単調性を用いたレプリカ交換モンテカルロ法の拡張と行列幾何学

渡辺　展正
(KEK → 9月よりYITP)

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(Work in progress)

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基研研究会　「熱場の量子論とその応用」

Contents

- Motivation from the gauge/gravity duality
    - How to identify the location of D-branes from QFT side
    - Notion of wave packet in operator/path-integral formalism
- How to solve the optimization problem
    - Replica-Exchange Monte Carlo method and its extension
- Numerical demonstration
- Summary & Prospectives

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- Motivation from the gauge/gravity duality (c.f. lectures by Hanada)
  - How to identify the location of D-branes from QFT side
  - Notion of wave packet in operator/path-integral formalism
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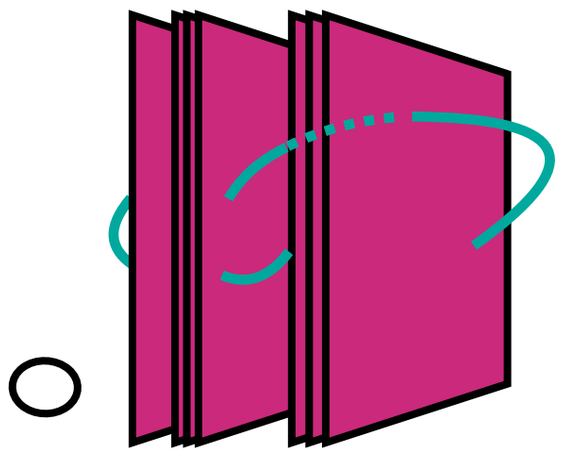
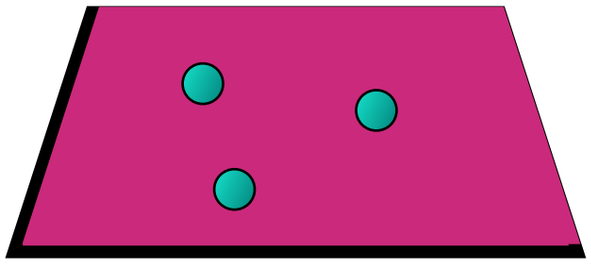
Introduction:gauge/gravity duality

conjecture from 2 descriptions of Dp-branes in string theory;

D-branes & string



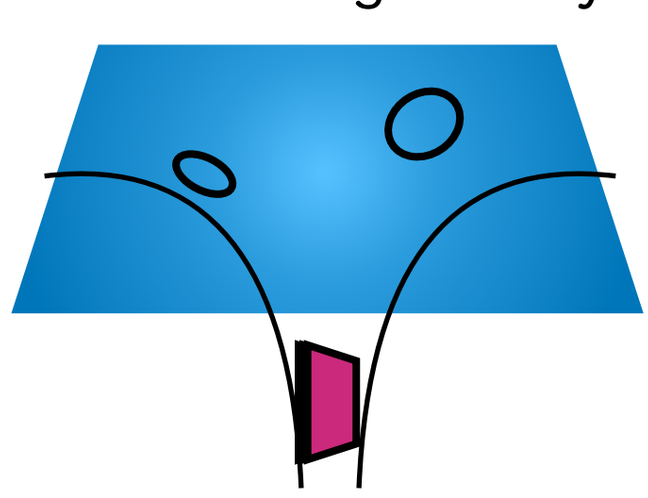
Effective theory of
open strings on branes



QFT

(Super Yang-Mills theory)

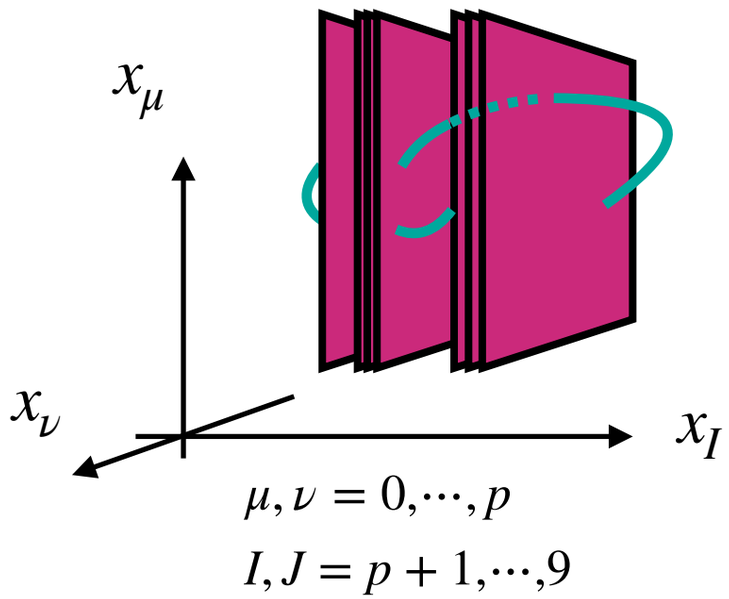
Theory of closed strings
in D-brane geometry



GR in curved spacetime

Expected to be obtained by the nonperturbative aspects of string theory

Position of D-branes & open strings



Effective action

$$\int \mathrm{d}^{p+1}x \, \mathrm{tr} \left(\frac{1}{4} F_{\mu\nu}^{\ 2} + \frac{1}{2} (D_\mu X_I)^2 + \frac{g^2}{4} [X_I, X_J]^2 + (\text{fermion terms}) \right)$$

$X_I(x)$: $N \times N$ hermitian matrices

$$X_I = \begin{pmatrix} & & \\ & \ddots & \\ & & \end{pmatrix}$$

Low-energy or classical states
→ X : simultaneously diagonal

diagonal : position of D-branes
off-diagonal : open strings among D-branes

[Witten, (1995)]

$$X_I = \begin{pmatrix} & & \\ & & \\ & & \end{pmatrix}$$

The above interpretation is also feasible

in the 't Hooft limit ($N \to \infty$, $\lambda = g^2 N \sim N^0$:fixed, $E \sim N^2$)

and strong coupling (:low energy),
where the dual gravity has been known.

[Polchinski, (1998/1999) / Susskind, (1999) / Hanada, (2021)]

Review: Matrix Quantum Mechanics

Quantum Mechanics with dN^2 degrees of freedom $\quad (I, J = p+1, \cdots, d+p+1)$

$\rightarrow$ each matrix element is **operator**

$$\hat{X}_{I,ij} = \sum_{a=1}^{N^2} \hat{X}_{I,a} \tau^a_{ij}, \quad \hat{P}_{I,ij} = \sum_{a=1}^{N^2} \hat{P}_{I,a} \tau^a_{ij}$$

τ^a : generator of $G = \mathrm{U}(N)$

$$\mathrm{tr}(\tau_a \tau_b) = \delta_{ab}$$

$$\sum_a (\tau^{ij}_a \tau^{kl}_a) = \frac{1}{N} \delta^{ik} \delta^{jl}$$

Uncertainty relation

$$[\hat{X}_{I,a}, \hat{P}_{J,b}] = \mathrm{i} \delta_{IJ} \delta_{ab}$$

- Hilbert space;

$$\mathscr{H} = \mathrm{Span} \left\{ |X\rangle;\ \hat{X}_{I,a} |X\rangle = X_{I,a} |X\rangle \right\} = \mathrm{Span} \left\{ |P\rangle;\ \hat{P}_{I,a} |P\rangle = P_{I,a} |P\rangle \right\}$$

“coordinate basis” “momentum basis”

- Partition function

$$Z(T) = \frac{1}{\mathrm{Vol} G} \int_G \mathrm{d}g\, \mathrm{Tr}_{\mathscr{H}} \left(\hat{g}\, \mathrm{e}^{-\hat{H}/T} \right) = \mathrm{Tr}_{\mathscr{H}_{\mathrm{inv}}} \left(\mathrm{e}^{-\hat{H}/T} \right)$$

Notion of wave packet

[Hanada (2021)]

How to identify the position of D-branes?

