# 符号問題と tempered Lefschetz thimble法

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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, to appear in PRD]
-- **MF**, **Matsumoto** and **Umeda**, " Implementing the HMC algorithm on the tempered Lefschetz thimble method" [arXiv:1912.xxxxx]

**Matsumoto's poster**

Also, for the geometrical optimization of tempering algorithms and its application to QG :

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

# 1. Introduction

# Overview

The **numerical 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

-- explain what the sign problem is

-- argue that **[MF-Umeda 1703.00861, MF-Matsumoto-Umeda 2019]**
a new algorithm "Tempered Lefschetz thimble method" (TLTM)
is a promising method towards solving the sign problem,
by exemplifying its effectiveness for:

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

# Sign problem

Our main concern is to estimate: $\langle \mathcal{O}(x) \rangle_S \equiv \dfrac{\int dx\, e^{-S(x)} \mathcal{O}(x)}{\int dx\, e^{-S(x)}}$

$$\begin{cases} x = (x^i) \in \mathbb{R}^N\text{: dynamical variable (real-valued)} \\ S(x)\text{: action, } \mathcal{O}(x)\text{: observable} \end{cases}$$

Markov chain Monte Carlo (MCMC) simulation:

probability distribution function

When $S(x) \in \mathbb{R}$, one can regard $p_{\text{eq}}(x) \equiv e^{-S(x)} / \int dx\, e^{-S(x)}$ as a PDF:

$$0 \le p_{\text{eq}}(x) \le 1, \quad \int dx\, p_{\text{eq}}(x) = 1$$

⇨ Generate a sample $\{x^{(k)}\}_{k=1,\ldots,N_{\text{conf}}}$ from $p_{\text{eq}}(x)$

⇨ $\langle \mathcal{O}(x) \rangle \approx \dfrac{1}{N_{\text{conf}}} \sum_{k=1}^{N_{\text{conf}}} \mathcal{O}(x^{(k)})$

Sign problem:

When $S(x) = S_R(x) + i\, S_I(x) \in \mathbb{C}$, one cannot regard $e^{-S(x)} / \int dx\, e^{-S(x)}$ as a PDF

⇨ Reweighting method :

# Sign problem

Our main concern is to estimate: $\langle \mathcal{O}(x) \rangle_S \equiv \dfrac{\int dx\, e^{-S(x)} \mathcal{O}(x)}{\int dx\, e^{-S(x)}} = \dfrac{\int dx\, e^{-S_R(x)} e^{-i S_I(x)} \mathcal{O}(x)}{\int dx\, e^{-S_R(x)} e^{-i S_I(x)}}$

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⇒ Reweighting method : treat $e^{-S_R(x)} / \int dx\, e^{-S_R(x)}$ as a PDF

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⇨ Reweighting method : treat $e^{-S_R(x)} / \int dx\, e^{-S_R(x)}$ as a PDF

⇨ $\langle \mathcal{O}(x) \rangle_S \equiv \dfrac{\left\langle e^{-i S_I(x)} \mathcal{O}(x) \right\rangle_{S_R}}{\left\langle e^{-i S_I(x)} \right\rangle_{S_R}} = \dfrac{e^{-O(N)}}{e^{-O(N)}} = O(1) \quad (N : \text{DOF})$

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$\Rightarrow$ Generate a sample $\{x^{(k)}\}_{k=1,\ldots,N_{\rm conf}}$ from $p_{\rm eq}(x)$

$\Rightarrow$ $\langle \mathcal{O}(x) \rangle \approx \dfrac{1}{N_{\rm conf}} \displaystyle\sum_{k=1}^{N_{\rm conf}} \mathcal{O}(x^{(k)})$

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$\Rightarrow$ Reweighting method : treat $e^{-S_R(x)} / \int dx\, e^{-S_R(x)}$ as a PDF

$\Rightarrow$ $\langle \mathcal{O}(x) \rangle_S \equiv \dfrac{\langle e^{-i S_I(x)} \mathcal{O}(x) \rangle_{S_R}}{\langle e^{-i S_I(x)} \rangle_{S_R}} \approx \dfrac{e^{-O(N)} \pm O(1/\sqrt{N_{\rm conf}})}{e^{-O(N)} \pm O(1/\sqrt{N_{\rm conf}})}$ $\quad \begin{pmatrix} N\text{ : DOF} \\ N_{\rm conf}\text{ : sample size} \end{pmatrix}$

$\Rightarrow$ Require $O(1/\sqrt{N_{\rm conf}}) < e^{-O(N)}$ $\Rightarrow$ $\boxed{N_{\rm conf} \simeq e^{O(N)}}$ sign problem!

# Approaches to the sign problem

Various approaches:

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

(2) (Generalized) Lefschetz thimble method ((G)LTM) **[Cristoforetti et al. 2012, ...] [Alexandru et al. 2015, ...]**

(3) ...

Advantages/disadvantages:

(1) CLM
Pros: fast $\propto O(N)$ $(N: \text{DOF})$
Cons: "wrong convergence problem" **[Ambjørn-Yang 1985, Aarts et al. 2011, Nagata-Nishimura-Shimasaki 2016]**

(2) LTM
Pros: No wrong convergence problem *iff* only a single thimble is relevant
Cons: Expensive $\propto O(N^3)$ ⇐ Jacobian determinant
Ergodicity problem if more than one thimble are relevant (wrong convergence de facto)

(2′) **TLTM** (Tempered Lefschetz thimble method) **[MF-Umeda 1703.00861, MF-Matsumoto-Umeda 1906.04243]**

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

Pros: Works well even when multiple thimbles are relevant
Cons: Expensive $\propto O(N^{3\sim 4})$ ⇐ 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. Some ongoing work
6. Conclusion and outlook

## 2. (Generalized) Lefschetz thimble method (GLTM)

[Cristoforetti et al. 1205.3996, 1303.7204, 1308.0233]
[Fujii-Honda-Kato-Kikukawa-Komatsu-Sano 1309.4371]
[Alexandru et al. 1512.08764]

# Lefschetz thimble method (1/2)

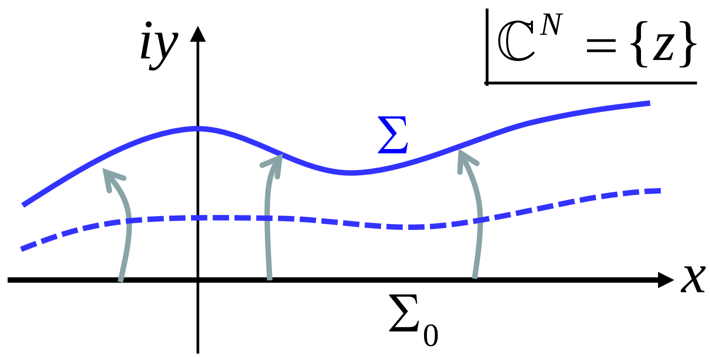
Complexify the variable: $x=(x^i)\in\mathbb{R}^N \;\Rightarrow\; z=(z^i=x^i+iy^i)\in\mathbb{C}^N$

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

Cauchy's theorem

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) :

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



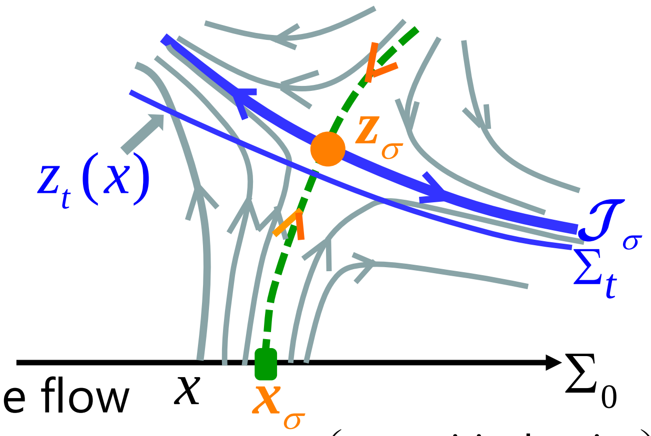

severe sign problem

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

# Lefschetz thimble method (2/2)

Prescription:

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




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

$\Rightarrow$ $\begin{cases} [\mathrm{Re}\,S(z_t)]^\cdot \geq 0 : \text{real part always increases along the flow} \\ [\mathrm{Im}\,S(z_t)]^\cdot = 0 : \text{imaginary part is kept fixed} \quad '' \end{cases}$

( $z_\sigma$ : critical point $(\partial_i S(z_\sigma)=0)$ )

$\Rightarrow$ In $t \to \infty$, $\Sigma_t$ 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:

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

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

$$\det(\partial z_t^i(x)/\partial x^j)\, e^{-S(z_t(x))} \equiv \boxed{e^{-S_t^{\mathrm{eff}}(x)}\, e^{i\theta_t(x)}}$$

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

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

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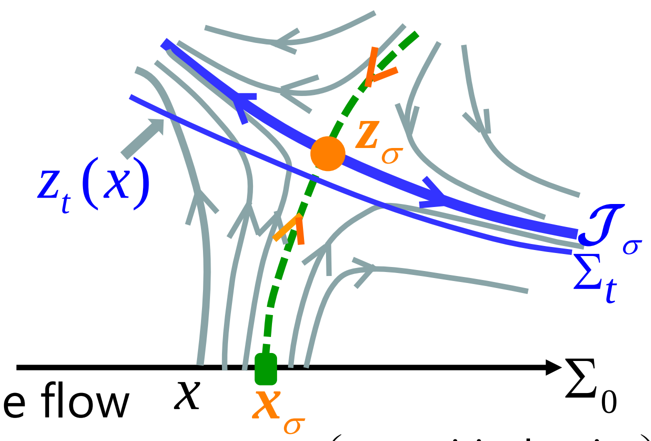


Property: $\left[S(z_t)\right]^\cdot = \partial_i S(z_t)\,\dot{z}_t^i = \left|\partial_i S(z_t)\right|^2 \geq 0$

$\Rightarrow$ $\left\{\begin{array}{l}[\mathrm{Re}\,S(z_t)]^\cdot \geq 0 : \text{real part always increases along the flow} \\ [\mathrm{Im}\,S(z_t)]^\cdot = 0 : \text{imaginary part is kept fixed} \quad ''\end{array}\right.$

$\left( z_\sigma : \dfrac{\text{critical point}}{(\partial_i S(z_\sigma) = 0)} \right)$

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$$\det(\partial z_t^i(x)/\partial x^j)\, e^{-S(z_t(x))} \equiv \boxed{e^{-S_t^{\mathrm{eff}}(x)}\, e^{i\theta_t(x)}}$$

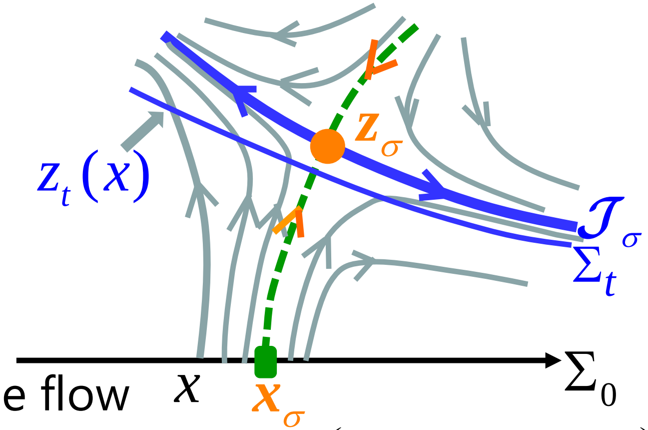
$$= \frac{\left\langle e^{i\theta_t(x)} \mathcal{O}(z_t(x)) \right\rangle_{S_t^{\mathrm{eff}}}}{\left\langle e^{i\theta_t(x)} \right\rangle_{S_t^{\mathrm{eff}}}} = \frac{e^{-e^{-\lambda t} O(N)}}{e^{-e^{-\lambda t} O(N)}}$$

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

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

$$= \frac{O(1)}{O(1)}$$ (no small numbers appear!)

