Complex Langevin simulation of finite density QCD

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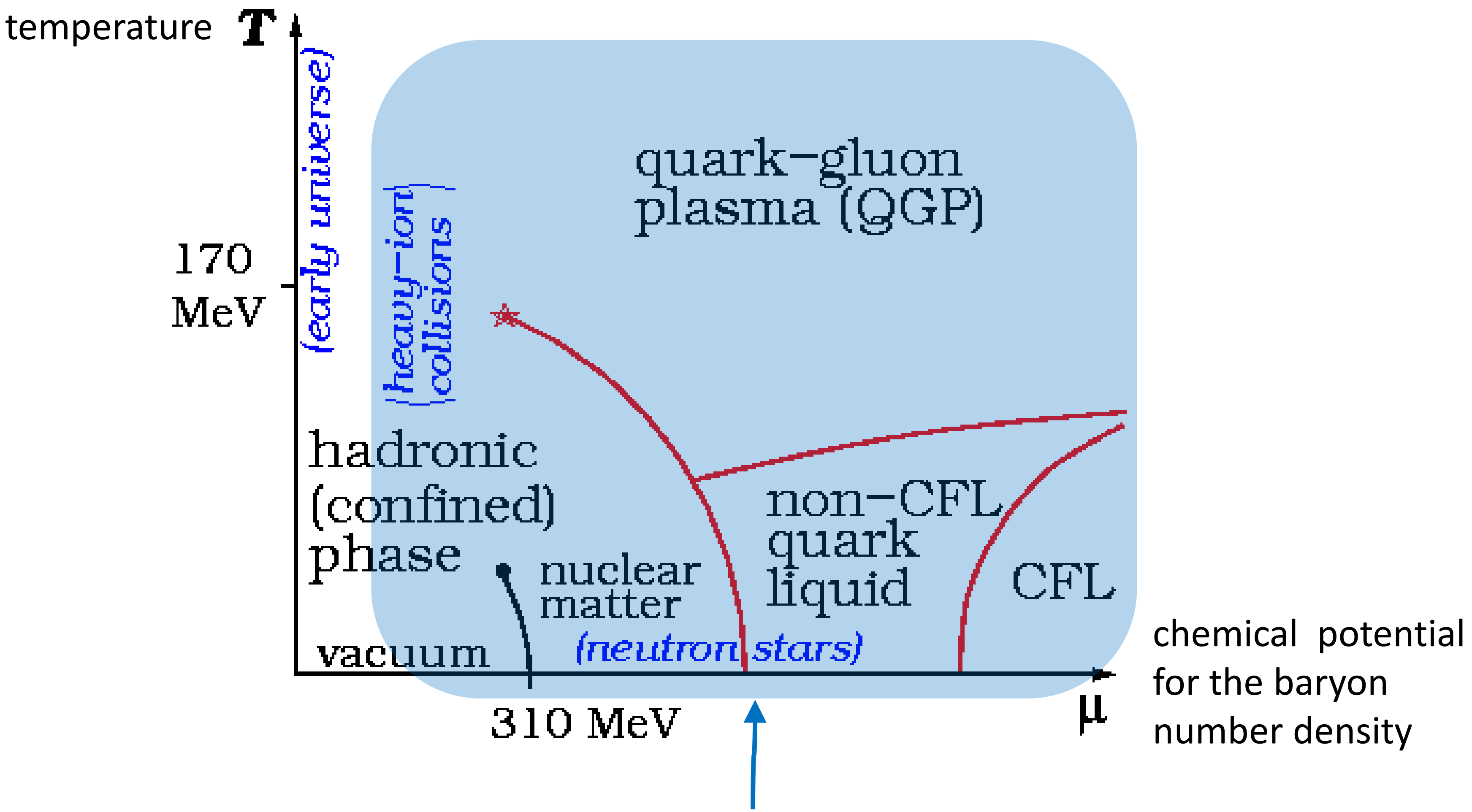
Invited talk at the YITP long-term workshop
"New Frontiers in QCD – Confinement, Phase Transition, Hadrons, and Hadron Interactions –"

May 28 - June 29, 2018

Yukawa Institute for Theoretical Physics, Kyoto University

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

QCD phase diagram at finite T and μ



First principle calculations are difficult due to the sign problem

The sign problem in Monte Carlo methods

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

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

The fermion determinant becomes complex in general.

