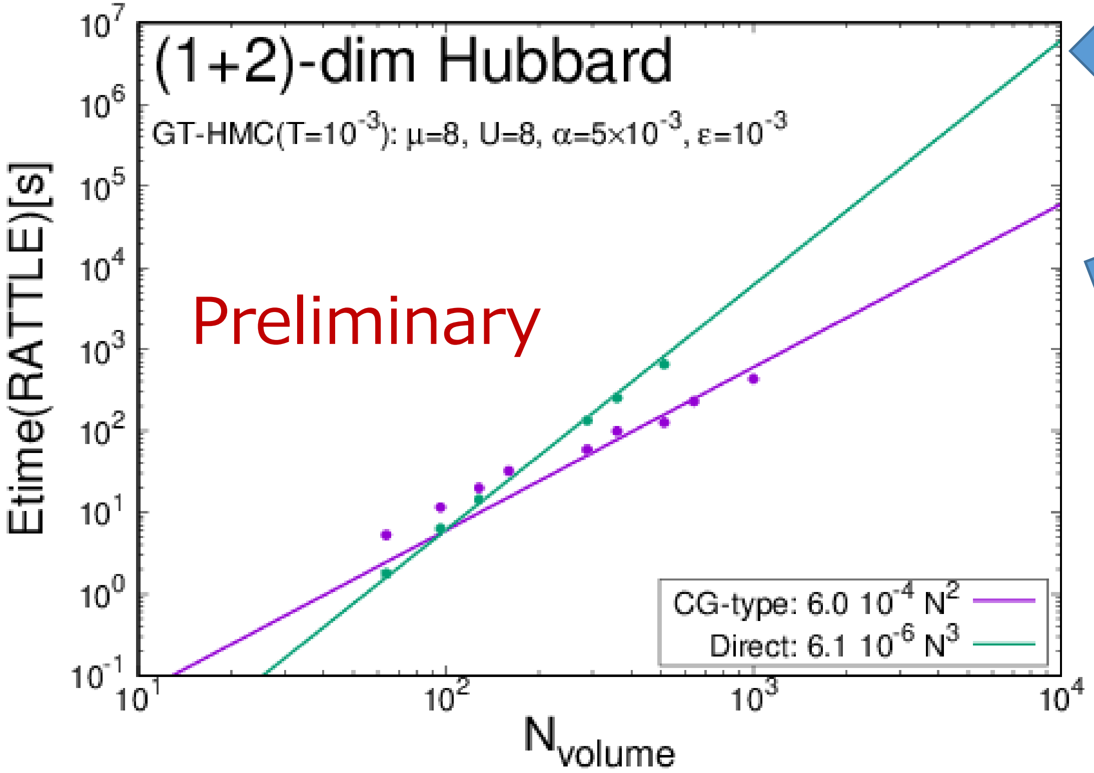


Result 1 : computational cost scaling

Fukuma and YN (in prep)

We evaluate the computational cost of RATTLE using GT-HMC (fixed flow time version of WV-HMC) with tuned α

Alexandru@Lattice2019, Fukuma et al. (2019)



