Tempered Lefschetz thimble method and its application to the Hubbard model away from half-filling

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@Wuhan (Lattice 2019)

Based on work with

Nobuyuki Matsumoto (Kyoto Univ) & **Naoya Umeda** (PwC)

-- **MF** and **Umeda**, "Parallel tempering algorithm for integration over Lefschetz thimbles" [arXiv:1703.00861, PTEP2017(2017)073B01]
-- **MF**, **Matsumoto** and **Umeda**, "Applying the tempered Lefschetz thimble method to the Hubbard model away from half-filling", [arXiv:1906.04243]

Also, for the geometrical optimization of tempering algorithms: → **Matsumoto's talk @14:20, Thu, June 20**

-- **MF**, **Matsumoto** and **Umeda**, [arXiv:1705.06097, JHEP1712(2017)001], [arXiv:1806.10915 JHEP1811(2018)060]

1. Introduction

Sign problem

The sign problem is one of the major obstacles
when performing numerical calculations in various fields of physics

Typical examples:

① Finite density QCD
② Quantum Monte Carlo simulations of quantum statistical systems
③ Real time QM/QFT

Today, I would like to talk about the sign problem in:

② Quantum Monte Carlo simulations
of strongly correlated electron systems,
especially the Hubbard model away from half-filling

and show that a new algorithm "Tempered Lefschetz thimble method" (TLTM) works well for this problem

Approaches to the sign problem

Two major approaches:

(1) Complex Langevin method (CLM) **[Parisi 1983]**

(2) (Generalized) Lefschetz thimble method ((G)LTM) **[Cristoforetti et al. 2012 Alexandru et al. 2016]**

Advantages/disadvantages:

(1) CLM Pros: fast $\propto O(N)$ (N : DOF)

Cons: "wrong convergence problem" **[Ambjørn-Yang 1985, Aarts et al. 2011, Nagata-Nishimura-Shimasaki 2016]**

(2) (G)LTM Pros: No wrong convergence problem *iff* only a single thimble is relevant

Cons: Expensive $\propto O(N^3)$ ⇐ Jacobian determinant

Multimodal problem if more than one thimble are relevant (wrong convergence de facto)

⇓

(2′) **TLTM** (Tempered Lefschetz thimble method) **[MF-Umeda 2017, MF-Matsumoto-Umeda 2019]**

"facilitate transitions among thimbles by tempering the system with the flow time"

Pros: Works well even when multi thimbles are relevant

Cons: Expensive $\propto O(N^{3\sim4})$ ⇐ Jacobian determinant + tempering

Plan

1. Introduction (done)
2. Generalized LTM (GLTM)
3. Tempered LTM (TLTM)
4. Applying the TLTM to the Hubbard model
   - 1D case
   - 2D case
5. Conclusion and outlook

2. Generalized Lefschetz thimble method (GLTM)

Generalized LTM (1/2)

[Cristoforetti et al. 2012
Alexandru et al. 2016]

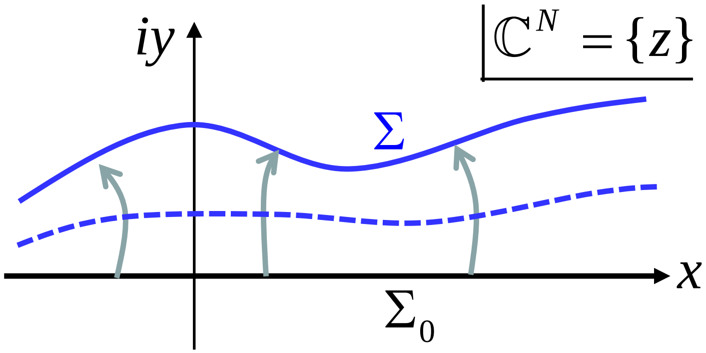
Complexify the variable: $x = (x^i) \in \mathbb{R}^N \;\Rightarrow\; z = (z^i = x^i + i y^i) \in \mathbb{C}^N$

Assumption: $e^{-S(z)}$, $e^{-S(z)}\mathcal{O}(z)$: entire functions over $\mathbb{C}^N$

⇩

Integral does not change under continuous deformations of the integration region from $\Sigma_0 = \mathbb{R}^N$ to $\Sigma \subset \mathbb{C}^N$ (with the boundary at infinity $|x| \to \infty$ kept fixed) :

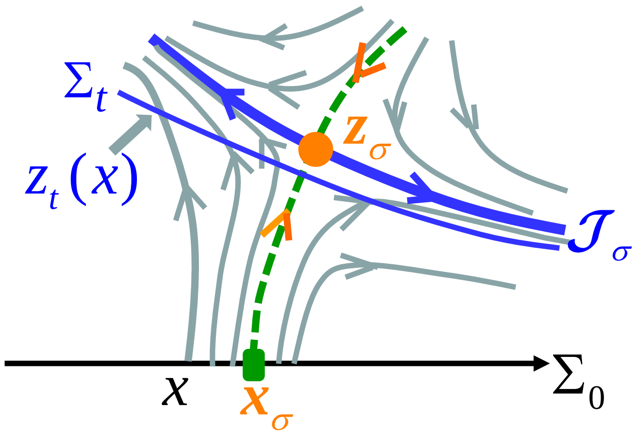
$$\langle \mathcal{O}(x) \rangle_S \equiv \frac{\int_{\Sigma_0} dx\, e^{-S(x)}\, \mathcal{O}(x)}{\int_{\Sigma_0} dx\, e^{-S(x)}} = \frac{\int_{\Sigma} dz\, e^{-S(z)}\, \mathcal{O}(z)}{\int_{\Sigma} dz\, e^{-S(z)}}$$



severe sign problem

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

Generalized LTM (2/2) [Alexandru et al. 2016]



Prescription:

antiholomorphic gradient flow $\dot{z}_t^i = \overline{\partial_i S(z_t)}$ with $z_{t=0}^i = x^i$

Property: $[S(z_t)]^{\bullet} = \partial_i S(z_t)\, \dot{z}_t^i = |\partial_i S(z_t)|^2 \geq 0$

⇨ $[\mathrm{Re}\, S(z_t)]^{\bullet} \geq 0$: real part always increases along the flow
$[\mathrm{Im}\, S(z_t)]^{\bullet} = 0$: imaginary part is kept fixed ″

⇨ In $t \to \infty$, Σ_t approaches a union of Lefschetz thimbles: $\Sigma_t \to \bigcup_\sigma \mathcal{J}_\sigma$

(on each of which $\mathrm{Im}\, S(z)$ is constant)

Expectation value:

$$\langle \mathcal{O}(x) \rangle_S \equiv \frac{\int_{\Sigma_0} dx\, e^{-S(x)} \mathcal{O}(x)}{\int_{\Sigma_0} dx\, e^{-S(x)}} = \frac{\int_{\Sigma_t} dz_t\, e^{-S(z_t)} \mathcal{O}(z_t)}{\int_{\Sigma_t} dz_t\, e^{-S(z_t)}} = \frac{\int_{\Sigma_0} dx\, \det(\partial z_t^i(x)/\partial x^j)\, e^{-S(z_t(x))}\, \mathcal{O}(z_t(x))}{\int_{\Sigma_0} dx\, \det(\partial z_t^i(x)/\partial x^j)\, e^{-S(z_t(x))}}$$

$$= \frac{\left\langle e^{i\theta_t(x)} \mathcal{O}(z_t(x)) \right\rangle_{S_t^{\mathrm{eff}}}}{\left\langle e^{i\theta_t(x)} \right\rangle_{S_t^{\mathrm{eff}}}}$$

$$e^{-S_t^{\mathrm{eff}}(x)} \equiv e^{-\mathrm{Re}\, S(z_t(x))} \left| \det(\partial z_t^i(x)/\partial x^j) \right|$$

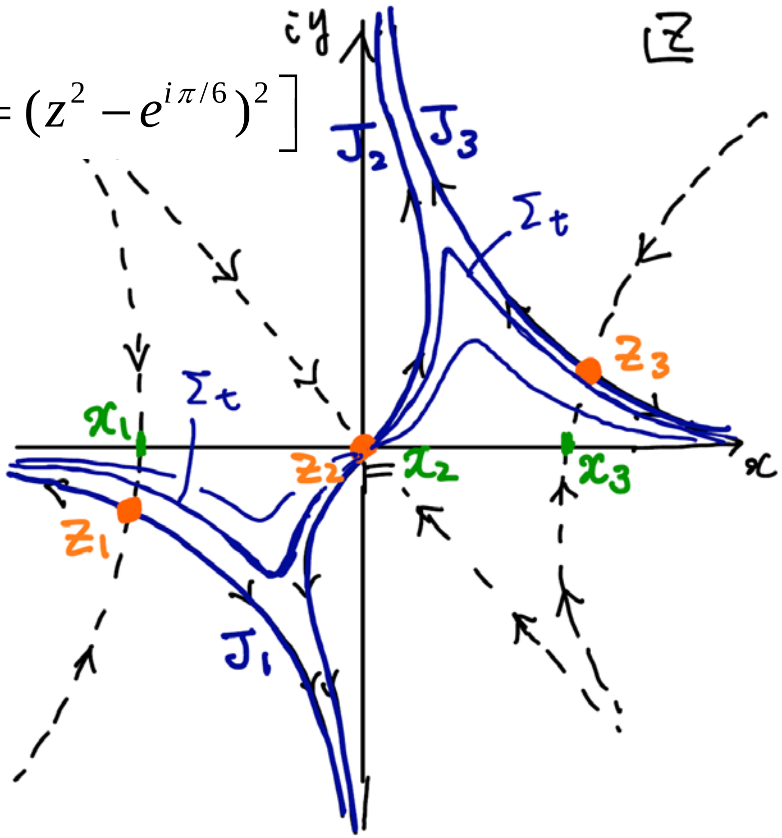
$$e^{i\theta_t(x)} \equiv e^{-i\, \mathrm{Im}\, S(z_t(x)) + i \arg \det(\partial z_t^i(x)/\partial x^j)}$$

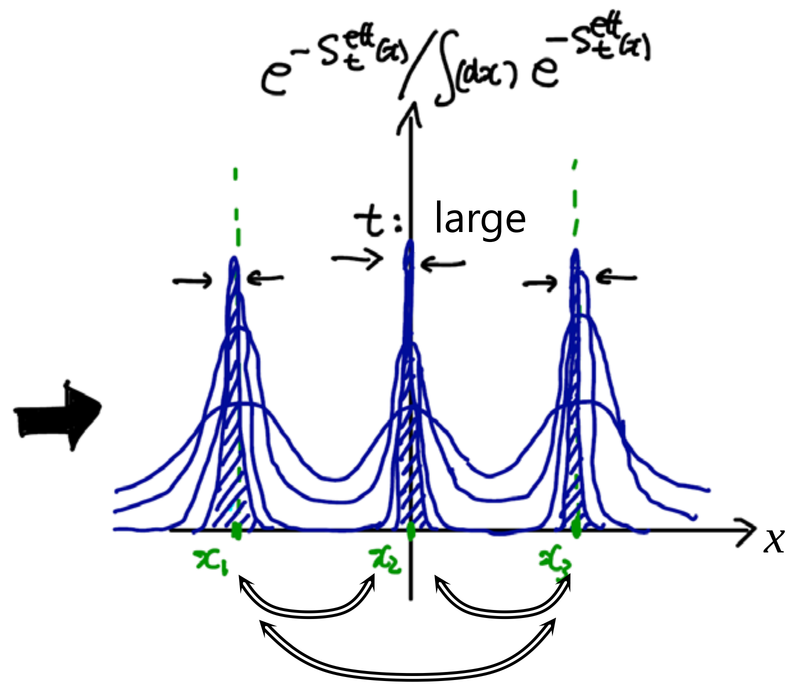
Multimodal problem in GLTM (1/2)

Flow time t needs to be large enough to solve the sign problem

However, this introduces a new problem ⇨ "multimodal problem"

$$\left[S(z) = (z^2 - e^{i\pi/6})^2 \right]$$





transitions among thimbles become indefinitely difficult as t increases

Dilemma between the sign problem and the multimodal problem

(for small t) (for large t)

Multimodal problem in GLTM (2/2)

Proposal in GLTM: **[Alexandru-Basar-Bedaque-Ridgway-Warrington 2016]**

Choose a middle value of T s.t. it is large enough for the sign problem but at the same time is not too large for the multimodal problem

flow time ($= T$)	small	medium	large
sign problem	NG	△	**OK**
multimodal problem	**OK**	△	NG

However, the existence of such T is not obvious a priori

Even when it exists, a very fine tuning will be needed

TLTM : **[MF-Umeda 2017] (cf. [Alexandru-Basar-Bedaque-Warrington 2017])**

Implement a tempering method by using the flow time *t* as a tempering parameter

flow time ($= T$)	small	medium	large
sign problem	NG	**OK**	**OK**
multimodal problem	**OK**	**OK**	**OK**

no fine tuning needed!