❌ $\hat{X}_{I,a}|X\rangle = X_{I,a}|X\rangle$: coordinate eigenvalue

Inconsistent in terms of the uncertainty relation and far from the classical picture…

In order to identify the location, consider the wave packet in dN^2-dim space

✔ $$|\Phi\rangle = \int_{\mathbb{R}^{dN^2}} \mathrm{d}X\,|X\rangle\langle X|\Phi\rangle = \int_{\mathbb{R}^{dN^2}} \mathrm{d}X\,\Phi(X)\,|X\rangle$$

and the center of $\Phi(X)$, $Y_{I,ij}$ (c.f. coherent state) [Hanada (2021)]

Wave packet in color space

[Hanada (2021)]

the wave packet in dN^2-dim space and the center of it

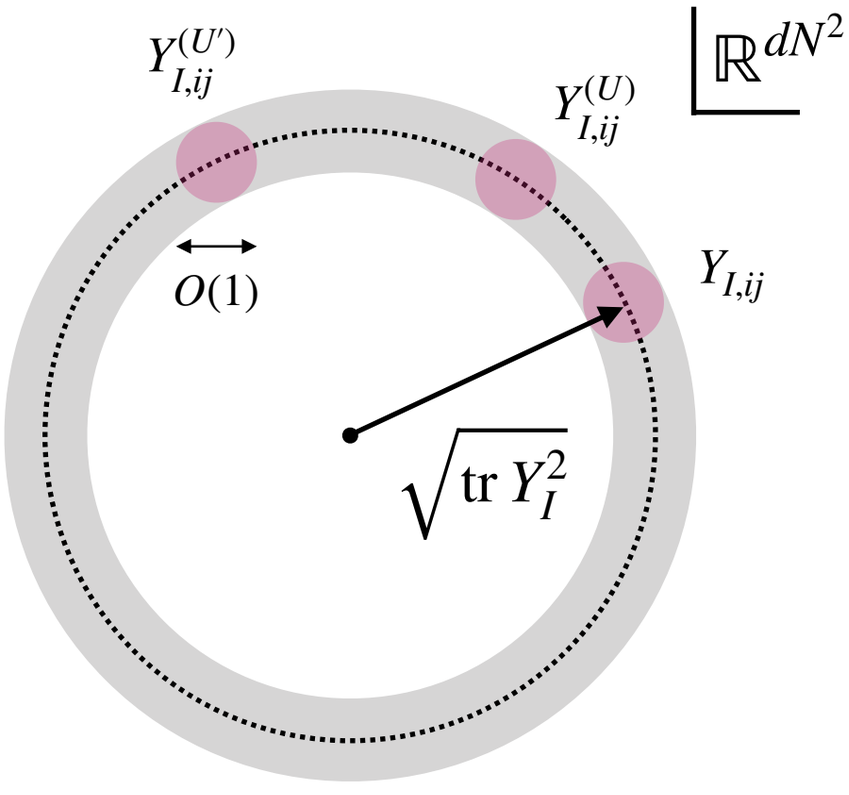
$$|\Phi\rangle = \int_{\mathbb{R}^{dN^2}} \mathrm{d}X\, |X\rangle\langle X|\Phi\rangle = \int_{\mathbb{R}^{dN^2}} \mathrm{d}X\, \Phi(X)\, |X\rangle \qquad Y_I = \begin{pmatrix} \blacksquare & & \\ & \ddots & \\ & & \blacksquare \end{pmatrix}$$

The center Y_I determines the location of D-branes!

Gauge transformation

$$\hat{X}_{I,ij} \to \left(U\hat{X}_I U^{-1}\right)_{ij} = \sum_{k,l=1}^{N} U_{ik}\hat{X}_{I,kl}U^{-1}_{lj} =: \hat{X}^{(U)}_{I,ij}$$

provides the gauge orbit of $Y_{I,a}$



- the position of the wave packet moves
  ⇔ “diagonalizability” of Y
- the shape and distance from origin
  of the wave packet are invariant

Determination of wave packet

How to identify the low-energy wave function for interacting theory?

Proposal 1 (Hamiltonian formalism) [Hanada (2021)]

$$\min_{\Phi} \langle \Phi | \hat{H} | \Phi \rangle \qquad \text{with given} \quad \langle \Phi | \hat{X}_I | \Phi \rangle = Y_I, \quad \langle \Phi | \hat{P}_I | \Phi \rangle = Q_I, \quad \cdots$$

If we set $Y_I = 0$, $Q_I = 0$, $|\Phi\rangle = |Y_I = 0,\, Q_I = 0\rangle$ is the ground state.

We can prepare such a state by the technique of quantum computation.

e.g.) Adiabatic state preparation

$$\hat{H}_A(s) = \mathrm{tr}\left(\frac{1}{2}\hat{P}_I^2 + \frac{m^2(s)}{2}\hat{X}_I^2 - \frac{g^2(s)}{4}[\hat{X}_I,\, \hat{X}_J]^2 \right)$$

$$\hat{H}_A(s=0) = \hat{H}_0$$
$$\hat{H}_A(s=s_{\mathrm{f}}) = \hat{H}_{\mathrm{target}}$$

ground state of $\hat{H}_{\mathrm{target}}$ is constructed from known & unique ground state of $\hat{H}_0$

$$|\,\text{ground state}\rangle = \lim_{s_{\mathrm{f}}\to\infty} \mathrm{T}\exp\left(-\mathrm{i}\int_0^{s_{\mathrm{f}}} \mathrm{d}s\, \hat{H}_A(s) \right) |\,\text{ground state}\rangle_0$$

Determination of wave packet

How to identify the low-energy wave function for interacting theory?

Proposal 1 (Hamiltonian formalism) [Hanada (2021)]

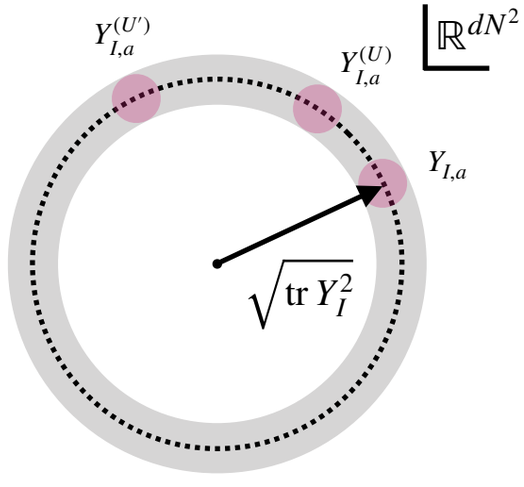
$$\min_{\Phi} \langle \Phi | \hat{H} | \Phi \rangle \qquad \text{with given} \quad \langle \Phi | \hat{X}_I | \Phi \rangle = Y_I, \quad \langle \Phi | \hat{P}_I | \Phi \rangle = Q_I, \quad \cdots$$

Proposal 2 (Path-integral formalism) [Hanada, Kanno, Matsuura, **HW**, in progress]

- Prepare $\{X_I\}$, and with given $Y_I^{(\mathrm{trial})}$ find a unitary matrix U minimizing R_∞

$$R_\infty(U, X, Y^{(\mathrm{trial})}) := \max_{I,a} \left| \left(X_I^{(U)} - Y_I^{(\mathrm{trial})} \right)_a \right|$$

: L_∞-distance or Chebyshev distance



- Vary $Y_I^{(\mathrm{trial})}$ searching $\min_Y R_\infty(U, X, Y)$

$\rightarrow$ $\langle R_\infty(U_{\min}, X, Y_{\min}) \rangle$ is gauge invariant

$\Leftrightarrow$ find the location and width of wave packet with guessing the center of it

