Complex Langevin simulations using the deformation technique

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Sign problem

For a given partition function

$$Z = \int dx \, e^{-S(x)}$$

In the Monte Carlo simulation

 $S(x) \in \mathbb{R}$

- x is generated with the probability distribution e^{-S} .
- $\langle O(x) \rangle$ can be obtained as the ensemble average.

 $S(x)\in \mathbb{C}$

• e^{-S} is no longer regarded as the Boltzmann weight factor.

Sign problem

• appears in finite density QCD, SYM theory, real time dynamics

Introduction

The complex Langevin method is a promising approach to the sign problem.

However, in finite density QCD at low temperature and high density, this method does not work due to the singular-drift problem.

- Singular-drift problem [Nishimura, Shimasaki '15]
 - associated with appearance of near-zero eigenvalues of the Dirac operator
- > We can avoid this problem by deforming the Dirac operator. [YI-Nishimura '16]

In this talk, I apply this technique to the simple matrix model.

◆ Note, however, that there are many ways to deform the Dirac operator.

Whether the final result is independent of the way to deformation or not?

Outline

- 1. Introduction
- 2. The complex Langevin method
- 3. A matrix model with the SSB of SO(4)
- 4. Improvement by deforming Dirac operator
- 5. Summary

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The complex Langevin method

Langevin eq.

$$\frac{d}{dt}x^{(\eta)}(t) = -\frac{\partial S}{\partial x} + \eta(t)$$

$$t : \text{Langevin time}$$

$$\eta : \text{ white noise}$$

$$\Rightarrow \text{ complexify } x \text{ and consider holomorphic extension of } S$$

$$x \to z = x + iy$$

$$S(x) \to S(x, y)$$

Complex Langevin eq. [Parisi '83] [Klauder '83]

$$\frac{d}{dt}x = -\operatorname{Re}\partial_{z}S(z) + \underline{\eta(t)}_{\text{real}} \qquad \qquad \begin{pmatrix} \langle \eta(t) \rangle = 0 \\ \langle \eta(t) \eta(t') \rangle = 2\delta(t-t') \\ \frac{d}{dt}y = -\operatorname{Im}\partial_{z}S(z) \end{pmatrix}$$

The probability distribution satisfies the Fokker-Planck equation

$$\partial_{t} \underline{P\left(x,y;t\right)} = \partial_{x} \left(\partial_{x} + \operatorname{Re}\left[\partial_{z}S\right]\right) P\left(x,y;t\right) + \partial_{y} \operatorname{Im}\left[\partial_{z}S\right] P\left(x,y;t\right)$$
real

Criteria for validity of the CLM

For holomorphic observables O(x+iy), the expectation values is given by

$$\langle O(x+iy)\rangle = \int dxdy P_{eq}(x,y) O(x+iy)$$

The crucial point is that there exists a real and non-negative weight P(x, y) such that

$$\int dx \,\rho\left(x\right) O\left(x\right) \stackrel{?}{=} \int dx dy \, P_{\text{eq}}\left(x,y\right) O\left(x+iy\right) \\ \xrightarrow{\sim e^{-S(x)}: \text{ complex}} \text{ real}$$

This is satisfied when

 $P_{eq}(x, y)$ damps rapidly [Aarts, James, Seiler, Stamateseu '11] [Nishimura, Shimasaki '15]

The CLM works successfully in finite density QCD and Random matrix theory.

at deconfined phase $T > T_c$ with quark mass at T = 0

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Definition of the toy model

♦ SO(4) symmetric Gaussian matrix model [Nishimura '02]

Partition function

$$Z = \int \prod_{\mu=1}^{4} dX_{\mu} \det D(X) e^{-S_{\rm b}[X_{\mu}]}$$

$$S_{\rm b} = \frac{1}{2} N \sum_{\mu=1}^{4} \operatorname{tr} (X_{\mu})^{2}$$

$$X_{\mu} : N \times N \text{ Hermitian matrices}$$

$$\mu = 1, \cdots, 4$$

• Diarc operator

$$D_{i\alpha,j\beta}(X) = \sum_{\mu=1}^{4} (\Gamma_{\mu})_{\alpha\beta} (X_{\mu})_{ij} \qquad \Gamma_{\mu} = \begin{cases} i\sigma_i & \text{for } \mu = i = 1, 2, 3, \\ \mathbf{1}_2 & \text{for } \mu = 4 \end{cases}$$

[Nishimura-Okubo-Sugino '05]