# Lefschetz thimble method (2/2)

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

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$$\det(\partial z_t^i(x)/\partial x^j)\, e^{-S(z_t(x))} \equiv \boxed{e^{-S_t^{\mathrm{eff}}(x)}\, e^{i\theta_t(x)}}$$

$$\boxed{\begin{aligned} e^{-S_t^{\mathrm{eff}}(x)} &\equiv e^{-\mathrm{Re}\,S(z_t(x))} \left| \det(\partial z_t^i(x)/\partial x^j) \right| \\ e^{i\theta_t(x)} &\equiv e^{-i\,\mathrm{Im}\,S(z_t(x)) + i \arg\det(\partial z_t^i(x)/\partial x^j)} \end{aligned}}$$

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

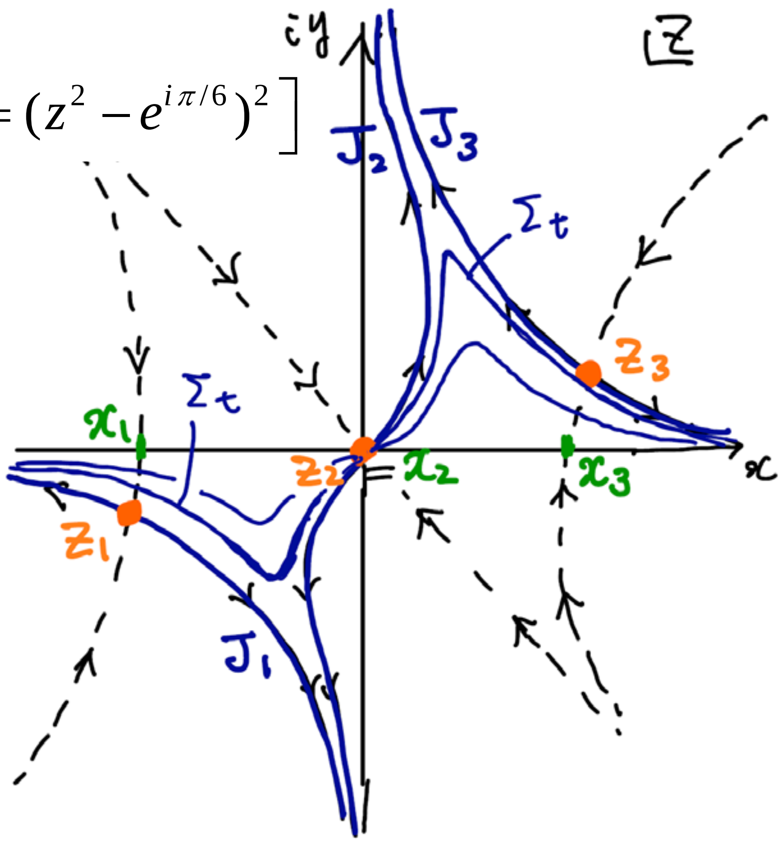
$$= \frac{O(1)}{O(1)} \approx \frac{O(1) + 1/\sqrt{N_{\mathrm{conf}}}}{O(1) + 1/\sqrt{N_{\mathrm{conf}}}}$$

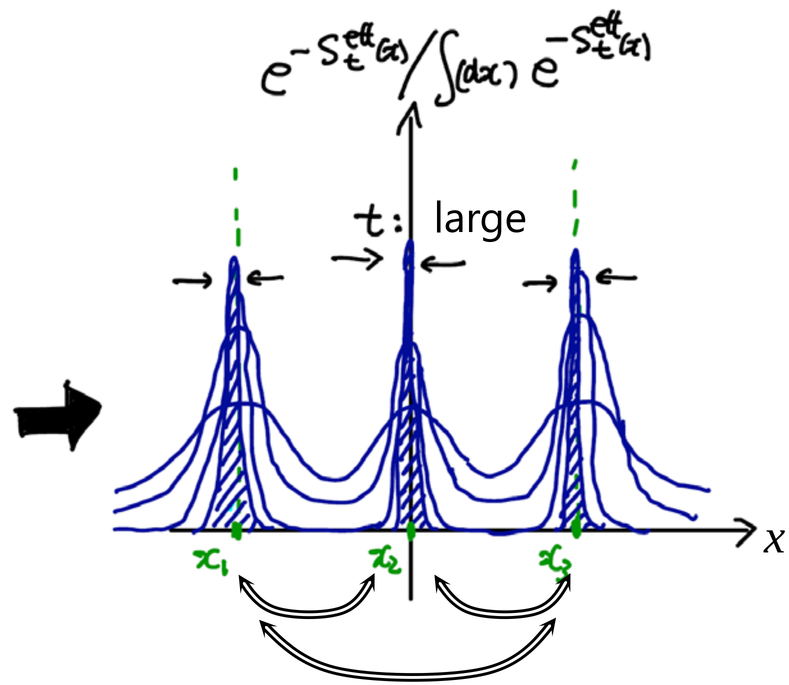
# Multimodal problem and Generalized LTM (1/2)

Flow time $t$ needs to be large enough to solve the sign problem $\left(t = O(\log N)\right)$

However, this introduces a new problem "ergodicity (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 ergodicity problem**

(for small $t$) (for large $t$)

# Multimodal problem and Generalized LTM (2/2)

**Proposal in Generalized LTM:** [Alexandru-Basar-Bedaque-Ridgway-Warrington 1512.08764]

Choose an intermediate value of $T$ s.t. it is large enough for the sign problem but at the same time is not too large for the ergodicity (multimodal) problem

| flow time $(= T)$ | small | medium | large |
|---|---|---|---|
| sign problem | NG | $\triangle$ | **OK** |
| ergodicity problem | **OK** | $\triangle$ | NG |

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

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

**Tempered LTM:** [MF-Umeda 1703.00861]

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

| flow time $(= T)$ | small | medium | large |
|---|---|---|---|
| sign problem | NG | **OK** | **OK** |
| ergodicity problem | **OK** | **OK** | **OK** |

**no fine tuning needed!**

# 3. Tempered Lefschetz thimble method (TLTM)

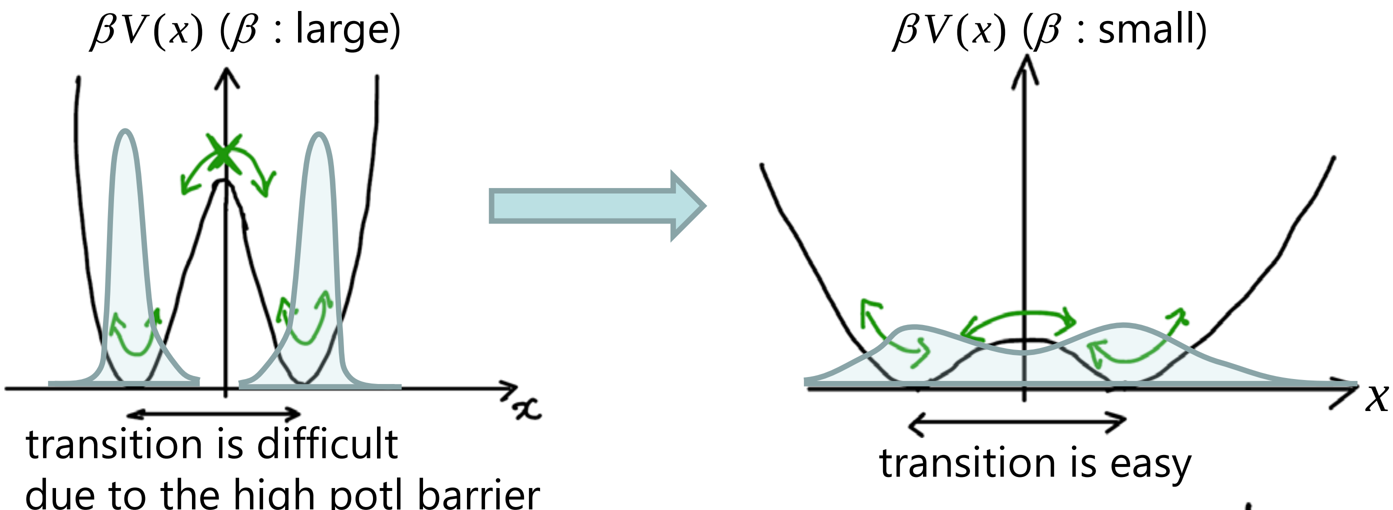
**[MF-Umeda 1703.00861, PTEP2017(2017)073B01]**
**[MF-Matsumoto-Umeda 1906.04243, to appear in PRD]**

# Idea of tempering

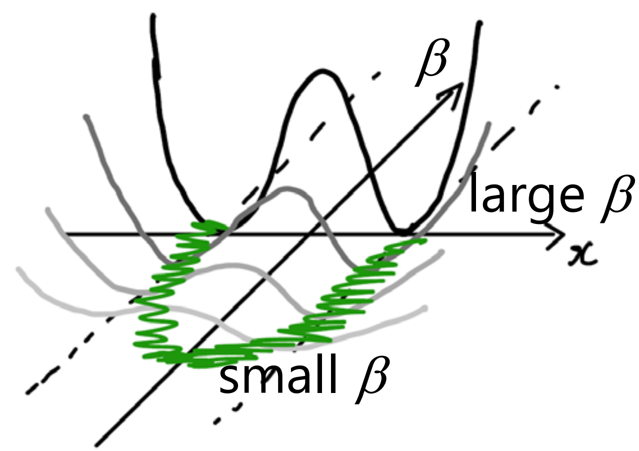
[Marinari-Parisi Europhys.Lett.19(1992)451]

Suppose that the action $S(x;\beta)$ gives a multimodal distribution for the value of $\beta$ in our main concern (e.g. $S(x;\beta)=\beta V(x)$ with $\beta \gg 1$)

It often happens that multimodality disappears if we take a different value of $\beta$ (e.g. for $\beta \ll 1$)




In the tempering method,
we extend the config space from $\{x\}$ to $\{(x,\beta)\}$.
Then, transitions between two modes become easy by passing through configs with smaller $\beta$



# Tempered LTM (1/3)

[MF-Umeda 1703.00861]

**Algorithm of TLTM**

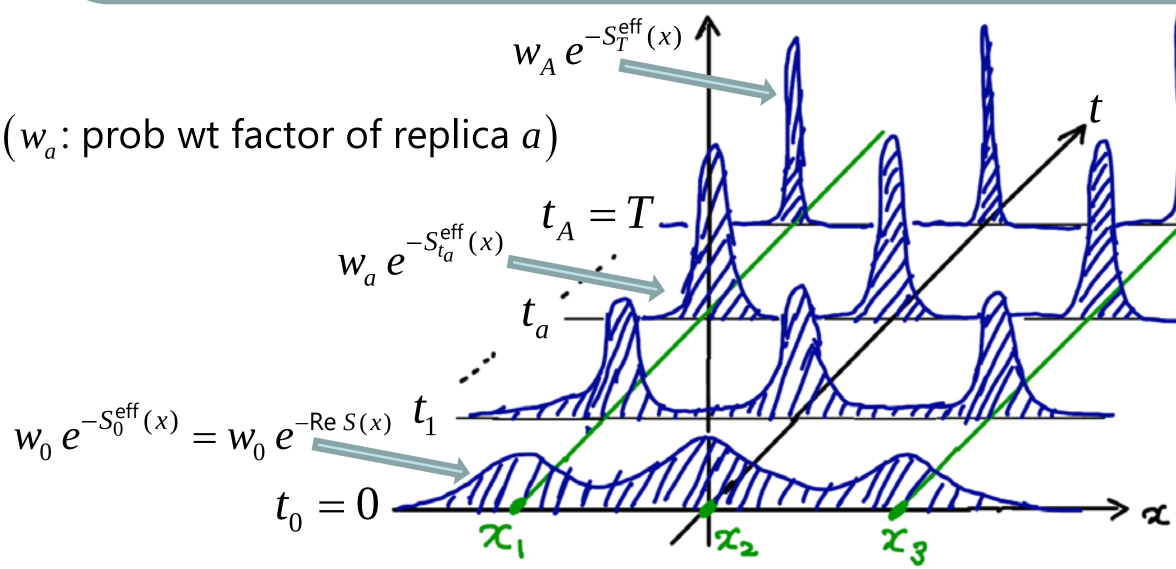
(1) Introduce copies of config space labeled by a finite set of flow times

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

and construct a Markov chain that drives the enlarged system

to global equilibrium $p_{\text{eq}}(x,t_a) \propto e^{-S^{\text{eff}}_{t_a}(x)}$

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




sign problem : **OK**
multimodality : NG

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multimodality : **OK**

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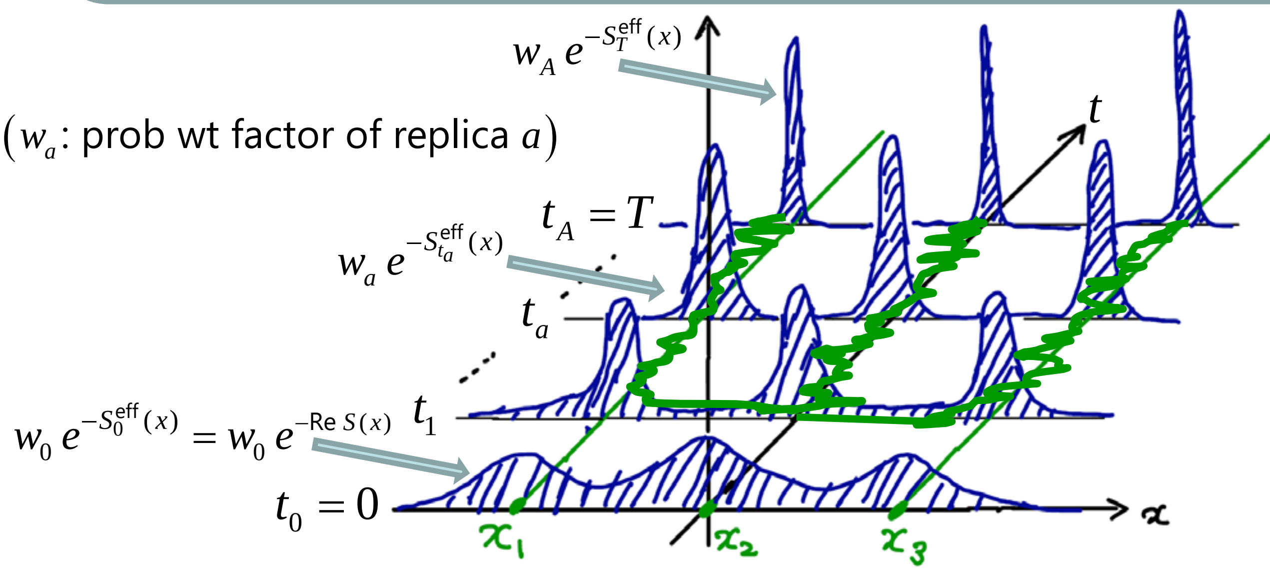