3. Tempered Lefschetz thimble method (TLTM)

[MF-Umeda 2017]

[MF-Matsumoto-Umeda 2019]

Tempered LTM (1/3) [MF-Umeda 2017]

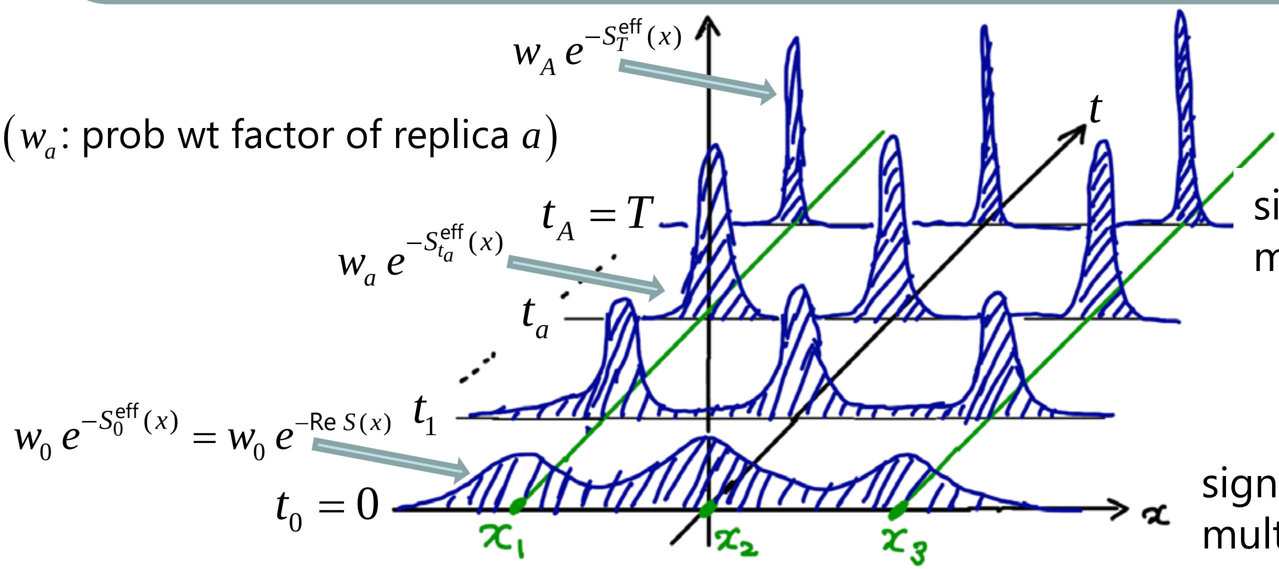
Algorithm of TLTM

(1) Introduce copies of config space labeled by a finite set of flow times

$$\mathcal{A} = \{t_a\}\ (a = 0, 1, \ldots, A) \quad \left(t_0 = 0 < t_1 < t_2 < \cdots < t_A = T\right),$$

and construct a Markov chain that drives the enlarged system to global equilibrium

$\left(w_a\text{: prob wt factor of replica } a\right)$



sign problem : **OK**
multimodality : NG

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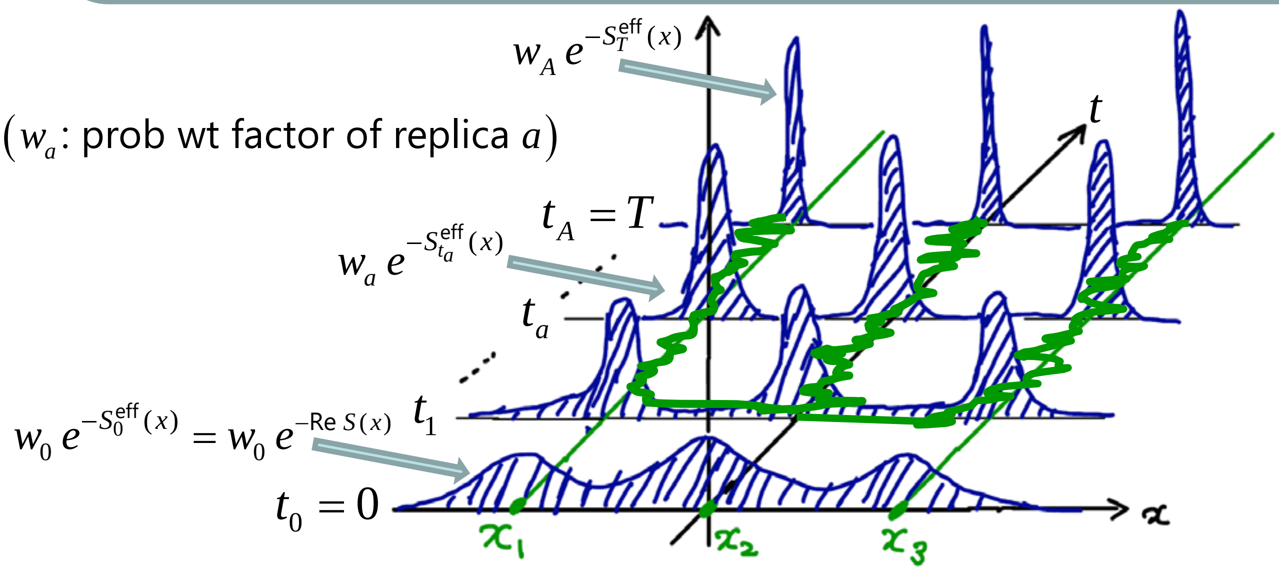
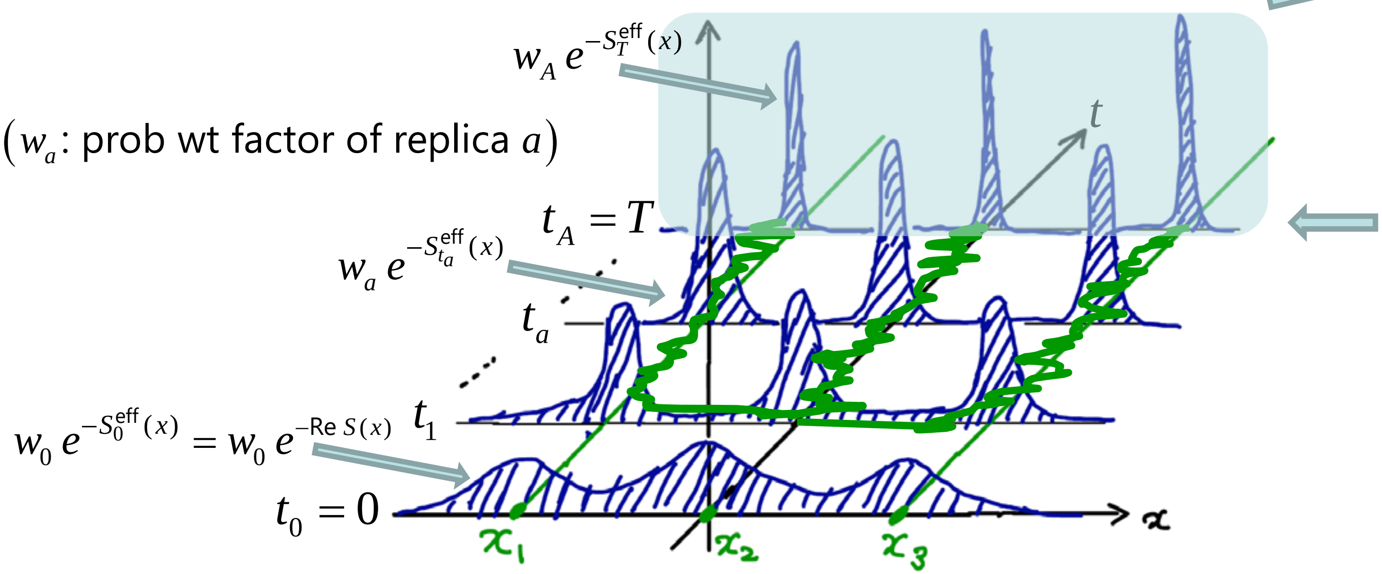


Algorithm of TLTM

(2) After the enlarged system is relaxed to global equilibrium, evaluate the expectation value by using the subsample at $t_A = T$ $(a = A)$



A-th replica

Tempered LTM (2/3) [MF-Umeda 2017]

