

# Monte Carlo Approach to String Theory

## —— An Overview

Jun Nishimura

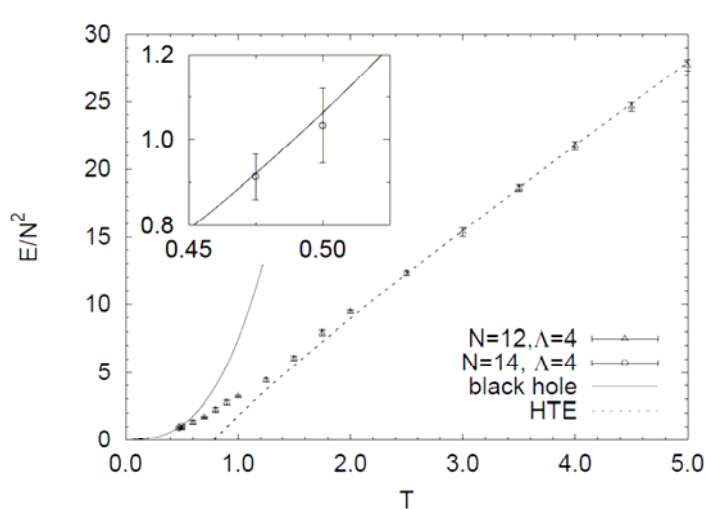
KEK & Graduate University for Advanced Studies  
(SOKENDAI)

Seminar at CQUEST, Sogang Univ. '08.4.28

# Why Monte Carlo simulations?

- Gauge/gravity duality:  
quantum field theories  $\simeq$  classical gravity  
strong coupling, large  $N$
- matrix models  
non-perturbative formulation of string theories  
play the role of lattice gauge theories for QCD
- I will explain the basic ideas and techniques  
necessary for matrix model simulations  
(in fact, simpler than field theories)

# Testing gauge/gravity duality from first principles AND understanding microscopic description of black hole



## “black hole thermodynamics”

$$\frac{E}{N^2} = C \left( \frac{T}{\lambda} \right)^p$$

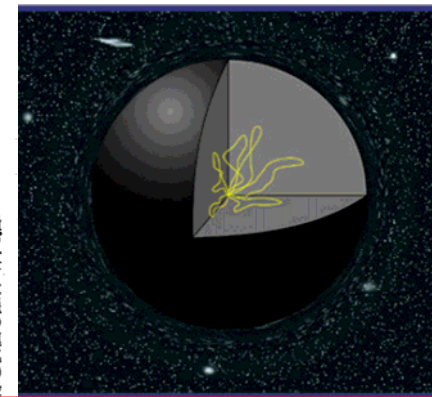
$$C = \frac{9}{14} \left( 4^{13} 15^2 \left( \frac{\pi}{7} \right)^{14} \right)^{1/5} = 7.407...$$

$$p = \frac{14}{5} = 2.8$$

Klebanov-Tseytlin '96

## ブラックホール内部 超弦理論で解明

高エネ研、スパコン使い再現



超弦理論が予測するブラックホール内部の様子。素粒子を表す多数の「弦」が、中心に端を持ちながら揺らいでいる。高エネルギー加速器研究機構提供

究極の理論とされる「超弦理論」に基づくブラックホール内部を、高エネルギー加速器研究機構（茨城県つくば市）などの研究チームがスーパーコンピュータで再現し、英国のホーキング博士の理論に一致することを確かめた。謎の多いブラックホール研究を進展させると共に、極めて困難な超弦理論の証明にスーパーコンピュータのシミュレーションが有効であることを初めて示した点でも注目されそうだ。ブラックホールは、質

量が大きな星の進化の最終段階などで作られる天体。重力が極めて強いため、光さえも抜け出せないと考えられていた。これに対し、ホーキング博士は74年、真空中でも粒子と反粒子が対になって生成と消滅を繰り返す量子効果と、アインシュタインの一般相対性理論を組み合わせ、外から見るとブラックホールから熱的な放射が生じているようになるという理論を提案。ブラックホールは最終的には「蒸発」すると主張し、大きく注目された。しかし、ブラックホールの中心付近は一般相対性理論を適用できず、超弦理論「すべての素粒子は「粒」ではなく、一次元的な広がりをを持った極めて微細な「弦」として考える理論。「弦」も理論とも呼ばれる。弦の振動の仕方などによってさまざまな素粒子を表すことができる。素粒子の間に働く基本的な相互作用には、電磁気力、弱い相互作用、強い相互作用、重力の4種類がある。重力以外の三つを記述する理論はあるが、重力まで含めた究極の理論はこれまでなかった。超弦理論では、重力を伝える素粒子「重力子」も含むため、四つの相互作用を統一して考えることが可能な理論として期待されている。しかし、弦の間に働く相互作用が強いという、具体的な計算が非常に難しく、実証された例はほとんどない。

研究責任者の西村淳岡機構素粒子原子核研究所准教授（素粒子物理学）は「ブラックホールの性質が超弦理論で理解できた」ということは、ほとんど明らかでなかった超弦理論の実在を示す有力な証拠になる。今後この理論に基づく計算機シミュレーションによって、宇宙の起源や素粒子の性質などを解明したい」と話している。

米科学誌「フィジカルレビュー・レターズ」（電子版）に15日掲載された。【河内敬一】

宇宙の起源  
解き明かせるか  
超弦理論によると、ブラックホールの内部は強い重力のため、素粒子を表す「弦」が中心に凝縮、中心に両端を持つ多数の弦が揺らいだ状態になっていると予測される。

どのような状態かは謎だった。

# Does 4d space-time emerge?

- IIB matrix model (Ishibashi-Kawai-Kitazawa-Tsuchiya '97)  
non-perturbative formulation of superstring theory

$$S = N \text{tr} \left\{ -\frac{1}{4} [X_\mu, X_\nu]^2 + \frac{1}{2} \psi_\alpha (\Gamma_\mu)_{\alpha\beta} [X_\mu, \psi_\beta] \right\}$$

- “moment of inertia” tensor

$$T_{\mu\nu} = \frac{1}{N} \text{Tr}(X_\mu X_\nu) \quad 10 \times 10 \text{ real symmetric matrix}$$

Eigenvalues :  $\lambda_1 > \lambda_2 > \cdots > \lambda_{10}$

order parameter for the SSB of SO(10)

Does a phenomenon such as

$$\langle \lambda_1 \rangle = \langle \lambda_2 \rangle = \langle \lambda_3 \rangle = \langle \lambda_4 \rangle \gg \langle \lambda_5 \rangle$$

occur in the  $N \rightarrow \infty$  limit

SO(10)  $\rightarrow$  SO(4)

# The aim of these lectures

- Satisfy **your curiosity**

Indeed MC studies of models with **16 SUSY** is made possible only recently.