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

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

$$\langle \mathcal{O}[U] \rangle = \frac{\langle \mathcal{O}[U]\, \mathrm{e}^{i\Gamma[U]} \rangle_0}{\langle \mathrm{e}^{i\Gamma[U]} \rangle_0}$$ (reweighting)

become exponentially small as the volume increases
due to violent fluctuations of the phase Γ

Number of configurations needed to evaluate <O> increases exponentially.

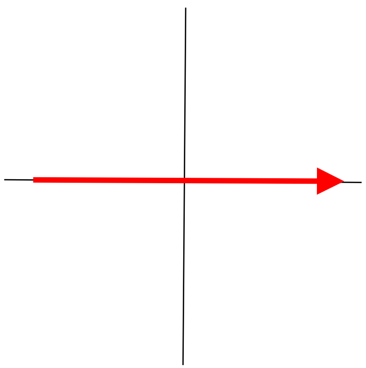
"sign problem"

A new development toward solution to the sign problem 2011〜

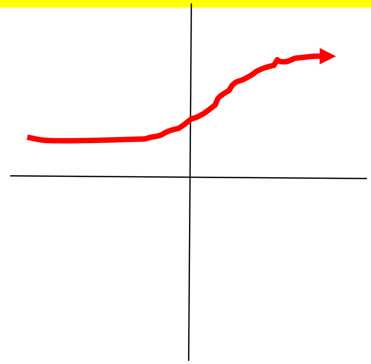
Key : complexification of dynamical variables

The original path integral

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



The phase of $w(x)$ oscillates violently (sign problem)

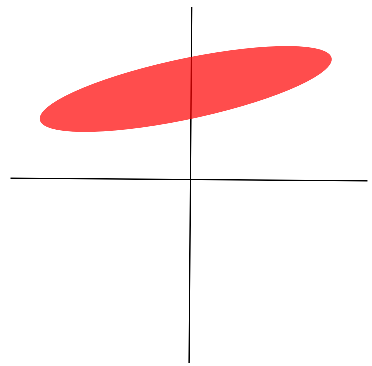


$$Z = \int dz \, w(z)$$

Minimize the sign problem by deforming the integration contour

“Lefschetz thimble approach”

This talk



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

“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

Parisi-Wu ('81)
For review, see
Damgaard-Huffel ('87)

$$Z = \int dx\, w(x) \qquad w(x) \geq 0$$

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" Gaussian noise

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

$$\langle \mathcal{O} \rangle = \lim_{t \to \infty} \langle \mathcal{O}(x^{(\eta)}(t)) \rangle_\eta \qquad \langle \cdots \rangle_\eta = \frac{\int \mathcal{D}\eta \cdots \mathrm{e}^{-\frac{1}{4}\int dt\, \eta^2(t)}}{\int \mathcal{D}\eta\, \mathrm{e}^{-\frac{1}{4}\int dt\, \eta^2(t)}}$$

Proof

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

Probability distribution of $x^{(\eta)}(t)$ $\qquad P(x,t) = \langle \delta(x - x^{(\eta)}(t)) \rangle_\eta$

Fokker-Planck eq.

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial x}\left(\frac{\partial}{\partial x} - \frac{1}{w(x)} \frac{\partial w(x)}{\partial x} \right) P \qquad \lim_{t \to \infty} P(x,t) = \frac{1}{Z} w(x)$$

The complex Langevin method

Parisi ('83), Klauder ('83)

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

complex

$v(x) \equiv \dfrac{1}{w(x)} \dfrac{\partial w(x)}{\partial x}$ becomes complex also.

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

$$\langle \mathcal{O} \rangle \stackrel{?}{=} \lim_{t\to\infty} \langle \mathcal{O}(z^{(\eta)}(t)) \rangle_\eta$$

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

Rem 2 : The drift term $v(x) \equiv \dfrac{1}{w(x)} \dfrac{\partial w(x)}{\partial x}$ 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

Ref.) Nagata-J.N.-Shimasaki,
Phys.Rev. D94 (2016) no.11, 114515, arXiv:1606.07627 [hep-lat]

The key identity for justification

$$\langle \mathcal{O} \rangle \stackrel{?}{=} \lim_{t\to\infty} \langle \mathcal{O}(z^{(\eta)}(t)) \rangle_\eta$$

$P(x, y; t)$: The probability distribution of the complexified variables $z = x + iy$ at Langevin time t.

$$= \int dx dy\, \mathcal{O}(x+iy) P(x, y; t)$$

$$\int dx dy\, \mathcal{O}(x+iy) P(x, y; t) \stackrel{?}{=} \int dx\, \mathcal{O}(x) \rho(x; t) \quad \cdots\cdots\text{(\#)}$$

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.