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

(Re det M)>0 and (Re M^{-1})>0 must be satisfied

Result 2 : number density

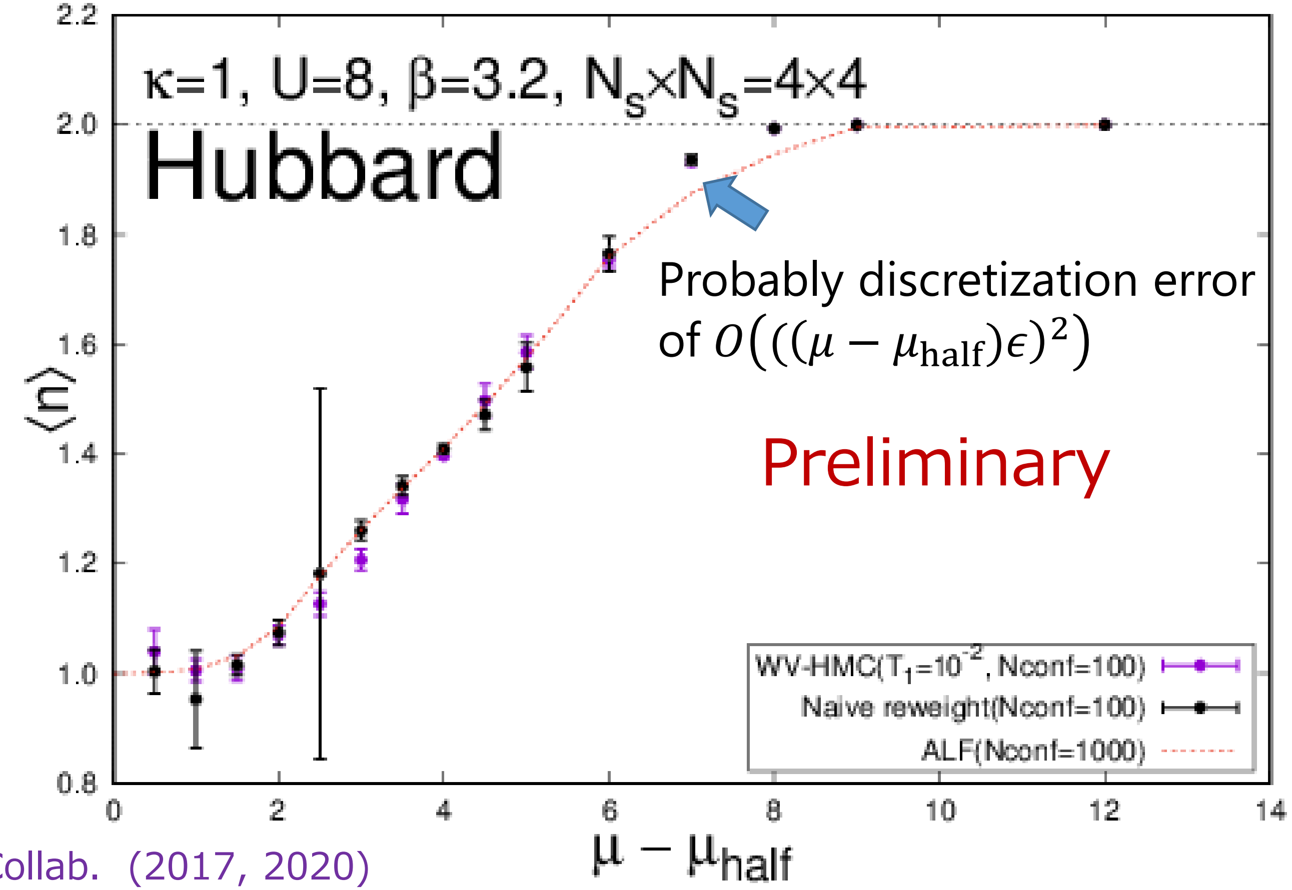
Fukuma and YN (in prep)

We measure number density $\langle n \rangle$ with naïve reweighting and WV-HMC

- Naïve reweighting suffers from large errors
  ➡ Tuning of α reduces sign problem, but does not completely resolve it

- WV-HMC gives small errors and is consistent with ALF

ALF is an established MC code in condensed matter physics



ALF Collab. (2017, 2020)