To observe the SSB

In order to see the SSB with finite N,

(

Introduce a symmetry breaking term in the boson action

 $\operatorname{tr}\left(X_{\mu}^{2}\right) \to \left(1 + \epsilon m_{\mu}\right) \operatorname{tr}\left(X_{\mu}^{2}\right)$

For example, we used here $m_{\mu} = (1,2,4,8)$

define the order parameters of SO(4) symmetry breaking

$$\langle \lambda_1 \rangle_{\epsilon} \equiv \frac{1}{N} \operatorname{tr} X_1 X_1, \quad \dots, \quad \langle \lambda_4 \rangle_{\epsilon} \equiv \frac{1}{N} \operatorname{tr} X_4 X_4. \quad \end{bmatrix}$$
 represent the extent in each direction

> After taking large N limit and $\epsilon \to 0$ limit,

• inequality of
$$\lim_{\epsilon \to 0} \langle \lambda_{\mu} \rangle_{\epsilon}$$
 implies the SSB of SO(4).

Applying the CLM to this model

complex Langevin equation

$$\frac{dX_{i}}{dt} = -\frac{\partial S}{\partial X_{i}} + \eta\left(t\right)$$

 $SU(N) \to SL(N,C)$

 X_{μ} : $N \times N$ Hermitian matrices $\rightarrow N \times N$ complex matrices

 $\eta(t): N \times N$ Hermitian matrices

action

$$S = \frac{N}{2} \left(1 + \epsilon m_{\mu}\right) \operatorname{tr} X_{\mu}^{2} - \ln \det D\left(X\right)$$

drift term

$$\frac{dS}{d\left(X_{\mu}\right)_{ij}} = N\left(1 + \epsilon m_{\mu}\right)\left(X_{\mu}\right)_{ji} - \operatorname{tr}_{\alpha}\left(D_{ji,\alpha\beta}^{-1}\Gamma_{\mu,\beta\gamma}\right)$$

Appearance of near-zero eigenvalues → the drift becomes too large "singular-drift problem" validity of the CLM is not guaranteed.

The eigenvalue distribution of the Dirac op.

- The eigenvalues around the singularity will cause the singular drift problem. zero-eigenvalue
- For small ϵ , the problem seems to become severe. $\operatorname{tr}(X_{\mu}^2) \to (1 + \epsilon m_{\mu}) \operatorname{tr}(X_{\mu}^2)$



SO(4) symmetry breaking?



It is necessary to obtain reliable results for smaller ϵ .

That can be improved by deforming the Dirac operator.

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Deformation of the Dirac operator





The singularity at the origin is avoided.

Extrapolation of the deformation parameter

order parameters for the SSB of SO(4)

$$\rho_{\mu}\left(\epsilon, m_{\rm f}\right) = \lim_{N \to \infty} \frac{\left\langle \frac{1}{N} {\rm tr} X_{\mu}^2 \right\rangle_{\epsilon, m_{\rm f}}}{\sum_{\nu=1}^4 \left\langle \frac{1}{N} {\rm tr} X_{\nu}^2 \right\rangle_{\epsilon, m_{\rm f}}}$$

1. $\epsilon \rightarrow 0$ limit

- confirm SO(3) \rightarrow SO(2)
- 2. $m_{\rm f}
 ightarrow 0$ limit
 - confirm this SSB in the original model. $(SO(4) \rightarrow SO(2))$

prediction from the Gaussian expansion method

$$\rho_{\mu} (\epsilon = 0, m_{\rm f} = 0) \simeq 0.35, 0.35, 0.167, 0.133$$

 \rightarrow This indicates the SSB from SO(4) to SO(2)

• Note that these results may contain uncontrollable systematic errors.

Extrapolation of ϵ to zero with finite m_f



This results clearly show the SSB from SO(3) to SO(2).

Extrapolation of the deformation parameter m_f

• Deformation 1A

$$D(X; m_{\rm f}) = \sum_{\mu=1}^{4} \Gamma_{\mu} \otimes X_{\mu} + m_{\rm f} \Gamma_{3} \otimes \mathbf{1}_{N} \quad \text{invariant under } m_{\rm f} \to -m_{\rm f}$$

> The lines are fits to $f(m_{\rm f}) = c_1 + c_2 m_{\rm f}^2 + c_3 m_{\rm f}^4$



Extrapolation of the deformation parameter m_f



These results are consistent with that of deformation 1A. This suggests that the GEM results have certain systematic errors.

Comparing with another type of deformation

Deformation 2



z=1 : undeformed model

 $z \in C \,$:deformation parameter



We restrict z to be real and approach z = 1.

The phase transition is expected to occur at some z within 0 < z < 1.