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

This is OK provided that eq.(#) holds and P(t=∞) is unique.

c.f.) J.N.-Shimasaki, PRD 92 (2015) 1, 011501 arXiv:1504.08359 [hep-lat]

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

c.f.) J.N.-Shimasaki, PRD 92 (2015) 1, 011501 arXiv:1504.08359 [hep-lat]

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

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

Aarts, James, Seiler, Stamatescu: Eur. Phys. J. C ('11) 71, 1756

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

$$= \int dxdy\, \mathcal{O}(x+iy) e^{tL^\top} P(x,y;0)$$

$$= \int dxdy\, \{e^{tL} \mathcal{O}(x+iy)\} P(x,y;0)$$

$$= \int dx\, \{e^{tL_0} \mathcal{O}(x)\} \rho(x;0)$$

$$= \int dx\, \mathcal{O}(x) e^{tL_0^\top} \rho(x;0)$$

$$= \int dx\, \mathcal{O}(x) \rho(x;t)$$

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

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

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

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

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

Nagata-J.N.-Shimasaki, Phys.Rev. D94 (2016) no.11, 114515, arXiv: 1606.07627 [hep-lat]

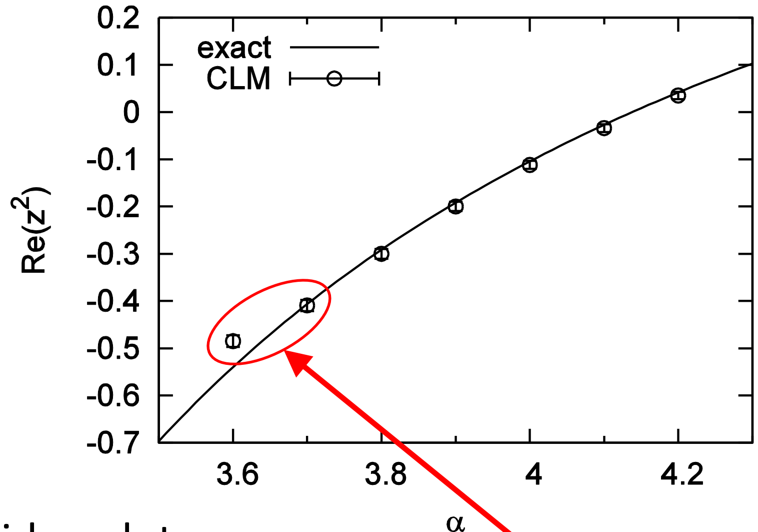
$$\int dxdy\{\mathrm{e}^{\tau L}\mathcal{O}(x+iy)\}P(x,y;t)$$
$$=\sum_{n=0}^{\infty}\frac{\tau^n}{n!}\int dxdy\{L^n\mathcal{O}(x+iy)\}P(x,y;t)$$

In order for this expression to be valid for finite τ ,
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. $L \sim v(z)\partial$

