Current status and perspectives of complex Langevin calculations in finite density QCD

Invited talk at XQCD2019

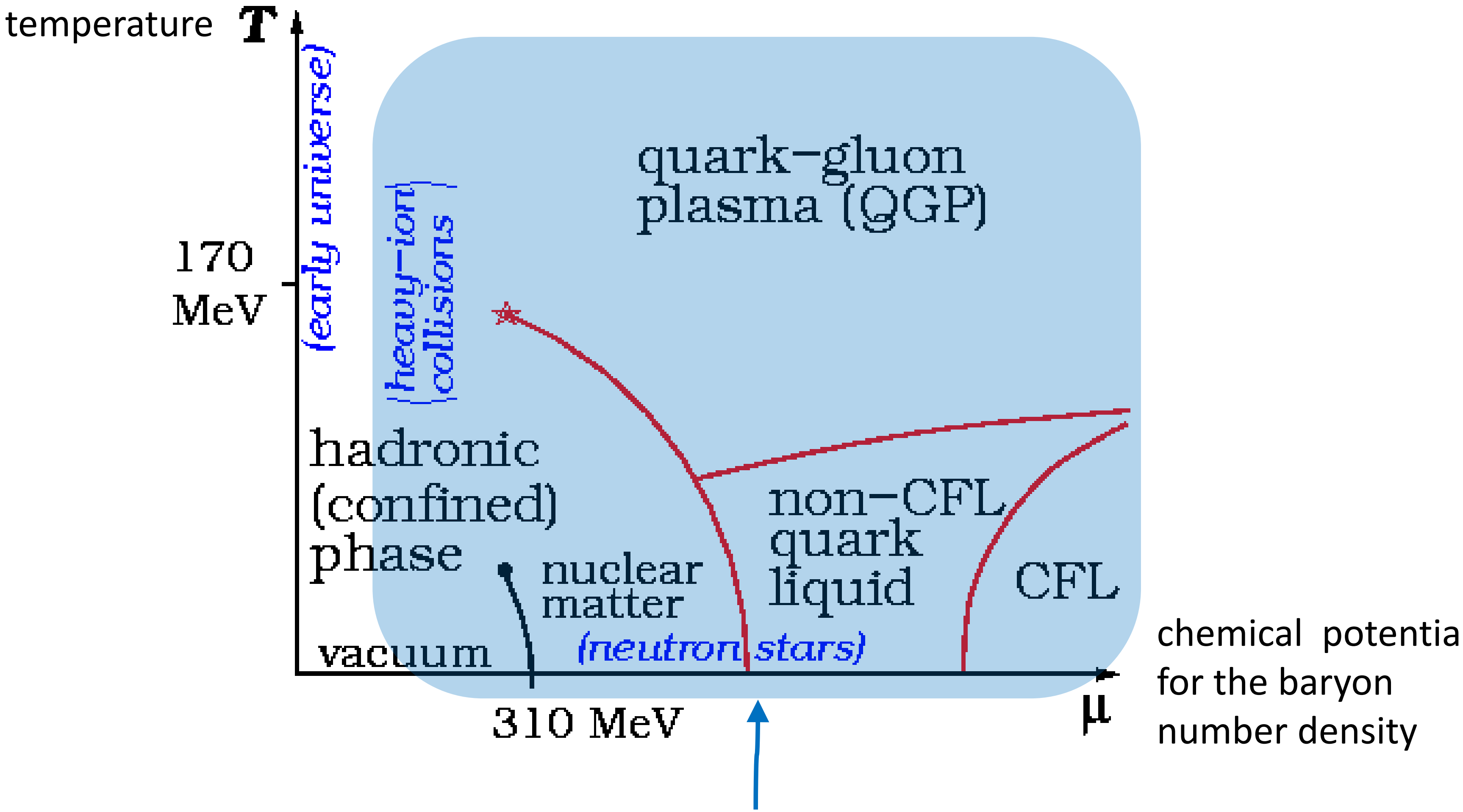
Bunkyo school building, University of Tsukuba,

Tokyo, Japan, Jun. 24, 2019

Jun Nishimura (KEK & SOKENDAI)

Ref.) Nagata, J.N., Shimasaki, Phys.Rev. D94 (2016) no.11, 114515, arXiv:1606.07627 [hep-lat]
Tsutsui, Ito, Matsufuru, J.N., Shimasaki, Tsuchiya, PoS LATTICE2018 (2018) 144, arXiv:1811.07647 [hep-lat]
Ito, Matsufuru, J.N., Shimasaki, Tsuchiya, Tsutsui, PoS LATTICE2018 (2018) 146, arXiv:1811.12688 [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 ($\mu \neq 0$),

$$
\begin{aligned}
Z &= \int dU\, d\Psi\, \mathrm{e}^{-S[U,\Psi]} \\
&= \int dU\, \mathrm{e}^{-S_{\mathrm{g}}[U]} \mathrm{det}\mathcal{M}[U]
\end{aligned}
$$

The fermion determinant becomes complex in general.

