Complex Langevin simulation of finite density QCD

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Invited talk at the YITP long-term workshop
“New Frontiers in QCD – Confinement, Phase Transition, Hadrons, and Hadron Interactions –”

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Ref.) Nagata, JN, Shimasaki : arXiv:1805.03964 [hep-lat]
QCD phase diagram at finite $T$ and $\mu$

First principle calculations are difficult due to the sign problem
The sign problem in Monte Carlo methods

• At finite baryon number density \((\mu \neq 0)\),

\[
Z = \int dU \, d\Psi \, e^{-S[U,\Psi]} \\
= \int dU \, e^{-S_g[U]} \det\mathcal{M}[U]
\]

The fermion determinant becomes complex in general.

\[
\det\mathcal{M}[U] = |\det\mathcal{M}[U]| \, e^{i\Gamma[U]}
\]

Generate configurations \(U\) with the probability \(e^{-S_g[U]} \, |\det\mathcal{M}[U]|\) and calculate

\[
\langle \mathcal{O}[U] \rangle = \frac{\langle \mathcal{O}[U] \, e^{i\Gamma[U]} \rangle_0}{\langle e^{i\Gamma[U]} \rangle_0}
\]

(reweighting)

become exponentially small as the volume increases due to violent fluctuations of the phase \(\Gamma\)

Number of configurations needed to evaluate \(\langle O \rangle\) increases exponentially.

“sign problem”
A new development toward solution to the sign problem

Key: complexification of dynamical variables

The original path integral

\[ Z = \int dx \, w(x) \]

Minimize the sign problem by deforming the integration contour

An equivalent stochastic process of the complexified variables (no sign problem !)

\[ Z = \int dz \, w(z) \]

"Lefschetz thimble approach"

"complex Langevin method"

The equivalence to the original path integral holds under certain conditions.
Brief history of the complex Langevin method

- 1983: proposal by Parisi ('83), Klauder ('83) as an extension of the Langevin method (stochastic quantization)

- 80s: tested in various complex-action systems. Works beautifully in some cases, but converges to wrong results in the other cases...

  (The reasons were not understood, and the interest in this method faded away.)

- 2011: argument for justification discussed by Aarts, James, Seiler, Stamatescu. Integration by parts can be invalid due to the excursion problem.

- 2012: “gauge cooling” Seiler, Sexty, Stamatescu

- 2013: finite density QCD in the deconfined phase succeeded Sexty

- 2016: QCD in the heavy dense limit succeeded Aarts, Attanasio, Jager, Sexty
Brief history of the CLM (cont’d)

- 2013: problems due to **poles in the drift** recognized  
  Mollgaard, Splittorff  
  (hinders finite density QCD at low T with light quarks)

- 2015: theoretical understanding of the **singular-drift problem**  
  JN, Shimasaki

- 2015: explicit justification of the **gauge cooling**  
  Nagata, JN, Shimasaki

- 2016: argument for justification refined,  
  → a useful criterion for correct convergence  
  Nagata, JN, Shimasaki

- 2016: **deformation technique** for the singular-drift problem  
  Ito, JN

- 2018: **finite QCD at low T with light quarks** succeeded  
  Nagata, JN, Shimasaki

I will explain how this was made possible.
The main message of this talk

Complex Langevin method used to be a subtle method, which has no guarantee to give correct results.

This is not true any more!

1. Complex Langevin method works beautifully in many interesting cases, including finite density QCD at low T with light quarks.

2. Now we have an explicit criterion which tells us whether the obtained results are correct or not.

3. Various techniques such as gauge cooling, deformation,... can be used to meet this criterion. (Further development in this direction is desired, though.)
Plan of the talk

1. Complex Langevin method
2. Argument for justification and the condition for correct convergence
3. Gauge cooling
4. Deformation technique
5. Application to lattice QCD at finite density
6. Summary and future prospects
1. Complex Langevin method
Stochastic quantization

\[ Z = \int dx \, w(x) \quad w(x) \geq 0 \]

Parisi-Wu (’81)

For review, see Damgaard-Huffel (’87)

View this as the stationary distribution of a stochastic process.