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

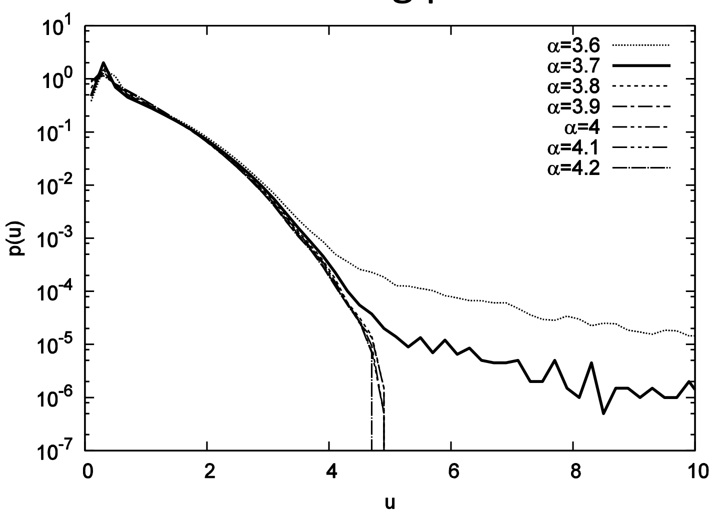
Demonstration of our condition



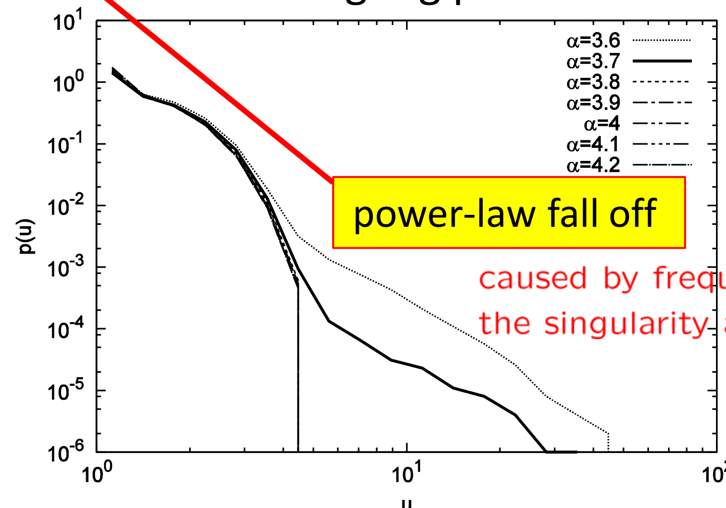
$$Z = \int dx\, w(x)$$
$$w(x) = (x+i\alpha)^p e^{-x^2/2}$$

$$p = 4$$

semi-log plot



log-log plot



power-law fall off

caused by frequent visits to the singularity at $z = -i\alpha$

The probability distribution of the magnitude of the drift term $u \equiv |v(z)| = \left|\frac{p}{z+i\alpha} - z\right|$

In this model, CLM fails at $\alpha \lesssim 3.7$ due to "the singular-drift problem"

3. Gauge cooling

"gauge cooling"

Seiler-Sexty-Stamatescu, PLB 723 (2013) 213
arXiv:1211.3709 [hep-lat]]

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 :

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

"gauge cooling"

$$z_k^{(\eta)}(t+\epsilon) = \tilde{z}_k^{(\eta)}(t) + \epsilon\, v_k(\tilde{z}^{(\eta)}(t)) + \sqrt{\epsilon}\, \eta_k(t)$$

Justification of the gauge cooling

Nagata-J.N.-Shimasaki, Phys.Rev. D94 (2016) no.11, 114515, arXiv: 1606.07627 [hep-lat]

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

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

$$\left(:\tilde{L}^n: \mathcal{O}(z) \right)\Big|_{z^{(g)}} = :\tilde{L}^n: \mathcal{O}(z)$$

The only effect of gauge cooling disappears from this expression !

$\mathcal{O}(z)$ and $\tilde{L} = \left(v_k(z) + \frac{\partial}{\partial z_k} \right) \frac{\partial}{\partial z_k}$ are invariant under complexified symmetry transformations.

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

Ref.) Ito, JN : JHEP 12 (2016) 009 [arXiv:1609.04501 [hep-lat]]

a simple matrix model motivated from string theory

J.N. PRD 65, 105012 (2002), hep-th/0108070

$$Z = \int \mathrm{d}A\, \mathrm{d}\psi\, \mathrm{d}\bar{\psi}\, \mathrm{e}^{-(S_\mathrm{b}+S_\mathrm{f})}$$

$$S_\mathrm{b} = \frac{1}{2} N \,\mathrm{tr}\, (A_\mu)^2 \qquad \mu = 1,2,3,4$$

$$S_\mathrm{f} = \bar{\psi}^f_\alpha (\Gamma_\mu)_{\alpha\beta} A_\mu \psi^f_\beta \qquad \alpha,\beta = 1,2 \quad f = 1,\cdots,N_\mathrm{f}$$

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

SSB of SO(4) rotational symmetry
in the $N \to \infty$ limit with fixed $r = \frac{N_\mathrm{f}}{N}$
due to the complex fermion determinant

c.f.) In matrix model formulation of superstring theory,
SSB : SO(10) → SO(4) is expected to occur.

Anagnostopoulos-Azuma-Ito-J.N.-Papadoudis : JHEP 02 (2018) 151.