- Convince you that “MC sim.” in general is **a powerful and (in fact) rather easy method**

Once you know how to use it, you can add it in **your “tool box”!**

**Not necessarily** mean that you have to do it yourself.

You can also ask **some students or experts to do it for you!**

- Enable you to **read papers** based on MC **with a lot of technical terms**  
some good ones must be useful for you to gain **new insights**  
into the physics you are interested in.

I believe, for further developments of string theory,  
Monte Carlo approach should really play **an important role**  
(Like **lattice simulation in QCD!**)

I hope these lectures help you participate in such a development.

# References

- H.J. Rothe (2005):  
**Lattice** Gauge Theories — An Introduction
- T. DeGrand, C. De Tar (2006):  
**Lattice** Methods For Quantum Chromodynamics

## Advertisement :

I am planning to write a review article on MC simulations focusing on **matrix models** based on the present lecture.

Any requests or suggestions would be very helpful!

# Plan of this lecture

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1. The principle of Monte Carlo simulation  
“Simulating” Gaussian matrix model
2. How to generate an ensemble for a general model  
—— algorithm  
detailed balance AND ergodicity
3. Basic algorithms for simulating bosonic models  
heat-bath algorithm, Metropolis algorithm  
examples: bosonic IKKT model, one-matrix model

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4. Basic algorithms for fermions  
hybrid Monte Carlo algorithms  
example: 4d version of IKKT model (supersymmetric)
5. An overview of previous works and future prospects

# *1. The principle of Monte Carlo simulation*



# 1. The principle of Monte Carlo simulation

- Generate configurations  $\{C\}$  with the probability  $\propto e^{-S[C]}$  ensemble  $\mathcal{E}$   
real positive

$$\langle \mathcal{O} \rangle \equiv \frac{\int d\phi \mathcal{O} e^{-S[\phi]}}{\int d\phi e^{-S[\phi]}} \simeq \frac{1}{n} \sum_{C \in \mathcal{E}} \mathcal{O}[C]$$

no. of configs. in the ensemble  $\mathcal{E}$

- By increasing  $n$ , one can obtain VEVs as accurate as one wishes.

Possible error due to finite  $n$  (finite statistics)

= statistical error

can be estimated from the fluctuations of  $\mathcal{O}[C]$

# “Simulating” Gaussian matrix model

—— the simplest possible example

$\phi$  :  $N \times N$  hermitian matrix

$$Z = \int d\phi e^{-S}, \quad S = \frac{1}{2} N \operatorname{tr} \phi^2$$

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int d\phi \mathcal{O} e^{-S}$$

**Vacuum Expectation Value**

Exact results :  $\left\langle \frac{1}{N} \operatorname{tr} \phi^2 \right\rangle = 1$  ,  $\left\langle \frac{1}{N} \operatorname{tr} \phi^4 \right\rangle = 2 + \frac{1}{N^2}$  , etc.

$$\phi_{ii} = \frac{A_i}{\sqrt{N}} \quad (1 \leq i \leq N)$$

$$\phi_{ij} = \frac{X_{ij} + iY_{ij}}{\sqrt{2N}} \quad (1 \leq i < j \leq N)$$

The ensemble can be obtained by just generating  $A_i, X_{ij}, Y_{ij}$  as Gaussian variables.

$$S = \frac{1}{2} \left[ \sum_{i=1}^N (A_i)^2 + \sum_{i < j} (X_{ij})^2 + \sum_{i < j} (Y_{ij})^2 \right]$$

$$\rho(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2}$$

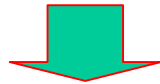
# Generating Gaussian variables

- Random number generator

—— the heart of MC sim.

generates a sequence of random numbers within the range  $[0,1)$  with **uniform probability**

Suppose  $x, y \in [0,1)$  are 2 such numbers.



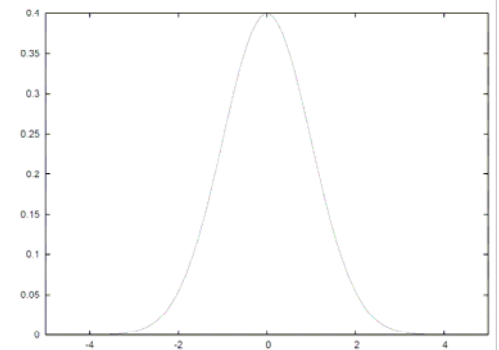
- Generating **Gaussian variables**

$$r = \sqrt{-2 \ln x} \quad \xi = r \cos \theta$$

$$\theta = 2\pi y \quad \eta = r \sin \theta$$

$$\begin{aligned} dx dy &= \frac{1}{2\pi} \exp\left(-\frac{r^2}{2}\right) r dr d\theta \\ &= \frac{1}{2\pi} \exp\left(-\frac{\xi^2 + \eta^2}{2}\right) d\xi d\eta \end{aligned}$$

$$\rho(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2}$$



$\xi, \eta$  are independent  
Gaussian variables

*2. How to generate an ensemble for a general model — algorithm*

# How to generate an ensemble for a general model? — “algorithm”

- Define the **transition probability**  $P[C \rightarrow C']$
- Given an **initial config.**  $C_0$   
one can generate (**probabilistically**)

$$C_0 \rightarrow C_1 \rightarrow \cdots \rightarrow C_{n-1} \rightarrow C_n \rightarrow C_{n+1} \rightarrow \cdots$$

$w_n[C]$  : probability of obtaining  $C$  at  $n$ -th step

$$w_{n+1}[C] = \sum_{C'} w_n[C'] P[C' \rightarrow C] , \quad w_0[C] = \delta_{C,C_0}$$

We want to choose  $P[C \rightarrow C']$  in such a way that

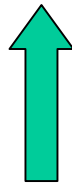
$$\lim_{n \rightarrow \infty} w_n[C] \propto e^{-S[C]}$$

# How to generate an ensemble for a general model? —“algorithm” (cont'd)

$$w_{n+1}[C] = \sum_{C'} w_n[C'] P[C' \rightarrow C]$$

Taking the  $n \rightarrow \infty$  limit,

$$e^{-S[C]} = \sum_{C'} e^{-S[C']} P[C' \rightarrow C] \quad \text{necessary condition}$$



summing over  $C'$

detailed balance :

$$e^{-S[C]} P[C \rightarrow C'] = e^{-S[C']} P[C' \rightarrow C] \quad \text{a stronger condition}$$

the flow of probability is balanced between  
**arbitrary pairs** of configurations