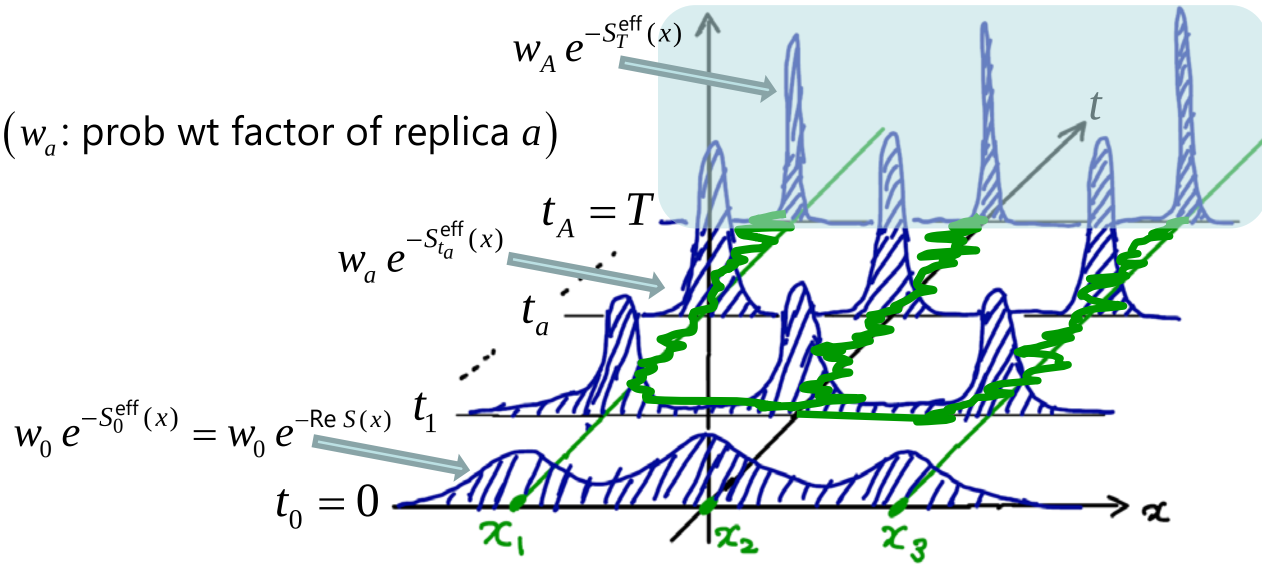
# Tempered LTM (2/3)

**Algorithm of TLTM**

[MF-Umeda 1703.00861]

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

$(w_a$: prob wt factor of replica $a)$




$A$-th replica

# Tempered LTM (2/3)

**[MF-Umeda 1703.00861]**

## Algorithm of TLTM

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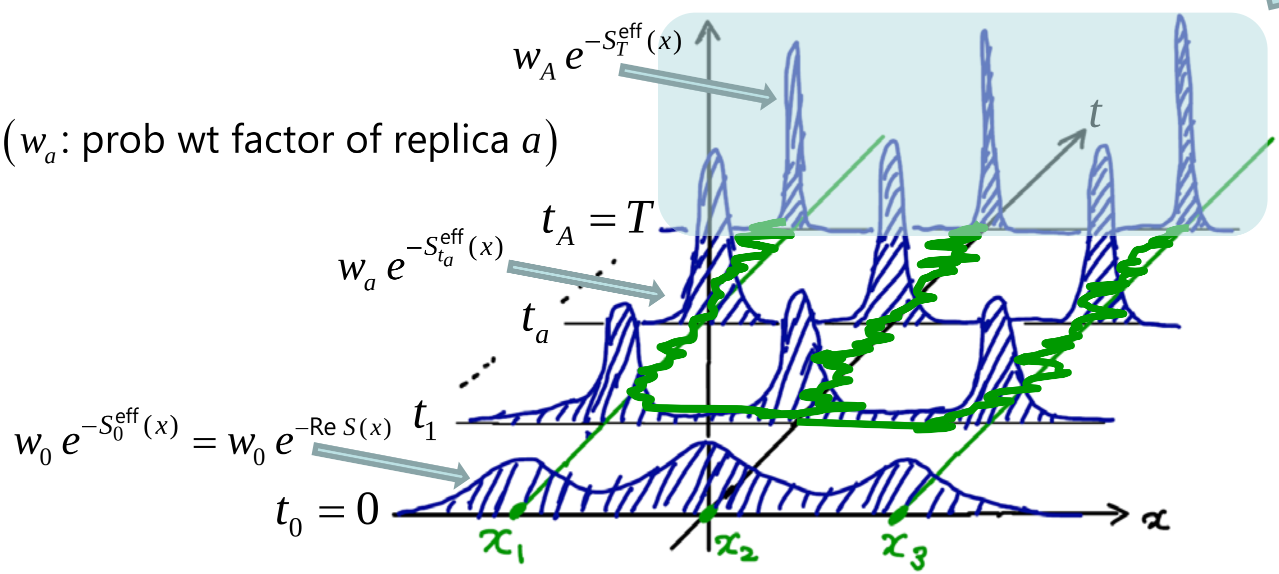


$A$-th replica

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

- 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 $\Leftrightarrow$ $\overbrace{\mathcal{M} \times \mathcal{M} \times \cdots \times \mathcal{M}}^{A+1} = \{(x_0, x_1, \ldots, x_A)\}$ ( ◯ )
  most of relevant steps can be done in parallel processes
  **[Swendsen-Wang 1986, Geyer 1991, Nemoto-Hukushima 1996]**

# Tempered LTM (2/3)

**Algorithm of TLTM**

**[MF-Umeda 1703.00861]**

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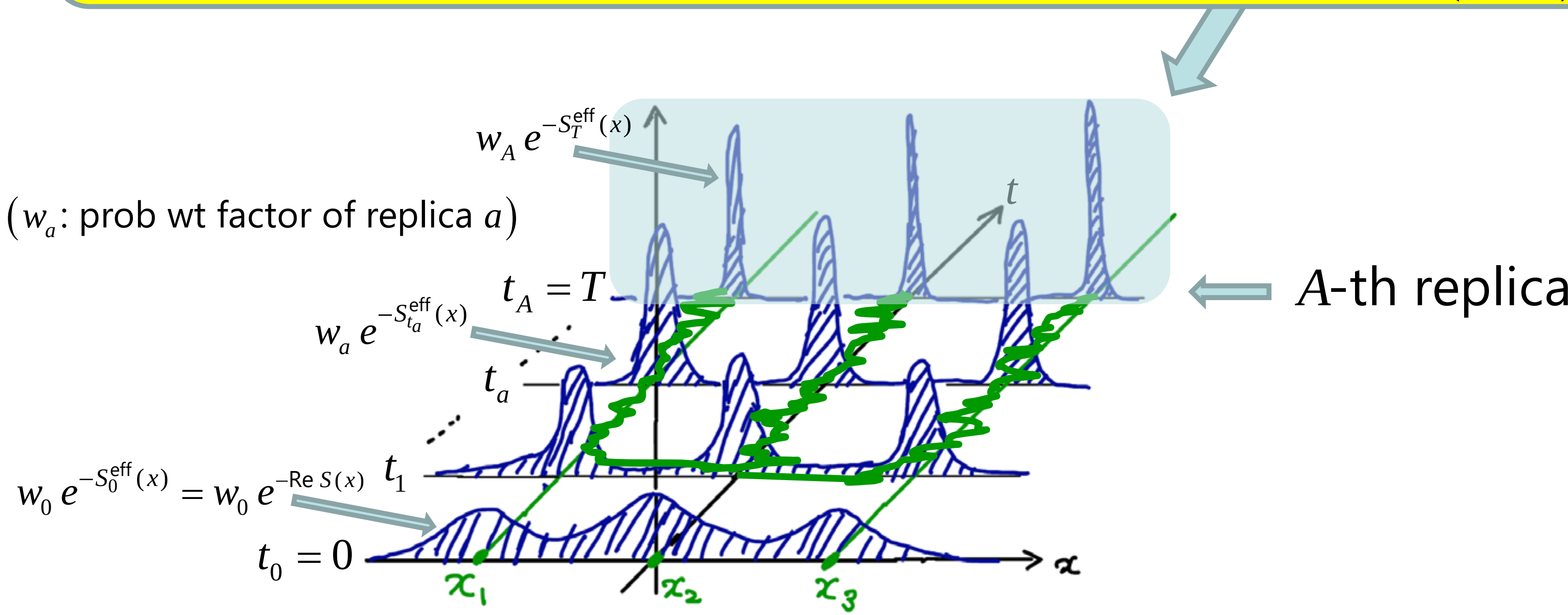


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- $\boxed{\text{parallel tempering}}$ : enlarged system $\Leftrightarrow$ $\overbrace{\mathcal{M} \times \mathcal{M} \times \cdots \times \mathcal{M}}^{A+1} = \{(x_0, x_1, \ldots, x_A)\}$ $(\bigcirc)$
  (replica exchange MCMC)
  **[Swendsen-Wang 1986, Geyer 1991, Nemoto-Hukushima 1996]**

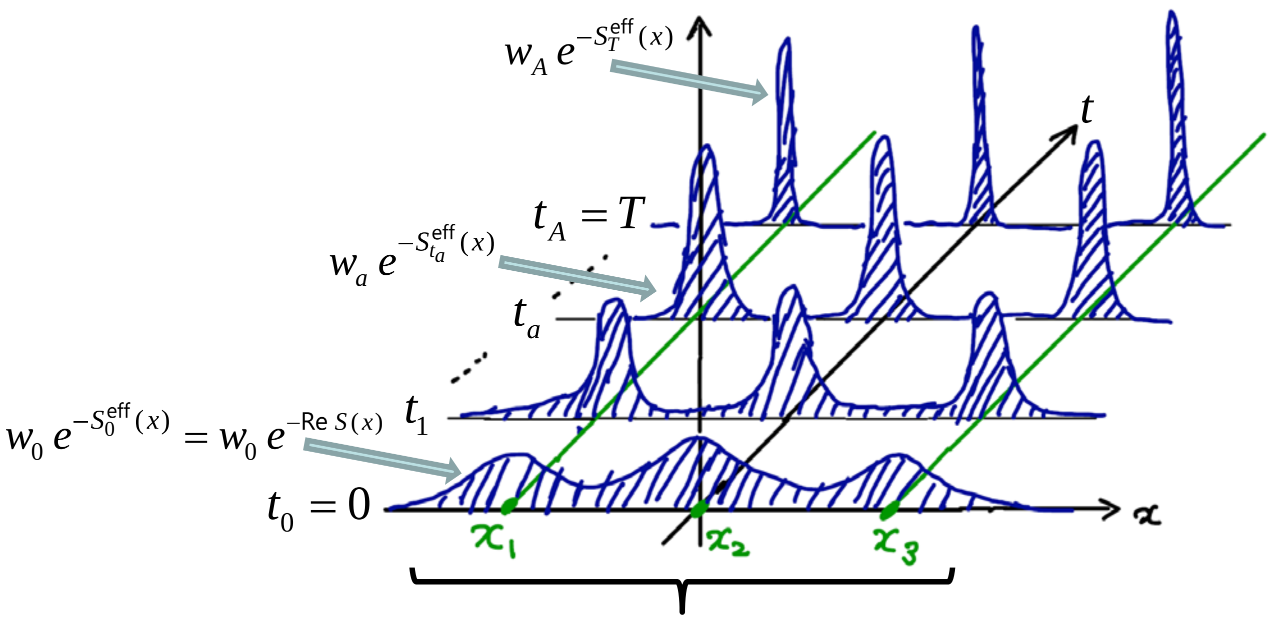
most of relevant steps can be done in parallel processes

# Tempered LTM (3/3)

[MF-Umeda 1703.00861, MF-Matsumoto-Umeda 1906.04243]

**Important points in TLTM:**

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




Distribution functions have peaks at the same positions $x_\sigma$
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**

# Example: (0+1)-dim Massive Thirring model (1/3)

Lorentzian action (dim reduction of (1+1)D model):

[Pawlowski-Zielinski 1302.1622, 1402.6042, Fujii-Kamata-Kikukawa 1509.08176]

$$S_M = \int dt \left[ i\bar{\psi}\gamma^0\partial_0\psi - m\bar{\psi}\psi - \frac{g^2}{2}(\bar{\psi}\gamma^0\psi)^2 \right] \quad \left( (\gamma^0)^2 = 1_2, \quad \gamma^{0\dagger} = \gamma^0 \right)$$

bosonization + discretization

Grand partition function $Z_{\beta,\mu} = \mathrm{tr}\ e^{-\beta(H-\mu Q)}$:

$$Z_{\beta,\mu} = \int_{\mathrm{PBC}} (d\phi)\, e^{-S(\phi)}$$

with

$$\begin{cases} (d\phi) = \prod_{n=1}^{N} \frac{d\phi_n}{2\pi}, \quad e^{-S(\phi)} = \det D(\phi) \exp\left[ \frac{-1}{2g^2} \sum_{n=1}^{N} (1 - \cos\phi_n) \right] \\ D_{nn'}(\phi) = \frac{1}{2}\left( e^{i\phi_n + \mu}\delta_{n+1,n'} - e^{-(i\phi_n+\mu)}\delta_{n-1,n'} - e^{i\phi_N+\mu}\delta_{n,N}\delta_{n',1} + e^{-(i\phi_N+\mu)}\delta_{n,1}\delta_{n',N} \right) + m\delta_{n,n'} \end{cases}$$