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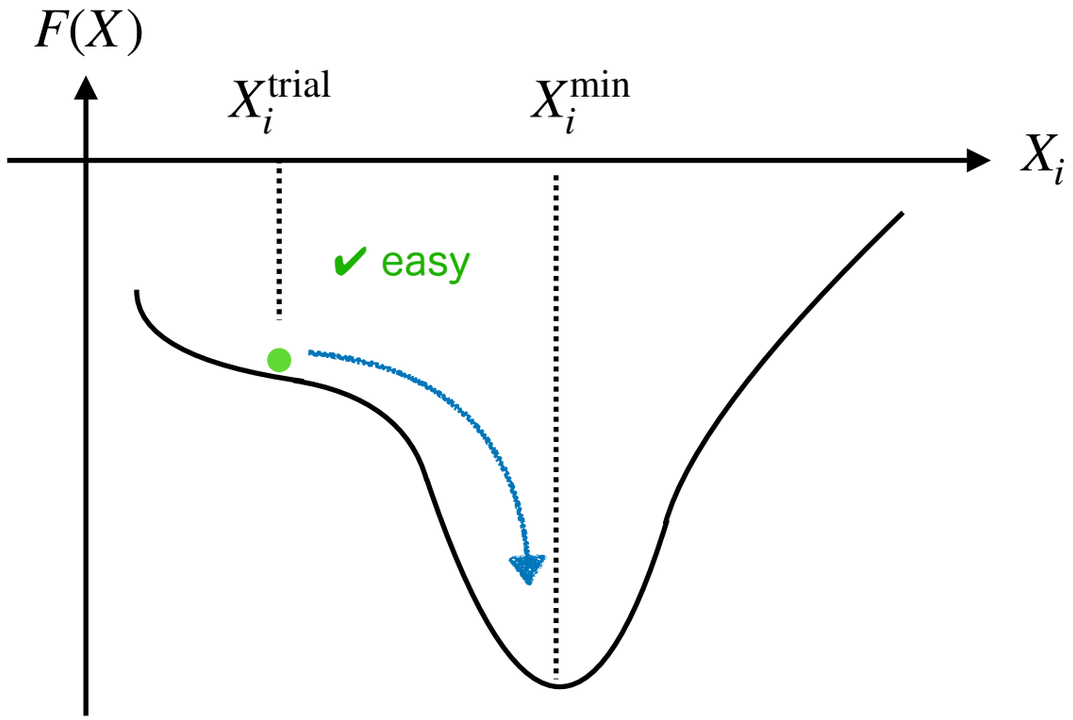
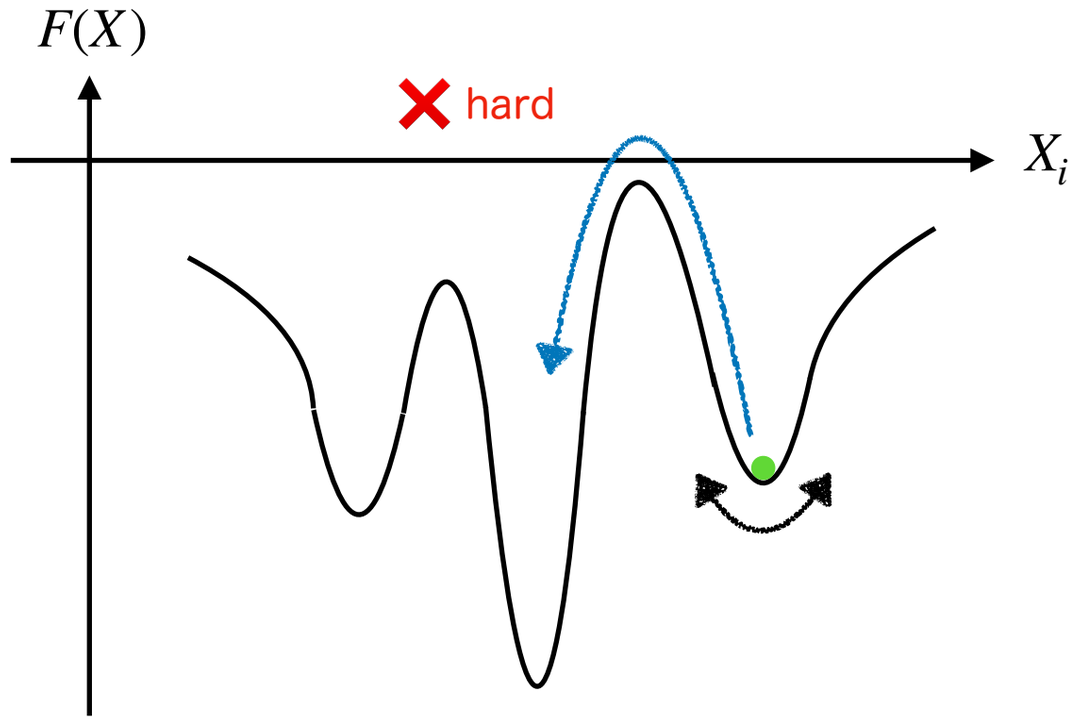
Search of minimum

A common problem we face; $F(X)$: some function to be minimized

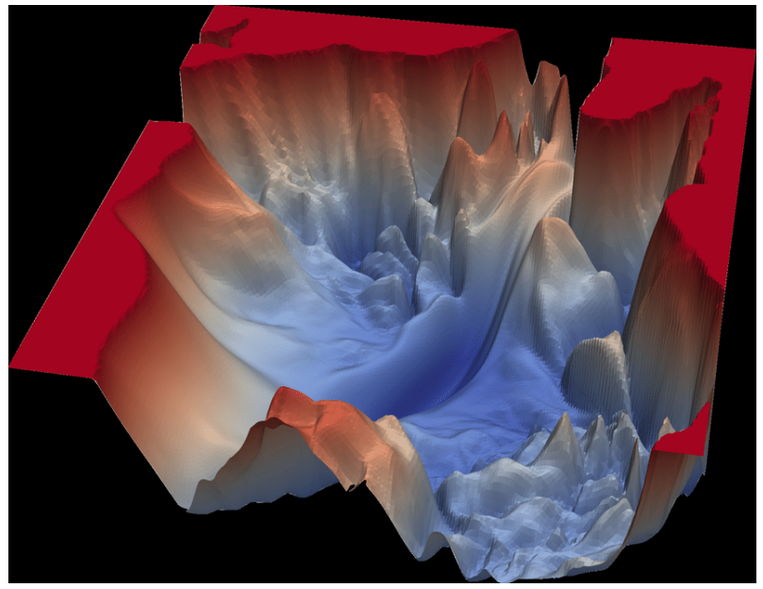




The idea of importance sampling (Monte Carlo method) is applicable and powerful to this problem.

However, it's often troublesome by being trapped in the local minima.
→ we sometimes give up to obtain the true minimum.

c.f. loss surface of DNN
from [Ulmer, (arXiv:2101.00674)]



Replica-Exchange Monte Carlo (REMC)

[Swendsen, Wang, (1986) / Geyer, (1991)]

known also as the parallel tempering, is good at searching global minimum config.;