Result 3 : energy density

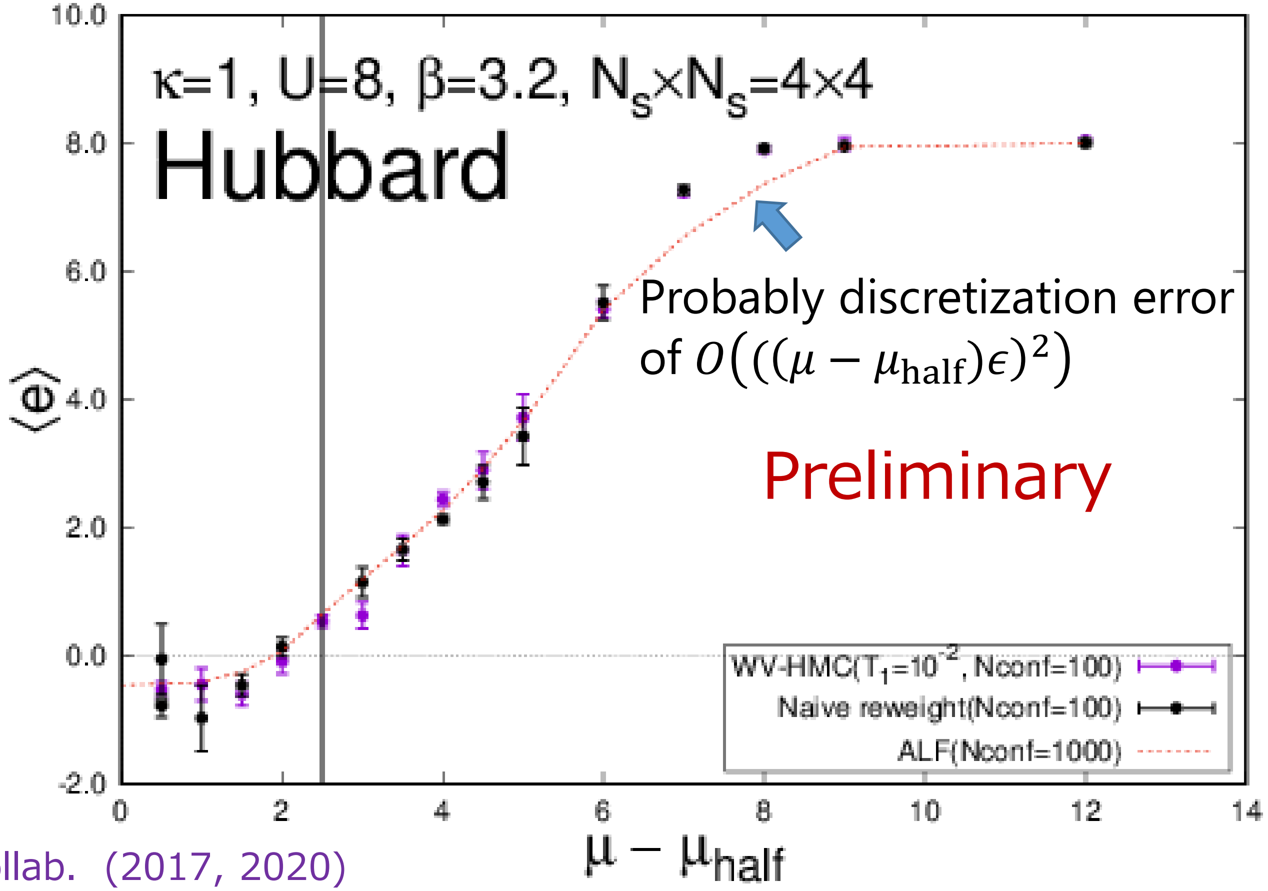
Fukuma and YN (in prep)

We measure energy density $\langle e \rangle$ with naïve reweighting and WV-HMC

- Naïve reweighting suffers from large errors
  ➡ Tuning of α reduces sign problem, but does not completely resolve it