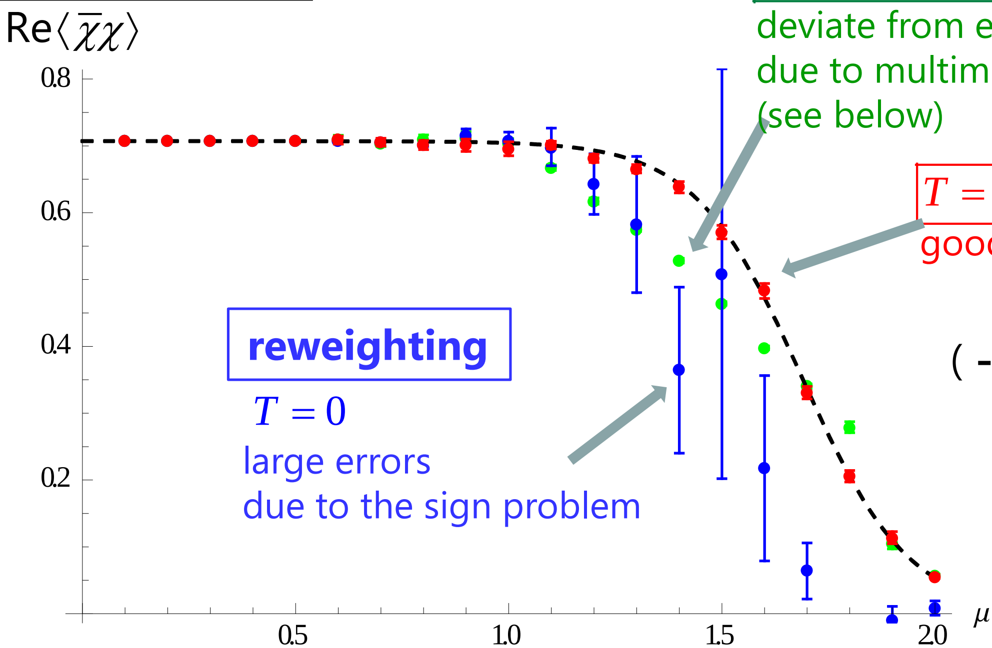
One can show $\boxed{[\det D(\phi;\mu)]^* = \det D(\phi;-\mu)}$ (thus, $\det D \notin \mathbb{R}$ for $\mu \in \mathbb{R}$)

⇨ Sign problem will arise when $N$ is very large

# Example: (0+1)-dim Massive Thirring model (2/3)

[MF-Umeda 1703.00861]

## Chiral condensate $\langle \bar{\chi}\chi \rangle$




$T = 2$ (w/o temp)
deviate from exact values
due to multimodality
(see below)

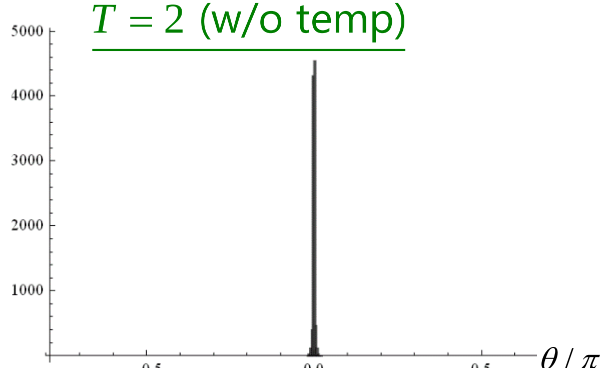
$T = 2$ (w/ temp)
good agreement

**reweighting**
$T = 0$
large errors
due to the sign problem

( ------ : exact values)

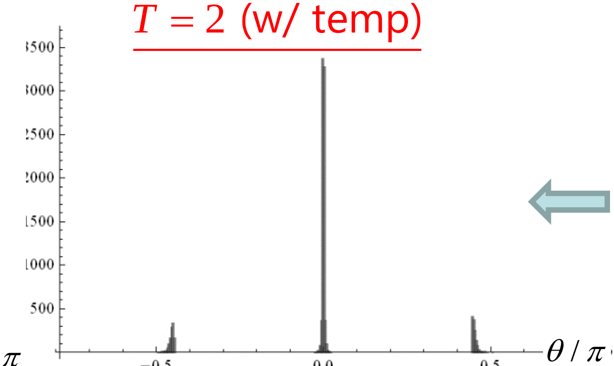
## Confirmation of the resolution of multimodality

$T = 2$ (w/o temp)



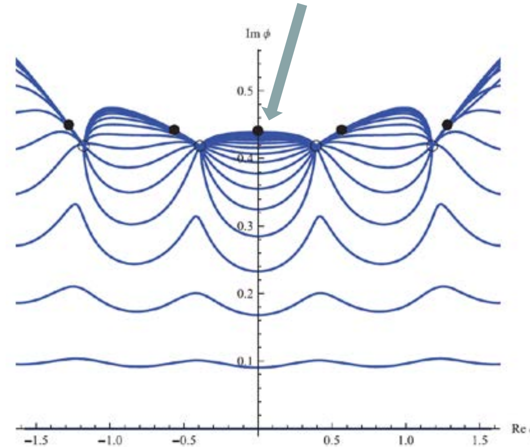

dominated by
a single thimble

$T = 2$ (w/ temp)




contributed by
multiple thimbles (i.e. config space is well explored)

dominant thimble



# Example: (0+1)-dim Massive Thirring model (3/3)

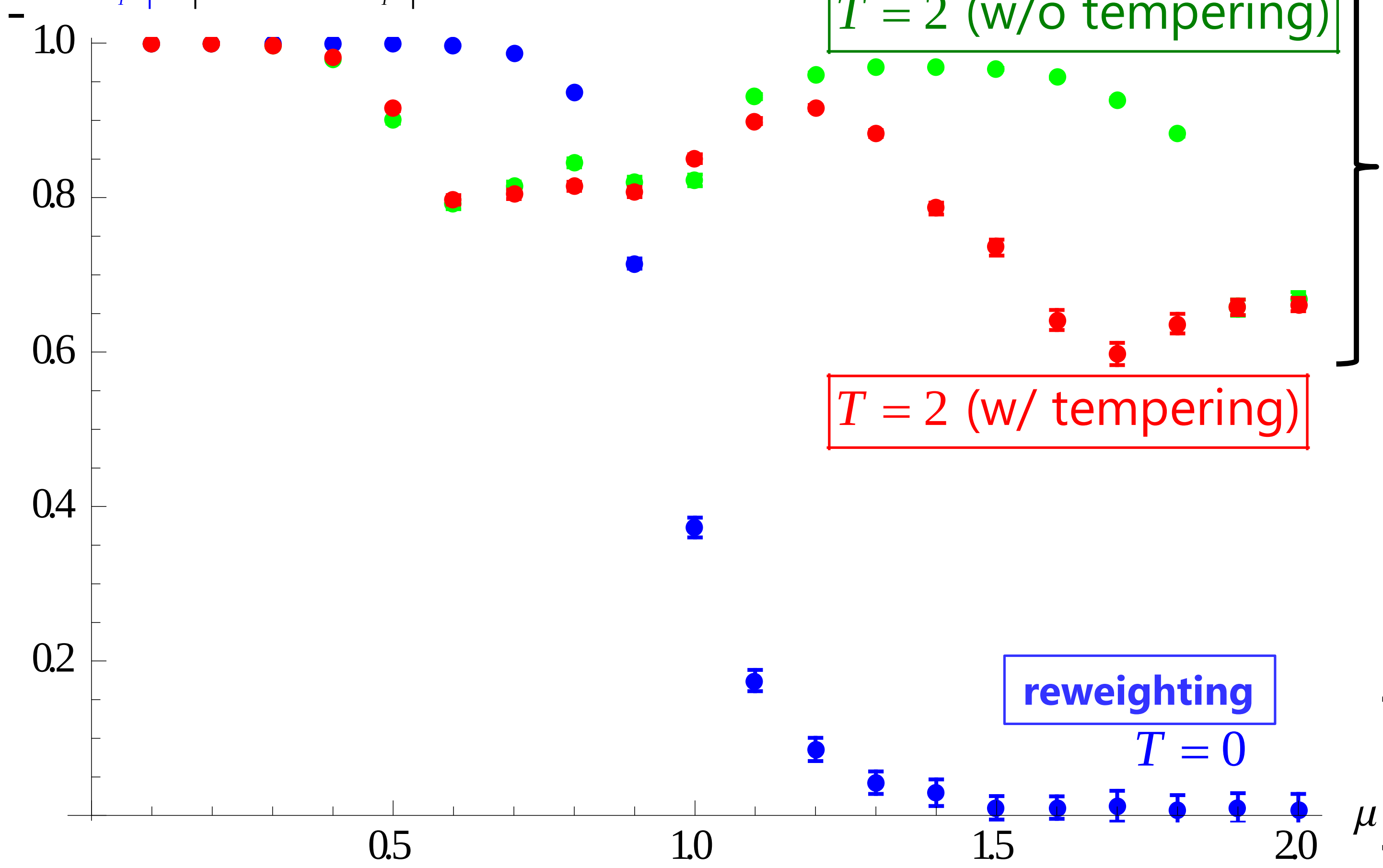
[MF-Umeda 1703.00861]

<u>Confirmation of the resolution of sign problem</u>

$$\left( \langle \mathcal{O}(\phi) \rangle = \frac{\langle e^{i\theta_T(\phi)}\, \mathcal{O}(\phi) \rangle_{S^{\rm eff}_{t_a}}}{\langle e^{i\theta_T(\phi)} \rangle_{S^{\rm eff}_T}} \right)$$

sign average

$$\left| \left\langle e^{i\theta_T(\phi)} \right\rangle_{S^{\rm eff}_T} \right| \sim \left| \left\langle e^{-iS_I(z_T(\phi))} \right\rangle_{S^{\rm eff}_T} \right|$$




no sign problem at $T = 2$

(<u>NB</u>: sign avarage $\left| \left\langle e^{i\theta_T(\phi)} \right\rangle_{S^{\rm eff}_T} \right|$ is smaller for the right sampling)

sign problem surely exists for the original action ($T = 0$)

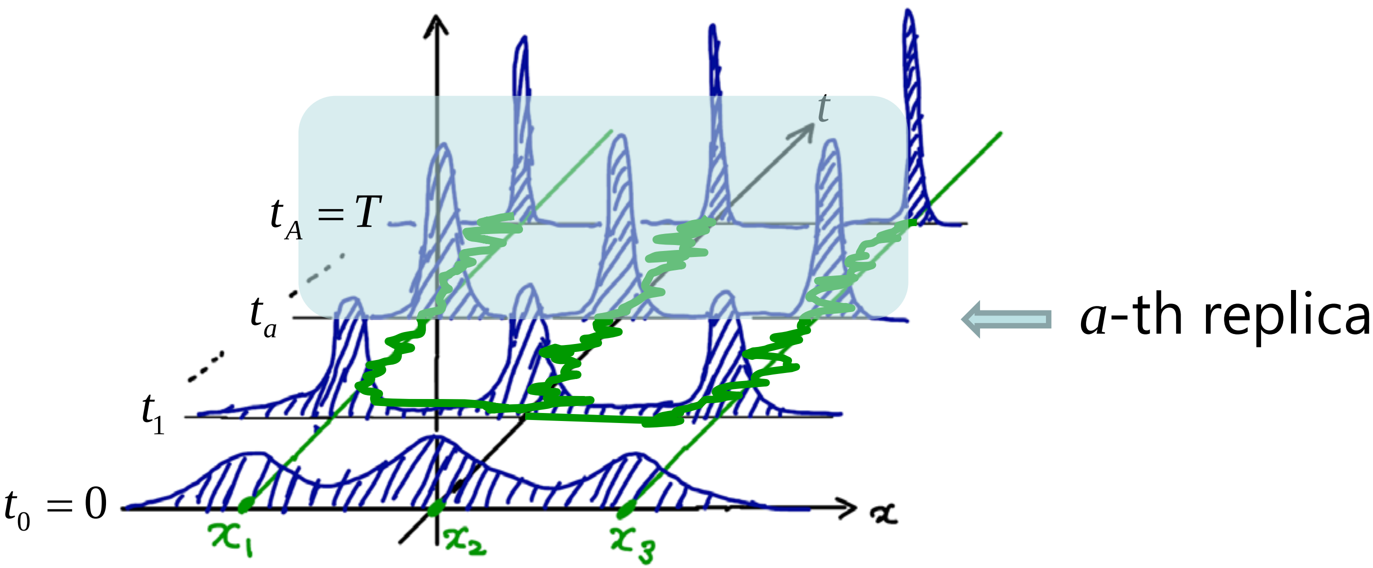
# We actually can go further…

[MF-Matsumoto-Umeda 1906.04243]

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

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

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



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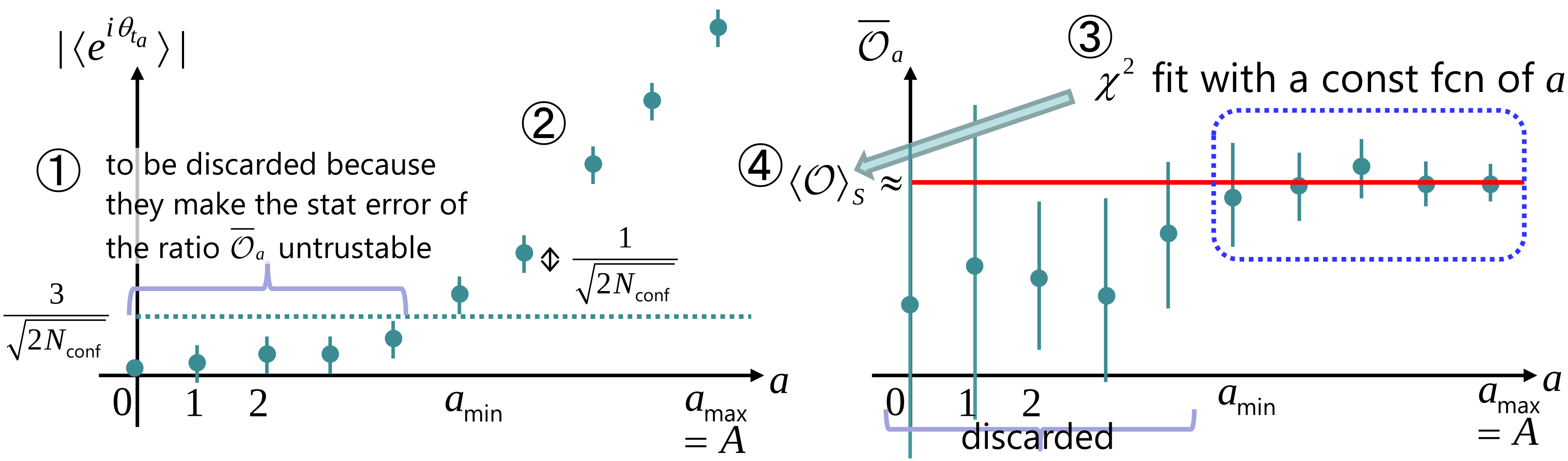
The LHS must be independent of $a$ due to Cauchy's theorem

**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 an algorithm with a criterion for precise estimation in the TLTM!