- Prepare M replica (copy of system) with different “temperature”

$$\beta_1 < \beta_2 < \cdots < \beta_M$$

which changes the scaling of pot. barrier

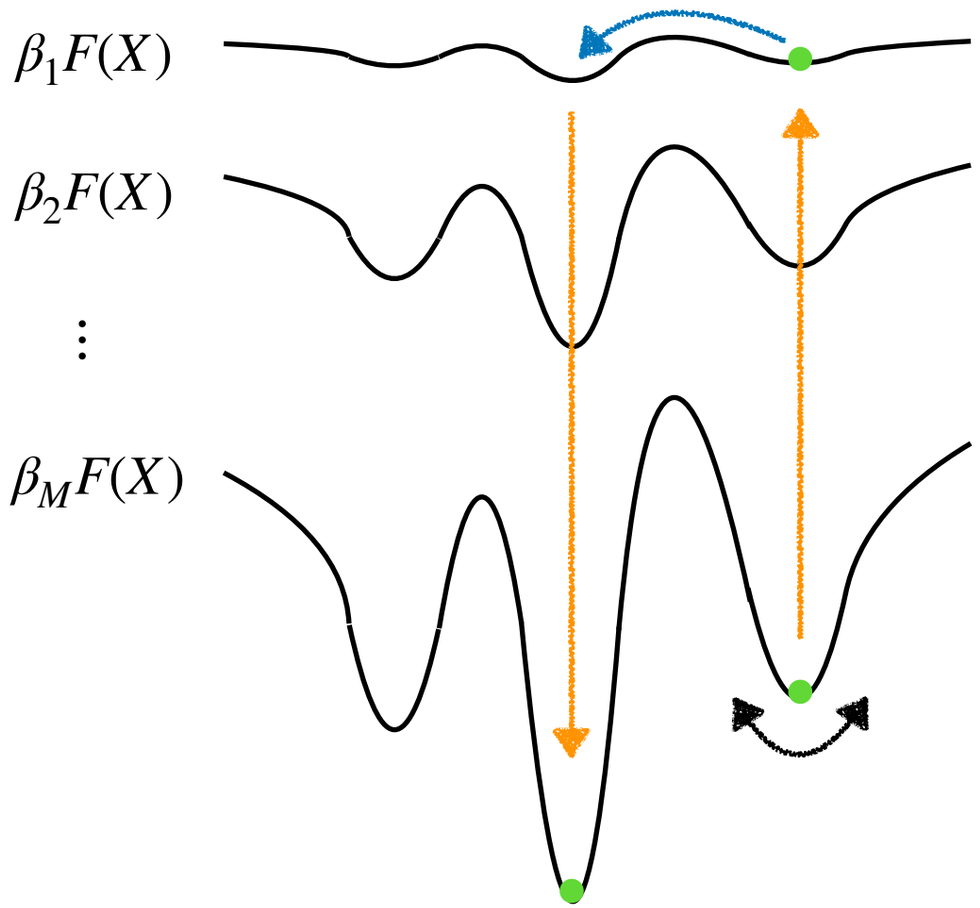
- Perform MCMC on each replica independently and generate

$$X_1,\ X_2,\ \cdots,\ X_M$$

- Exchange configurations X_m & X_{m+1} ($m = 1, \cdots, M-1$) with weight (:Metropolis test)

$$\begin{aligned}\Delta S := &\beta_m F(X_{m+1}) + \beta_{m+1} F(X_m) \\ &-\beta_m F(X_m) - \beta_{m+1} F(X_{m+1})\end{aligned}$$

$F(X)$: same function among replicas



Escapable from minima via high-T replica
→sampling efficiency has been improved!

c.f. [textbook by Hanada, Matsuura, (2021/2022)]

An extension of REMC

Still severe to minimize the L_∞-distance due to the huge #local minima

original problem

$$R_\infty(X^{(U)}) = \max_{I,a} |X_I^{(U)} - Y_I|_a$$

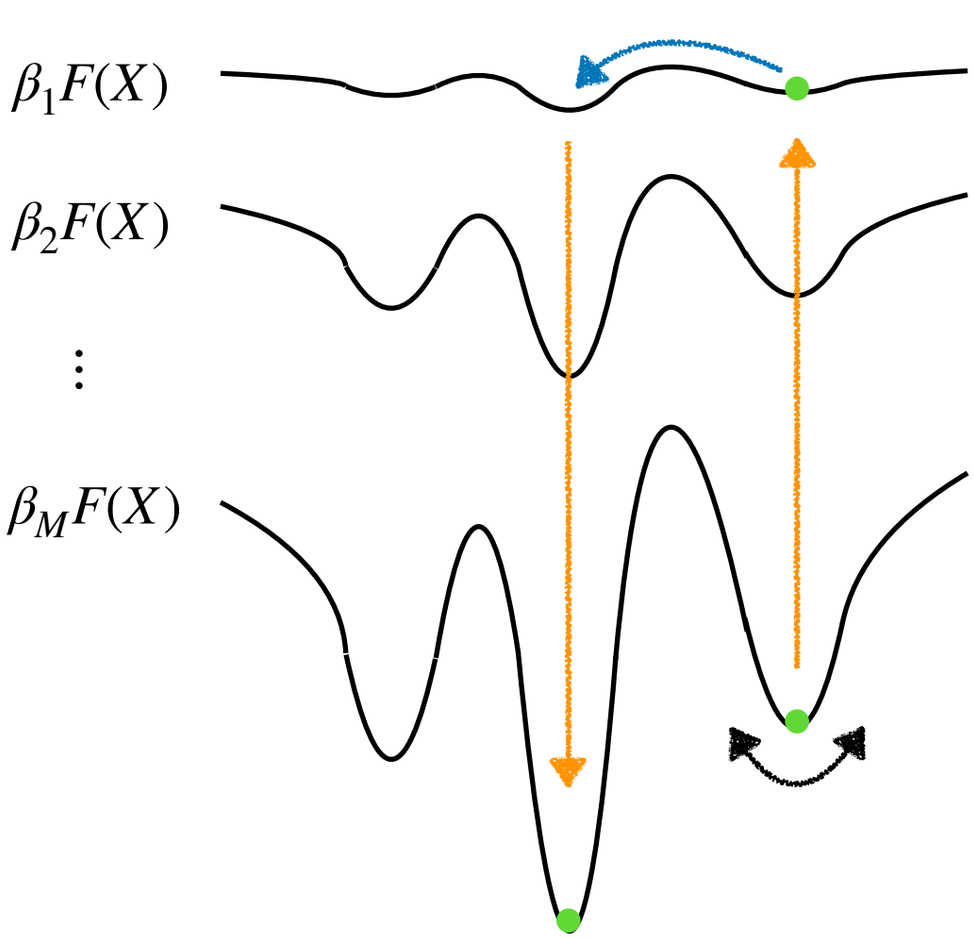
: L_∞-distance

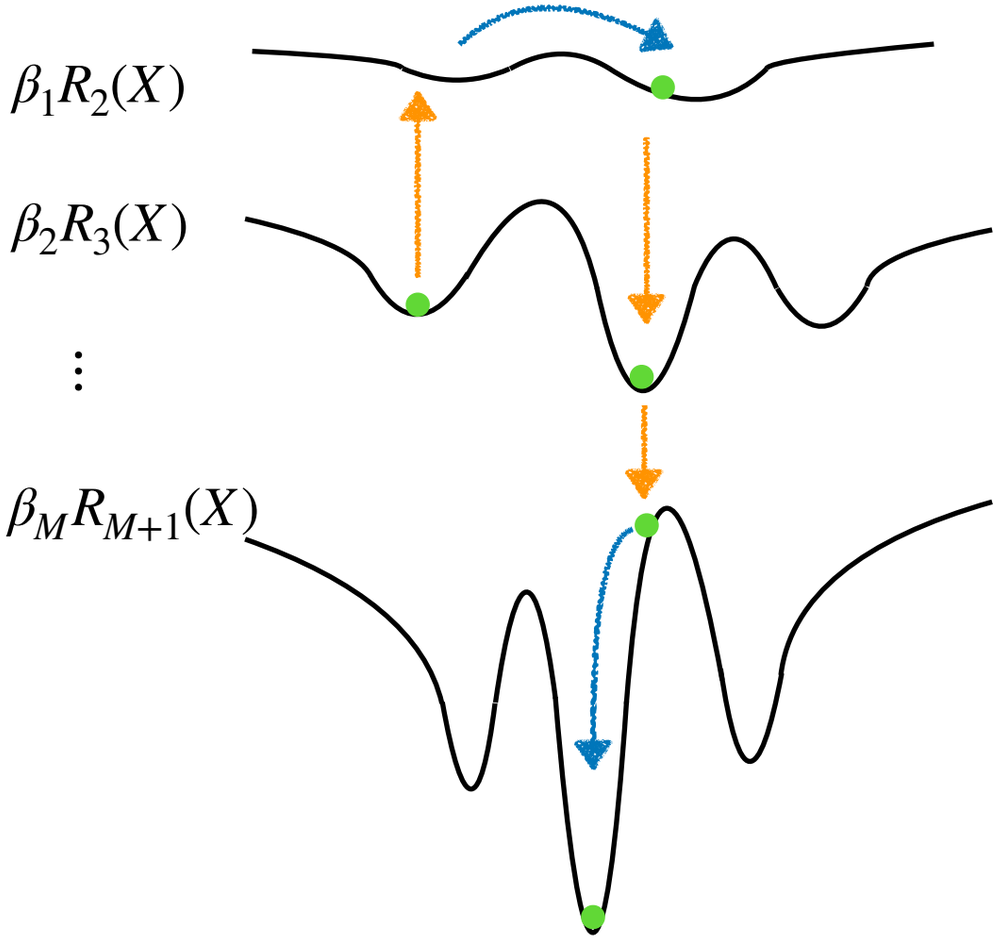
new problem

$$R_p(X^{(U)}) = \left(\sum_a |X_I^{(U)} - Y_I|_a^{\,p} \right)^{1/p}$$

: L_p-distance

extend by introducing “evaluation function” on each replica





Algorithm of extended REMC

- Prepare M replica (copy of system) with different “temperature”