Application of the complex Langevin method

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

$$A_\mu \ : \ \text{Hermitian} \ \mapsto \mathcal{A}_\mu \ : \ \text{general complex}$$

$$S_{\text{eff}} = \frac{1}{2} N \, \text{tr} \, (\mathcal{A}_\mu)^2 - \log \det (\Gamma_\mu \mathcal{A}_\mu)$$

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

$$S_{\text{breaking}} = \frac{1}{2} \varepsilon N \sum_{i=1}^{4} m_i \, \text{tr} \, (\mathcal{A}_i)^2$$

$$m_1 < m_2 < m_3 < m_4$$

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

and calculate :

$$\langle \lambda_i \rangle = \lim_{\varepsilon \to 0} \lim_{N \to \infty} \left\langle \frac{1}{N} \text{tr} \, (\mathcal{A}_i)^2 \right\rangle_{\text{CL}}$$

no sum over $i = 1, 2, 3, 4$

Results of the CLM

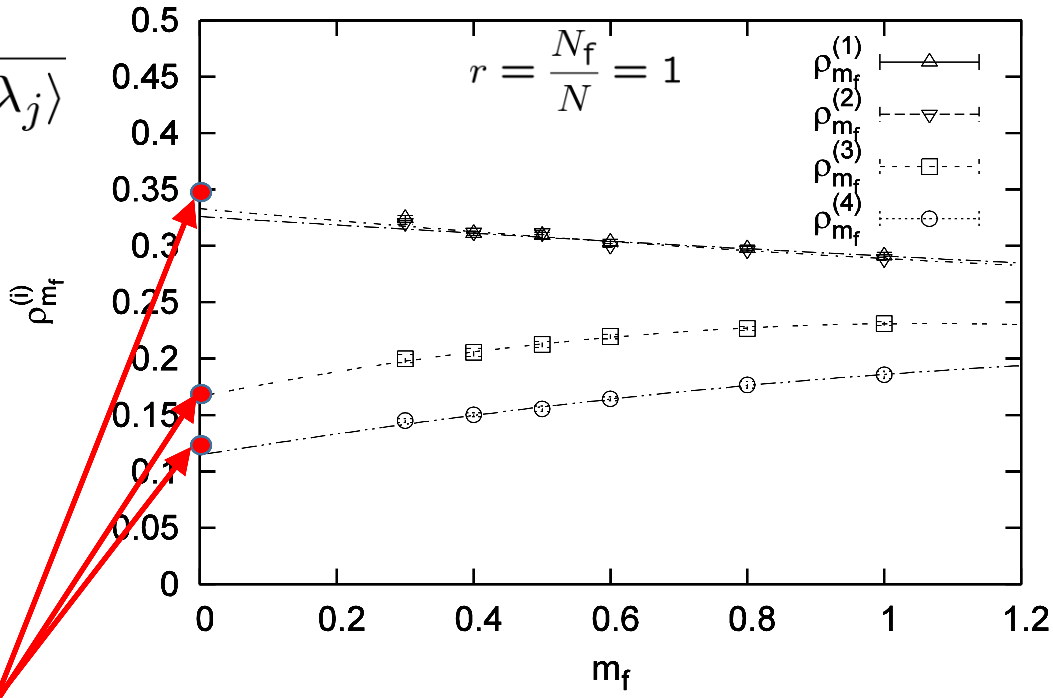
Ito-J.N., JHEP 12 (2016) 009

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

$$S_{\mathsf{f}} = \bar{\psi}^f_\alpha (\Gamma_\mu)_{\alpha\beta} A_\mu \psi^f_\beta \boxed{+ m_{\mathsf{f}} \bar{\psi}^f_\alpha (\Gamma_4)_{\alpha\beta} \psi^f_\beta}$$

Explicitly breaks $SO(4) \mapsto SO(3)$

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



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

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

$$S_{\mathrm{plaq}}(U) = -\beta \sum_n \sum_{\mu\neq\nu} \mathrm{tr}\,(U_{n\mu} U_{n+\hat{\mu},\nu} U^{-1}_{n+\hat{\nu},\mu} U^{-1}_{n\nu})$$

generators of SU(3)

$$v_{an\mu}(U) = \frac{1}{w(U)} D_{an\mu} w(U) \qquad D_{an\mu} f(U) = \frac{\partial}{\partial x} f(\mathrm{e}^{ixt_a} U_{n\mu})\Big|_{x=0}$$

Complexification of dynamical variables : $U_{n\mu} \mapsto \mathcal{U}_{n\mu} \in \mathrm{SL}(3,\mathbb{C})$

Discretized version of complex Langevin eq.