Algorithm of TLTM

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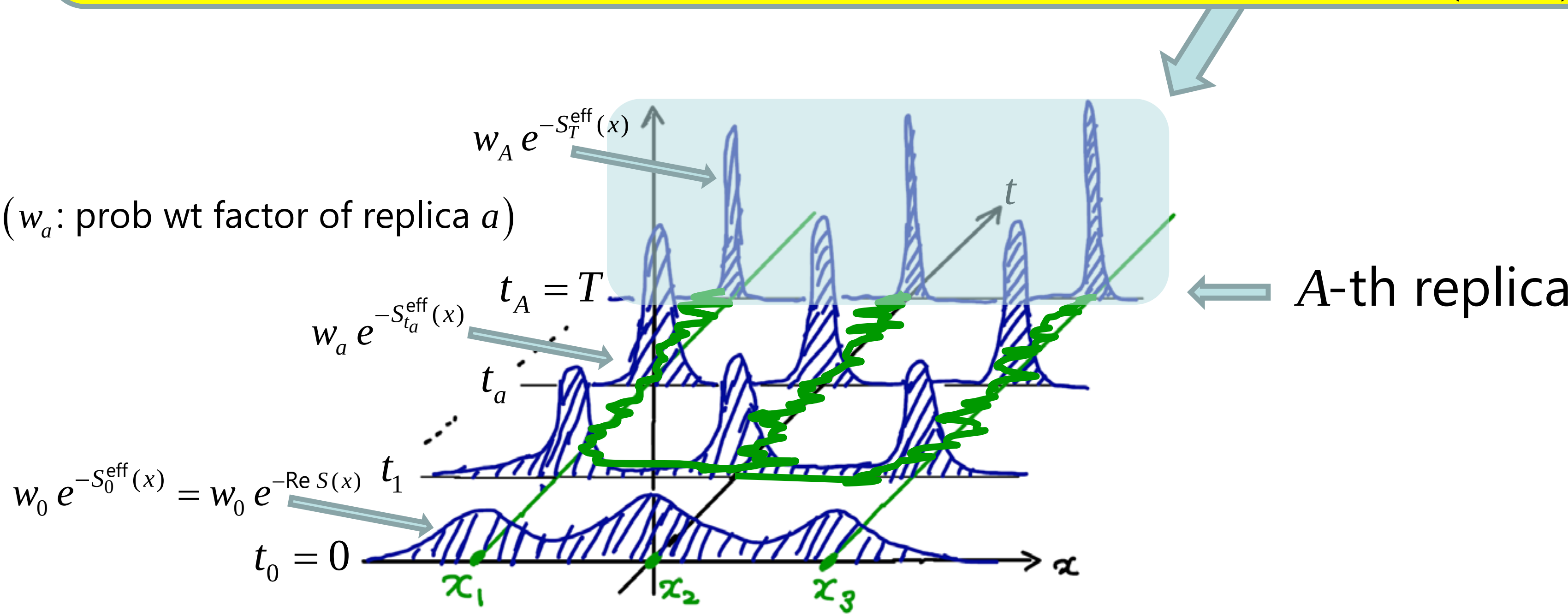

NB: various tempering methods $(\mathcal{M} \equiv \{x\}$: original config space$)$

- simulated tempering : enlarged system $\Leftrightarrow$ $\mathcal{M} \times \mathcal{A} = \{(x, t_a)\}$ $\left(\triangle \left[\text{tedious task to detemine the weights } w_a \right] \right)$
  [Marinari-Parisi 1992]
- parallel tempering (replica exchange MCMC) : enlarged system $\Leftrightarrow$ $\overbrace{\mathcal{M} \times \mathcal{M} \times \cdots \times \mathcal{M}}^{A+1} = \{(x_0, x_1, \ldots, x_A)\}$ (◯)
  [Swendsen-Wang 1986, Geyer 1991]
  most of relevant steps can be done in parallel processes

Tempered LTM (2/3) [MF-Umeda 2017]

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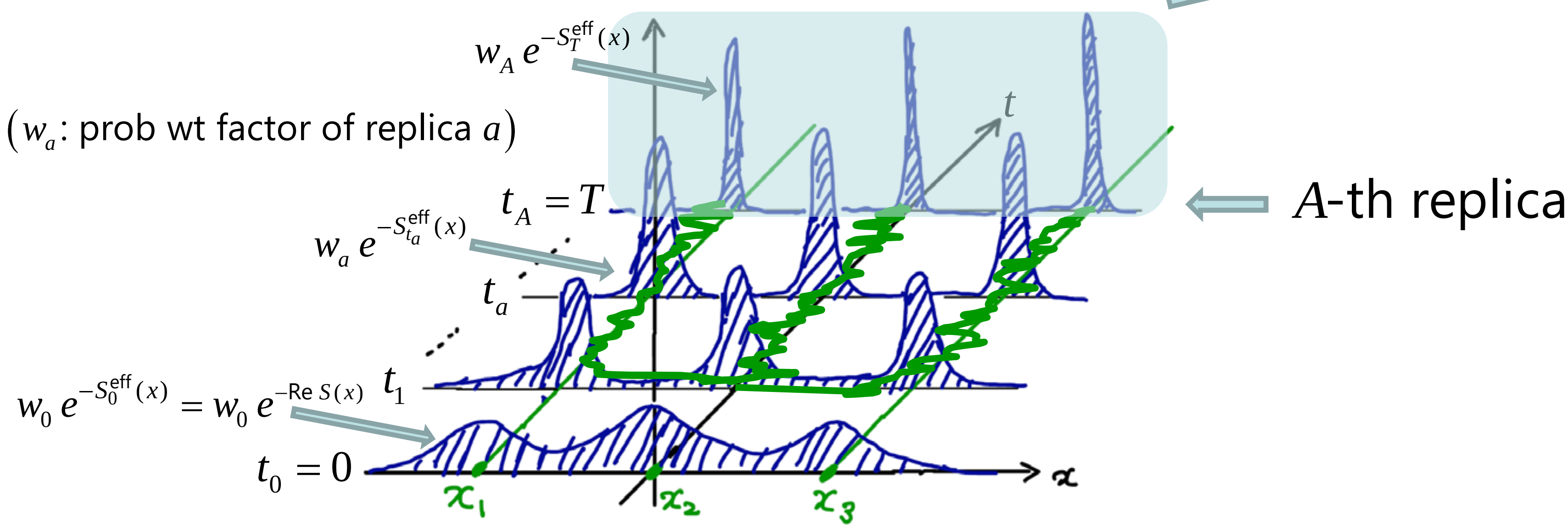

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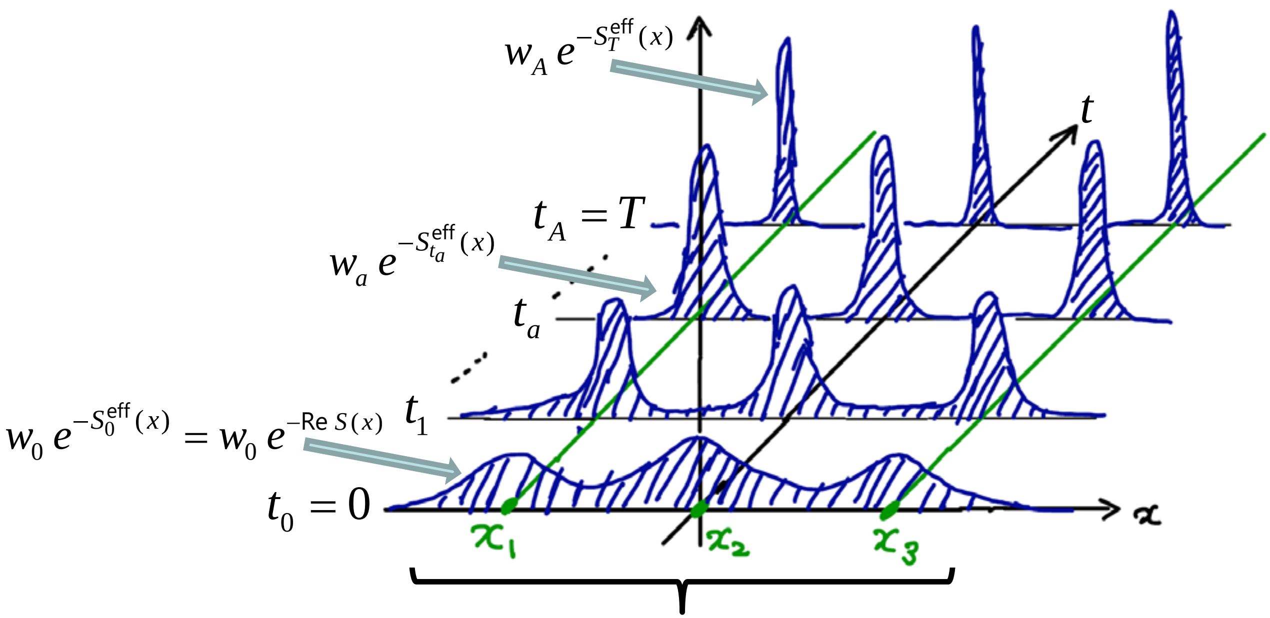
  [Swendsen-Wang 1986, Geyer 1991]

Tempered LTM (3/3)

[MF-Umeda 2017, MF-Matsumoto-Umeda 2019]

Important points in TLTM:

(1) **NO "tiny overlap problem" in TLTM**



Distribution functions have peaks at the same positions x_σ for varying tempering parameter (which is t in our case)

⇨ We can expect significant overlap between adjacent replicas!

(2) **The growth of computational cost due to the tempering can be compensated by the increase of parallel processes**

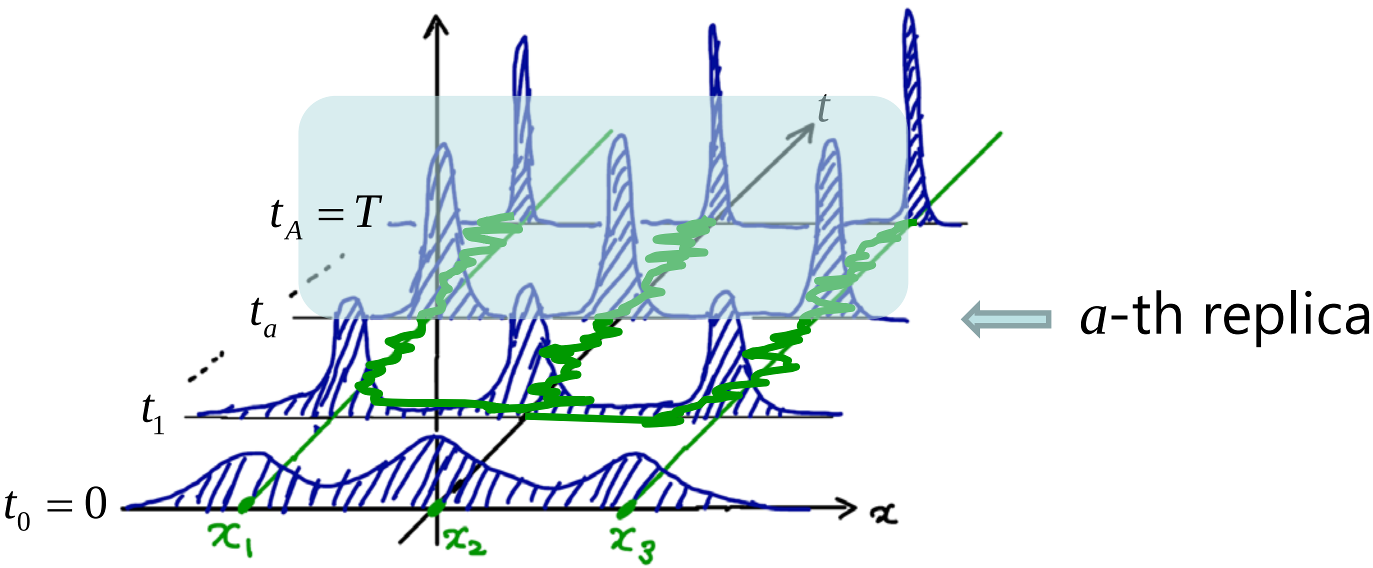
We actually can go further...