$$\beta_1 < \beta_2 < \cdots < \beta_M$$

which changes the scaling of pot. barrier

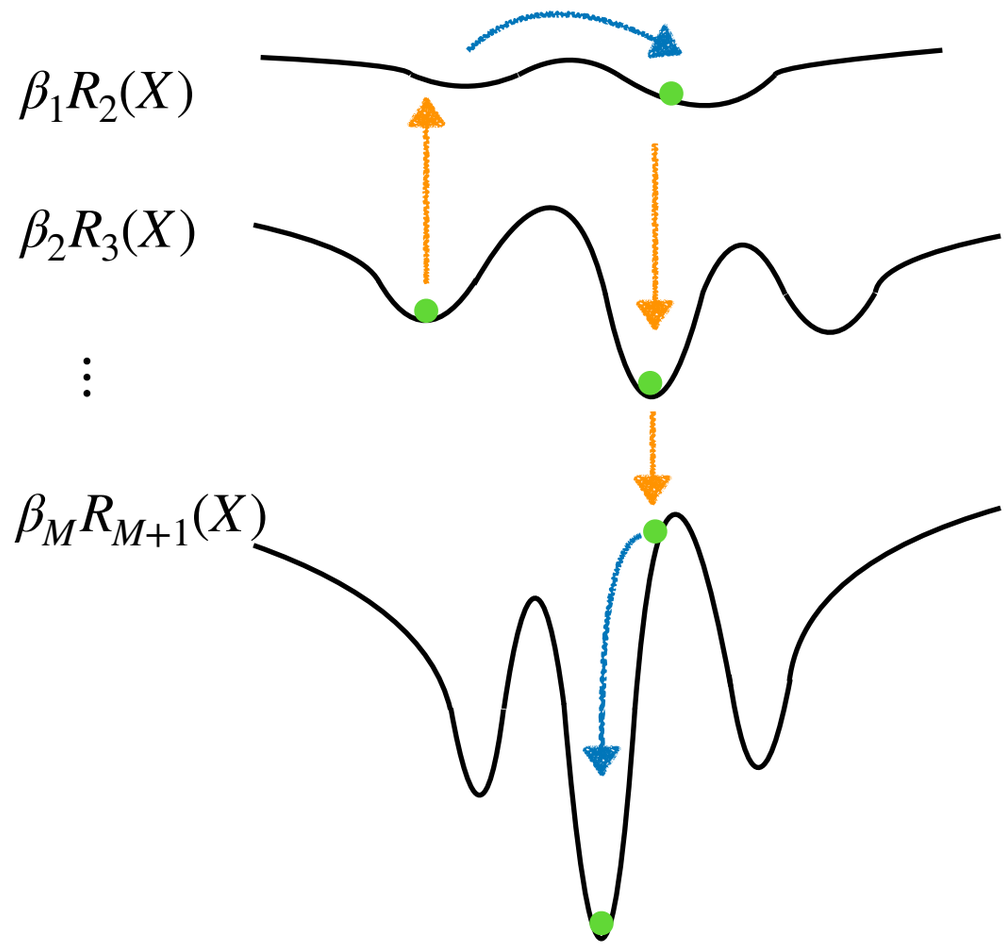
- Perform MCMC on each replica independently and generate

$$X_1,\ X_2,\ \cdots,\ X_M$$

- Exchange configurations X_m & X_{m+1} $(m = 1, \cdots, M-1)$ with weight by p

$$\Delta S_p := \beta_m R_p(X_{m+1}) + \beta_{m+1} R_{p+1}(X_m) - \beta_m R_p(X_m) - \beta_{m+1} R_{p+1}(X_{m+1})$$

$$R_p(X^{(U)}) = \left(\sum_a |X_I^{(U)} - Y_I|_a^{\,p} \right)^{1/p}$$



- Introducing some ‘cutoff’ M
- optimizing R_p on each replica

Properties of extended REMC

- MCMC algorithm in each replica → guaranteed it could work
- Different pot. structure among replicas → many minimizing path

  ∵) for an X

  $$R_2(X) \geq R_3(X) \geq \cdots \geq R_\infty(X) \geq 0$$: monotonic series of X

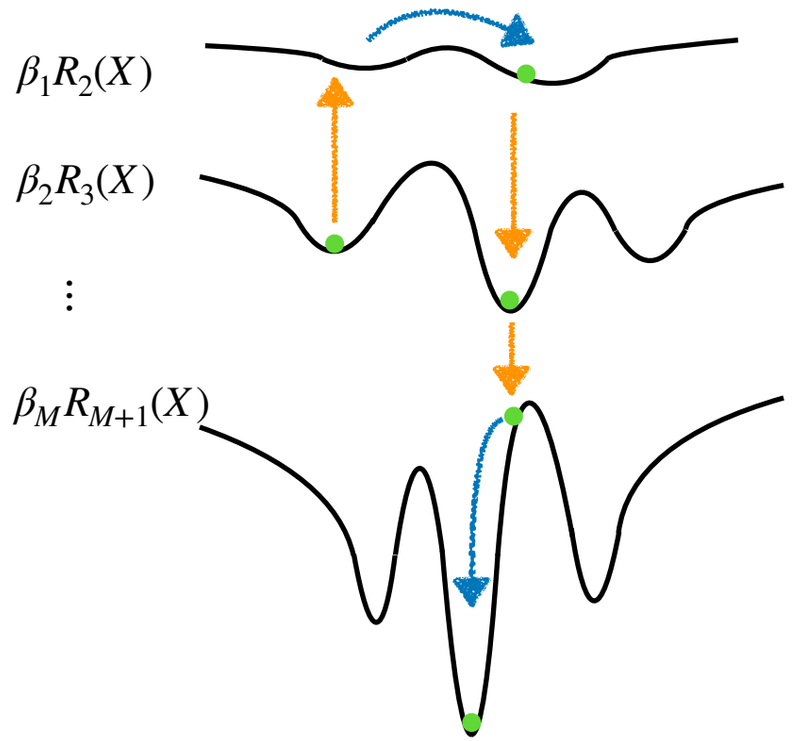
  but not satisfied

  $$\beta_2 R_2(X) \geq \beta_3 R_3(X) \geq \cdots \geq \beta_M R_M(X), \qquad \beta_2 < \beta_3 < \cdots < \beta_M$$

- Less local minima for smaller p

  ∵) $F_2(X^{(U)}) = \sqrt{\mathrm{tr}(X_I^{(U)} - Y_I)^2}$ is gauge inv.