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

The drift term can become large when :

1) link variables $\mathcal{U}_{n\mu}$ become far from unitary (excursion problem)

"gauge cooling"

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

Rem.) The fermion determinant gives rise to a drift $\mathrm{tr}\,(M[\mathcal{U}]^{-1} \mathcal{D}_{an\mu} M[\mathcal{U}])$

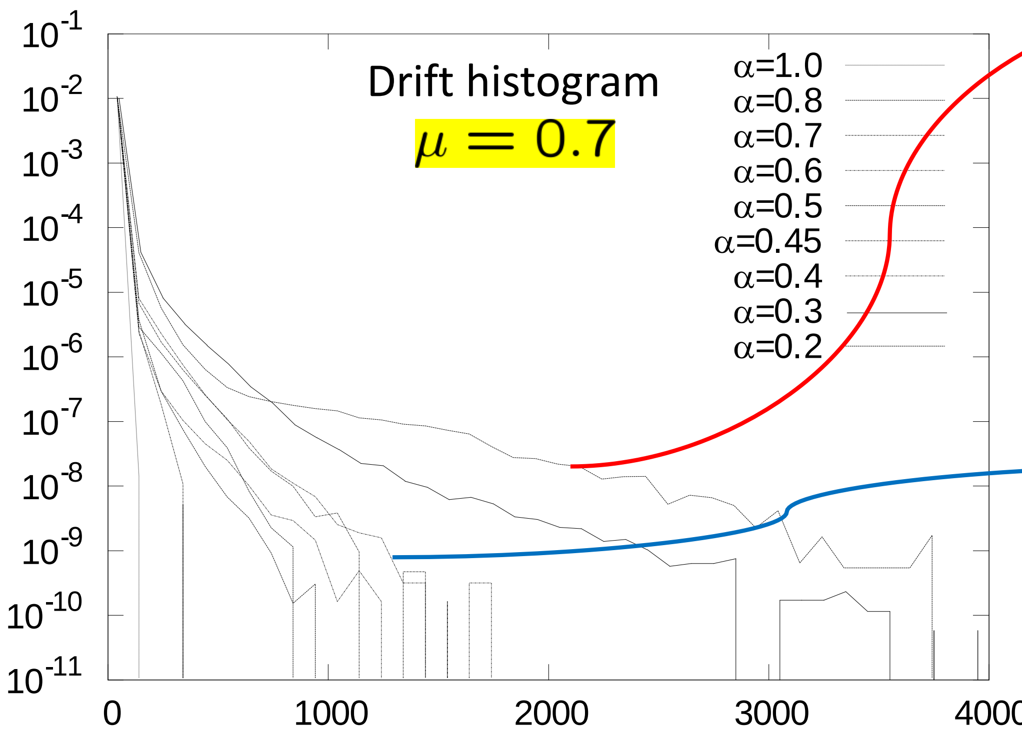
"deformation technique"

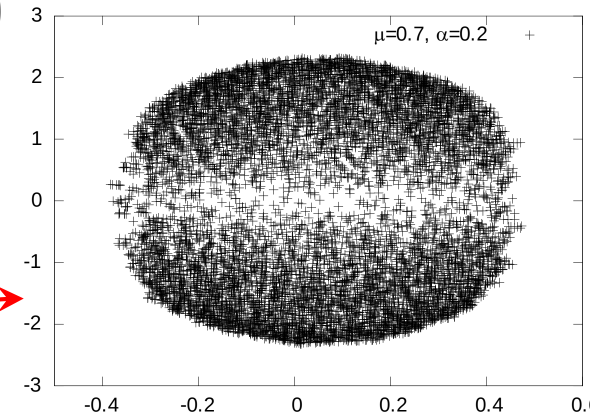
Deformation technique

Staggered fermion (4 quark flavors)

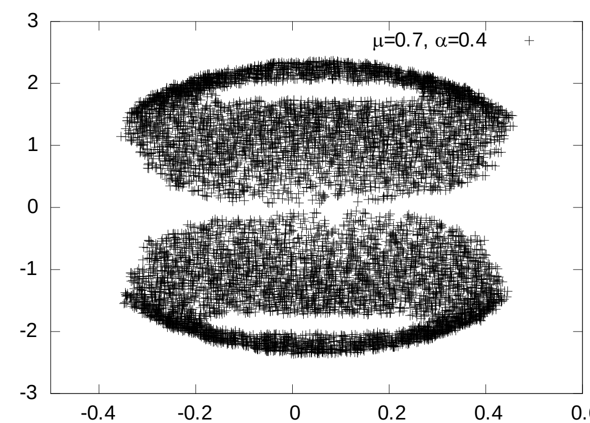
$$S_f = \sum_x \Big[\sum_{\nu=1}^{4} \frac{1}{2} \eta_\nu(x) \left(e^{\mu\delta_{\nu 4}} \bar\psi(x) U_{x\nu} \psi(x+\hat\nu) - e^{-\mu\delta_{\nu 4}} \bar\psi(x) U^{-1}_{x-\hat\nu,\nu} \psi(x-\bar\nu) \right) + m\bar\psi(x)\psi(x) + i\alpha\eta_4(x)\bar\psi(x)\psi(x) \Big]$$