Langevin eq.

\[ \frac{d}{dt} x(\eta)(t) = v(x(\eta)(t)) + \eta(t) \]

“drift term”

\[ v(x) = \frac{1}{w(x)} \frac{\partial w(x)}{\partial x} \]

Gaussian noise

\[ \langle \mathcal{O} \rangle = \lim_{t \to \infty} \langle \mathcal{O}(x(\eta)(t)) \rangle_\eta \]

\[ \langle \cdots \rangle_\eta = \frac{\int D\eta \cdots e^{-\frac{1}{4} \int dt \, \eta^2(t)}}{\int D\eta \, e^{-\frac{1}{4} \int dt \, \eta^2(t)}} \]

Proof

\[ \langle \mathcal{O}(x(\eta)(t)) \rangle_\eta = \int dx \, \mathcal{O}(x) P(x, t) \]

Probability distribution of \( x(\eta)(t) \)

\[ P(x, t) = \langle \delta(x - x(\eta)(t)) \rangle_\eta \]

Fokker-Planck eq.

\[ \frac{\partial P}{\partial t} = \frac{\partial}{\partial x} \left( \frac{\partial}{\partial x} - \frac{1}{w(x)} \frac{\partial w(x)}{\partial x} \right) P \]

\[ \lim_{t \to \infty} P(x, t) = \frac{1}{Z} w(x) \]
The complex Langevin method

Parisi ('83), Klauder ('83)

\[ Z = \int dx \, w(x) \]

Complexify the dynamical variables, and consider their (fictitious) time evolution:

\[ z^{(\eta)}(t) = x^{(\eta)}(t) + i y^{(\eta)}(t) \]

defined by the complex Langevin equation

\[ \frac{d}{dt} z^{(\eta)}(t) = v(z^{(\eta)}(t)) + \eta(t) \]

Gaussian noise (real)

probability \( \propto e^{-\frac{1}{4} \int dt \eta(t)^2} \)

\[ \langle \mathcal{O} \rangle \overset{?}{=} \lim_{t \to \infty} \langle \mathcal{O}(z^{(\eta)}(t)) \rangle_{\eta} \]

Rem 1: When \( w(x) \) is real positive, it reduces to one of the usual MC methods.

Rem 2: The drift term \( v(x) \equiv \frac{1}{w(x)} \frac{\partial w(x)}{\partial x} \) and the observables \( \mathcal{O}(x) \).

should be evaluated for complexified variables by analytic continuation.
2. Argument for justification and the condition for correct convergence

The key identity for justification

\[ \langle \mathcal{O} \rangle \equiv \lim_{t \to \infty} \langle \mathcal{O}(z^{(\eta)}(t)) \rangle_{\eta} \]

\[ P(x, y; t) : \text{The probability distribution of the complexified variables } z = x + iy \text{ at Langevin time } t. \]

\[ = \int dxdy \mathcal{O}(x + iy) P(x, y; t) \]

\[ \int dxdy \mathcal{O}(x + iy) P(x, y; t) \overset{?}{=} \int dx \mathcal{O}(x) \rho(x; t) \cdots \cdots (#) \]

where \( \rho(x; t) \in \mathbb{C} \) obeys

\[ \frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x} \left( \frac{\partial}{\partial x} - \frac{1}{w(x)} \frac{\partial w(x)}{\partial x} \right) \rho \]

Fokker-Planck eq.

\[ \lim_{t \to \infty} \rho(x; t) = \frac{1}{Z} w(x) \]

This is OK provided that eq.(#) holds and

\[ P(t=\infty) \text{ is unique.} \]

The eigenvalue spectrum of the Fokker-Planck Ham. is NOT an issue!


\[ \frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x} \left( \frac{\partial}{\partial x} - \frac{1}{w(x)} \frac{\partial w(x)}{\partial x} \right) \rho \]  
Fokker-Planck eq.

\[ -H \]  
Fokker-Planck Hamiltonian

\[ \rho(x; t) \propto w(x) \] is a zero mode of \( H \)

When \( w(x) \geq 0 \), all the other eigenvalues are real positive.