[MF-Matsumoto-Umeda 2019]

Consider the estimates of $\langle \mathcal{O} \rangle_S$ at various flow times t_a:

$$\langle \mathcal{O} \rangle_S = \frac{\langle e^{i\theta_{t_a}(x)} \mathcal{O}(z_{t_a}(x)) \rangle_{S^{\text{eff}}_{t_a}}}{\langle e^{i\theta_{t_a}(x)} \rangle_{S^{\text{eff}}_{t_a}}} \approx \frac{\sum_{k=1}^{N_{\text{samp}}} e^{i\theta_{t_a}(x^{(k)})} \mathcal{O}(z_{t_a}(x^{(k)}))}{\sum_{k=1}^{N_{\text{samp}}} e^{i\theta_{t_a}(x^{(k)})}} \equiv \overline{\mathcal{O}}_a \quad (a = 0, 1, \ldots, A)$$

Here the estimation on the RHS is made by using the subsample at t_a:



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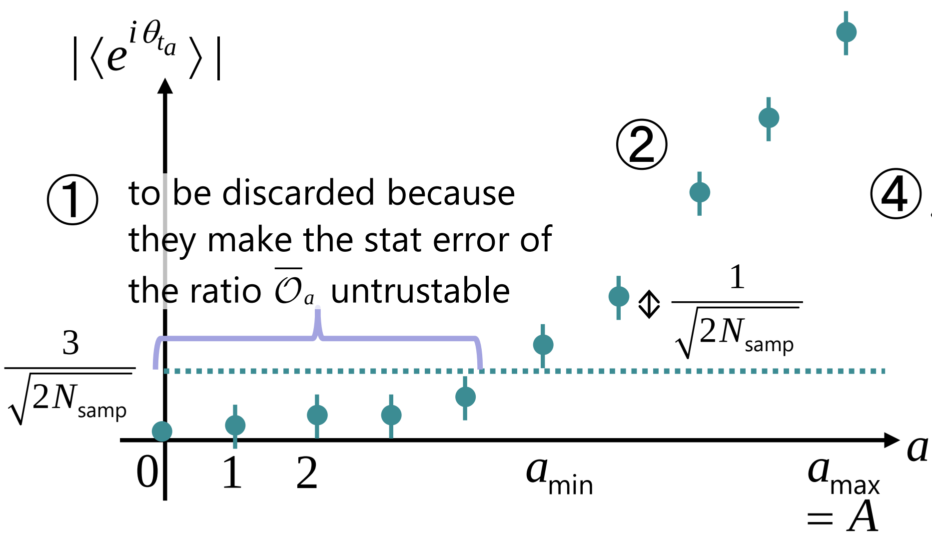
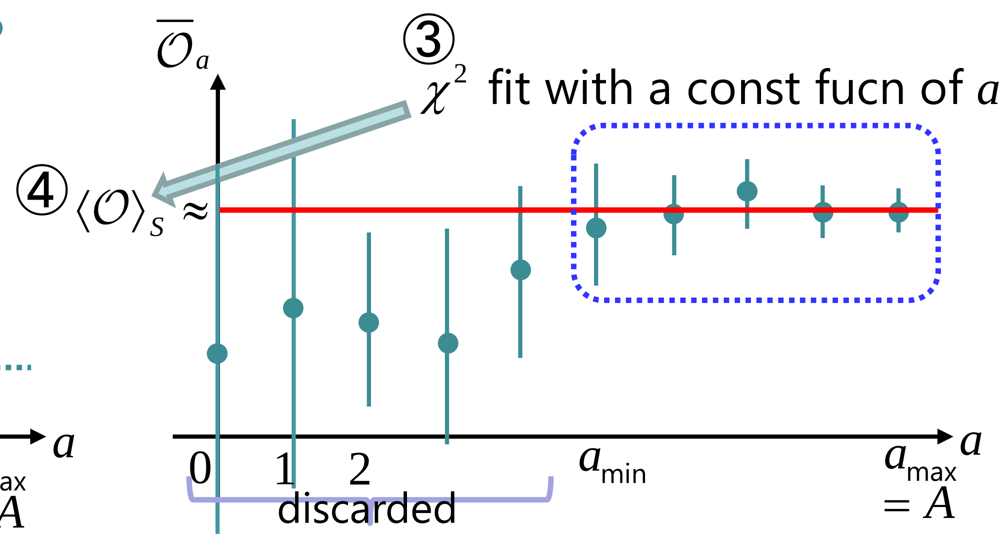
The LHS must be independent of a due to Cauchy's theorem

The RHS must be the same for all a's within the statistical error margin if the system is in global equilibrium and the sample size is large enough

This gives a method with criteria for precise estimation in the TLTM!





4. Applying the TLTM to the Hubbard model

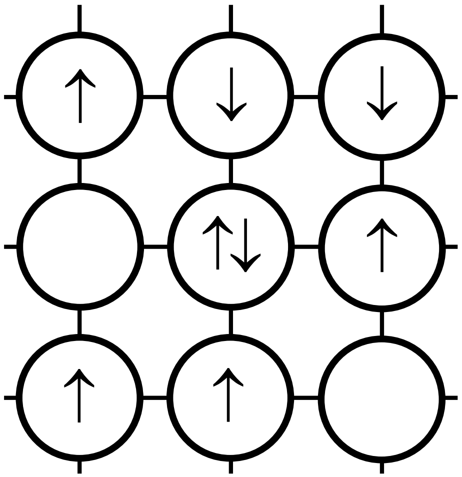
[MF-Matsumoto-Umeda 2019]

Hubbard model (1/2)

Hubbard model **[Hubbard 1963]**

modeling electrons in a solid

- $c^\dagger_{\mathbf{x},\sigma},\ c_{\mathbf{x},\sigma}$: creation/anihilation op of an electron
  on site $\mathbf{x}$ with spin $\sigma(=\uparrow,\downarrow)$



$(N_S$: # of sites$)$

- Hamiltonian

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

$n_{\mathbf{x},\sigma}\equiv c^\dagger_{\mathbf{x},\sigma}c_{\mathbf{x},\sigma}$

$\kappa(>0)$: hopping parameter

μ : chemical potential

$U(>0)$: strength of on-site replusive potential

$n_{\mathbf{x},\sigma}\to n_{\mathbf{x},\sigma}-1/2$ s.t. $\mu=0\Leftrightarrow$ half-filling $\sum_{\sigma=\uparrow,\downarrow}\left\langle n_{\mathbf{x},\sigma}-1/2\right\rangle=0$

$$H=\underbrace{-\kappa\sum_{\mathbf{x},\mathbf{y}}\sum_{\sigma}K_{\mathbf{xy}}\,c^\dagger_{\mathbf{x},\sigma}c_{\mathbf{y},\sigma}-\mu\sum_{\mathbf{x}}\left(n_{\mathbf{x},\uparrow}+n_{\mathbf{x},\downarrow}-1\right)}_{H_1}+\underbrace{U\sum_{\mathbf{x}}\left(n_{\mathbf{x},\uparrow}-\frac{1}{2}\right)\left(n_{\mathbf{x},\downarrow}-\frac{1}{2}\right)}_{H_2}$$

(fermion bilinear) (four fermion)

Hubbard model (2/2)

- Grand partition function (continuous imaginary time) : $Z^{\text{cont}}_{\beta,\mu} = \mathrm{tr}\, e^{-\beta H}$

- Quantum Monte Carlo

$$e^{-\beta H} = e^{-\beta(H_1+H_2)} = \left(e^{-\epsilon(H_1+H_2)}\right)^{N_t} \cong \left(e^{-\epsilon H_1} e^{-\epsilon H_2}\right)^{N_t} \quad (\beta = N_t \epsilon)$$

⇨ Transform $e^{-\epsilon H_2} = \prod_{\mathbf{x}} e^{-\epsilon U \left(n_{\mathbf{x},\uparrow} - 1/2\right)\left(n_{\mathbf{x},\downarrow} - 1/2\right)}$ to a fermion bilinear using a boson ϕ

⇨ $$Z_{\beta,\mu} = \int [d\phi] e^{-S[\phi_{\ell,\mathbf{x}}]} \equiv \int \prod_{\ell=1}^{N_t} \prod_{\mathbf{x}} d\phi_{\ell,\mathbf{x}}\, e^{-(1/2)\sum_{\ell,\mathbf{x}} \phi_{\ell,\mathbf{x}}{}^2} \det M_{\uparrow}[\phi] \det M_{\downarrow}[\phi]$$

$$M_{\uparrow/\downarrow}[\phi] \equiv 1_{N_s} + e^{\pm\beta\mu} \prod_{\ell} \left(e^{\epsilon\kappa K} \,\mathrm{diag}[e^{\pm i\sqrt{\epsilon U}\phi_{\ell,\mathbf{x}}}] \right) \; : \; N_s \times N_s \text{ matrix}$$

This gives complex actions for non half-filling states $(\mu \neq 0)$

(NB: For half filling $(\mu = 0)$

$$\det M_{\uparrow}[\phi] \det M_{\downarrow}[\phi] = \left|\det M_{\uparrow}[\phi]\right|^2 \geq 0$$

$\Rightarrow$ No sign problem)

⇨ We apply the Tempered LTM to this system $\left(\begin{array}{l} x = (x^i) = (\phi_{\ell,\mathbf{x}}) \in \mathbb{R}^N \\ i = 1, \ldots, N \;\; (N = N_s N_t) \end{array} \right)$

[MF-Matsumoto-Umeda 2019]

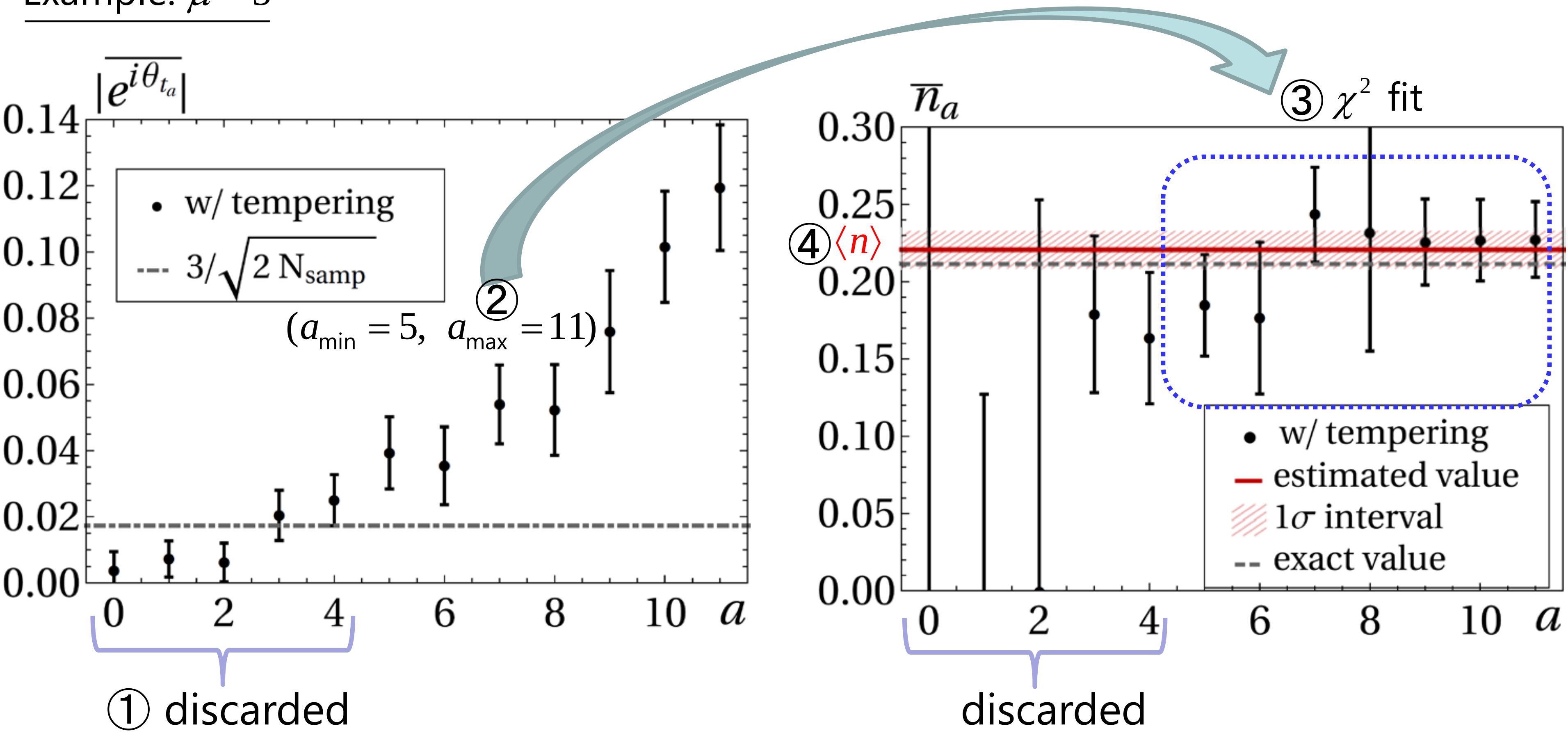
Results for 2D lattice (1/4)