Results (Preliminary)



Im z SO(3)/ SO(2)? 0 1 Re z

> The lines are fits to $g(z) = c_1 + c_2 z + c_3 z^2$





Results (Preliminary)

Deformation 2

Im z SO(3)/ SO(2)? 0 1 Re z

 \succ Fit using the results obtained by the "deformation 1Å".

 $D(X;z) = \sum \Gamma_i \otimes X_i + z\Gamma_4 \otimes X_4$





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Summary

- In order to avoid the singular-drift problem in the CLM, we have deformed the Dirac operator.
- We considered two types of deformation and compared the results.
- ➢ After taking $m_f \rightarrow 0$ limit, the results obtained for deformation 1A are consistent with that for deformation 1B, and both the results show the SSB from SO(4) to SO(2).
- However, there is a slight deviation from the prediction by the GEM, which indicates that the result of GEM contains certain systematic errors.
- As for the second deformation, further calculation is needed, although we expect that the result is consistent with the deformation 1.
- ➤ This consistency is important for usefulness of the deformation technique.
 → finite density QCD, IKKT matrix model …

Usual Monte Carlo sampling (Metropolis method)

$$Z = \int dx \, e^{-S(x)}$$

Markov chain

$$\begin{array}{ccc} x_0 \to \cdots \to x_n \to x_{n+1} \to \cdots \\ T & T & T \end{array}$$

transition probability

$$T(x_n \to x_{n+1}) = f(x_n \to x_{n+1}) P_{\text{acc}}$$

1. generating a proposal with the probability

$$f(x_n \to x_{n+1})$$
 , where $f(x_n \to x_{n+1}) = f(x_{n+1} \to x_n)$

ex) Gaussian distribution

2. Metropolis test

accept or reject the proposals with acceptance rate

$$P_{\text{acc}} = \min\left\{1, e^{-\Delta S}\right\} \qquad \Delta S = S\left(x_{n+1}\right) - S\left(x_n\right)$$

Reweighting method

Regarding the imaginary part as the observable, we can evaluate the expectation values.

$$\begin{split} \langle O\left(x\right)\rangle &= \frac{\int dx \, e^{-S[x]} O\left(x\right)}{\int dx \, e^{-S[x]}} &= \frac{\int dx \, e^{-\operatorname{Re}S[x]} e^{-i\operatorname{Im}S[x]} O\left(x\right) / \int dx \, e^{-\operatorname{Re}S[x]}}{\int dx \, e^{-\operatorname{Re}S[x]} e^{-i\operatorname{Im}S[x]} / \int dx \, e^{-\operatorname{Re}S[x]}} \\ &= \frac{\left\langle O\left(x\right) e^{-i\operatorname{Im}S[x]}\right\rangle_{\operatorname{Re}S}}{\left\langle e^{-i\operatorname{Im}S[x]}\right\rangle_{\operatorname{Re}S}} \end{split}$$

- This method is successful as long as the fluctuation of the phase $e^{-i \text{Im}S[x]}$ is small.
- The fluctuation increases exponentially with the system size.
- promising approaches
 - Holomorphic gradient flow (Lefschetz thimble)
 - Complex Langevin method

Stochastic process

When it is difficult to generate x directly with the distribution $e^{-s(x)}$, one can obtain the configurations by a stochastic process.

Brownian motion

Velocity of the particle is described as

$$m\frac{d}{dt}\boldsymbol{v}\left(t\right) = -\alpha\boldsymbol{v}\left(t\right) + \boldsymbol{\eta}\left(t\right)$$



m : mass of the particle α : friction coefficient of the fluid $\eta(t)$: force due to the collision with the molecules

Langevin equation

$$\frac{d}{dt}x^{(\eta)}(t) = -\frac{\partial S}{\partial x} + \eta(t)$$

 $x^{(\eta)}(t)$ is obtained by the stochastic process with the $\eta\left(t
ight)$

Stochastic quantization

Langevin eq.

$$\frac{d}{dt}x^{(\eta)}(t) = -\frac{\partial S}{\partial x} + \eta(t)$$

t : Langevin time $\eta\left(t
ight)$: noise

 $\eta\left(t
ight)$ is generated with the Gaussian distribution

 $\langle \eta (t) \eta (t') \rangle_{\eta} = 2\delta (t - t')$

$$\left\langle \mathcal{O} \right\rangle_{\eta} \equiv \frac{\int D\eta \, \mathcal{O}e^{-\frac{1}{4} \int dt \, \eta^{2}(t)}}{\int D\eta \, e^{-\frac{1}{4} \int dt \, \eta^{2}(t)}}$$

probability distribution function of x

$$P(x;t) = \left\langle \delta\left(x - x^{(\eta)}(t)\right) \right\rangle_{\eta} \qquad \Longrightarrow \qquad \lim_{t \to \infty} \left\langle O\left(x^{(\eta)}(t)\right) \right\rangle_{\eta} = \left\langle O(x) \right\rangle$$