## 4. Applying the TLTM to the Hubbard model

**[MF-Matsumoto-Umeda 1906.04243, to appear in PRD]**

# Hubbard model (1/2)

## Hubbard model [Hubbard 1963]

modeling NR electrons in a solid

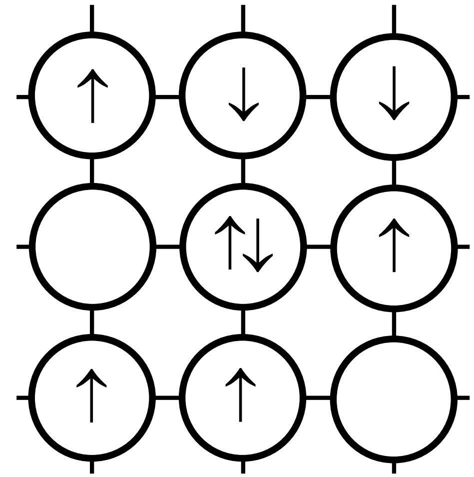
- $c^\dagger_{\mathbf{x},\sigma},\ c_{\mathbf{x},\sigma}$ : creation/anihilation op of an electron

  on site $\mathbf{x}$ with spin $\sigma(=\uparrow,\downarrow)$

- Hamiltonian

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

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




bipartite lattice

$(N_S$ : # of sites$)$

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

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

(fermion bilinear) (four fermion)

# Hubbard model (2/2)

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

- Quantum Monte Carlo

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

⇨ 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 $\phi$

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

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

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

<u>NB</u>: 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

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

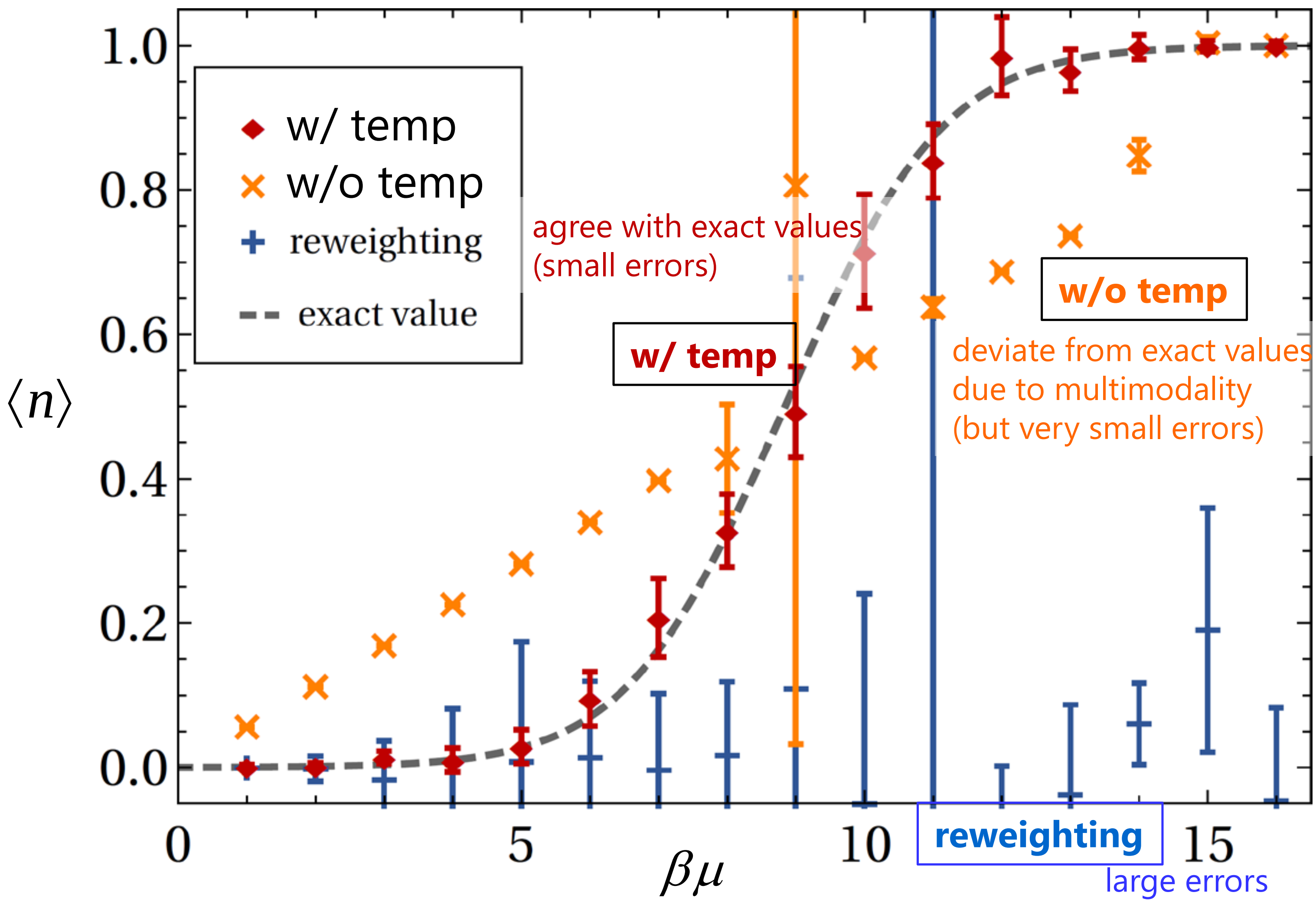
**[MF-Matsumoto-Umeda 1906.04243]**

# Results for 1D lattice (1/3)

[MF-Matsumoto-Umeda 2019]

imaginary time : 2 steps $(N_\tau = 2)$
spatial lattice: 1D periodic lattice with $N_s = 2$
$\beta\kappa = 1, \quad \beta U = 16, \quad$ max flow time $T = 0.4$
sample size: 5,000

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




large errors
due to the sign problem

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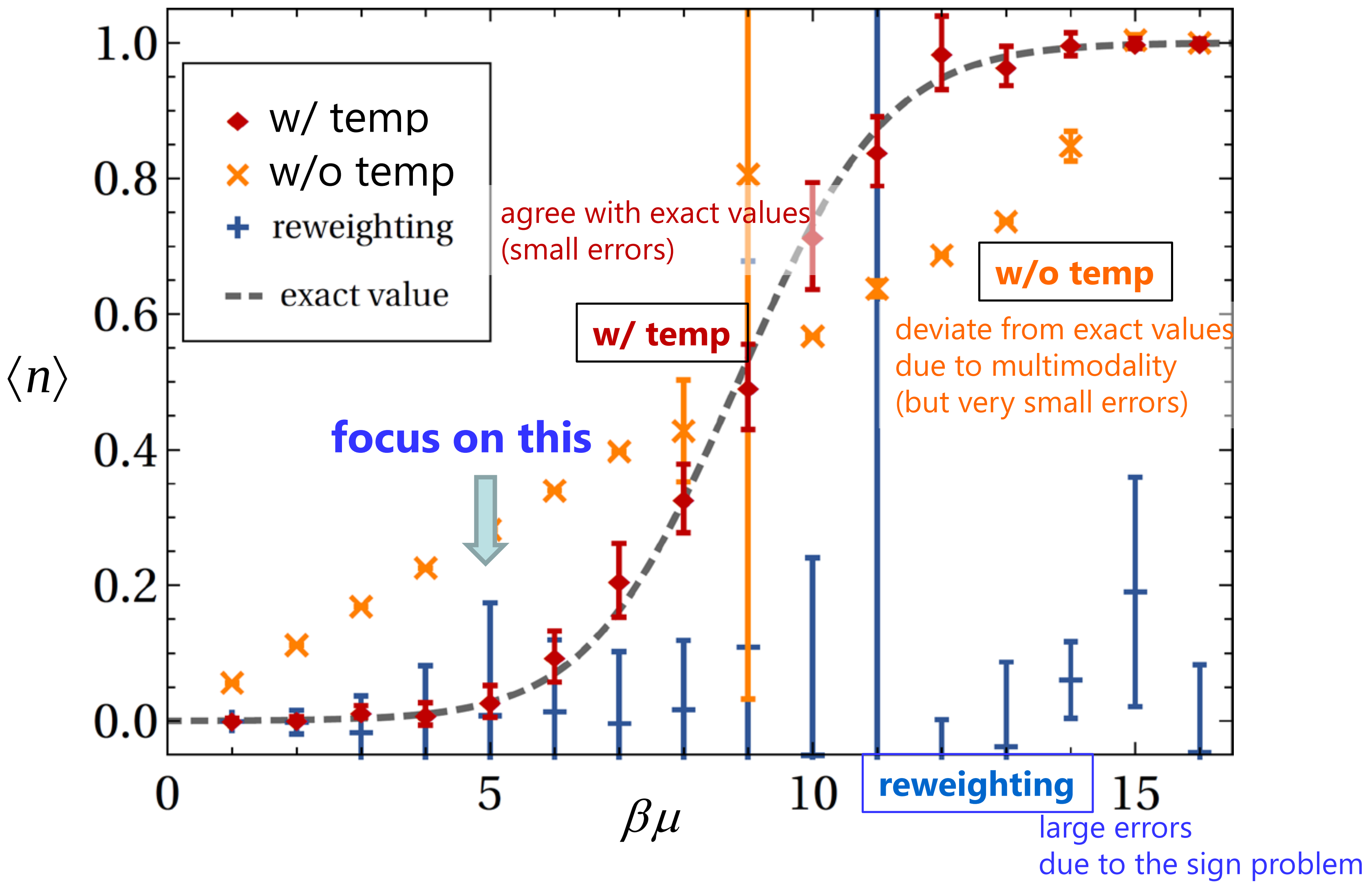
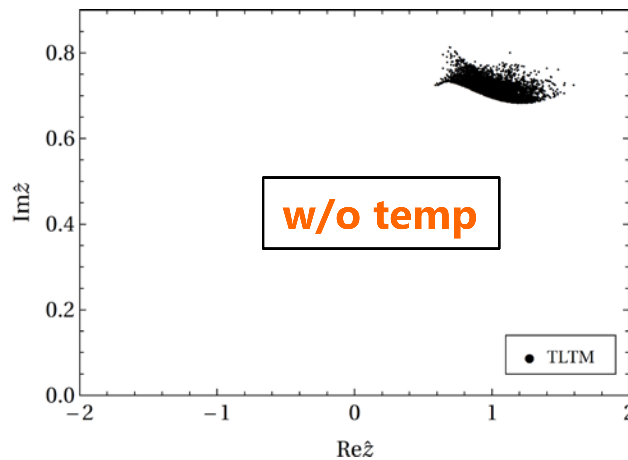
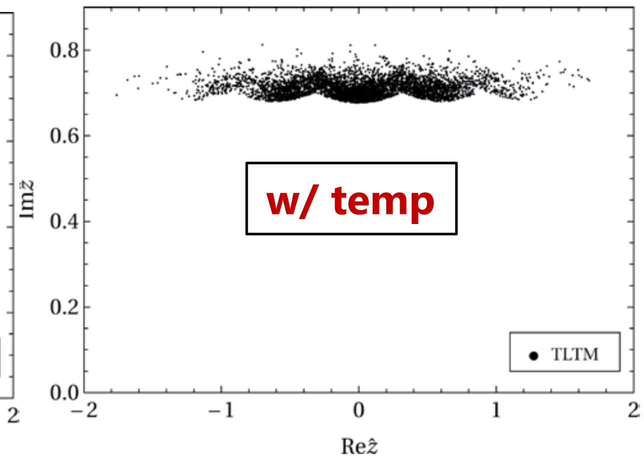


# Results for 1D lattice (2/3)

**[MF-Matsumoto-Umeda 2019]**

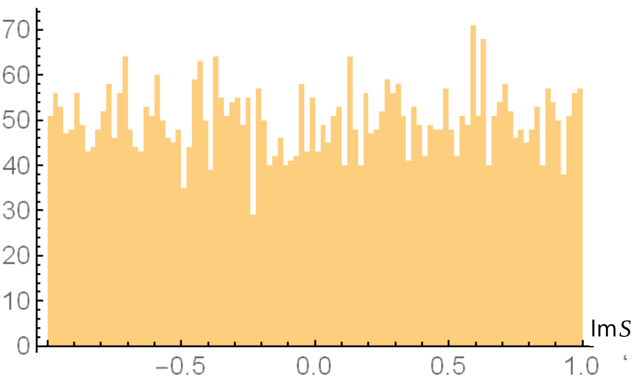
Distribution of flowed configs at flow time $T = 0.4$
(projected on a plane)