# How to generate an ensemble for a general model? — “algorithm” (cont’d)

Choose  $P[C \rightarrow C']$  to satisfy also :

## Ergodicity

For arbitrary pairs of configs.  $C, C'$   
there is a finite probability of moving from  $C$  to  $C'$   
within finite steps unless  $e^{-S[C']} = 0$

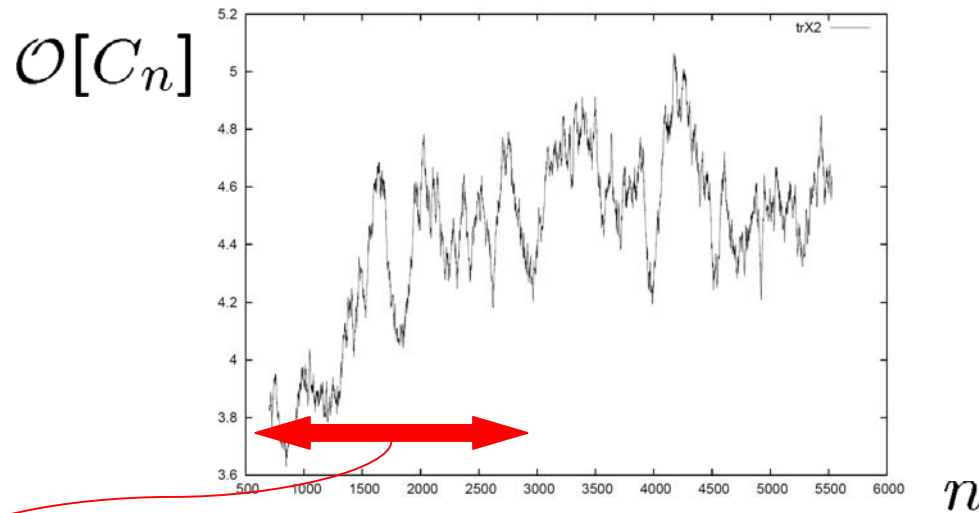
## Theorem:

If  $\left\{ \begin{array}{l} \text{the detailed balance} \\ \text{the ergodicity} \end{array} \right\}$  are satisfied,

$$\lim_{n \rightarrow \infty} w_n[C] \propto e^{-S[C]}$$

Various choices for  $P[C \rightarrow C']$  lead to various [algorithms](#).

# Thermalization and auto-correlation



history of an observable

$$\langle \mathcal{O} \rangle \simeq \frac{1}{n} \sum_{C \in \mathcal{E}} \mathcal{O}[C]$$

- thermalization

$$\lim_{n \rightarrow \infty} w_n[C] \propto e^{-S[C]}$$

One has to discard sufficiently many configs.  
generated before “thermal equilibrium” is achieved

- auto-correlation

should be taken into account in estimating statistical errors  
jack-knife method

Efficiency = CPU time required to produce an independent config.



### *3. The basic algorithms for simulating bosonic models*

# Heat bath algorithm

- Divide the whole system into **sub-systems**

$$C = \{C^{(1)}, C^{(2)}, \dots, C^{(k)}\}$$

- Update  $C^{(1)}$  fixing the rest

$$C' = \{\tilde{C}^{(1)}, C^{(2)}, \dots, C^{(k)}\}$$

with the probability  $P_1[C \rightarrow C'] \propto e^{-S[C']}$  ,  
which satisfies the detailed balance

$$e^{-S[C]} P_1[C \rightarrow C'] = e^{-S[C']} P_1[C' \rightarrow C]$$

- Repeat this for each sub-system ➡ **One sweep**

# bosonic IKKT model

(Hotta-J.N.-Tsuchiya NPB 545 ('99))

$A_\mu$  ( $\mu = 1, \dots, D$ )  $N \times N$  traceless hermitian

$$\begin{aligned} S &= -\frac{1}{4} N \operatorname{tr} [A_\mu, A_\nu]^2 \\ &= N \sum_{\mu < \nu} \left[ -\frac{1}{2} \operatorname{tr} (G_{\mu\nu})^2 + 2 \operatorname{tr} (A_\mu^2 A_\nu^2) \right] \\ &\quad G_{\mu\nu} \equiv \{A_\mu, A_\nu\} : \text{hermitian} \end{aligned}$$

introduce auxiliary variables:

$Q_{\mu\nu}$  ( $\mu < \nu$ ) :  $N \times N$  hermitian

$$\tilde{S} = N \sum_{\mu < \nu} \left[ \frac{1}{2} \operatorname{tr} (Q_{\mu\nu})^2 - \operatorname{tr} (Q_{\mu\nu} G_{\mu\nu}) + 2 \operatorname{tr} (A_\mu^2 A_\nu^2) \right]$$

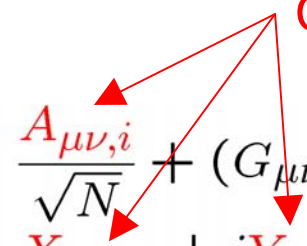
# bosonic IKKT model (cont'd)

- Updating  $Q_{\mu\nu}$

$$\begin{aligned}\tilde{S} &= N \sum_{\mu < \nu} \left[ \frac{1}{2} \text{tr}(Q_{\mu\nu})^2 - \text{tr}(Q_{\mu\nu} G_{\mu\nu}) + 2 \text{tr}(A_\mu^2 A_\nu^2) \right] \\ &= \frac{1}{2} N \sum_{\mu < \nu} \text{tr}(Q_{\mu\nu} - G_{\mu\nu})^2 + (Q\text{-indep.})\end{aligned}$$

Just the same as in the Gaussian matrix model !