• P(x; t) satisfies the Fokker-Planck eq.

$$\frac{\partial}{\partial t}P\left(x;t\right) = \frac{\partial}{\partial x}\left(\frac{\partial S}{\partial x} + \frac{\partial}{\partial x}\right)P\left(x;t\right)$$

Equivalence to the path integral

We assume

 $P(x,t) = \psi(x,t) e^{-S/2}$

Then, the FP eq. becomes



Thus, we obtain

 $\lim_{t \to \infty} P\left(x, t\right) = a_0 e^{-S}$

up to normalization

dominant

The expectation value

$$\lim_{t \to \infty} \left\langle O\left(x^{(\eta)}\left(t\right)\right) \right\rangle_{\eta} = \lim_{t \to \infty} \int dx \, O\left(x\right) P\left(x;t\right) = \left\langle O\left(x\right) \right\rangle,$$

Proof of the relation

$$\int dx \,\rho\left(x;t\right) O\left(x\right) = \int dx dy \,P\left(x,y;t\right) O\left(x+iy\right)$$

• at t = 0, we can choose $P(x, y; 0) = \rho(x; 0) \delta(y) \longrightarrow$ The relation holds.

• for an arbitrary t, we need to show the below relations

$$\int dx O(x) \rho(x;t) = \int dx O(x;t) \rho(x;0)$$
$$\int dx dy O(x+iy) P(x,y;t) = \int dx dy O(x+iy;t) P(x,y;0)$$

the time-dependent observable is defined by

$$\frac{\partial}{\partial t}O\left(z;t\right) = \tilde{L}O\left(z;t\right)$$
$$\tilde{L} = \left(\frac{\partial}{\partial z} - \frac{\partial S}{\partial z}\right)\frac{\partial}{\partial z}$$

$$P_{eq}(x, y)$$
 damps rapidly
in the imaginary direction.
around singularities of the drift term.

consider time interpolating function

$$F(t,\tau) = \int dx dy O(x+iy;\tau) P(x,y;t-\tau)$$

• We show that $F(t, \tau)$ is independent of τ

$$egin{aligned} & rac{\partial}{\partial au}F\left(t, au
ight) = & \int dxdy \, rac{\partial}{\partial au}O\left(x+iy; au
ight) P\left(x,y;t- au
ight) + \int dxdy \, O\left(x+iy; au
ight) rac{\partial}{\partial au}P\left(x,y;t- au
ight) \ & iggin{aligned} & iggin{aligned$$

$$=\int dxdy\, ilde{L}O\left(x+iy; au
ight)P\left(x,y;t- au
ight)-\int dxdy\,O\left(x+iy; au
ight)L^{ op}P\left(x,y;t- au
ight),$$

partial derivative

 \checkmark

$$= \int dx dy \,\tilde{L}O(x+iy;\tau) P(x,y;t-\tau) - \int dx dy \,LO(x+iy;\tau) P(x,y;t-\tau),$$
$$\downarrow \quad LO(z) = \tilde{L}O(z) \quad \text{for a holomorphic function}$$
$$= 0$$

Example of the singular-drift

[Nishimura, Shimasaki '15]

partition function

$$Z = \int dx \, w(x) \, , \quad w(x) = (x + i\alpha)^p \, \mathrm{e}^{-x^2/2} \, ,$$

action

$$S(z) = -\log w(z) = -p\log(z + i\alpha) + z^2/2$$

drift term

$$\frac{dz}{dt} = \frac{p}{z+i\alpha} - z + \eta(t)$$

The pole exists at $(x, y) = (0, -\alpha)$





Improvement by means of the fermion bilinear term

introduce a bilinear term to fermions

$$D \to D' = \sum_{\mu=1}^{4} \Gamma^{\mu} \otimes (X_{\mu} + \alpha_{\mu} \mathbf{1})$$

here, we used

$$\alpha_{\mu} = (0,0,0,m_{\rm f})$$

This term shifts the eigenvalue distribution to the real direction.

 \rightarrow we can extrapolate using much smaller ϵ .

It explicitly breaks the SO(4) symmetry.

SO(3) symmetry still remains.