- $R_p(X) \approx R_{p+1}(X)$ for sufficiently large p



Contents

Mock-data setup

Consider the simple setup ($I = 1$ case)

$$X_{ij} = \sum_{a=1}^{N^2-1} X_a \tau^a_{ij}, \qquad X_a = 1$$

$\mathrm{tr}\, \tau^a \tau^b = \delta^{ab}$ τ^a : $\mathrm{SU}(N)$ generator

and prepare the mock data Z by randomly generating the unitary matrices V

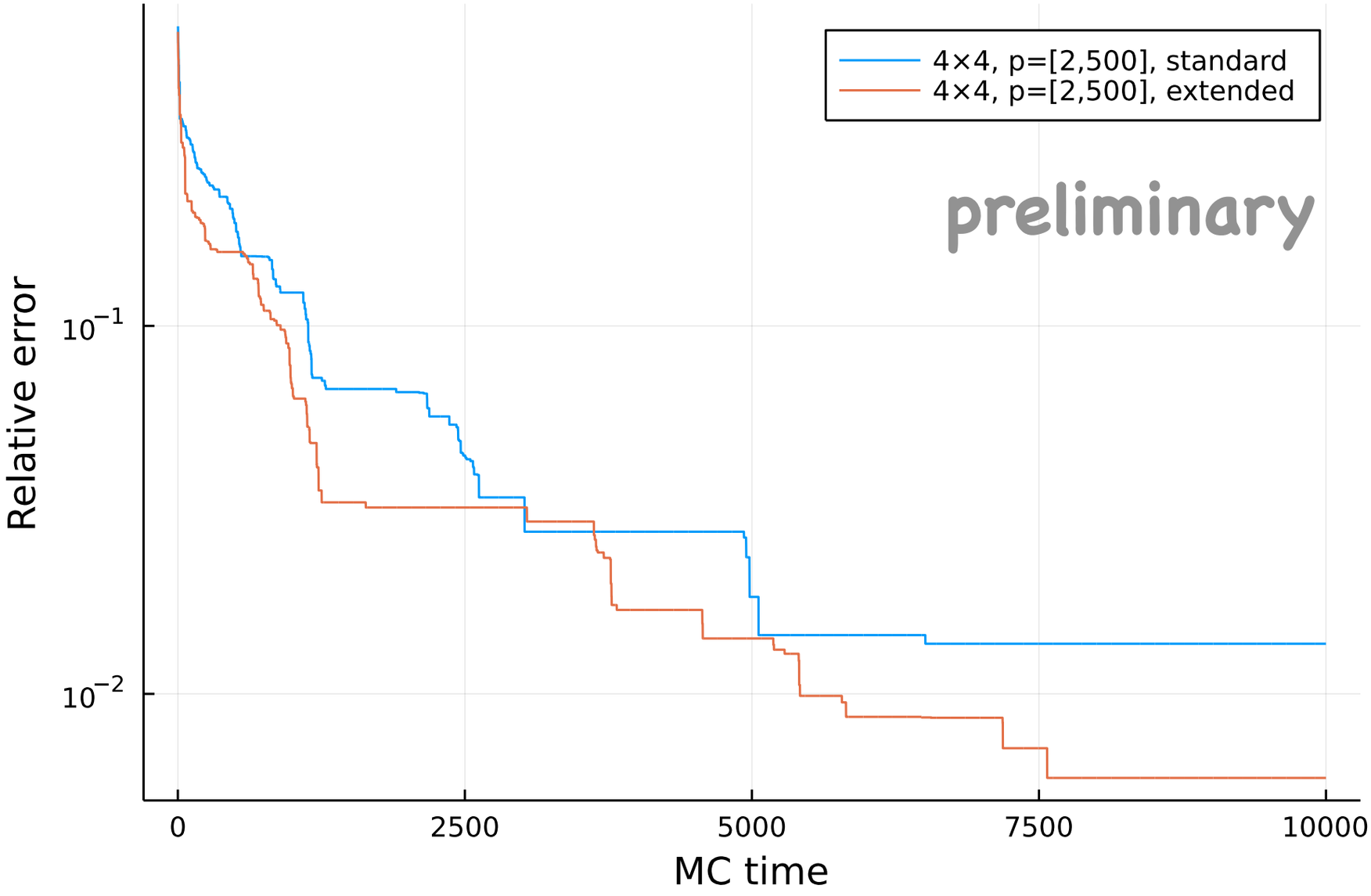
$$Z = VXV^{-1} \qquad (C = \mathbf{O})$$

$$R_\infty(U, Z) := \max_a \left| Z^{(U)} \right|_a \qquad R_\infty(U, X) = 1$$

- Demonstration that the algorithm works well and optimize the distance
- Comparison with the standard REMC

Minimization : 4×4 matrix

Demonstration: 4×4 matrix $\quad (p_{\min}, p_{\max}) = (2, 500),\ \beta_p = p$



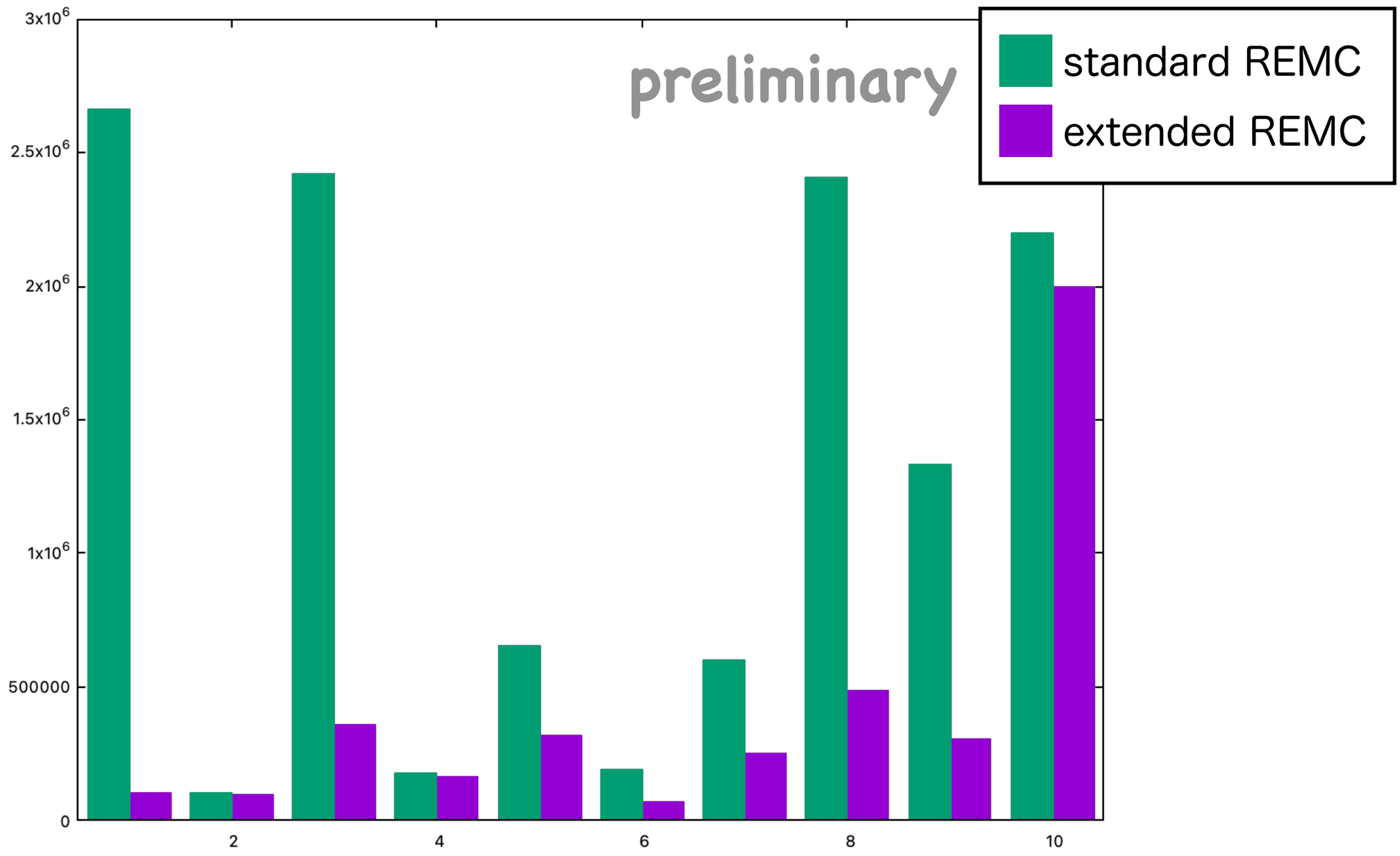
Z_a (exact value : $X_a = 1$)

standard	extended
0.974580	0.990662
0.982464	0.991926
0.985314	0.994632
0.989367	0.997921
0.993501	1.000019
0.994553	1.000333
1.000397	1.000921
1.002344	1.001330
1.003228	1.001429
1.009786	1.001482
1.010196	1.001692
1.012892	1.002493
1.013082	1.003807
1.013474	1.005307
1.013684	1.005908