[MF-Matsumoto-Umeda 2019]

imaginary time : 5 steps $(N_t = 5)$
spatial lattice: 2D periodic lattice with $N_s = 2\times 2$
$\beta = 1, \quad \kappa = 3, \quad U = 13$
sample size: 5,000~25,000 depending on μ

$$\langle n \rangle = \frac{\langle e^{i\theta_{t_a}(x)}\, n(z_{t_a}(x))\rangle_{S^{\rm eff}_{t_a}}}{\langle e^{i\theta_{t_a}(x)}\rangle_{S^{\rm eff}_{t_a}}} \approx \overline{n}_a$$

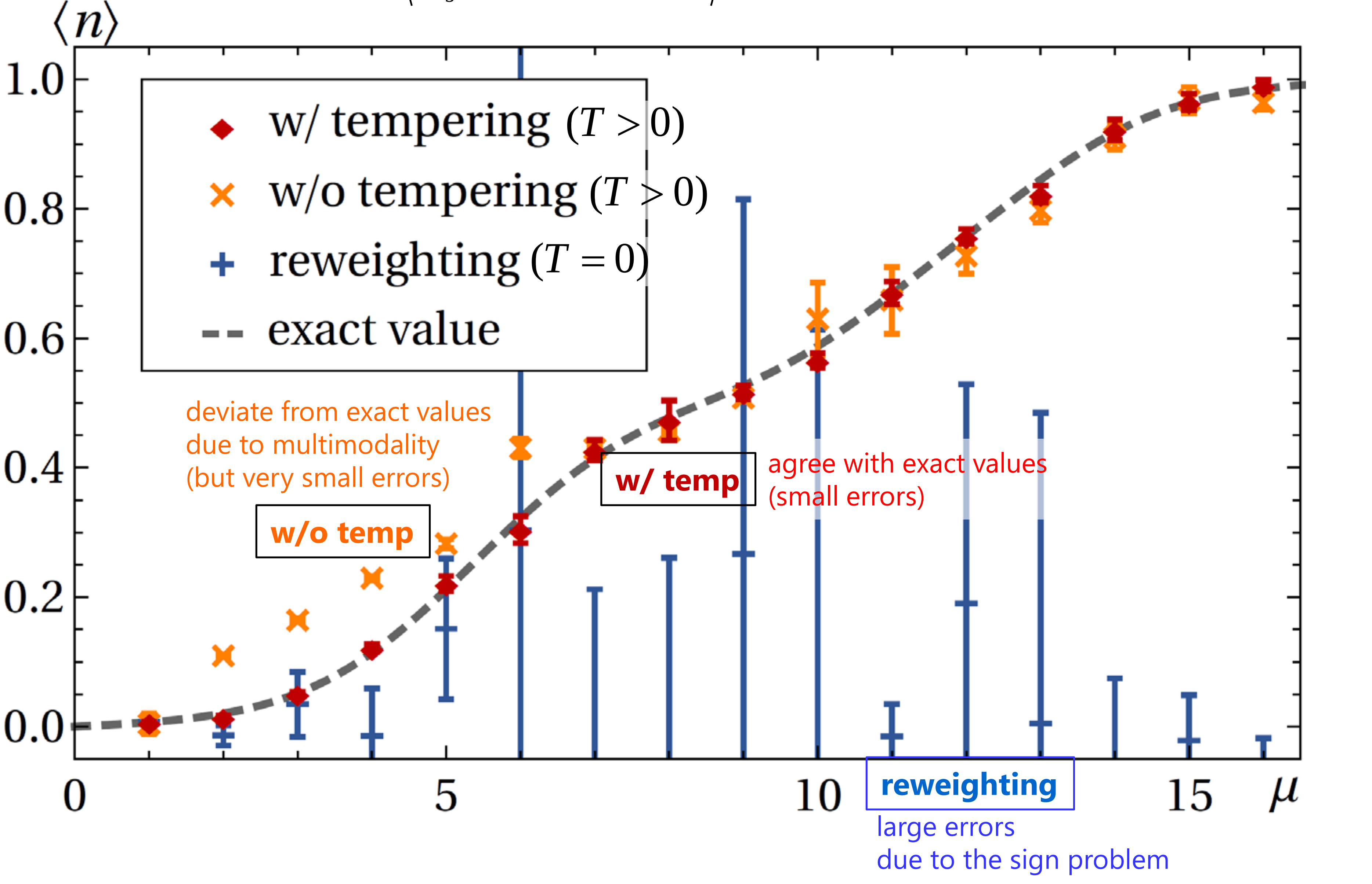
Example: $\mu = 5$



Results for 2D lattice (2/4)

[MF-Matsumoto-Umeda 2019]

$\begin{bmatrix} N_t = 5, N_s = 2\times 2 \\ \beta = 1, \quad \kappa = 3, \quad U = 13 \end{bmatrix}$ $\quad \langle n \rangle = \left\langle \frac{1}{N_s} \sum_{\mathbf{x}} \left(n_{\mathbf{x},\uparrow} + n_{\mathbf{x},\downarrow} - 1 \right) \right\rangle$



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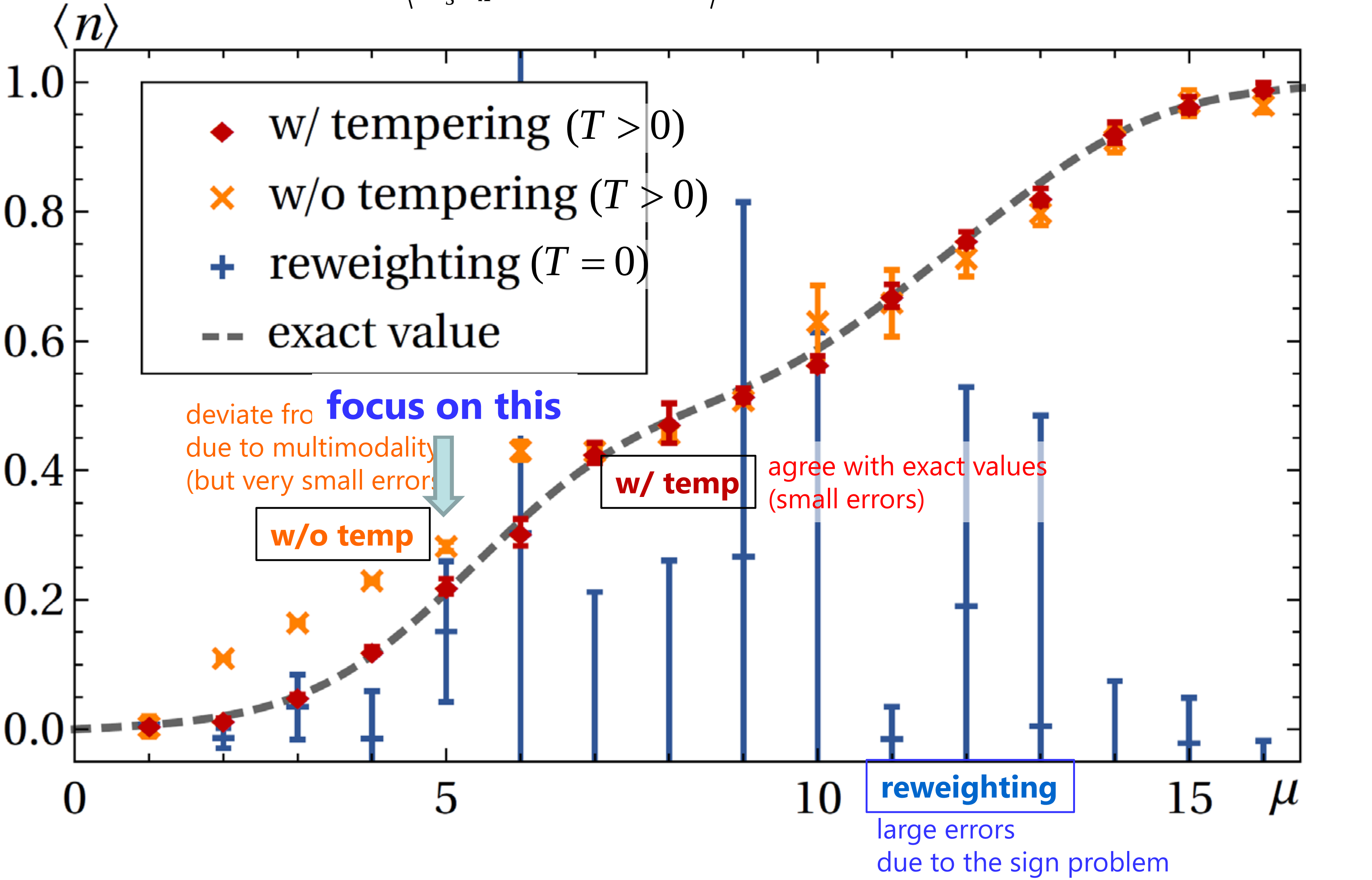
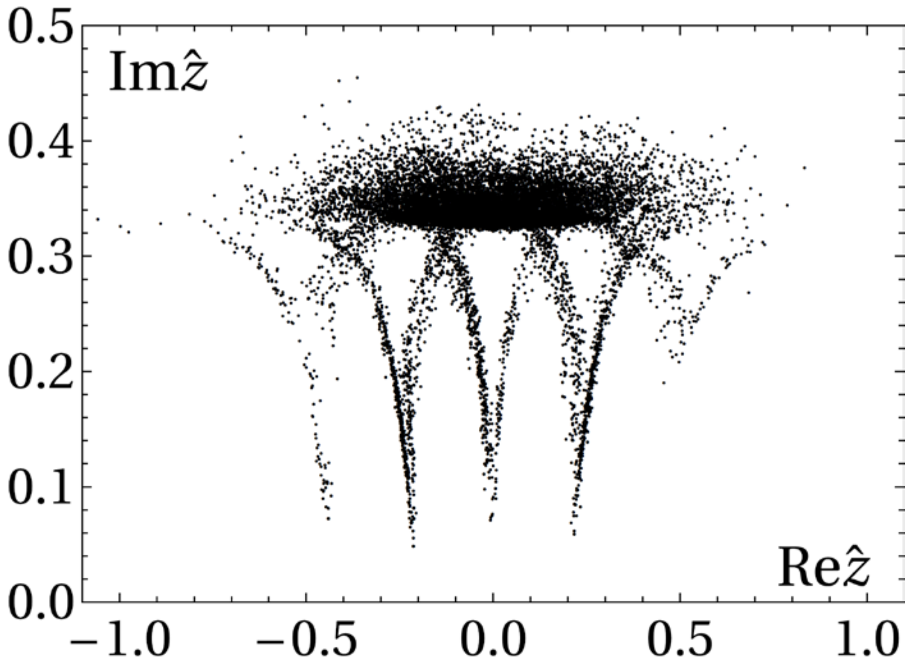