We can investigate the SSB of SO(3).



Improvement by means of the fermion bilinear term

$$\rho_{m_{\rm f}}^{(i)} = \lim_{\epsilon \to 0} \frac{\langle \lambda_i \rangle_{\epsilon,m_{\rm f}}}{\sum_{i=1}^4 \langle \lambda_i \rangle_{\epsilon,m_{\rm f}}} = \frac{\langle \lambda_i \rangle_{m_{\rm f}}}{\sum_{i=1}^4 \langle \lambda_i \rangle_{m_{\rm f}}} \qquad 0.5$$

$$\square \text{ In the } m_f \to 0 \text{ limit} \qquad 0.4$$

$$\rho^{(i)} = \lim_{m_{\rm f} \to 0} \rho_{m_{\rm f}}^{(i)} = \frac{\langle \lambda_i \rangle}{4 + 2r}. \qquad 0.3$$

$$0.25$$

$$0.2$$

$$0.2$$

$$0.15$$

$$\langle \lambda_1 \rangle = 2.10(7) \langle \lambda_2 \rangle = 2.03(5) \langle \lambda_3 \rangle = 1.02(2) \langle \lambda_4 \rangle = 0.74(2)$$

 $ho_{m_{f}}^{(1)}
ho_{m_{f}}^{(2)}
ho_{m_{f}}^{(3)}
ho_{m_{f}}^{(3)}
ho_{m_{f}}^{(4)}
ho_{m_{f}}^{(4)}$ 0.1 0.05 0 0.2 0.4 0.6 0.8 1.2 0 1 m_f

SSB from SO(4) to SO(2)

previous result

$$\langle \lambda_1 \rangle = \langle \lambda_2 \rangle \simeq 2.1$$

 $\langle \lambda_3 \rangle \simeq 1.0 \quad \langle \lambda_4 \rangle \simeq 0.8$

Summary

The complex Langevin method

For holomorphic action, P(x, y, t) has to

- damp rapidly in the imaginary direction
- avoid singularities of the drift term

■ The matrix model with the SSB of SO(4)

$$Z = \int dX \, \left(\det D\right)^{N_{\rm f}} e^{-S_{\rm b}[X]}$$

- The pole arises in the drift term due to the zero-eigenvalues of Dirac op..
- we introduce the fermion bilinear term in the action

$$D \to D' = \sum_{\mu=1}^{4} \Gamma^{\mu} \otimes (X_{\mu} + \alpha_{\mu} \mathbf{1})$$

- This term makes the probability distribution P(X, t) to avoid the pole of Dirac op..
- The result clearly shows the SSB from SO(4) to SO(2).

Future Works

Application to the IKKT matrix model which has the SO(10) symmetry.

- The non-perturbative formulation of superstring theory.
- It is expected that 4d space emerges from compact 10d space.

It is suggested that the SO(10) breaks down to SO(3) by the Gaussian expansion method.

It is based on the systematic calculation, and using approximations.

[Nishimura, Okubo, Sugino '05]

We need to study this from first-principle calculation using the CLM.

The finite density QCD

In the high density low temperature phase, introducing an external source as we did here may help reduce the singular-drift problem.

Improvement by means of fermion mass terms

Introducing a mass term to fermions

$$D \to D' = \sum_{\mu=1}^{4} \Gamma^{\mu} \otimes (X_{\mu} + \alpha_{\mu} \mathbf{1})$$

Here, we used

 $\alpha_{\mu} = (0, 0, m_{\rm f}, 0)$

This term makes the eigenvalue distribution of *D* to avoid the pole.

 \rightarrow we can extrapolate the values of $\langle \lambda_i \rangle$ using much smaller ϵ .



Improvement by means of fermion mass terms

- 1. taking the $\epsilon \rightarrow 0$ limit with m_f fixed.
- 2. taking the $m_f \rightarrow 0$ limit.



The result clearly shows the SSB from SO(4) to SO(2).





Idea of "gauge cooling"

For lattice gauge theory,

Link variables $U_{x,\mu}$

$$SU(N) \to SL(N,\mathbb{C})$$

Considering unitarity norm.

$$rac{1}{N} \mathrm{tr} \left(U U^{\dagger} - \mathbf{1}
ight)$$
 It is no longer zero.

• It is necessary to control the norm to be small.

→ "gauge cooling"

 $U_{x,\mu} \to \Omega_x U_{x,\mu} \Omega_{x+\hat{\mu}}^{-1} \qquad \Omega_x \in SL(N,\mathbb{C})$

• Gauge inv. observables are independent of the gauge cooling.