MC time : 4×4 matrix

(#replica = 100, (threshold) = 1.025)

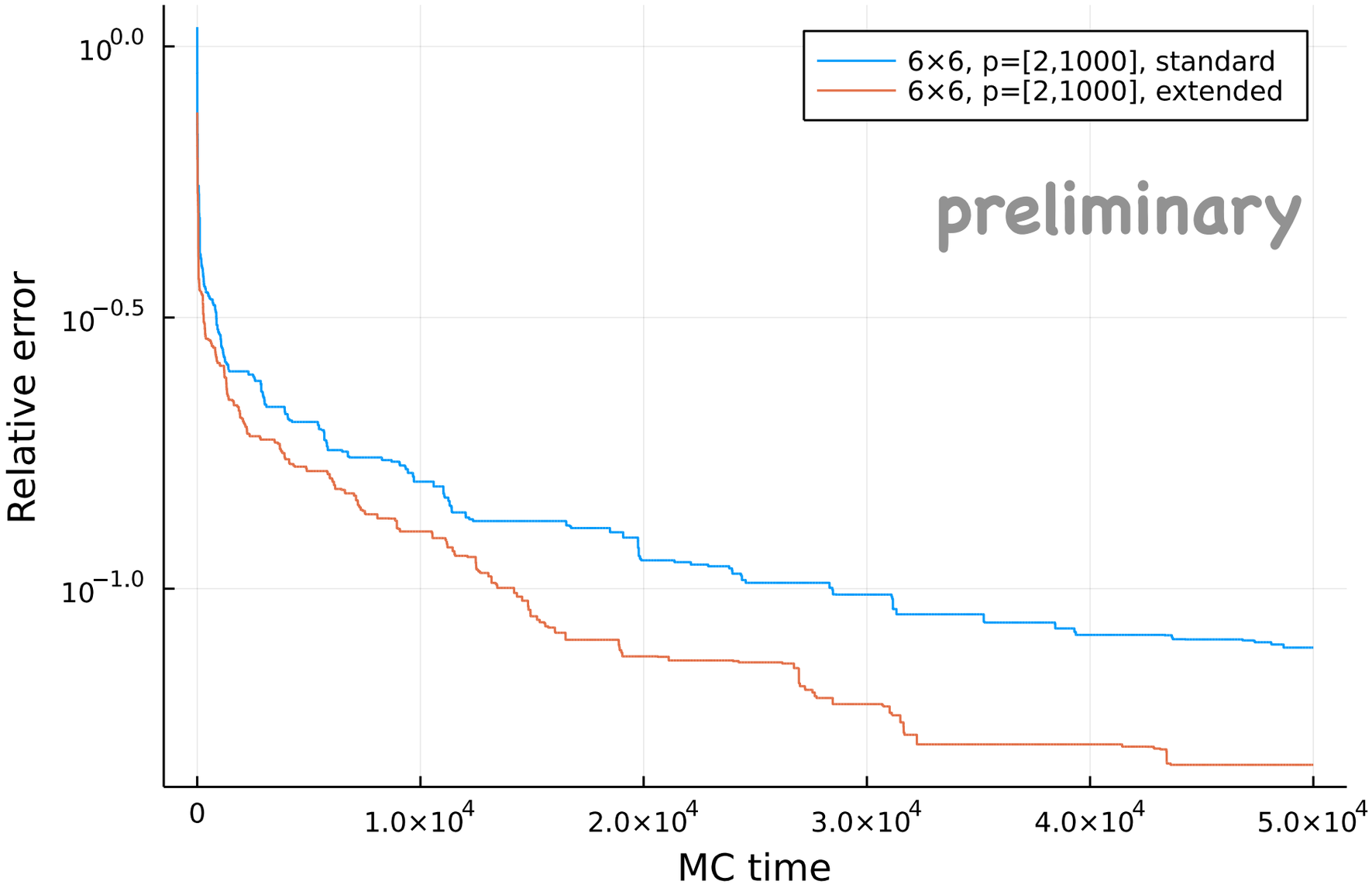
MC time (iteration)



Z constructed by 10 different unitary matrix V

Minimization : 6×6 matrix

Demonstration: 6×6 matrix $\quad (p_{\min}, p_{\max}) = (2,\ 1000),\ \beta_p = p$



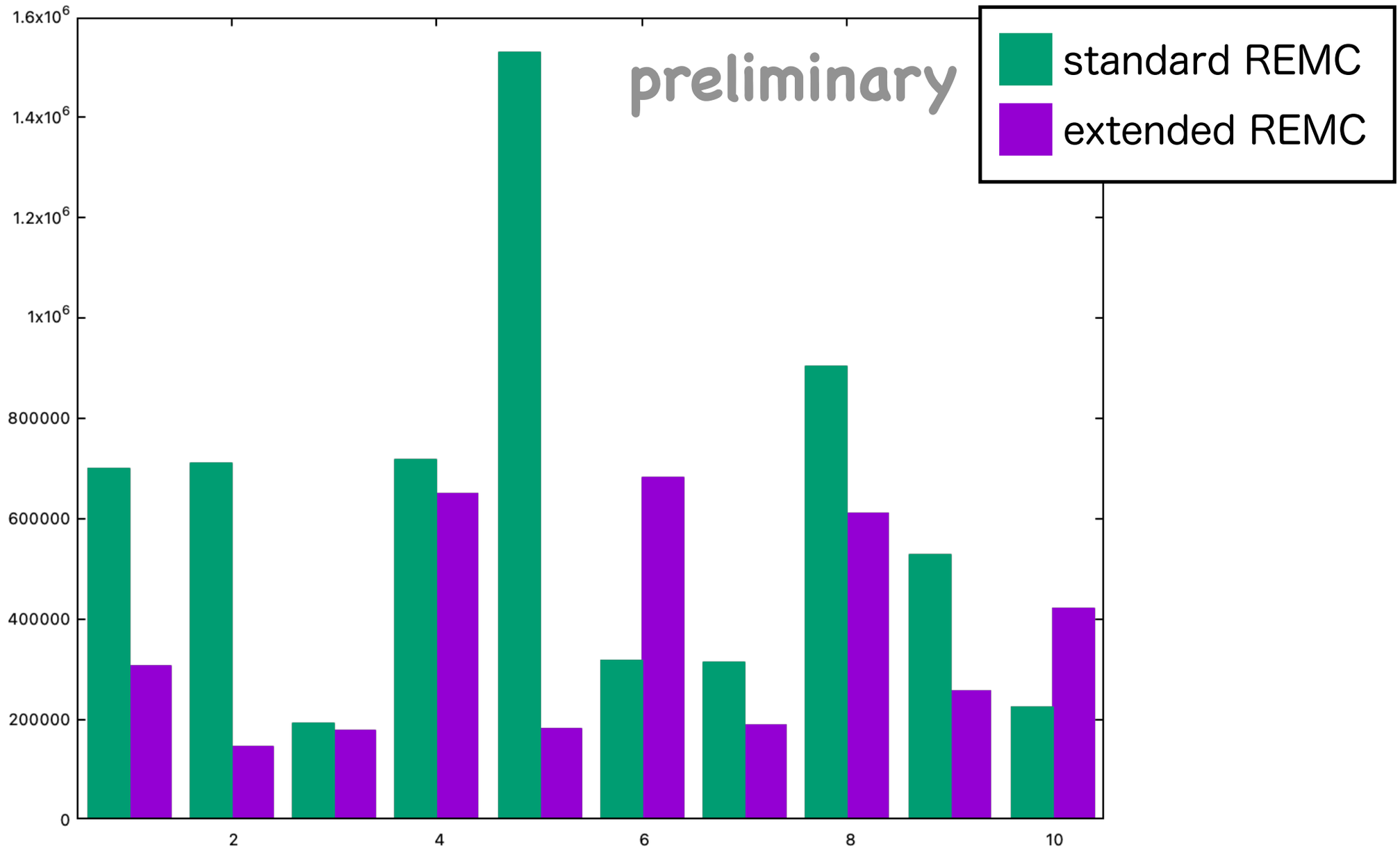
Z_a (exact value : $X_a = 1$)