"imaginary chemical pot." in the continuum



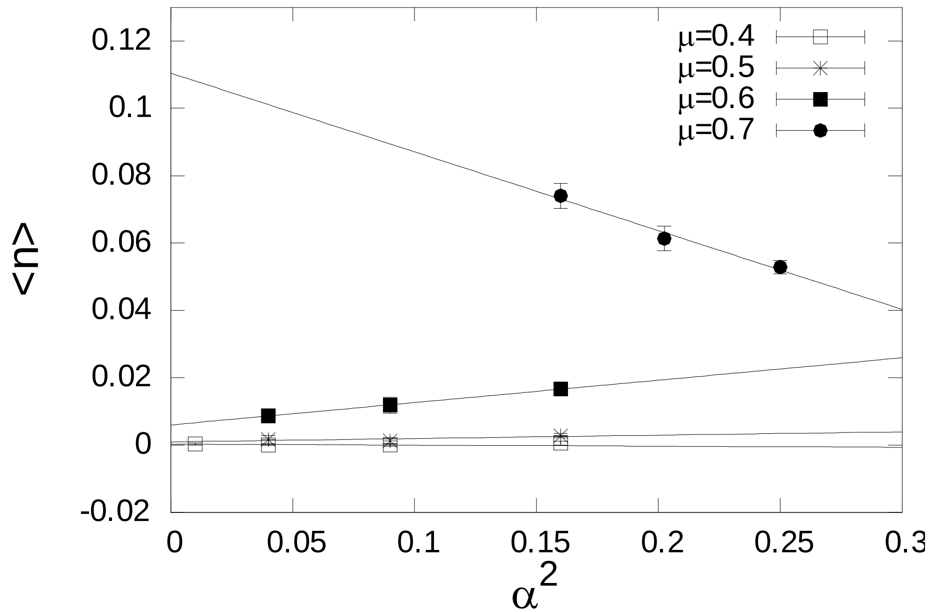


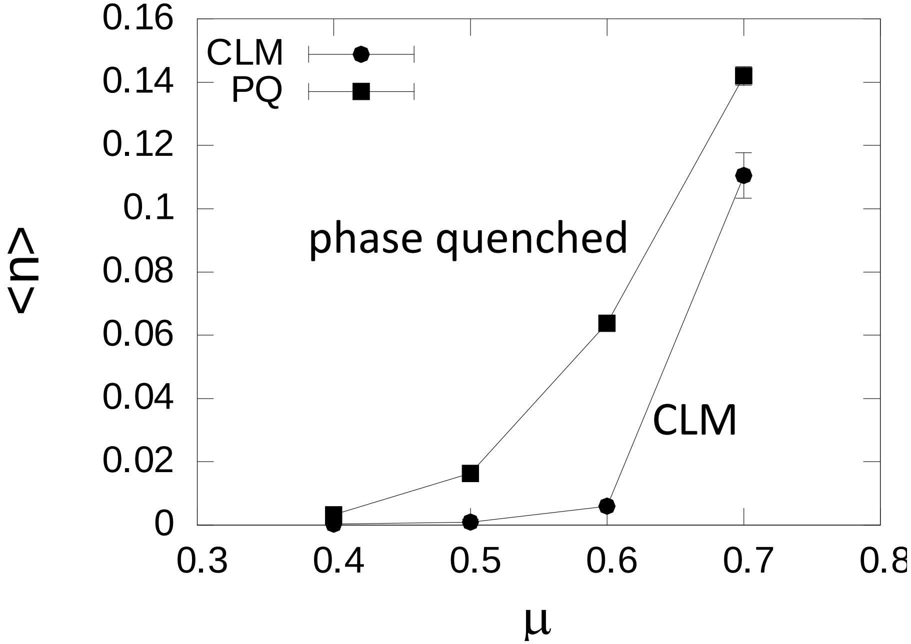
eigenvalue distribution of Dirac matrix $M[\mathcal{U}]$



baryon number density

$$\langle n \rangle = \frac{1}{3N_{\mathrm{V}}}\frac{\partial}{\partial \mu}\log Z$$