Results for 2D lattice (3/4)

[MF-Matsumoto-Umeda 2019]

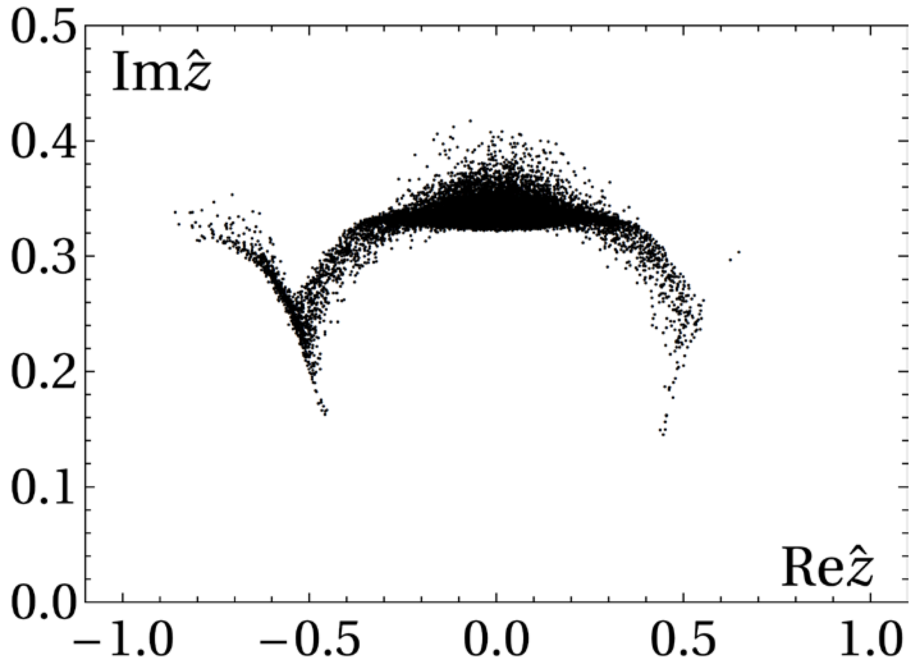
Distribution of flowed configs at flow time $T = 0.5$ $(\mu = 5)$
(projected on a plane)

w/ temp



distributed widely
over many thimbles

w/o temp

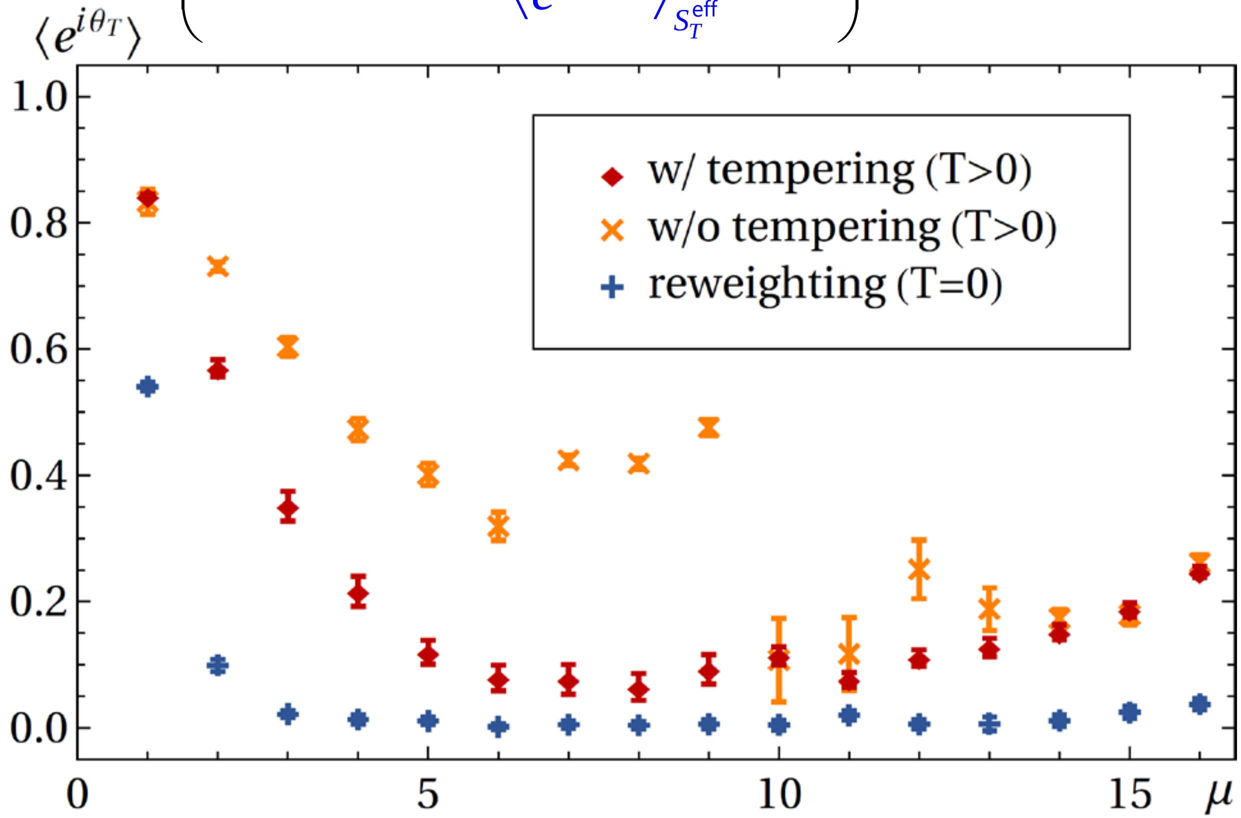


distributed over only
a small number of thimbles

Results for 2D lattice (4/4)

[MF-Matsumoto-Umeda 2019]

phase average $\left(\langle \mathcal{O}(x) \rangle = \frac{\langle e^{i\theta_T(x)}\, \mathcal{O}(z_T(x)) \rangle_{S_T^{\rm eff}}}{\langle e^{i\theta_T(x)} \rangle_{S_T^{\rm eff}}} \right)$



When only a single (or very few) thimble(s) is sampled, the phase average can become larger than that in the correct sampling due to the absence of phase mixtures among thimbles

It is generally dangerous to regard the phase average as an index of the "resolution of the sign problem"

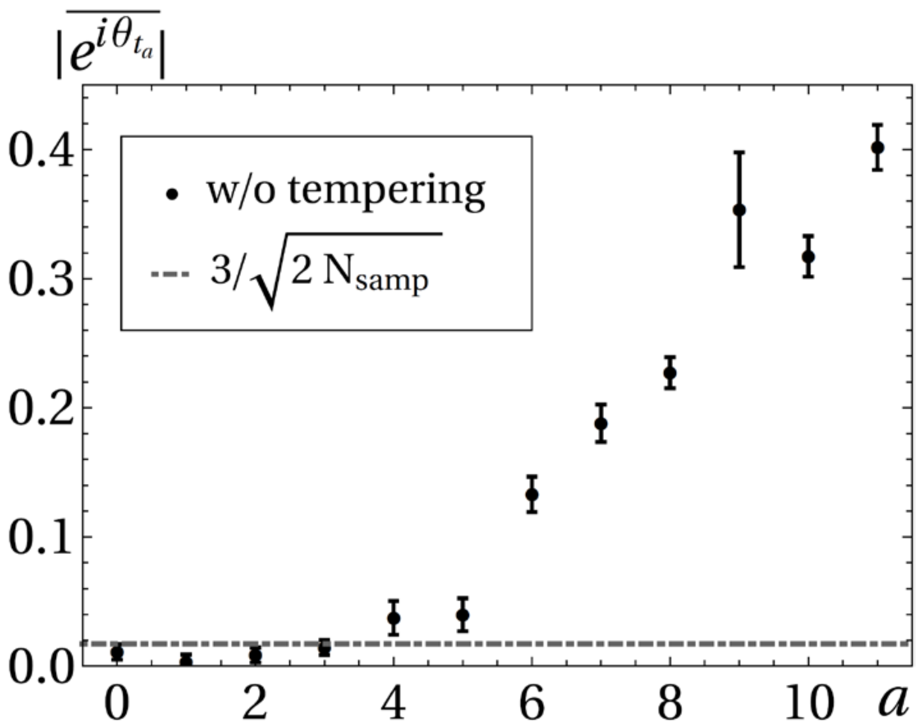
Comment on the GLTM

[MF-Matsumoto-Umeda 2019]

imaginary time : 5 steps ($N_t = 5$)
spatial lattice: 2D periodic lattice with $N_s = 2\times 2$
$\beta = 1, \quad \kappa = 3, \quad U = 13$
sample size: 5,000~25,000 depending on μ

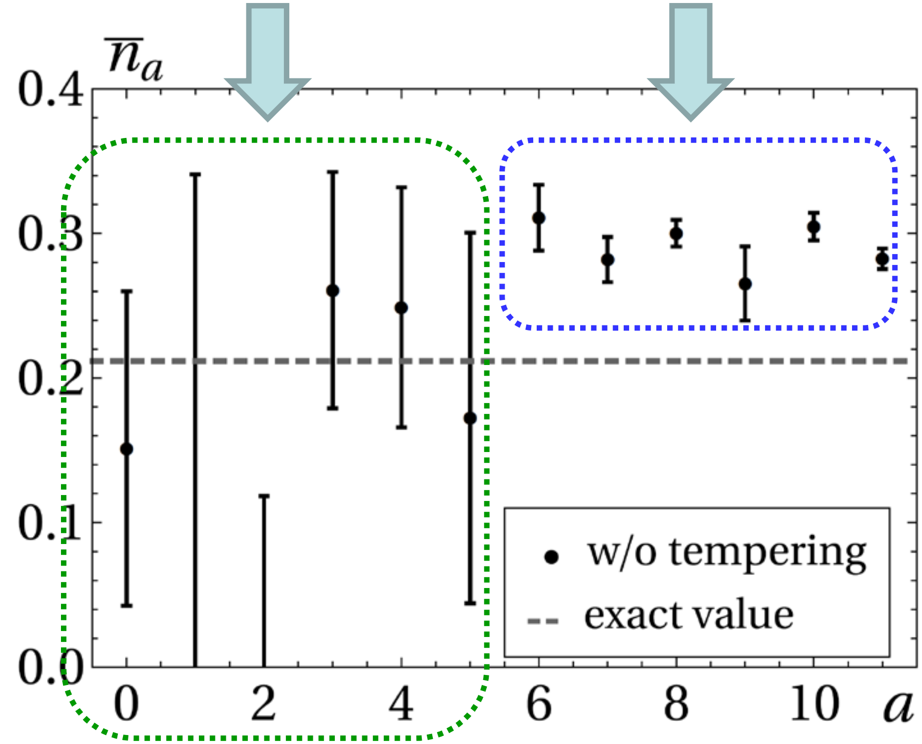
$$\left(\langle n \rangle = \frac{\langle e^{i\theta_{t_a}(x)}\, n(z_{t_a}(x)) \rangle_{S^{\mathrm{eff}}_{t_a}}}{\langle e^{i\theta_{t_a}(x)} \rangle_{S^{\mathrm{eff}}_{t_a}}} \approx \overline{n}_a \right)$$