This guarantees \( \rho(x; t) \to w(x) \) for \( t \to \infty \).

When \( w(x) \in \mathbb{C} \), the eigenvalues become complex.

All the EV (except for the zero mode) should have a positive real part.

This follows if \((\#)\) holds and \( P(t = \infty) \) is unique.
Previous argument for the key identity

\[
\int dxdy \mathcal{O}(x + iy) P(x, y; t) = \int dxdy \mathcal{O}(x + iy) e^{tL^\top} P(x, y; 0) = \int dxdy \{e^{tL} \mathcal{O}(x + iy)\} P(x, y; 0) = \int dx \{e^{tL_0} \mathcal{O}(x)\} \rho(x; 0) = \int dx \mathcal{O}(x) e^{tL_0^\top} \rho(x; 0) = \int dx \mathcal{O}(x) \rho(x; t)
\]

\[
\frac{\partial P}{\partial t} = L^\top P(x, y; t)
\]

\[
\frac{\partial \rho}{\partial t} = (L_0)^\top \rho(x; t)
\]

\[
P(x, y; 0) = \rho(x; 0) \delta(y)
\]

\[
L \mathcal{O}(z)|_{y=0} = L_0 \mathcal{O}(x)
\]

for holomorphic functions \(v(z)\) and \(\mathcal{O}(z)\)

There are 2 subtle points in this argument!

- **Subtlety 1**: The integration by parts used here cannot be always justified.
  
  e.g.) when \(P(x,y;t)\) does not fall off fast enough at large \(y\).

- **Subtlety 2**: It was implicitly assumed that this expression is well-defined for infinite \(t\).
The condition for the time-evolved observables to be well-defined


\[ \int dx dy \{ e^{\tau L} \mathcal{O}(x + iy) \} P(x, y; t) \]

\[ = \sum_{n=0}^{\infty} \frac{\tau^n}{n!} \int dx dy \{ L^n \mathcal{O}(x + iy) \} P(x, y; t) \]

In order for this expression to be valid for finite \( \tau \), the infinite series should have a finite convergence radius.

This requires that the probability of the drift term should be suppressed exponentially at large magnitude. \( L \sim v(z) \delta \)

This is slightly stronger than the condition for justifying the integration by parts; hence it gives a necessary and sufficient condition.
Demonstration of our condition

The probability distribution of the magnitude of the drift term

\[ u \equiv |v(z)| = \left| \frac{p}{z + i\alpha} \right| \]

In this model, CLM fails at \( \alpha \lesssim 3.7 \) due to "the singular-drift problem"
3. Gauge cooling
E.g.) a system of $N$ real variables $x_k$

$$Z = \int dx \, w(x) = \int \prod_k dx_k \, w(x)$$

$$v_k(x) \equiv \frac{1}{w(x)} \frac{\partial w(x)}{\partial x_k}$$

Symmetry properties of the drift term $v_k(z)$ and the observables $\mathcal{O}(z)$

$$x_j' = g_{jk} x_k$$

enhances upon complexification of variables

$$z_j' = g_{jk} z_k$$

$g \in$ complexified Lie group

One can modify the Langevin process as:

$$\tilde{z}_k^{(\eta)}(t) = g_{kl} z_l^{(\eta)}(t)$$

$$z_k^{(\eta)}(t + \epsilon) = \tilde{z}_k^{(\eta)}(t) + \epsilon v_k(\tilde{z}^{(\eta)}(t)) + \sqrt{\epsilon} \eta_k(t)$$
Justification of the gauge cooling


\[
\langle \mathcal{O}(z^{(\eta)}(t + \epsilon)) \rangle_\eta = \sum_{n=0}^{\infty} \frac{1}{n!} \epsilon^n \int dx \, dy \left( :\bar{L}^n : \mathcal{O}(z) \right) |_{z^{(g)}} P(x, y; t)
\]

\[
\left( :\bar{L}^n : \mathcal{O}(z) \right) |_{z^{(g)}} = :\bar{L}^n : \mathcal{O}(z)
\]

\[
z_k^{(g)} = g_{kl}(x, y) z_l
\]