Generate normal Gaussian variables



$$\begin{aligned}(Q_{\mu\nu})_{ii} &= \frac{A_{\mu\nu,i}}{\sqrt{N}} + (G_{\mu\nu})_{ii} & (1 \leq i \leq N) \\ (Q_{\mu\nu})_{ij} &= \frac{X_{\mu\nu,ij} + iY_{\mu\nu,ij}}{\sqrt{2N}} + (G_{\mu\nu})_{ij} & (1 \leq i < j \leq N)\end{aligned}$$

# bosonic IKKT model (cont'd)

- Updating  $A_\mu$

$$\tilde{S} = N \sum_{\mu < \nu} \left[ \frac{1}{2} \text{tr}(Q_{\mu\nu})^2 - \text{tr}(Q_{\mu\nu} G_{\mu\nu}) + 2 \text{tr}(A_\mu^2 A_\nu^2) \right]$$

$$= N \left[ 2 \text{tr}(S_\mu A_\mu^2) - \text{tr}(T_\mu A_\mu) \right] + (A_\mu\text{-indep.})$$

$$S_\mu = \sum_{\nu \neq \mu} A_\nu^2$$

$$T_\mu = \sum_{\nu \neq \mu} (A_\nu Q_{\mu\nu} + Q_{\mu\nu} A_\nu)$$

$O(N^3)$   
calculations

$(A_\mu)_{11}, \dots, (A_\mu)_{NN}$  can be updated simultaneously.

$(A_\mu)_{i_1 i_2}, \dots, (A_\mu)_{i_{n-1} i_n}$ , where  $i_1, \dots, i_n$  are all different, can be updated simultaneously\*.

Both by generating Gaussian variables.

(\* Repeat until all the off-diagonal elements get updated.)

# bosonic IKKT model (cont'd)

dynamical variables	no. of arithmetic operations for updating
$Q_{\mu\nu}$	$O(N^2)$
$A_\mu$ $\left\{ \begin{array}{l} \text{diagonal} \\ \text{off-diagonal} \end{array} \right.$	$O(N^2)$ $O(N^3)$
	<div style="display: flex; align-items: center;"> <div style="font-size: 3em; margin-right: 10px;">}</div> <div style="border: 1px solid black; background-color: yellow; padding: 5px;">one sweep</div> </div> <div style="margin-left: 150px;"> <span style="color: red; font-size: 1.5em;">←</span> <span style="color: red;">dominant part</span> </div>

exact result:  $\left\langle \frac{1}{N} \text{tr}(F_{\mu\nu})^2 \right\rangle = D \left( 1 - \frac{1}{N^2} \right) \quad F_{\mu\nu} \equiv i [A_\mu, A_\nu]$

*Exercise* 1) Write a code and plot the **history** of  $\frac{1}{N} \text{tr}(F_{\mu\nu})^2$   
 2) Check that the ensemble average agrees with the exact result within **the statistical error**

See Hotta-J.N.-Tsuchiya ('99) for  $\left\langle \frac{1}{N} \text{tr}(A_\mu)^2 \right\rangle$  etc.

# Metropolis algorithm

Less efficient than heat bath algorithm,  
but applicable to any model.  
Important idea for including fermions.

- Generate a trial config.  $C'$   
from the previous config.  $C$   
with the probability  $f(C \rightarrow C')$   
obeying  $f(C \rightarrow C') = f(C' \rightarrow C)$  reversibility
- Accept  $C'$  with the probability  $\min(1, e^{-\Delta S})$   
 $\Delta S \equiv S[C'] - S[C]$   
otherwise stay with  $C$
- One can again divide the system into  
sub-systems, and visit each of them sequentially.

# One-matrix model

Kawahara-J.N.-Yamaguchi, JHEP 0706 ('07)

Solvable in the large  $N$  limit.

$$S = \frac{N}{g} \left( -\text{tr} \phi^2 + \frac{1}{4} \text{tr} \phi^4 \right)$$

$$\phi = U \Lambda U^\dagger, \quad \Lambda = \text{diag}(\lambda_1, \dots, \lambda_n)$$

Integrating over  $U$ , one obtains

$$\tilde{S} = \frac{N}{g} \sum_i \left( -\lambda_i^2 + \frac{1}{4} \lambda_i^4 \right) - \sum_{i < j} \log |\lambda_i - \lambda_j|^2$$

Update  $\lambda_1$

Choose the trial value for  $\lambda'_1$   
randomly within a fixed interval  $[-X, X]$ .

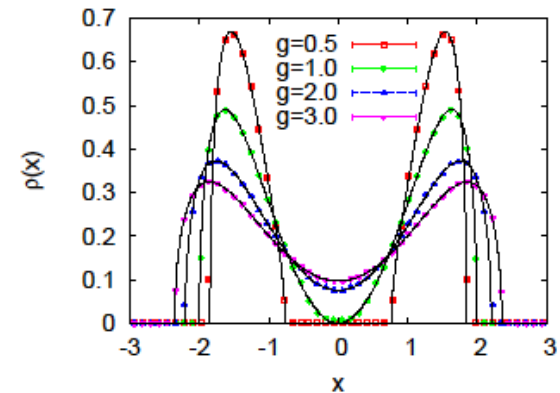
Calculate  $\Delta S$  and perform the **Metropolis reject/accept**.

Repeat this for  $\lambda_2, \dots, \lambda_N$

$O(N^2)$  calculations

Eigenval. Dist.

$$\rho(x) \equiv \frac{1}{N} \sum_{i=1}^N \delta(x - \lambda_i)$$



**Figure 1:** The eigenvalue distribution  $\rho(x)$  is plotted for  $g = 0.5, 1.0, 2.0, 3.0$  with  $N = 32$ . The curves represent the exact results (3.2), (3.3) obtained in the planar large- $N$  limit.



# Summary of the first part

- Monte Carlo simulation  
Euclidean path integral formalism  
Calculation of VEVs, correlation fns, etc.  
by generating configs. and taking average.
- heat bath algorithm : efficient, but not general  
Metropolis algorithm : less efficient, but general  
important idea for including fermions
- Simulating bosonic models is very easy.  
Do try : Gaussian matrix model (< a few hours)  
bosonic IKKT model, one-matrix model

# Pedagogical Lectures on Monte Carlo Simulations and Its Application to Matrix Models

Jun Nishimura

KEK & Graduate University for Advanced Studies  
(SOKENDAI)

Seminar at CQUEST, Sogang Univ. '08.4.30

# A brief review of the first part (Ch.1,2,3)

- Generate configurations  $\{C\}$   
with the probability  $\propto e^{-S[C]}$  ensemble  $\mathcal{E}$   
real positive

$$\langle \mathcal{O} \rangle \equiv \frac{\int d\phi \mathcal{O} e^{-S[\phi]}}{\int d\phi e^{-S[\phi]}} \simeq \frac{1}{n} \sum_{C \in \mathcal{E}} \mathcal{O}[C]$$

no. of configs. in the ensemble  $\mathcal{E}$

- Define the transition probability  $P[C \rightarrow C']$
- Given an initial config.  $C_0$

one can generate (probabilistically)

$$C_0 \rightarrow C_1 \rightarrow \cdots \rightarrow C_{n-1} \rightarrow C_n \rightarrow C_{n+1} \rightarrow \cdots$$

detailed balance :

$$e^{-S[C]} P[C \rightarrow C'] = e^{-S[C']} P[C' \rightarrow C]$$

# Various "algorithm"

—— the choice of  $P[C \rightarrow C']$

- Heat bath algorithm

$$C = \{C^{(1)}, C^{(2)}, \dots, C^{(k)}\}$$

$$C' = \{\tilde{C}^{(1)}, C^{(2)}, \dots, C^{(k)}\}$$

with the probability  $P_1[C \rightarrow C'] \propto e^{-S[C']}$

- Metropolis algorithm

propose a **trial config.**  $C'$  with probability  $f(C \rightarrow C')$   
**such that**  $f(C \rightarrow C') = f(C' \rightarrow C)$  **reversibility**