Histogram of Im$S(z)/\pi$

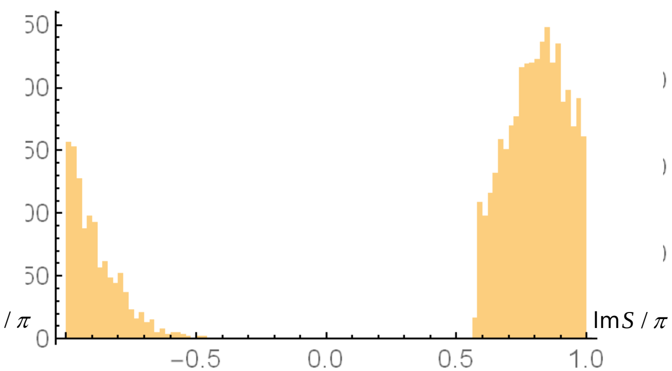
**reweighting**




distributing uniformly from $-\pi$ to $+\pi$

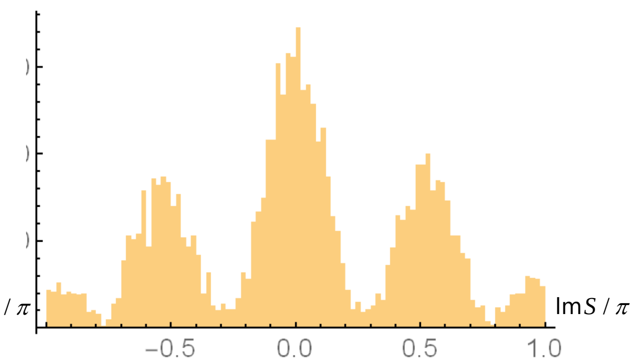
⇨ severe sign problem

**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)

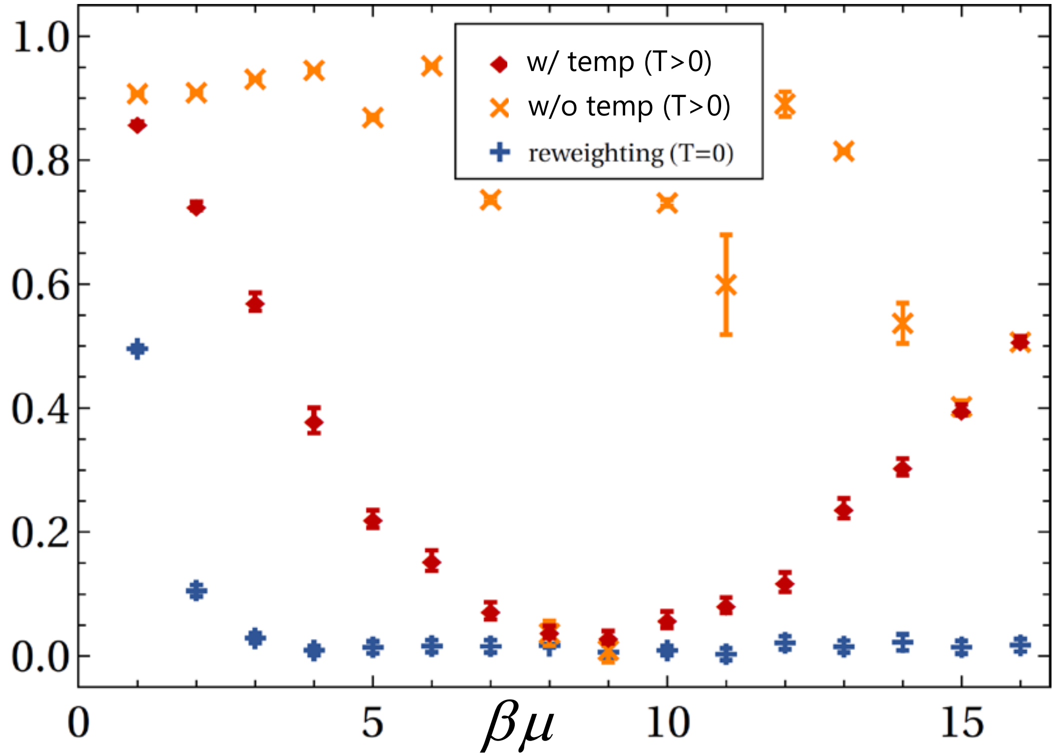
# Results for 1D lattice (3/3)

**[MF-Matsumoto-Umeda 2019]**

<u>sign average</u>

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

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




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

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

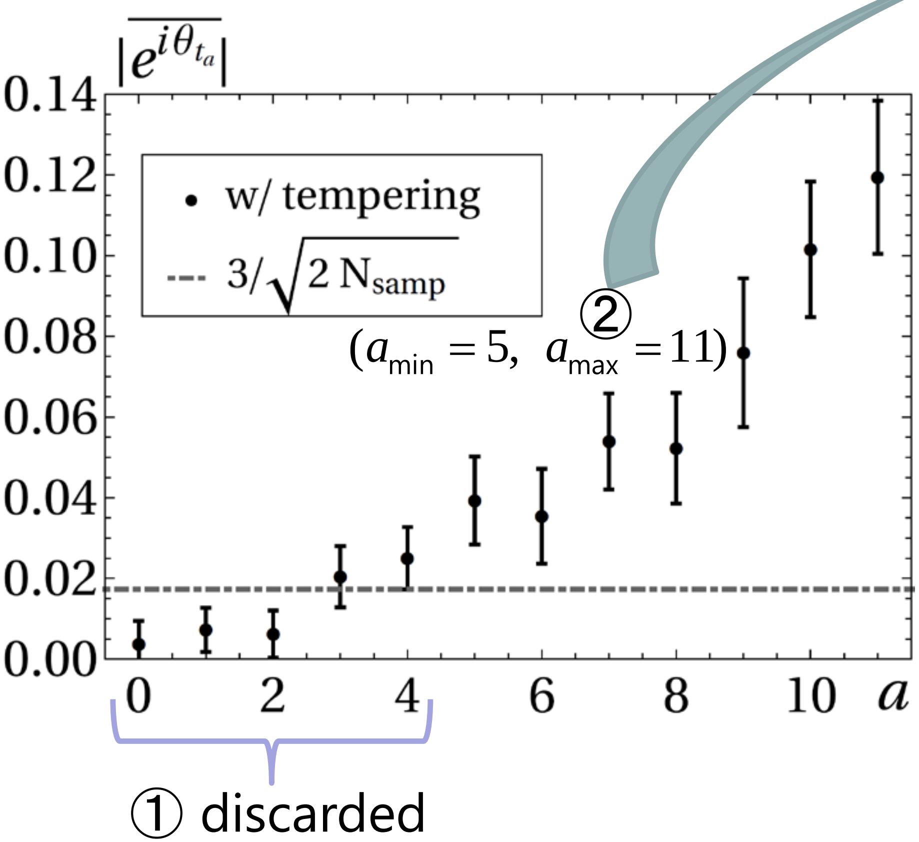
# Results for 2D lattice (1/5)

[MF-Matsumoto-Umeda 1906.04243]

imaginary time : 5 steps ($N_\tau = 5$)
spatial lattice: 2D periodic lattice with $N_s = 2\times 2$
$\beta\kappa = 3$ $\beta U = 13$, max flow time $T = 0.5$
sample size: 5,000~25,000 depending on $\beta\mu$

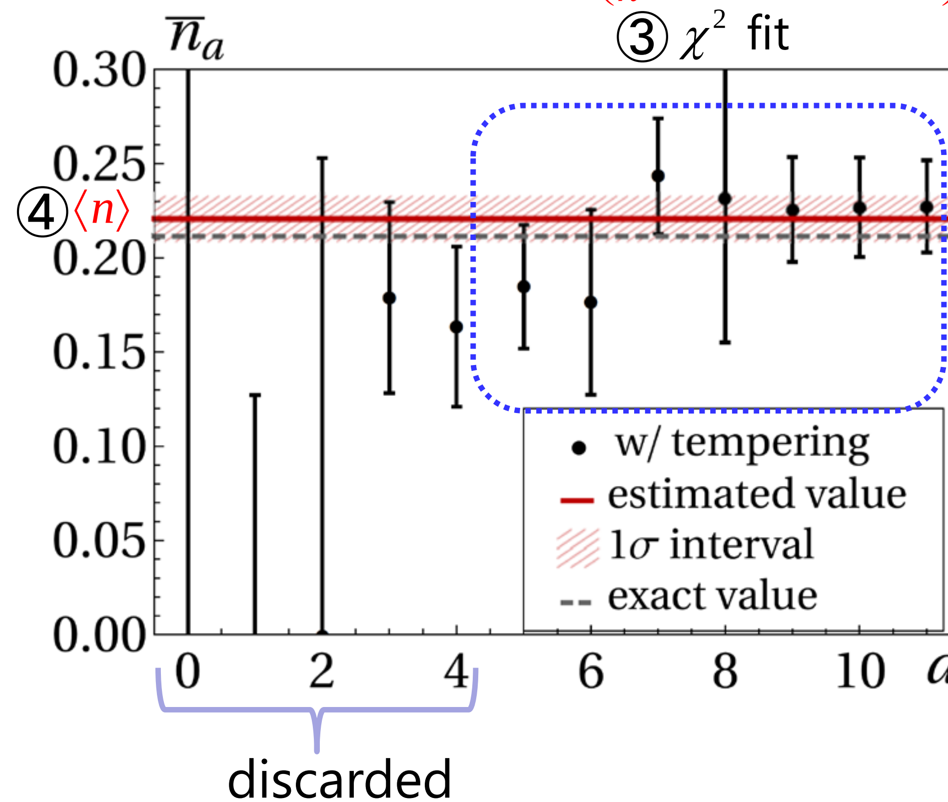
$$\left( \langle n\rangle = \frac{\langle e^{i\theta_{t_a}(x)}\, n(z_{t_a}(x))\rangle_{S^{\rm eff}_{t_a}}}{\langle e^{i\theta_{t_a}(x)}\rangle_{S^{\rm eff}_{t_a}}} \approx \overline{n}_a \right)$$

Example: $\beta\mu = 5$




$\left(\begin{array}{l}\langle n\rangle \approx 0.221 \pm 0.012 \\ \chi^2/\mathrm{DOF} = 0.45\end{array}\right)$

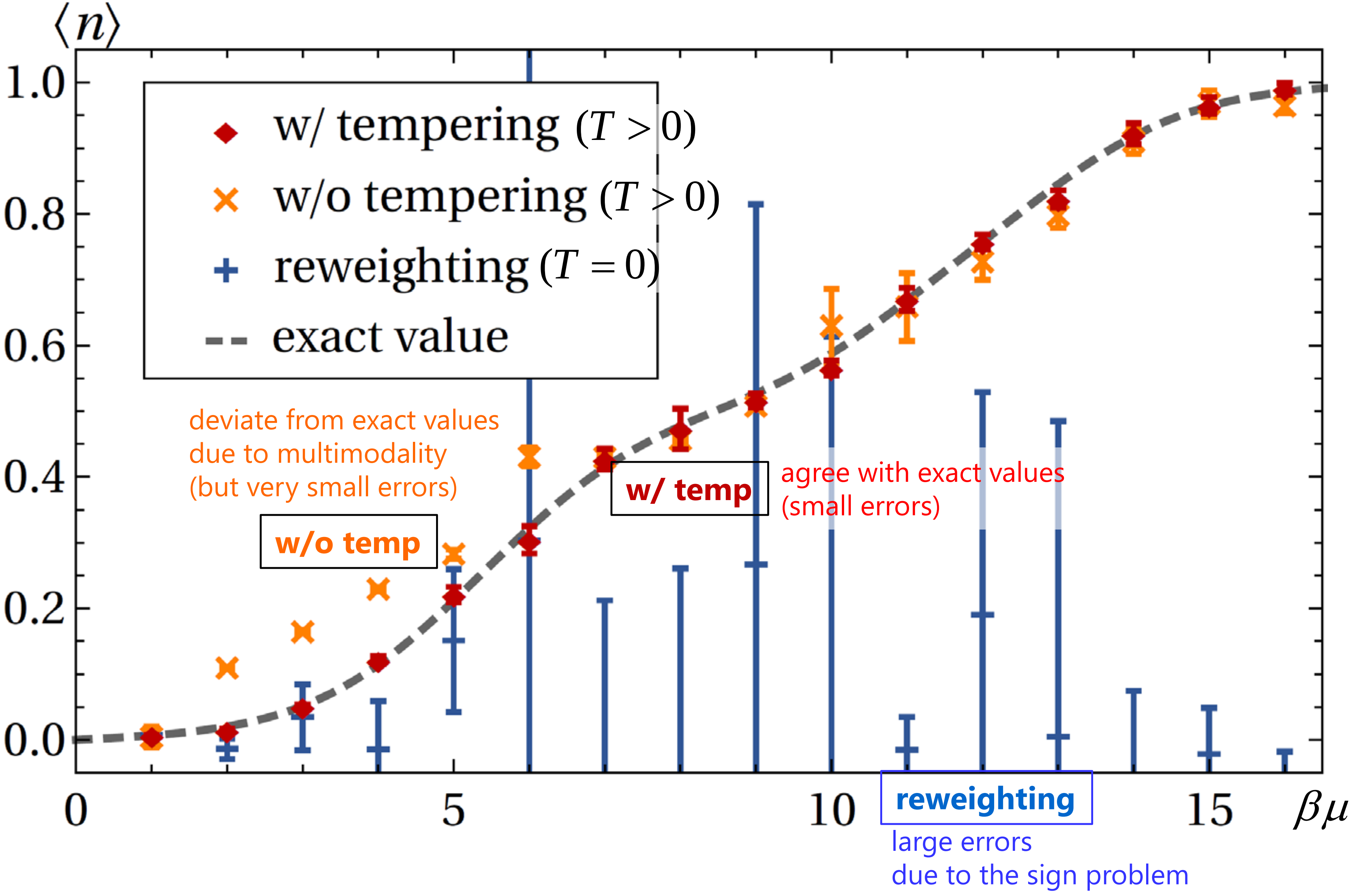
③ $\chi^2$ fit



# Results for 2D lattice (2/5)

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

[MF-Matsumoto-Umeda 1906.04243]