The only effect of gauge cooling disappears from this expression!

\[
\begin{align*}
\mathcal{O}(z) \text{ and } \bar{L} = \left( v_k(z) + \frac{\partial}{\partial z_k} \right) \frac{\partial}{\partial z_k} \text{ are invariant} \\
\text{under complexified symmetry transformations.}
\end{align*}
\]

Note, however, that \( P(x,y;t) \) changes non-trivially because the noise term does not transform covariantly under the complexified symmetry.

One can use this freedom to satisfy the condition for correct convergence!
4. Deformation technique

a simple matrix model motivated from string theory

\[ Z = \int dA \, d\psi \, d\bar{\psi} \, e^{-(S_b + S_f)} \]

\[ S_b = \frac{1}{2} N \text{tr} \,(A_\mu)^2 \]

\[ S_f = \bar{\psi}_\alpha^f \left( \Gamma_\mu \right)_{\alpha\beta} A_\mu \psi_\beta^f \]

\[ \Gamma_1 = i \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \Gamma_2 = i \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \Gamma_3 = i \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \Gamma_4 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \]

SSB of SO(4) rotational symmetry
in the \( N \to \infty \) limit with fixed \( r = \frac{N_f}{N} \)
due to the complex fermion determinant
c.f.) In matrix model formulation of superstring theory,
SSB : SO(10) \( \rightarrow \) SO(4) is expected to occur.

**Application of the complex Langevin method**

Ito-J.N., JHEP 12 (2016) 009

\[ A_\mu : \text{Hermitian} \quad \rightarrow \quad A_\mu : \text{general complex} \]

\[ S_{\text{eff}} = \frac{1}{2} N \ tr (A_\mu)^2 - \log \det (\Gamma_\mu A_\mu) \]

In order to investigate the SSB, we introduce an infinitesimal SO(4) breaking terms:

\[ S_{\text{breaking}} = \frac{1}{2} \varepsilon N \sum_{i=1}^{4} m_i \ tr (A_i)^2 \]

\[ m_1 < m_2 < m_3 < m_4 \]

in this work, \( \vec{m} = (1, 2, 4, 8) \)

and calculate:

\[ \langle \lambda_i \rangle = \lim_{\varepsilon \rightarrow 0} \lim_{N \rightarrow \infty} \left\langle \frac{1}{N} \tr (A_i)^2 \right\rangle_{\text{CL}} \]

no sum over \( i = 1, 2, 3, 4 \)
Results of the CLM

In order to cure the singular-drift problem, we deform the fermion action as:

\[ S_f = \bar{\psi}^f_\alpha (\Gamma_\mu)_{\alpha\beta} A_\mu \psi^f_\beta + m_f \bar{\psi}^f_\alpha (\Gamma_4)_{\alpha\beta} \psi^f_\beta \]

Explicitly breaks \( \text{SO}(4) \leftrightarrow \text{SO}(3) \)

\[ \rho_i \equiv \frac{\langle \lambda_i \rangle}{\sum_{j=1}^{4} \langle \lambda_j \rangle} \]

GEM result: \( \rho_1 = \rho_2 = 0.35 \), \( \rho_3 = 0.17 \), \( \rho_4 = 0.13 \)

\( \langle \lambda_1 \rangle = \langle \lambda_2 \rangle = 2.1 \), \( \langle \lambda_3 \rangle = 1.0 \), \( \langle \lambda_4 \rangle = 0.8 \) at \( r = 1 \)

CLM reproduces the SSB of SO(4) induced by complex fermion determinant!
5. Application to lattice QCD at finite density

Ref.) Nagata, JN, Shimasaki : arXiv:1805.03964 [hep-lat]
Set up of our calculations

Nagata, JN, Shimasaki : arXiv:1805.03964 [hep-lat]