**Accept**  $C'$  with the probability  $\min(1, e^{-\Delta S})$

$$\Delta S \equiv S[C'] - S[C]$$

otherwise **stay with C**

# Plan of this lecture

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1. The principle of Monte Carlo simulation  
“Simulating” Gaussian matrix model
2. How to generate an ensemble for a general model  
—— algorithm  
detailed balance AND ergodicity
3. Basic algorithms for simulating bosonic models  
heat-bath algorithm, Metropolis algorithm  
examples: bosonic IKKT model, one-matrix model

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4. Basic algorithms for fermions  
hybrid Monte Carlo algorithms  
example: 4d version of IKKT model (supersymmetric)
5. An overview of previous works and future prospects

## *4. The basic algorithms for fermions*

# How to treat fermions in simulations

$$S_f = -\bar{\psi}_i \mathcal{M}_{ij}[\phi] \psi_j$$

There is **no way** to put **Grassmann variables**, as they are, on a computer!

$$\begin{aligned} Z_f &= \int d\psi d\bar{\psi} e^{-S_f[\psi, \bar{\psi}, \phi]} \\ &= \det \mathcal{M}[\phi] \end{aligned}$$

fermion determinant

One has to simulate :

size :  $\mathcal{N} \propto$  no. of d.o.f.

$$S_{\text{eff}}[\phi] = S_b[\phi] - \ln \det \mathcal{M}[\phi]$$

requires  $O(\mathcal{N}^3)$  arithmetic operations

$$\begin{cases} \text{matrix models :} & \mathcal{N} \propto N^2 \\ \text{field theories :} & \mathcal{N} \propto V \equiv L^D \end{cases}$$

One needs **clever techniques** to deal with them efficiently.

# Hybrid Monte Carlo (HMC) algorithm

e.g.) bosonic IKKT model

$$S[A] = -\frac{1}{4} N \operatorname{tr}[A_\mu, A_\nu]^2$$

introduce auxiliary variables

$$X_\mu \quad (\mu = 1, \dots, D) : N \times N \text{ hermitian}$$

$$\tilde{S}[A, X] = \frac{1}{2} \operatorname{tr}(X_\mu)^2 + S[A]$$

As a particular way of proposing a **trial config.**  
in Metropolis algorithm, we consider  
an auxiliary **classical dynamics** regarding

$X_\mu$  : the **conjugate momentum** of  $A_\mu$   
 $\tilde{S}[A, X]$  : the **Hamiltonian**



# HMC algorithm (cont'd)

$$\tilde{S}[A, X] = \frac{1}{2} \text{tr}(X_\mu)^2 + S[A]$$

Hamiltonian eq.

Molecular Dynamics

$$\begin{cases} \frac{dA_\mu}{d\tau} = \frac{\partial \tilde{S}[A, X]}{\partial X_\mu} = X_\mu^* \\ \frac{dX_\mu}{d\tau} = -\frac{\partial \tilde{S}[A, X]}{\partial A_\mu} = -\frac{\partial S[A]}{\partial A_\mu} \end{cases}$$

→ "force term"  
main part of  
The calculation

Solve it for a fixed "time" interval  $T$

$$(A, X) \rightarrow (A', X')$$

old config.      trial config.

One trajectory

$$\left\{ \begin{array}{l} \text{reversibility OK} \\ \tilde{S}[A, X] = \tilde{S}[A', X'] \end{array} \right. \Rightarrow \text{always accepted}$$

# HMC algorithm (cont'd)

- Can one keep on generating new configs. by the **Molecular Dynamics** alone?

NO! Ergodicity problem

e.g.) Configs. with different  $\tilde{S}$  cannot be reached.

➡ **refresh** momenta  $X$  after each **trajectory**

$$\tilde{S}[A, X] = \frac{1}{2} \text{tr}(X_\mu)^2 + S[A]$$

One can update  $X$  by generating Gaussian variables.

Hence the name : **"hybrid"** Monte Carlo

# HMC algorithm (cont'd)

- In practice, Hamilton eq. should be discretized.

$\left\{ \begin{array}{ll} \text{reversibility} & \rightarrow \text{should be respected} \\ \tilde{S}[A, X] = \tilde{S}[A', X'] & \rightarrow \text{will be sacrificed} \end{array} \right.$



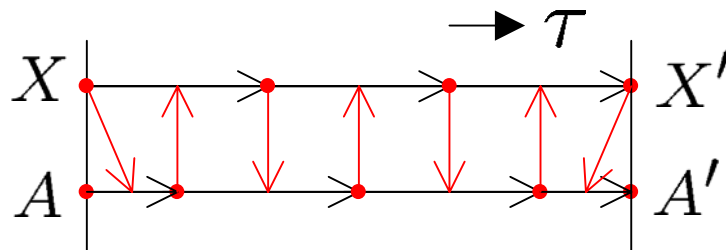
Metropolis procedure :

accept (  $A', X'$  ) with the probability  $\min(1, e^{-\Delta\tilde{S}})$

$$\Delta\tilde{S} = \tilde{S}[A', X'] - \tilde{S}[A, X]$$

Then the **detailed balance** will still be satisfied.

leap-frog discretization



# 4d version of IKKT model

Ambjorn-Anagnostopoulos-Bietenholz-  
Hotta-J.N. JHEP07,013 ('00)