Example: $\mu = 5$



large stat errors (due to sign problem)

wrong value (due to multimodality)



It is a hard task to find an intermediate flow time that solves both sign problem and multimodality

5. Conclusion and outlook

Conclusion and outlook

What we have done:

- We proposed the tempered Lefschetz thimble method (TLTM) as a versatile method to solve the numerical sign problem
- We further developed it and found an algorithm to estimate expec. values with a criterion ensuring global equilibrium and the sample size (the key: $\overline{\mathcal{O}}_a$ should not depend on replica a due to Cauchy's theorem)
- GLTM can easily give incorrect results or large ambiguities
- TLTM works for the Hubbard model and gives correct results, avoiding both the sign and multimodal problems simultaneously

Outlook:

- Investigate the Hubbard model of larger temporal and spatial sizes to understand the phase structure [computational cost: $O(N^{3\sim4})$]
- More generally, apply the TLTM to the following three typical subjects: **[MF-Matsumoto-Umeda, work in progress]**

  ① Finite density QCD
  ② Quantum Monte Carlo (incl. the Hubbard model)
  ③ Real time QM/QFT
- Develop a more efficient algorithm with less computational cost

Thank you.

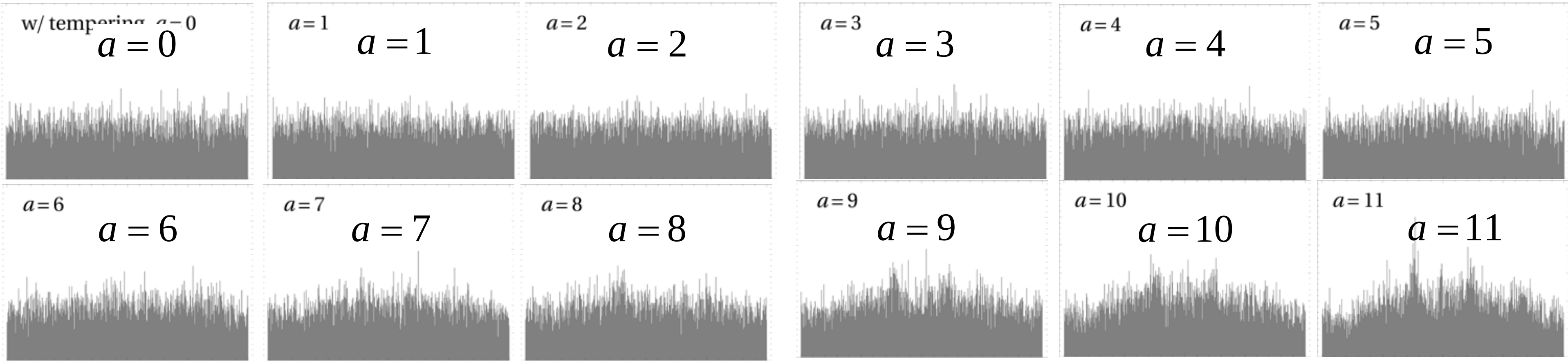
Backups

Results for 2D lattice (4/5)

[MF-Matsumoto-Umeda 2019]

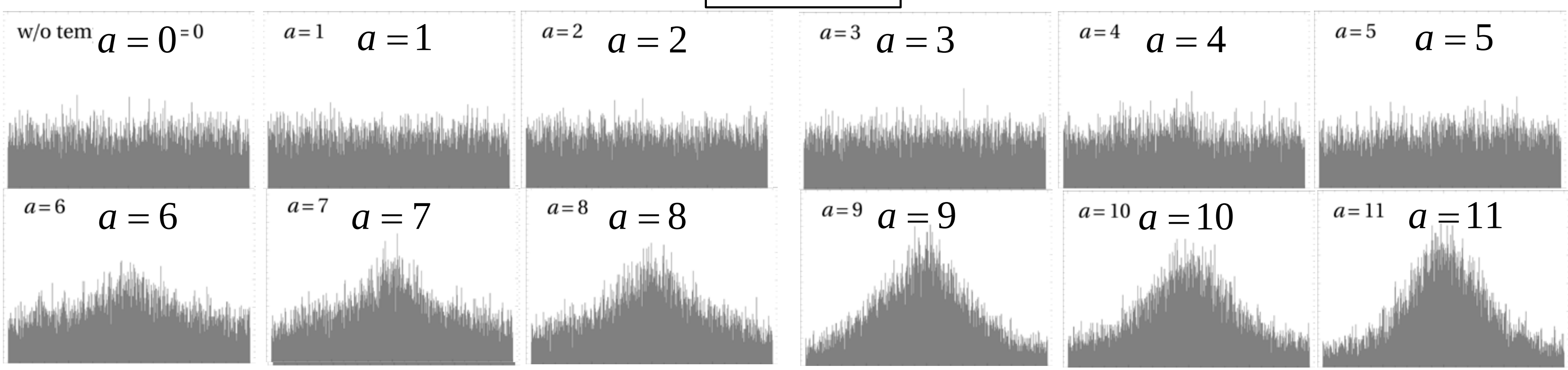
Histogram of $\theta_{t_a} \in [-\pi, \pi]$

w/ temp



many peaks (may not be so obvious because there are so many peaks and the peaks are broadened by Jacobian)

w/o temp



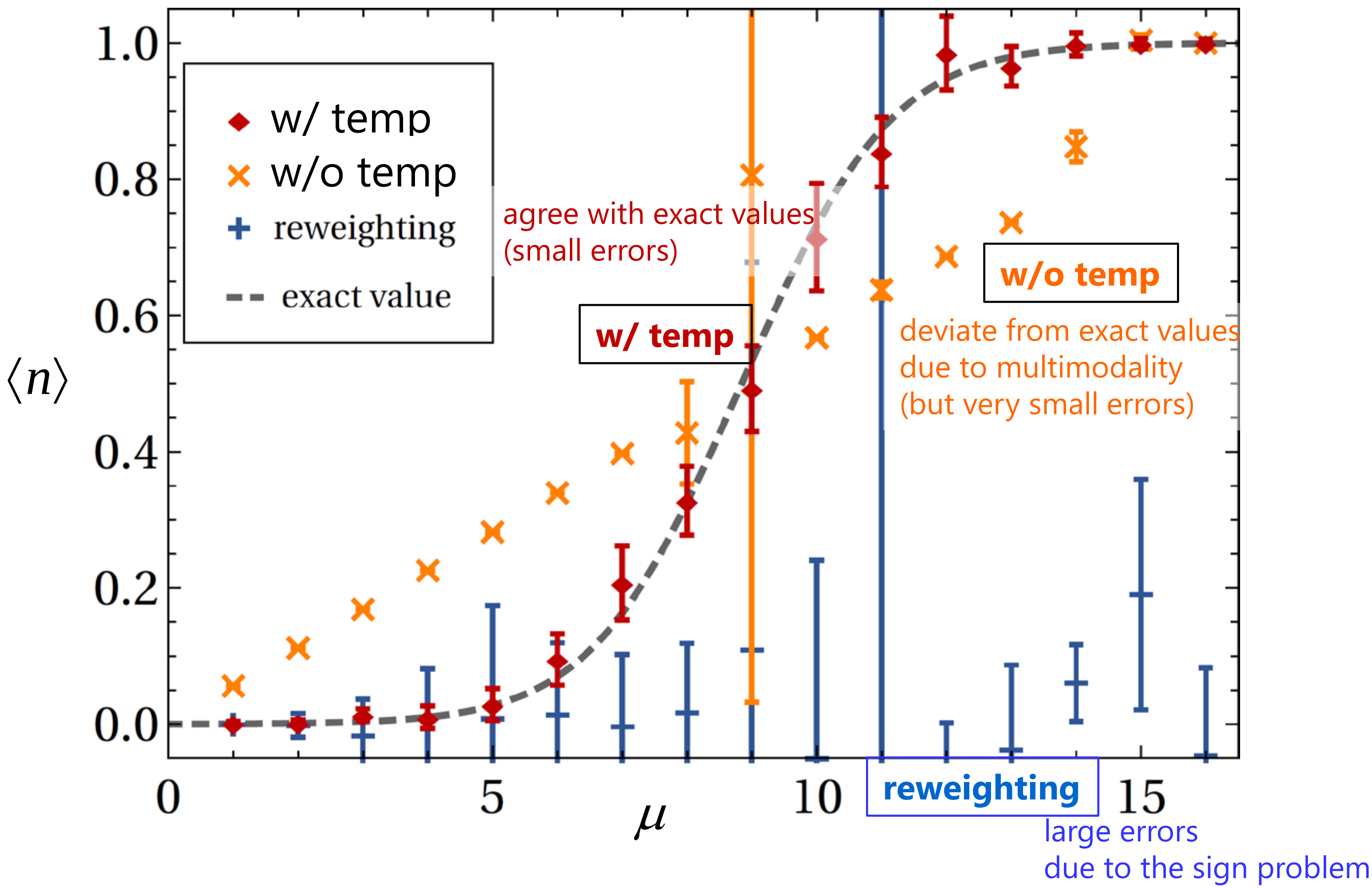
unimodal distribution

Results for 1D lattice (1/3)

[MF-Matsumoto-Umeda 2019]

imaginary time : 2 steps $(N_t = 2)$
spatial lattice: 1D periodic lattice with $N_s = 2$
$\beta = 1, \quad \kappa = 1, \quad U = 16$
sample size: 5,000

number density $n = \frac{1}{N_s} \sum_x (n_{x,\uparrow} + n_{x,\downarrow} - 1)$