- WV-HMC gives small errors and is consistent with ALF

ALF is an established MC code in condensed matter physics

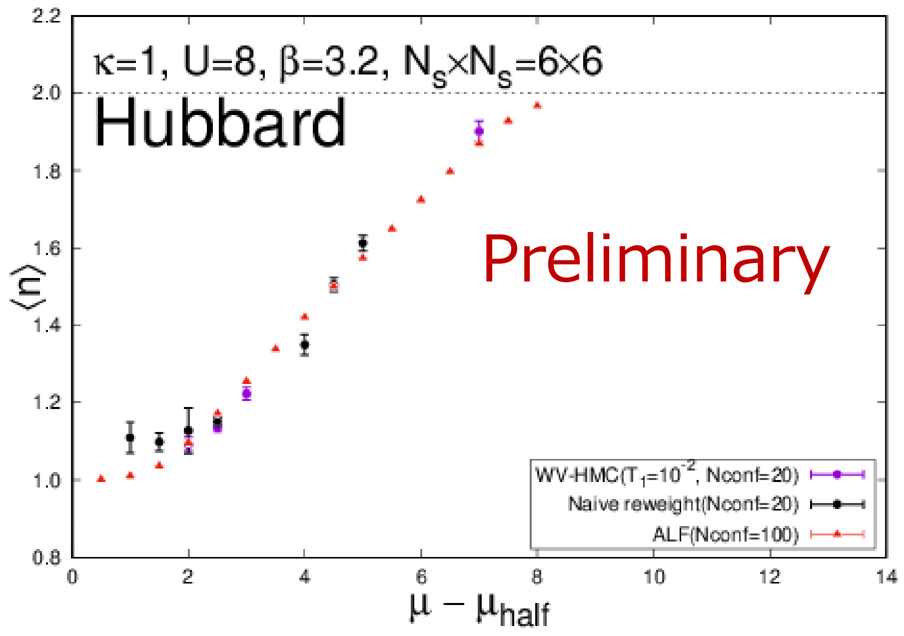


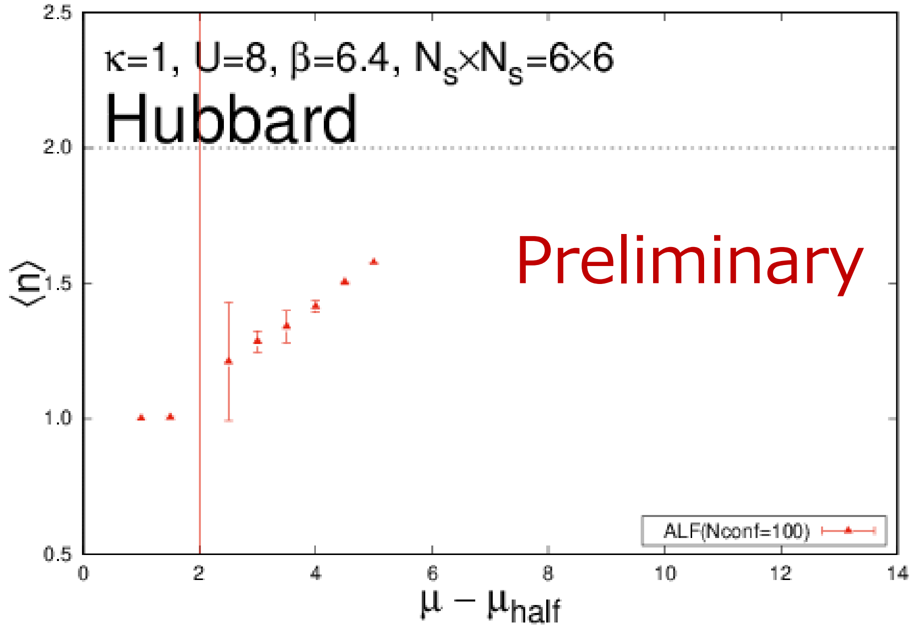
ALF Collab. (2017, 2020)

Results 4:
larger lattice and lower temperature (ongoing)

Fukuma and YN (in prep)

We move on to a larger lattice (6×6) and a lower temperature ($\beta = 6.4$), where it becomes harder to evaluate observables with other algorithms





Summary

We applied WV-HMC to the sign problem in (1+2)-dim Hubbard model as a step toward finite density QCD Fukuma and YN (in prep)

- Computational cost scaling
  - Direct solver : $O(N^3)$ N ≡Degrees of Freedom
  - CG-type solver : $O(N^2)$
- Estimates of observables
  - WV-HMC give consistent results with those of well-established ALF code with small statistical errors in the parameter region where the sign problem is severe