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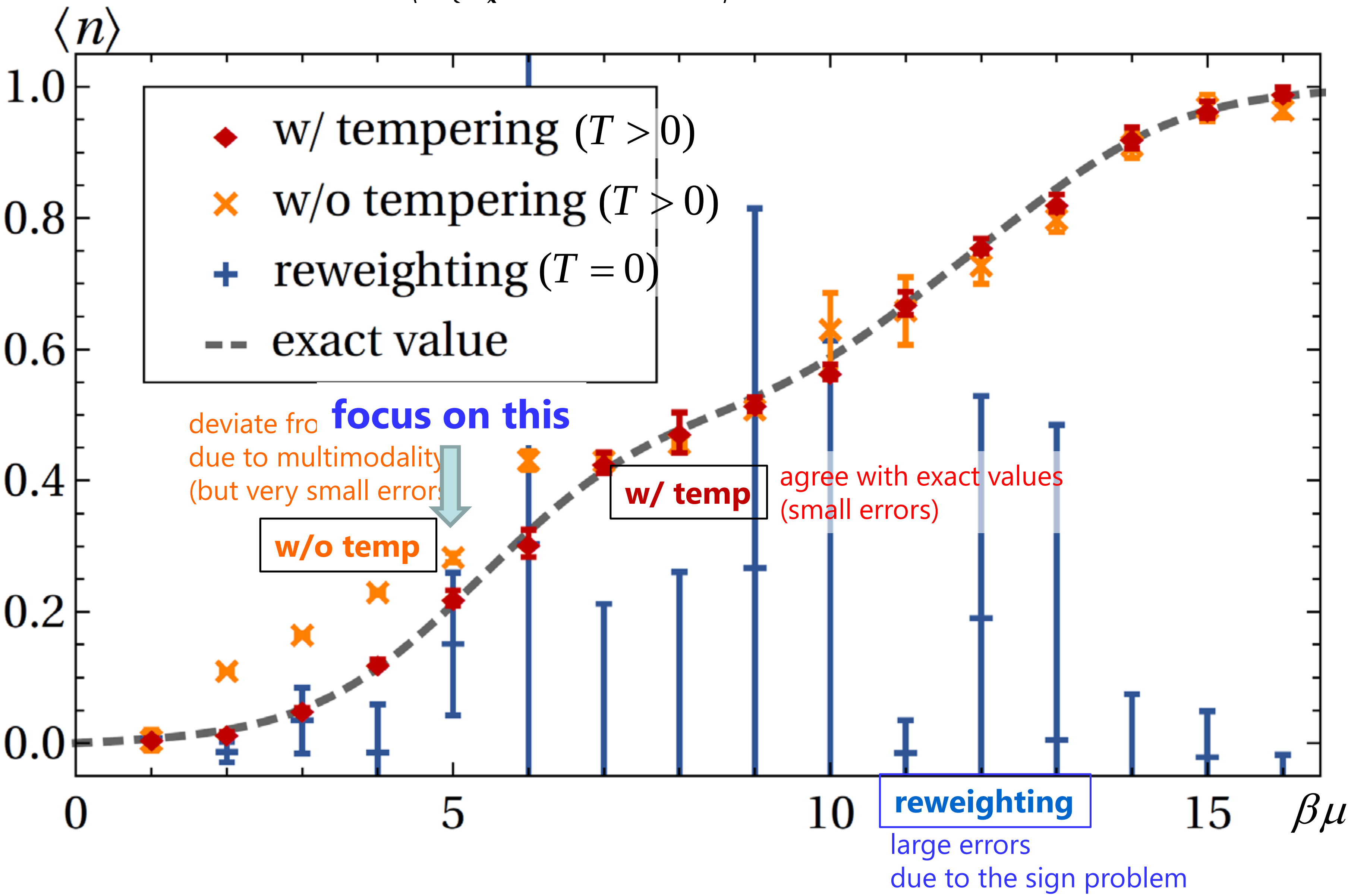
**[MF-Matsumoto-Umeda 1906.04243]**

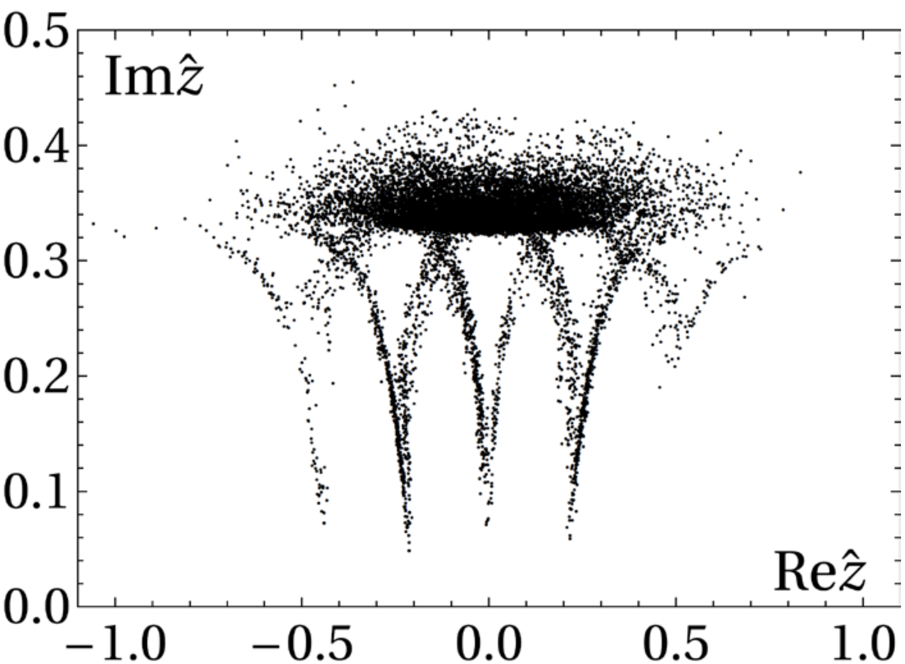


# Results for 2D lattice (3/5)

[MF-Matsumoto-Umeda 1906.04243]

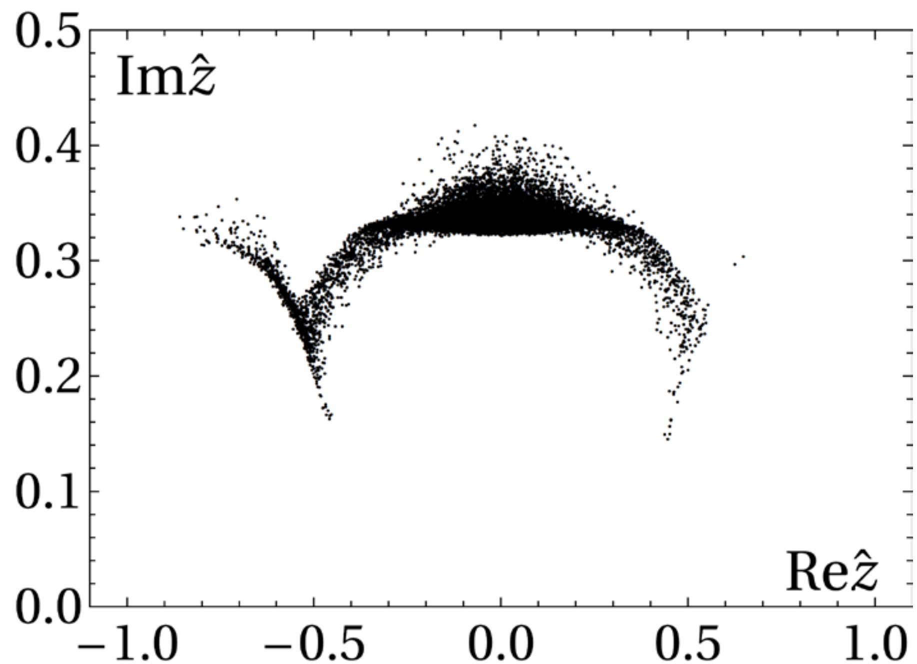
Distribution of flowed configs at flow time $T = 0.5$ $(\beta\mu = 5)$
(projected on a plane)

**w/ temp**




distributed widely
over many thimbles

**w/o temp**



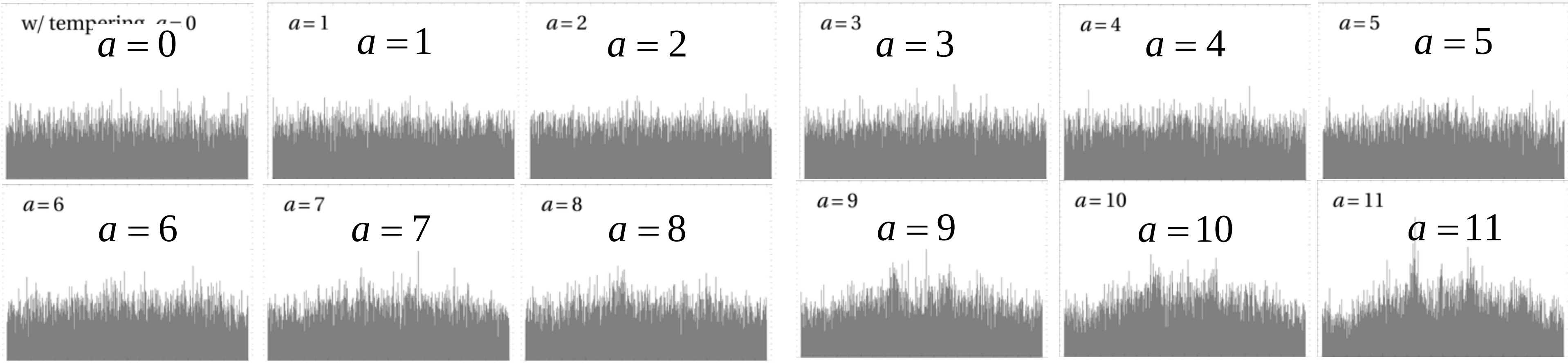

distributed over only
a small number of thimbles

# Results for 2D lattice (4/5)

[MF-Matsumoto-Umeda 1906.04243]

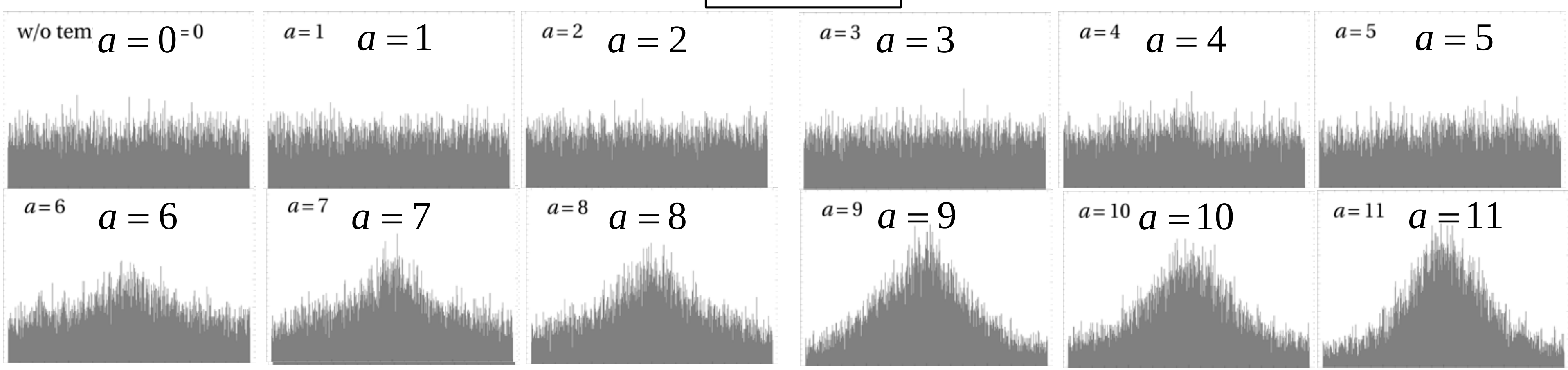
Histogram of $\theta_{t_a} \in [-\pi,\pi)$