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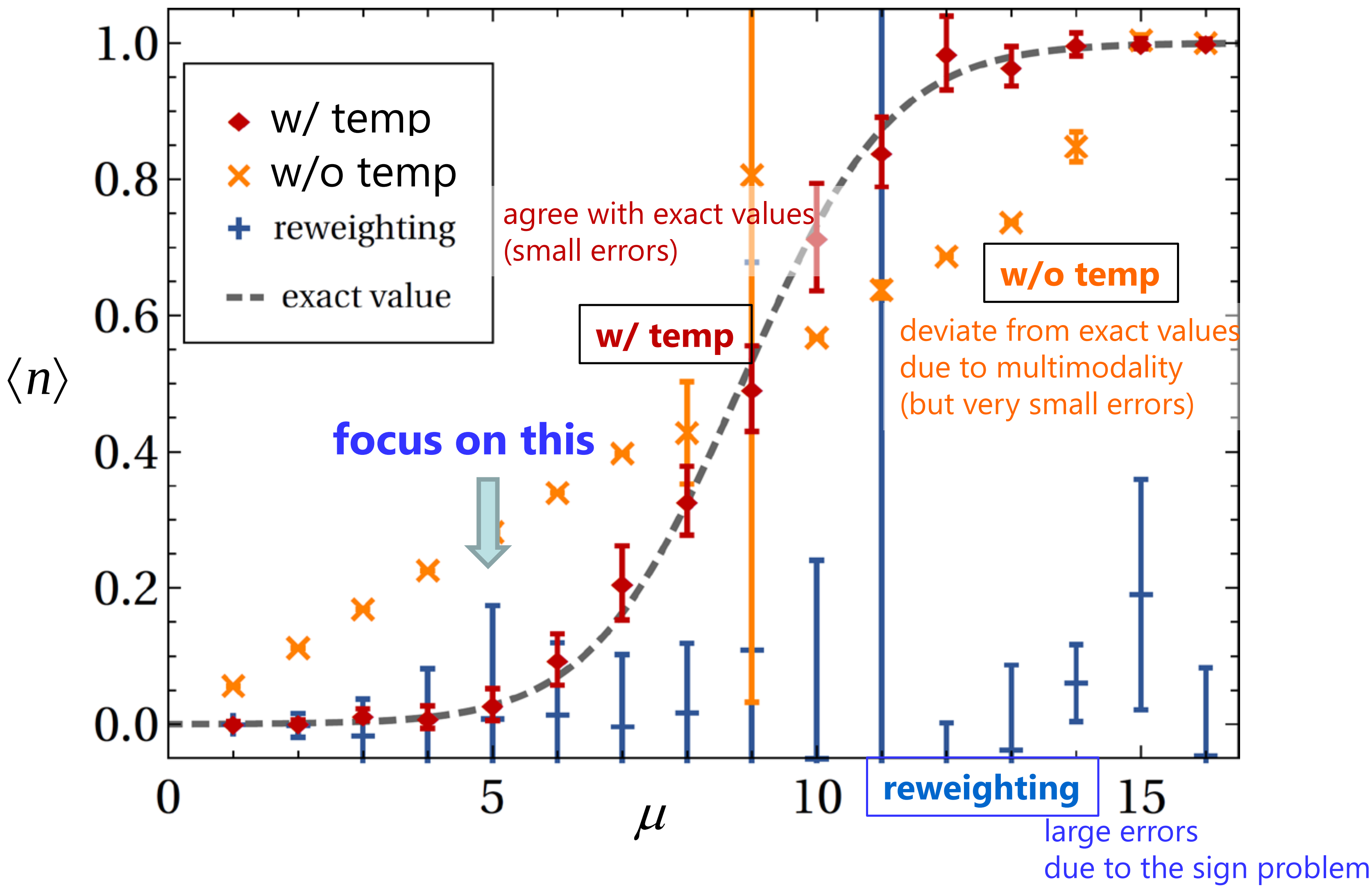


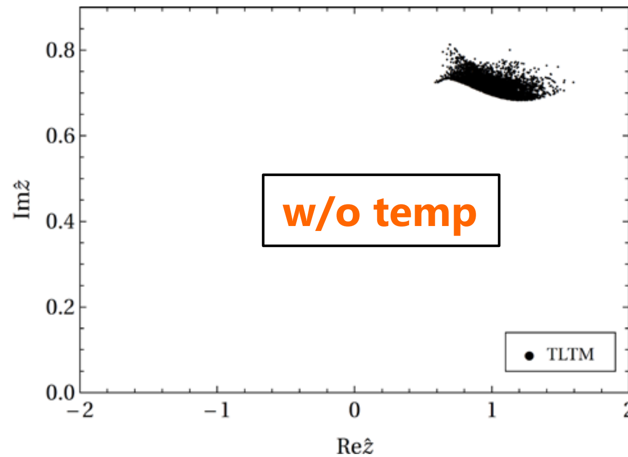
Results for 1D lattice (2/3)

[MF-Matsumoto-Umeda 2019]

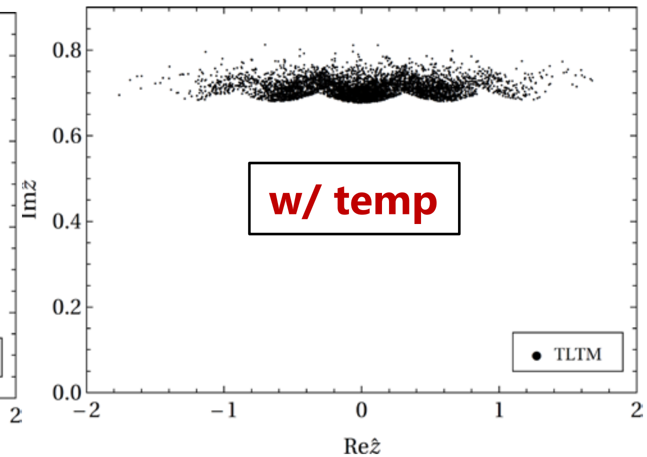
Distribution of flowed configs at flow time $T = 0.4$

(projected on a plane)

w/o temp

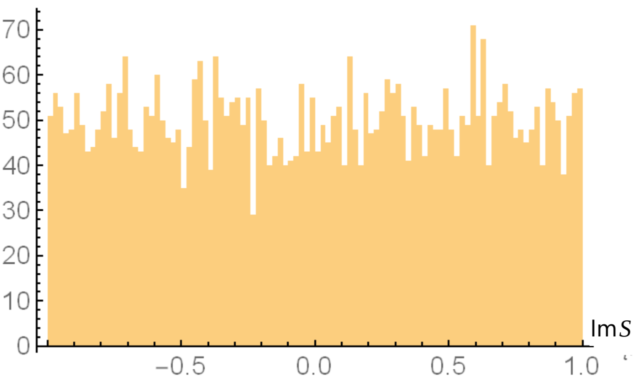


w/ temp



Histogram of ImS(z)/π

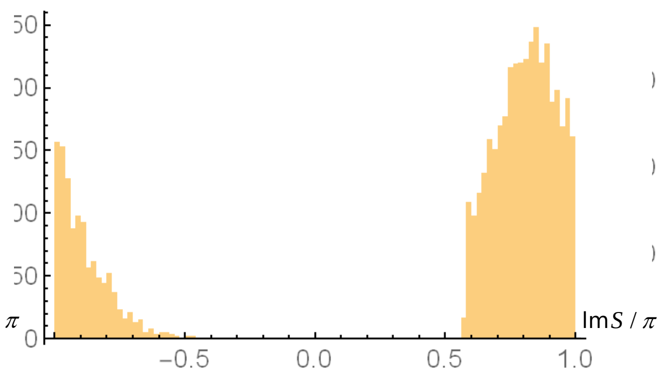
reweighting



distributing uniformly
from −π to +π

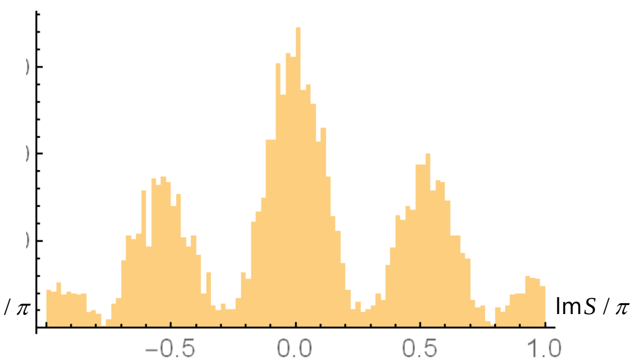
⇨ severe sign problem

w/o temp



peaked at a single angle ~0.8 π
due to the trap to a single thimble
(errors become small
because the thimble is well sampled)

w/ temp



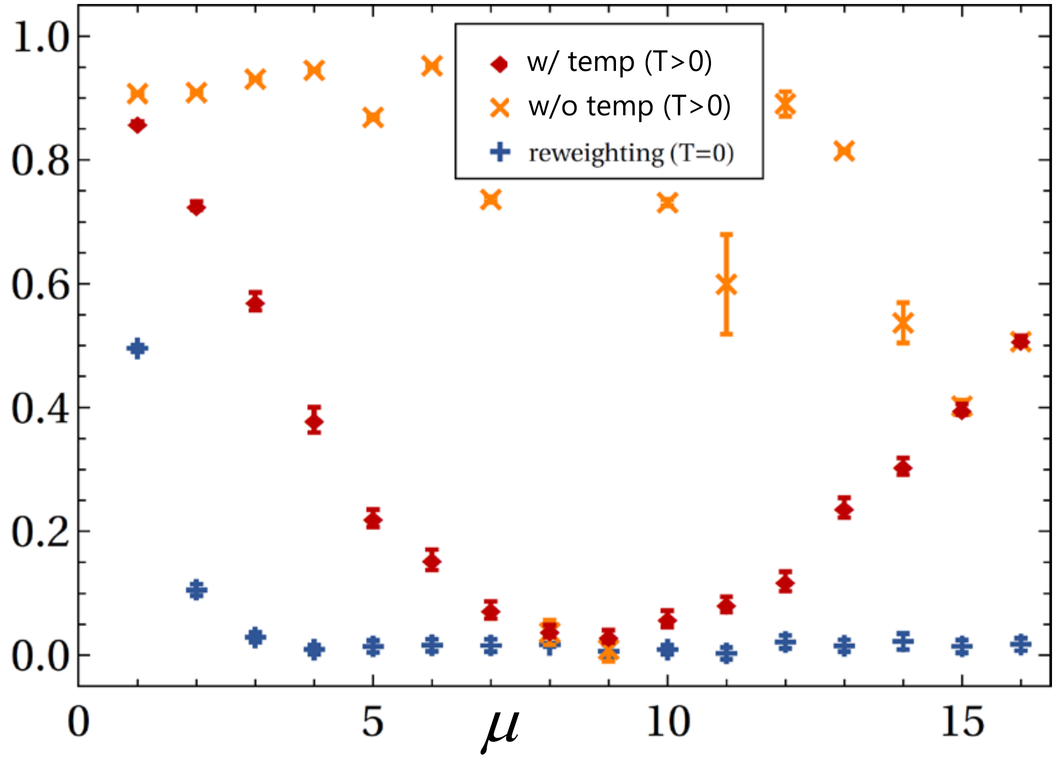
peaked at several angles
because of sufficient transitions
among thimbles
(errors become a bit larger
due to the small size of sampling)

Results for 1D lattice (3/3)

[MF-Matsumoto-Umeda 2019]

phase average $\left(\langle \mathcal{O}(x) \rangle = \dfrac{\langle e^{i\theta_T(x)}\, \mathcal{O}(z_T(x)) \rangle_{S_T^{\mathrm{eff}}}}{\langle e^{i\theta_T(x)} \rangle_{S_T^{\mathrm{eff}}}} \right)$

$\left| \langle e^{i\theta_T(x)} \rangle_{S_T^{\mathrm{eff}}} \right|$



When only a single (or very few) thimble(s) is sampled, the phase average can become larger than the correct sampling due to the absence of phase mixtures among thimbles

⇨ It is generally dangerous to regard the phase average as an index of the "resolution of the sign problem"