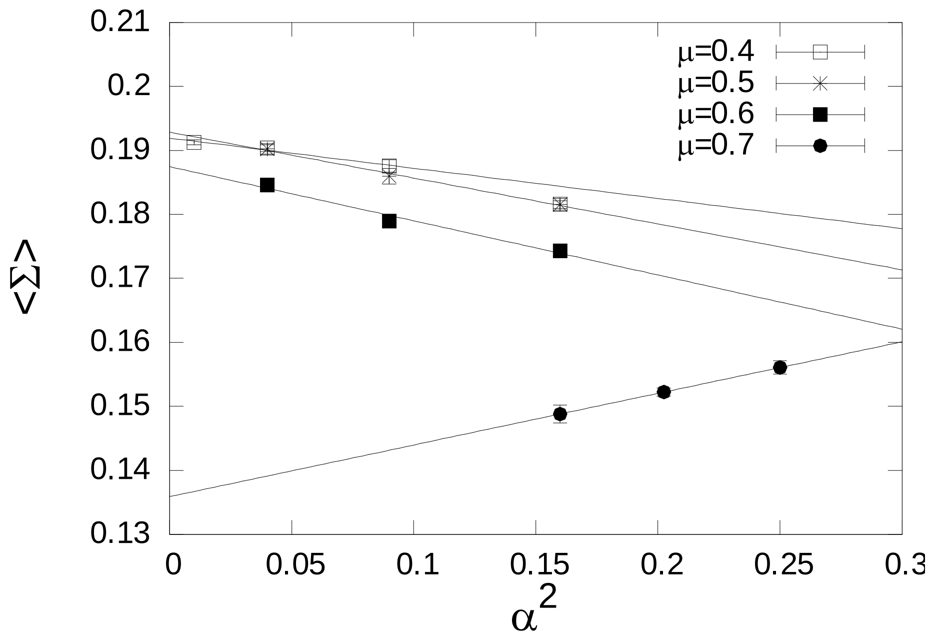


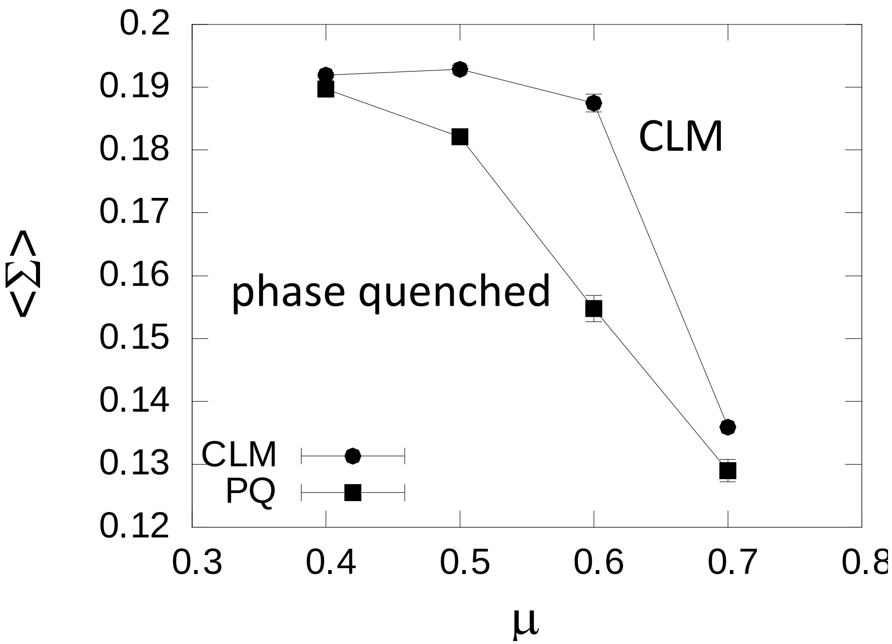
linear extrapolation w.r.t. α^2
considering symmetry under $\alpha \leftrightarrow -\alpha$

Silver Blaze phenomenon suggested

chiral condensate

$$\langle \Sigma \rangle = \frac{1}{N_{\mathsf{V}}} \frac{\partial}{\partial m} \log Z$$





linear extrapolation w.r.t. α^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 (refers to the first two future directions)