$A_\mu$  ( $\mu = 1, \dots, 4$ ) :  $N \times N$  traceless hermitian

$\psi_\alpha, \bar{\psi}_\alpha$  ( $\alpha = 1, 2$ ) :  $N \times N$  traceless matrices  
with Grassmann entries

$$S_b[A] = -\frac{1}{4} N \text{tr}[A_\mu, A_\nu]^2$$

$$\begin{aligned} S_f[A] &= -(\Gamma_\mu)_{\alpha\beta} \text{tr}(\bar{\Psi}_\alpha[A_\mu, \Psi_\beta]) \\ &= -\bar{\psi}_{a\alpha} \mathcal{M}_{a\alpha b\beta} \psi_{b\beta} \end{aligned}$$

$$\begin{aligned} \mathcal{M}_{a\alpha, b\beta} &\equiv (\Gamma_\mu)_{\alpha\beta} \text{tr}(t_a[A_\mu, t_b]) \\ &2(N^2 - 1) \times 2(N^2 - 1) \text{ matrix} \end{aligned}$$

$$\begin{aligned} \Psi_\alpha &= \sum_a \psi_{a\alpha} t^a \\ \bar{\Psi}_\alpha &= \sum_a \bar{\psi}_{a\alpha} t^a \end{aligned}$$

generators of  $SU(N)$

$$Z = \int dA e^{-S_b[A]} \det \mathcal{M}[A]$$

real positive

# 4d version of IKKT model (cont'd)

- apply HMC

$$S[A] = S_b[A] - \ln \det \mathcal{M}[A]$$

$$\begin{aligned} \frac{dX_\mu}{d\tau} &= -\frac{\partial S}{\partial A_\mu} \\ &= -\frac{\partial S_b}{\partial A_\mu} - \text{tr} \left( \mathcal{M}^{-1} \frac{\partial \mathcal{M}}{\partial A_\mu} \right) \end{aligned}$$

"force term"

needs to be calculated  
at each Molecular Dynamics step

At the end of each trajectory,

$\det \mathcal{M}$  needs to be calculated

comp. effort | c.f.) bosonic models

matrix models :	$\mathcal{N} \propto N^2$	$O(N^6)$	$O(N^3)$
field theories :	$\mathcal{N} \propto V \equiv L^D$	$O(V^2)$	$O(V)$

# pseudo-fermions

a crucial trick for further efficiency

- Represent **fermion determinant** by integration over **auxiliary bosonic variables**

$$\det \mathcal{M}[A] \propto \int dF dF^* e^{-F^* \mathcal{K}[A] F}$$

real positive

$$\mathcal{D} = \mathcal{M}^\dagger \mathcal{M} \quad : \quad \text{all the eigenvalues} > 0$$

$$\mathcal{K}[A] = \mathcal{D}[A]^{-1/2}$$

rational approx.

$$x^{-1/2} \simeq a_0 + \sum_{i=1}^Q \frac{a_i}{x + b_i}$$

$a_i, b_i$  : real positive

can be optimized

for  $\epsilon \leq x \leq 1$

$$\mathcal{K} = \mathcal{D}^{-1/2} \simeq a_0 + \sum_{i=1}^Q a_i (\mathcal{D} + b_i)^{-1}$$

# pseudo-fermions (cont'd)

- Apply HMC to the whole system

$$S_{\text{PF}}[A, F, F^*] = S_{\text{b}}[A] - a_0 F^* F - \sum_{i=1}^Q a_i F^* (\mathcal{D}[A] + b_i)^{-1} F \equiv G_i$$

the main task boils down to solving **linear eq.**

$$(\mathcal{D}[A] + b_i) G_i = \textcolor{red}{F} \quad \text{for a given } \textcolor{red}{F}$$

instead of calculating  $\det \mathcal{M}$ ,  $\mathcal{M}^{-1}$

## Conjugate gradient method



iterative multiplication of  $(\mathcal{D}[A] + b_i)$

$$\begin{cases} \text{matrix models : } O(N^3) \\ \text{field theories : } O(V) \end{cases} \text{ arithmetic operations}$$

comparable to bosonic models!

# Multi-mass CG solver

- Actually, one does not have to solve

$$(\mathcal{D}[A] + b_i) G_i = F$$

for each of  $b_i$  ( $i = 1, \dots, Q$ ) separately.

Solve it for the smallest  $b_i$  with the CG method

➡ The solution for larger  $b_i$  can be obtained as a **by-product** of the CG procedure.

Jegerlehner, hep-lat/9612014

Thus, one can **save the factor of  $Q$** .

c.f.) typically  $Q \sim 10$

Hybrid Monte Carlo  
rational approximation  
multi-mass CG solver



Clark-Kennedy-Sroczynski('05)

**Rational Hybrid Monte Carlo**

**The standard algorithm for  
QCD, SUSY theories**



*5. An overview of previous works  
and future prospects*

# An overview of previous works and future prospects

- **Bosonic models** can be studied very easily.

- applications:

including Myers terms to bosonic IKKT model

$$S_3 = \frac{2}{3} i \alpha N \epsilon_{\mu\nu\lambda} \text{tr}(A_\mu A_\nu A_\lambda)$$



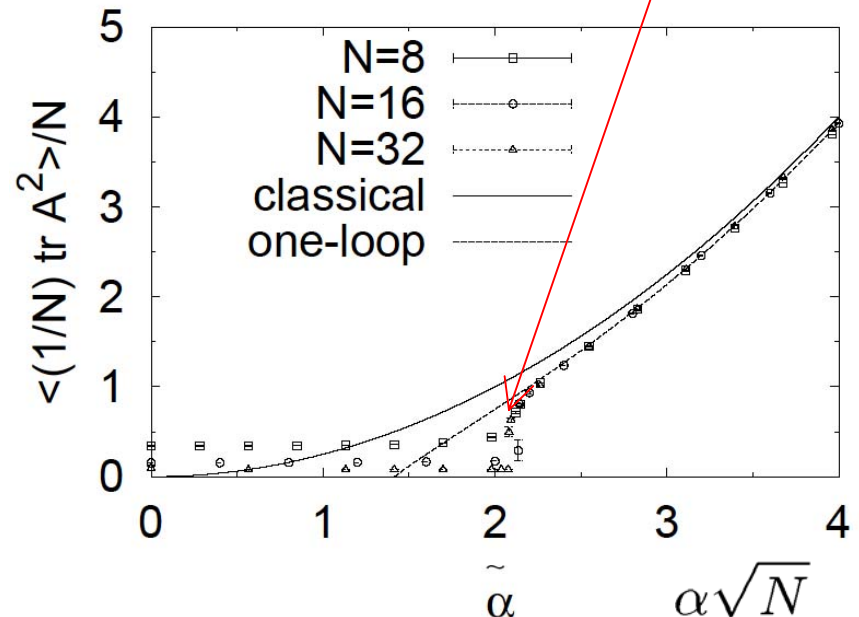
gauge theories on a **fuzzy sphere**

Iso-Kimura-Tanaka-Wakatsuki,  
Nucl.Phys.B604,121 ('01)

fuzzy sphere becomes unstable  
as the coupling becomes strong.