**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**



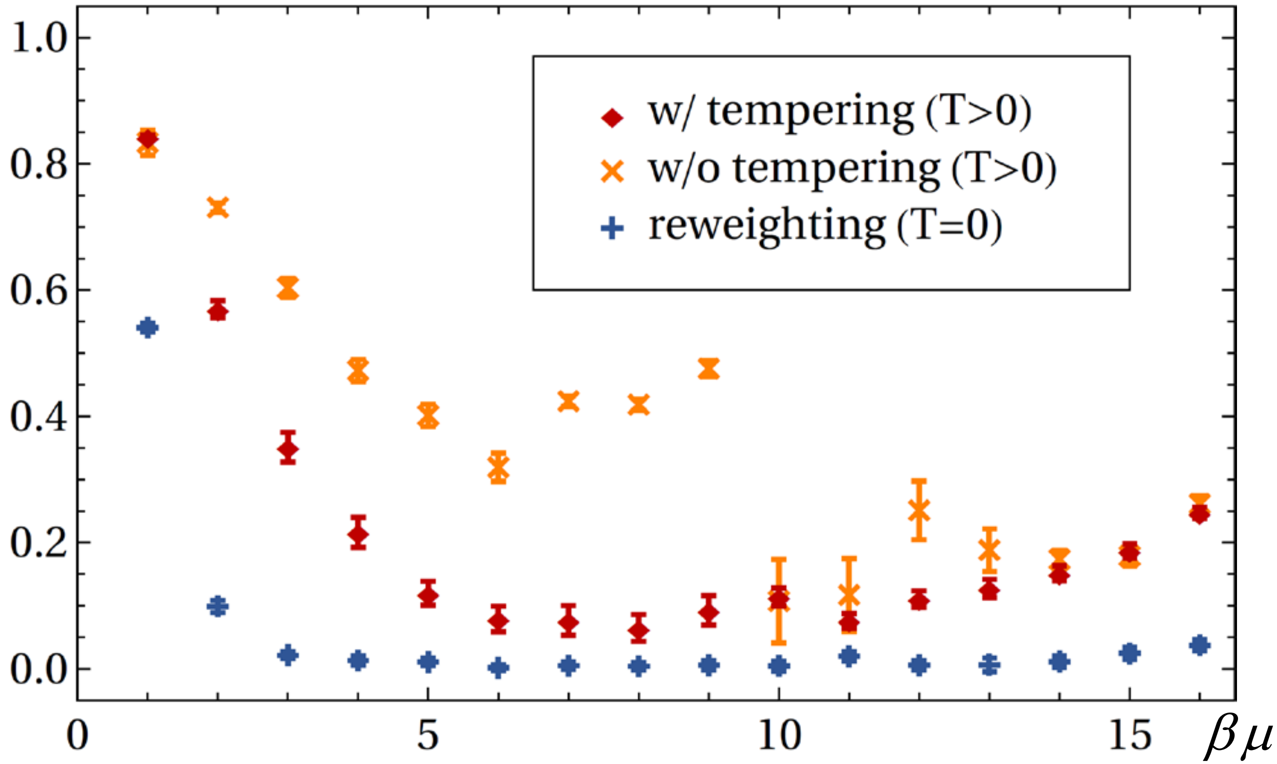

unimodal distribution

# Results for 2D lattice (5/5)

**[MF-Matsumoto-Umeda 1906.04243]**

sign average

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




When only a single (or very few) thimble(s) is sampled,
the sign 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 sign average
as an index of the "resolution of the sign problem"

# Comment on the Generalized LTM

[MF-Matsumoto-Umeda 1906.04243]

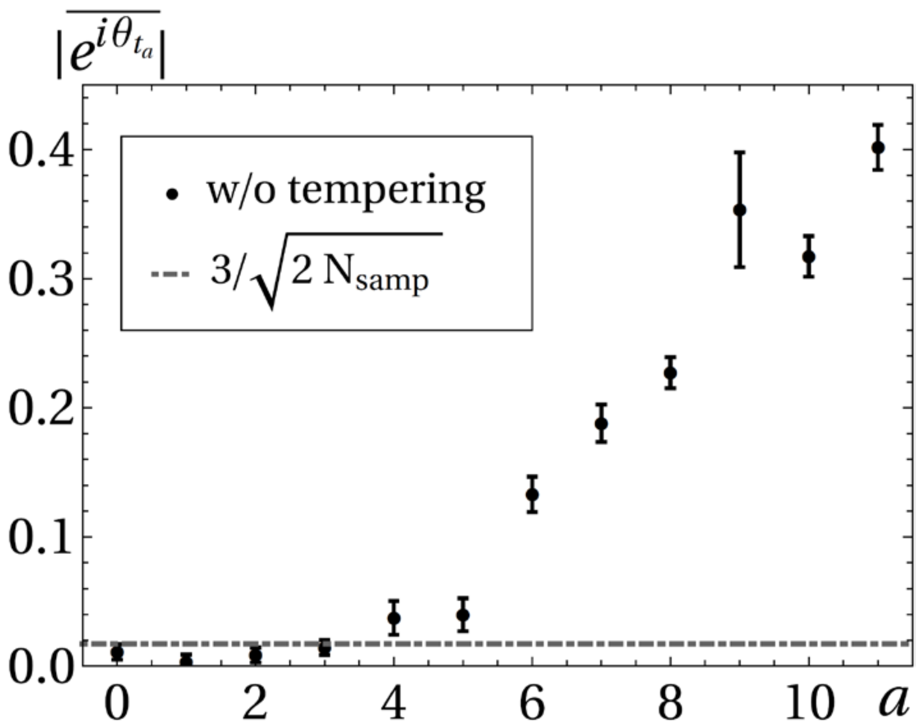
imaginary time : 5 steps ($N_\tau = 5$)
spatial lattice: 2D periodic lattice with $N_s = 2 \times 2$
$\beta\kappa = 3, \quad \beta U = 13, \quad 0 \le T \le 0.4 \left( \Leftrightarrow 0 \le a \le 10 \right)$
sample size: 5,000~25,000 depending on $\beta\mu$

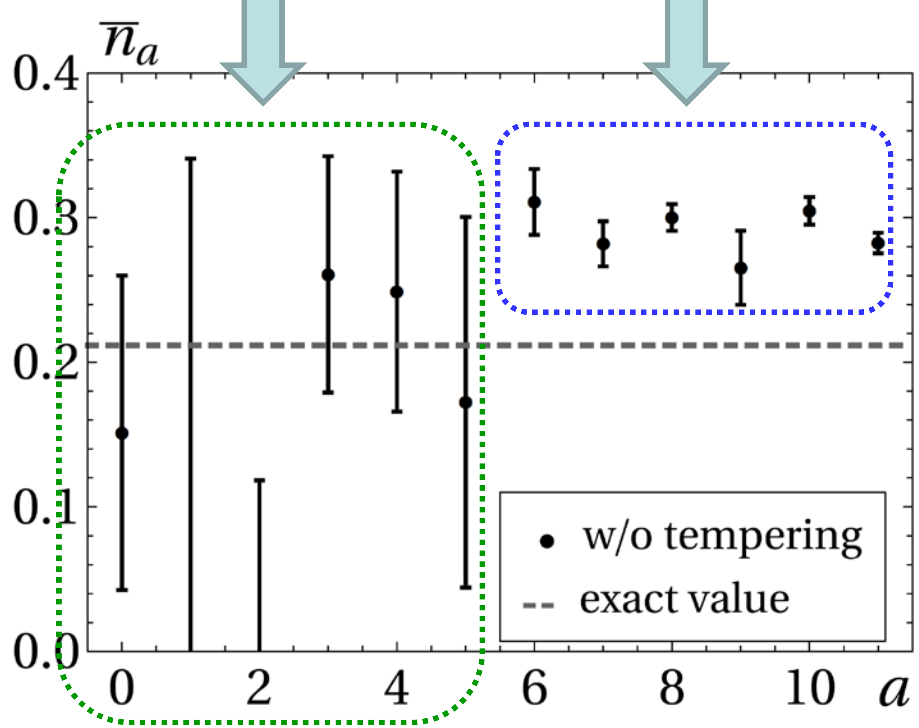
$$\left( \langle n \rangle = \frac{\langle e^{i\theta_{t_a}(x)}\, n(z_{t_a}(x)) \rangle_{S^{\mathrm{eff}}_{t_a}}}{\langle e^{i\theta_{t_a}(x)} \rangle_{S^{\mathrm{eff}}_{t_a}}} \approx \overline{n}_a \right)$$

Example: $\beta\mu = 5$

large stat errors
(due to sign problem)

wrong values
(due to multimodality)




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

## 5. Some ongoing work

**[MF-Matsumoto-Umeda, in preparation]**

# Some ongoing work (1/2)

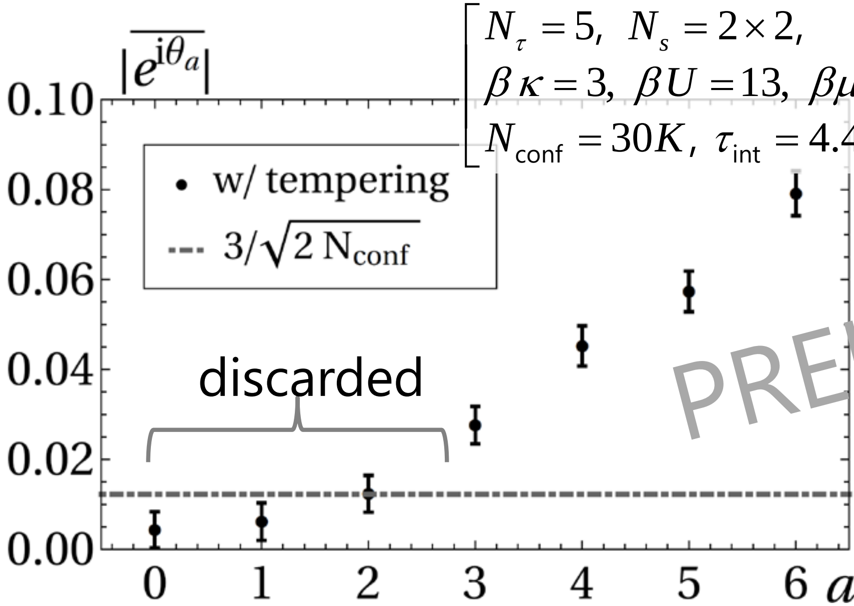
Implementation of HMC on the TLTM:

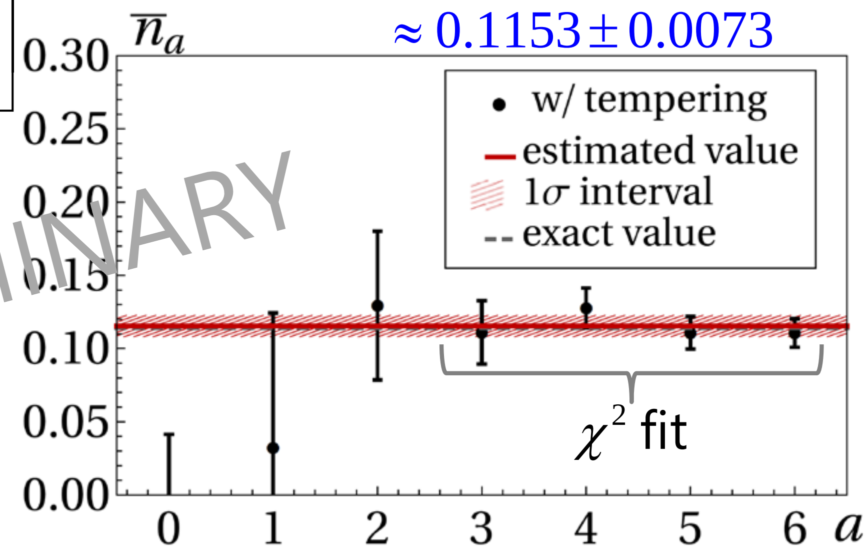
**[MF-Matsumoto-Umeda, in prep]** ⇨ **Matsumoto's poster**

- We implemented the HMC algorithm for transitions at each replica
  **[cf. Fujii-Honda-Kato-Kikukawa-Komatsu-Sano 2013, Alexandru in Lattice 2019]**
  (our crucial improvement: handling of configs near det zeros + tempering)
- Computational cost gets much reduced with short autocorrelation times
  (at least a few times faster than the Metropolis even for small $N$)
- We no longer need to tune parameters that required long-term test runs
  (such as determining the variance of the proposal distribution)
- Good features in the TLTM are all preserved
  (such as the sufficient overlaps between adjacent replicas)

$$\begin{bmatrix} N_\tau = 5,\ N_s = 2\times 2, \\ \beta\kappa = 3,\ \beta U = 13,\ \beta\mu = 4, \\ N_{\text{conf}} = 30K,\ \tau_{\text{int}} = 4.47 \pm 0.35 \end{bmatrix}$$

$\langle n \rangle = 0.1143$ (exact)
$\approx 0.1153 \pm 0.0073$



# Some ongoing work (2/2)

Application of TLTM to Stephanov models (chiral matrix models):

Dirac operator $D \Rightarrow 2N \times 2N$ dense complex matrix $D = \begin{pmatrix} m1_N & * \\ * & m1_N \end{pmatrix}$

- It has been known that the CLM does not work for this model even for small $N$ (Gauge cooling is not applicable for this model)
- Multiple Lefschetz thimbles again become relevant around critical points
- GLTM gives wrong results or large ambiguities for some parameter region
- TLTM seems to work for all the region of parameters $(T, \mu, m)$, producing numerical results that agree with exact values $(N = 4, 8, 12, \ldots)$

# 6. Conclusion and outlook

# Conclusion and outlook

## What we have done:

- We proposed the tempered Lefschetz thimble method (TLTM) as a versatile method towards solving the numerical sign problem
- We further developed it and found an algorithm for a precise estimation 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 ergodicity problems simultaneously

## Outlook: **[MF-Matsumoto, work in progress]**

- 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:
  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 (e.g. HMC at each replica **[MF-Matsumoto-Umeda, in prep]**)

Thank you.