standard	extended
0.552661	0.576161
0.683123	0.736379
0.710418	0.824971
0.824777	0.882625
0.862196	0.910872
0.939672	0.918226
0.959044	1.003542
…	…
1.068943	1.043846
1.072758	1.045241
1.072943	1.045690
1.075320	1.045949
1.075803	1.046511
1.077198	1.047045
1.077872	1.047336

MC time : 6×6 matrix

(#replica = 500, (threshold) = 1.025)

MC time (iteration)



Z constructed by 10 different unitary matrix V

Summary & Prospectives

- Locations of D-branes can be determined by identifying the center of the wave packet in the color space.
- In the path-integral formalism, it corresponds to find

$$\min_{U\in \mathrm{SU}(N)} \max_{I,a} \left| \left(U^\dagger X_I U - Y_I \right)_a \right|$$

  for the field X_I.

- We employ the Replica-exchange Monte Carlo method and its extended version to solve the optimization problem.

- Application to more physically-meaningful models.
  - (0+0)-dim, (0+1)-dim matrix model (e.g. w/ 3 matrices)
- Application to more generic setup (including outside the physics)

Backup

A puzzle

[Polchinski, (1998/1999) / Susskind, (1999)]

e.g.) $p = 3$ case; D3-brane effective theory

$$\langle \mathrm{tr}\, X_I^2 \rangle \sim N^2 \qquad \text{: 't Hooft counting}$$

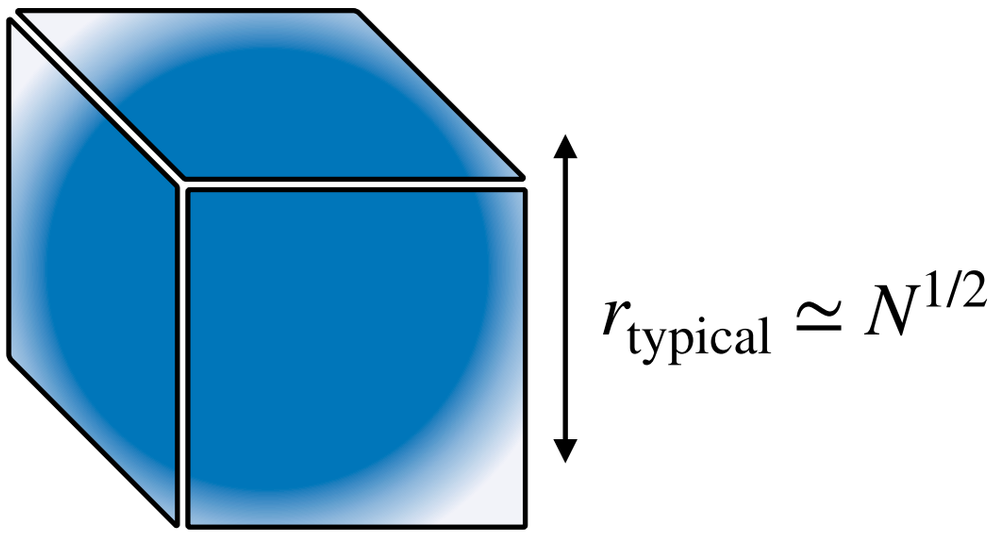
☆ eigenvalues of X_I^2 is of order $N \to$ eigenvalues of X_I is of order $\sqrt{N}$

Note also that X_I are not diagonalized simultaneously.

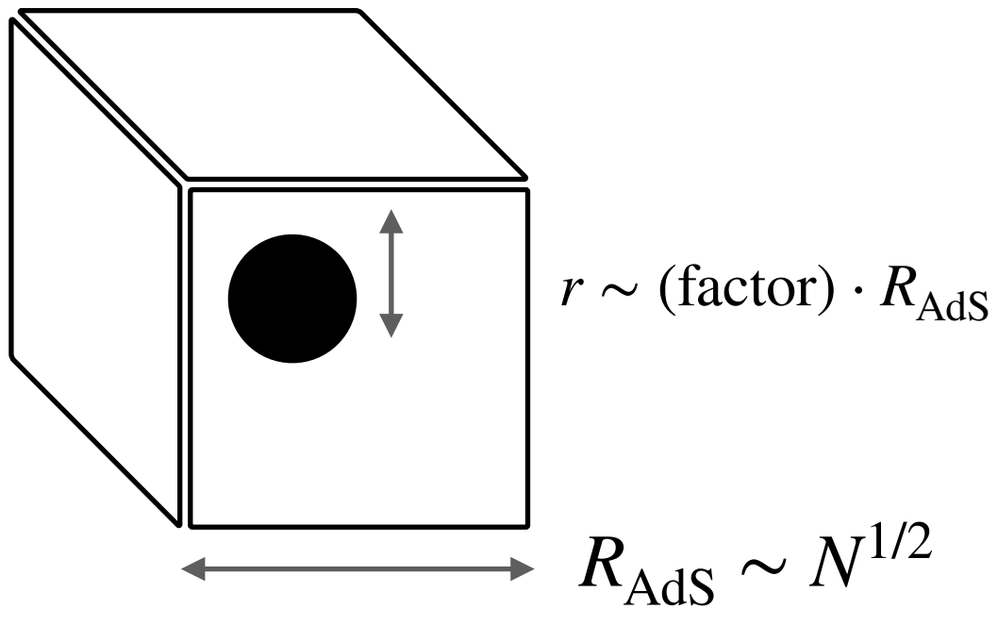
AdS5/CFT4 correspondence

[Maldacena, (1997) / Gubser, Klebanov, Polyakov, (1998) / Witten, (1998)]

QFT side



gravity (string theory) side



Reason for the discrepancy

[Hanada (2021)]

✔

❌Wrong! $\langle \mathrm{tr}\, X_I^2 \rangle \sim N^2$: 't Hooft counting

☆ eigenvalues of X_I^2 is of order N $\rightarrow$ ✔ eigenvalues of X_I is of order $\sqrt{N}$

Assumption;

The operator $\hat{X}_I$ s.t. $\hat{X}_{I,a}|X\rangle = X_{I,a}|X\rangle$ provides the Hermitian matrix X_I.

$$\hat{X}_{I,ij} = \sum_{a=1}^{N^2} \hat{X}_{I,a}\tau^a_{ij}, \quad \hat{P}_{I,ij} = \sum_{a=1}^{N^2} \hat{P}_{I,a}\tau^a_{ij} \qquad \tau^a : \mathrm{U}(N) \text{ generators}$$

However, uncertainty relation

$$\left[\hat{X}_{I,a}, \hat{P}_{J,b}\right] = \mathrm{i}\delta_{IJ}\delta_{ab}, \qquad \Delta X_{I,a}\Delta P_{J,b} \gtrsim N^0\delta_{IJ}\delta_{ab}$$

the coordinate eigenstate $|X\rangle$ contains **various momentum modes**

and therefore it is inappropriate for the low-energy state!