Azuma-Bal-Nagao-J.N.,  
JHEP 05,005 ('04)

fuzzy sphere  
collapses



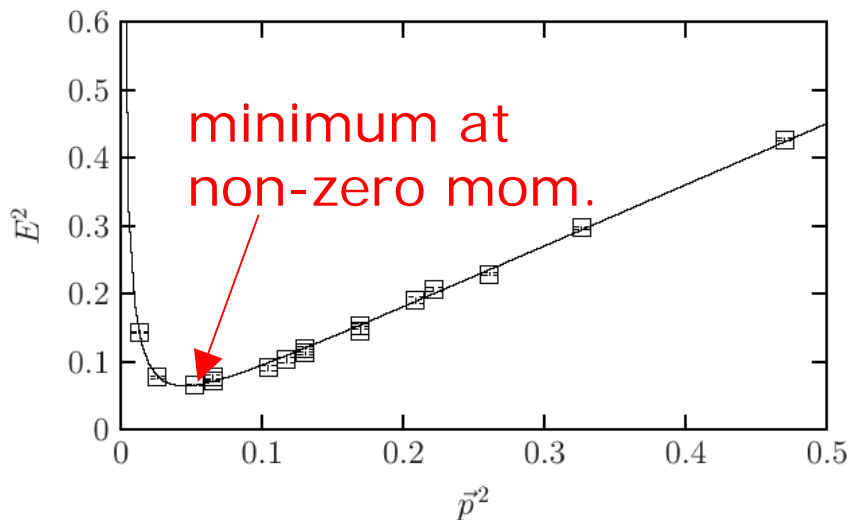
# An overview of previous works and future prospects (cont'd)

Field theories on a **non-commutative torus**  
can be formulated non-perturbatively using matrix models

Ambjorn-Makeenko-J.N.-Szabo, JHEP 05,023 ('00)

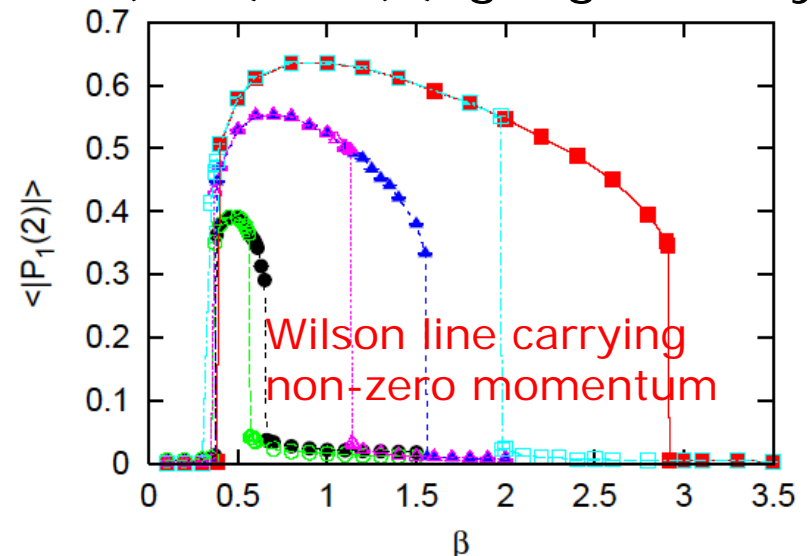
Spontaneous breakdown of translational symmetry  
due to **UV/IR mixing** effect

(2+1)d scalar field theory



Bietenholz-Hofheinz-J.N.,  
JHEP 06,042 ('04)

(2+2)d U(1) gauge theory



Bietenholz-J.N.-Susaki-Volkholz,  
JHEP 10,042 ('06)

# An overview of previous works and future prospects (cont'd)

- 1d SUSY gauge theories at finite temperature

Anagnostopoulos-Hanada-J.N.-Takeuchi, Phys.Rev.Lett.100,021601('08)

Fourier mode simulation using RHMC algorithm



The first non-perturbative studies of a system with 16 supercharges

Gauge/gravity correspondence

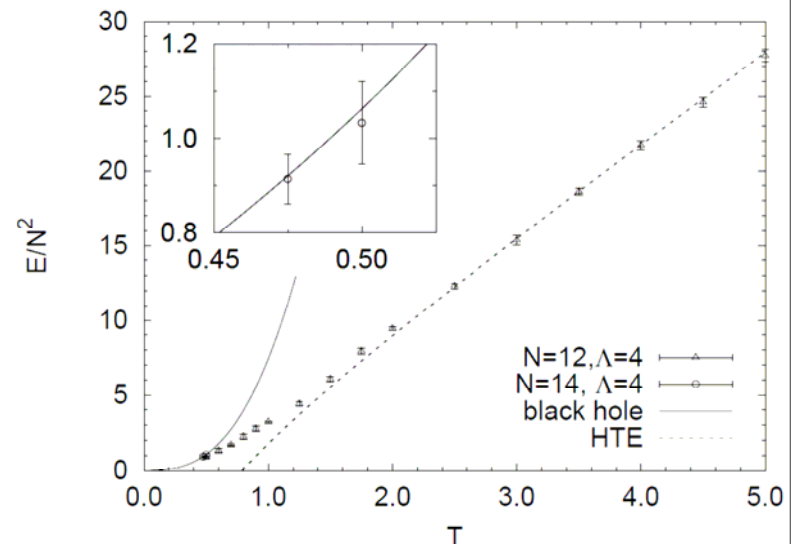
We can “study” gravity from gauge theory !

Testing the correspondence

{ at the operator level  
in the case with less SUSY

Extension to higher dimensions  
various proposals  
using lattice approach

Kaplan, Sugino, Catterall,...