- lattice size : $4^3 \times 8$
- plaquette action with $\beta = 5.7$
- staggered fermion (4 quark flavors)
- quark chemical pot.: $\mu a = 0.4, 0.5, 0.6, 0.7$
  corresponding to $3.2 \leq \mu/T \leq 5.6$
- quark mass : $ma = 0.05$
- total Langevin time = 50 $\sim$ 150
  with stepsize $\epsilon = 10^{-4}$
the complex Langevin method for QCD

\[ w(U) = e^{-S_{\text{plaq}}[U]} \det M[U] \]

\[ S_{\text{plaq}}(U) = -\beta \sum_n \sum_{\mu \neq \nu} \text{tr} \left( U_{n\mu} U_{n+\bar{\mu},\nu} U_{n+\bar{\nu},\mu}^{-1} U_{n\nu}^{-1} \right) \]

\[ v_{an\mu}(U) = \frac{1}{w(U)} D_{an\mu} w(U) \]

\[ D_{an\mu} f(U) = \left. \frac{\partial}{\partial x} f(e^{ix a_{n\mu}} U_{n\mu}) \right|_{x=0} \]

Complexification of dynamical variables: \( U_{n\mu} \mapsto U_{n\mu} \in \text{SL}(3, \mathbb{C}) \)

Discretized version of complex Langevin eq.

\[ \mathcal{U}_{n\mu}^{(\eta)}(t+\epsilon) = \exp \left\{ i \sum_a \left( \epsilon v_{an\mu}(U) + \sqrt{\epsilon} \eta_{an\mu}(t) \right) t_a \right\} \mathcal{U}_{n\mu}^{(\eta)}(t) \]

The drift term can become large when:

1) link variables \( U_{n\mu} \) become far from unitary (excursion problem) \[ \text{“gauge cooling”} \]

2) \( M[U] \) has eigenvalues close to zero (singular drift problem)

Rem.) The fermion determinant gives rise to a drift \[ \text{tr} \left( M[U]^{-1} D_{an\mu} M[U] \right) \]

\[ \text{“deformation technique”} \]
Deformation technique

Staggered fermion (4 quark flavors)

\[ S_f = \sum_x \left[ \sum_{\nu=1}^{4} \frac{1}{2} \eta_\nu(x) \left( e^{\mu \delta_{\nu 4}} \bar{\psi}(x) U_{x \nu} \psi(x + \nu) - e^{-\mu \delta_{\nu 4}} \bar{\psi}(x) U_{x - \nu, \nu}^{-1} \psi(x - \nu) \right) + m \bar{\psi}(x) \psi(x) + i \alpha \eta_4(x) \bar{\psi}(x) \psi(x) \right] \]

"imaginary chemical pot." in the continuum

Drift histogram

\[ \mu = 0.7 \]

Eigenvalue distribution of Dirac matrix \( M[U] \)
baryon number density

\[ \langle n \rangle = \frac{1}{3N} \frac{\partial}{\partial \mu} \log Z \]

linear extrapolation w.r.t. \( \alpha^2 \)
considering symmetry under \( \alpha \leftrightarrow -\alpha \)

Silver Blaze phenomenon suggested
chiral condensate

$$\langle \Sigma \rangle = \frac{1}{N \sqrt{\partial}} \log Z$$

linear extrapolation w.r.t. $\alpha^2$
considering symmetry under $\alpha \leftrightarrow -\alpha$
6. Summary and future prospects
Summary and future prospects

- The complex Langevin method is a powerful tool to investigate interesting systems with complex action.
  - The argument for justification was refined, and the condition for correct convergence was obtained.
  - The singular-drift problem may be avoided by the deformation technique.

- Finite density QCD at low temperature with light quarks
  - The singular drift problem can be avoided by the deformation technique.
    (Also successful applications in matrix models related to superstring theory.)

- Future directions
  - Larger lattices with lighter quarks
  - Exploration of “the critical end point” at finite T
  - Cases with 2 quark flavors
  - Applications to other complex-action systems

S.Tsutsui’s talk in the afternoon