# An overview of previous works and future prospects (cont'd)

- “Partial use” of Monte Carlo simulation

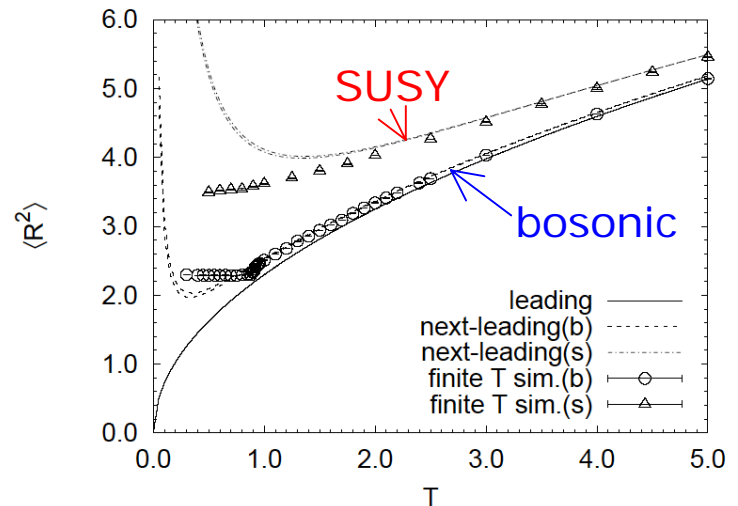
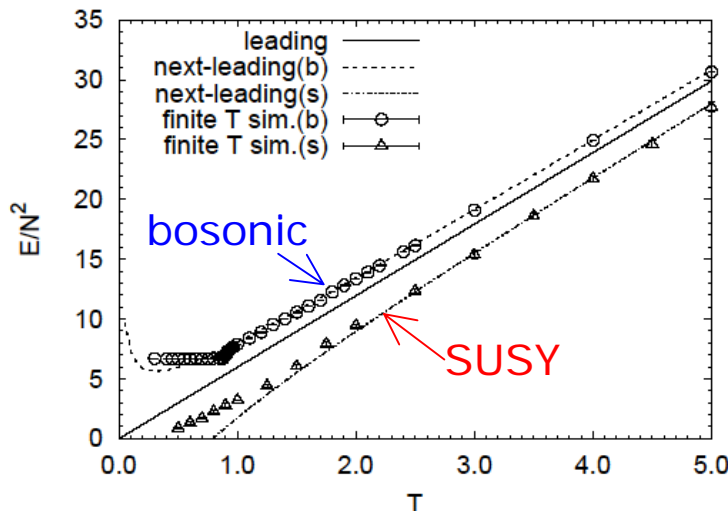
High temperature expansion of **1d SUSY gauge theory**

Kawahara-J.N.-Takeuchi, JHEP 12,103 ('07)

$$\frac{\partial}{\partial t} \rightarrow \begin{cases} 2\pi i n T & (n = 0, \pm 1, \pm 2, \dots) \quad \text{bosons} \\ 2\pi i r T & (r = \pm \frac{1}{2}, \pm \frac{3}{2}, \dots) \quad \text{fermions} \end{cases}$$

At high  $T$ , one can integrate out all the modes except **the bosonic zero mode**

➡ **bosonic IKKT model**



# An overview of previous works and future prospects (cont'd)

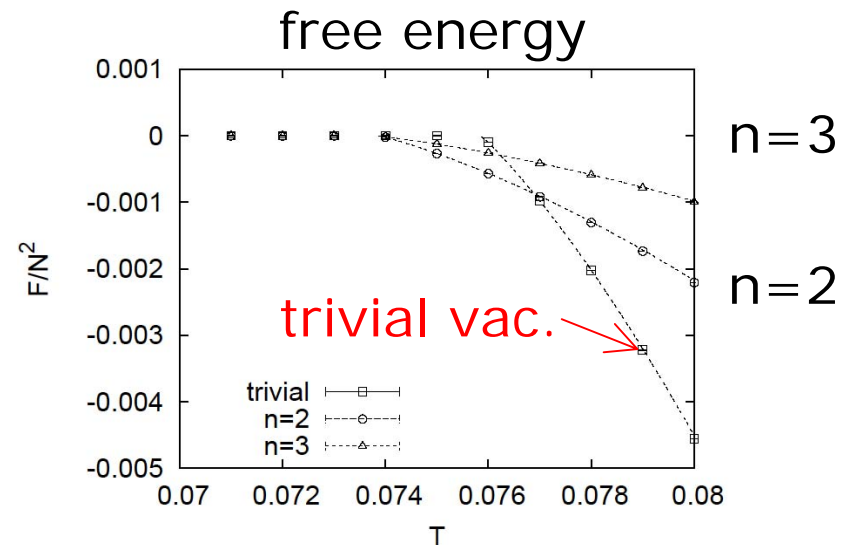
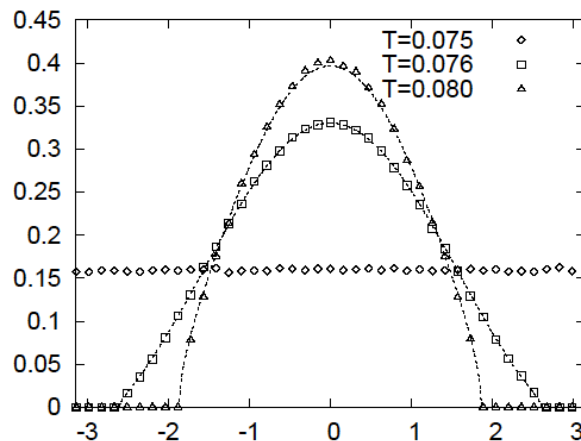
plane wave matrix model

$\mu$  : mass parameter

At large  $\mu$ , one can integrate out all the modes except the gauge field moduli.

only  $O(N)$  d.o.f.

distribution of the gauge field moduli (trivial vac.)



# An overview of previous works and future prospects (cont'd)

- IKKT model, BFSS model

Fermion determinant (Pfaffian) becomes **complex**, but

$$Z_0 = \int dA e^{-S_b[A]} |\det \mathcal{M}[A]|$$

can be simulated in the same way (e.g., RHMC).

The effect of the phase can be included by **the reweighting method**, but

sign problem

$$\langle \mathcal{O} \rangle = \frac{\langle \mathcal{O} e^{i\Gamma} \rangle_0}{\langle e^{i\Gamma} \rangle_0}$$

both  $\langle \mathcal{O} e^{i\Gamma} \rangle_0$  and  $\langle e^{i\Gamma} \rangle_0$   
becomes exponentially small  
as  $N$  increases

An idea to sample efficiently the region in the config. space,  
**where the fluctuation of  $\Gamma$  is not so violent.**

# An overview of previous works and future prospects (cont'd)

- Monte Carlo simulation

a powerful method to study **strongly coupled systems**  
from first principles

As such, one should be able to find many more places  
for applications in **string theory**.

If you think you've found one,  
you can **try it out yourself**  
(I gave you all the basics. More details in text books)  
or you can **contact us**.  
(We can tell you **whether it is feasible or not**.  
We may also collaborate if you wish.)

I hope MC sim has the potential to **revolutionize**  
the research of **string theory** (as in the case of QCD) !