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

Generate configurations *U* with the probability $\mathrm{e}^{-S_{\mathrm{g}}[U]}\, |\mathrm{det}\mathcal{M}[U]|$
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.

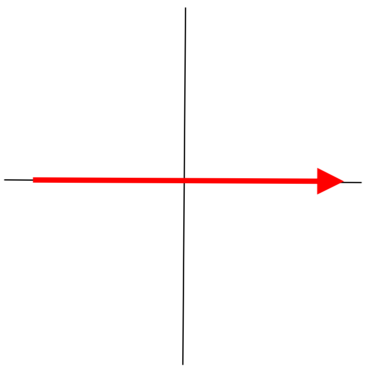
"sign problem"

A new development toward solution to the sign problem 2011～

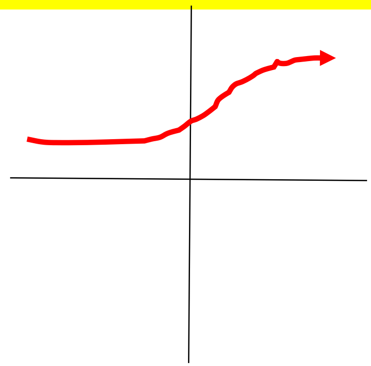
Key : complexification of dynamical variables

The original path integral

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



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

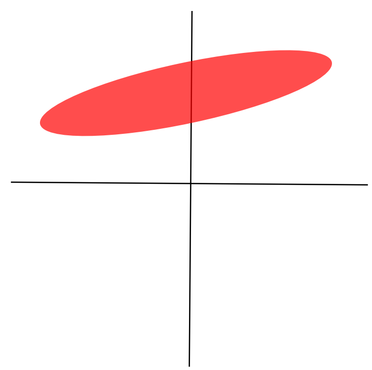


$$Z = \int dz\, w(z)$$

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 only under certain conditions.

The current status and perspectives of the complex Langevin calculations in finite density QCD

Unfortunately, there is still a lot of skepticism in this method due to the "wrong convergence problem".

However,

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

I will discuss the parameter region of finite density QCD, in which the criterion is satisfied.

I will show explicit results, which reveal highly nontrivial properties in the high density region.

I will discuss what we can do in the near future.

Plan of the talk

1. Complex Langevin method
2. Argument for justification and
   the condition for correct convergence
3. Application to lattice QCD at finite density
   - 3.1 Can we see the deconfining transition?
   - 3.2 Studies of the low-T high density region
4. Summary and future prospects

1. Complex Langevin method

The real Langevin method

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

Parisi-Wu ('81)
Damgaard-Huffel ('87)

View this as the stationary distribution of a stochastic process.

Langevin eq. $$\frac{d}{dt}x^{(\eta)}(t) = v(x^{(\eta)}(t)) + \eta(t)$$

Gaussian noise

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

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

Proof

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

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

Probability distribution of $x^{(\eta)}(t)$

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

$$v(x) \equiv \frac{1}{w(x)} \frac{\partial w(x)}{\partial x}$$ 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 $\propto e^{-\frac{1}{4}\int dt\, \eta(t)^2}$

$$\lim_{t\to\infty} \langle \mathcal{O}(z^{(\eta)}(t)) \rangle_\eta \stackrel{?}{=} \frac{1}{Z} \int dx\, \mathcal{O}(x) w(x)$$

Rem 1 : When w(x) is real positive, it reduces to the real Langevin method.

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

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

The key identity for justification

$$\lim_{t\to\infty} \langle \mathcal{O}(z^{(\eta)}(t))\rangle_\eta \stackrel{?}{=} \frac{1}{Z}\int dx\, \mathcal{O}(x) w(x)$$

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

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

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

where $\rho(x;t) \in \mathbb{C}$ obeys $\dfrac{\partial \rho}{\partial t} = \dfrac{\partial}{\partial x}\left(\dfrac{\partial}{\partial x} - \dfrac{1}{w(x)}\dfrac{\partial w(x)}{\partial x}\right)\rho$ 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]

Condition for justifying the CLM

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

Proof of this identity was discussed for the first time in

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

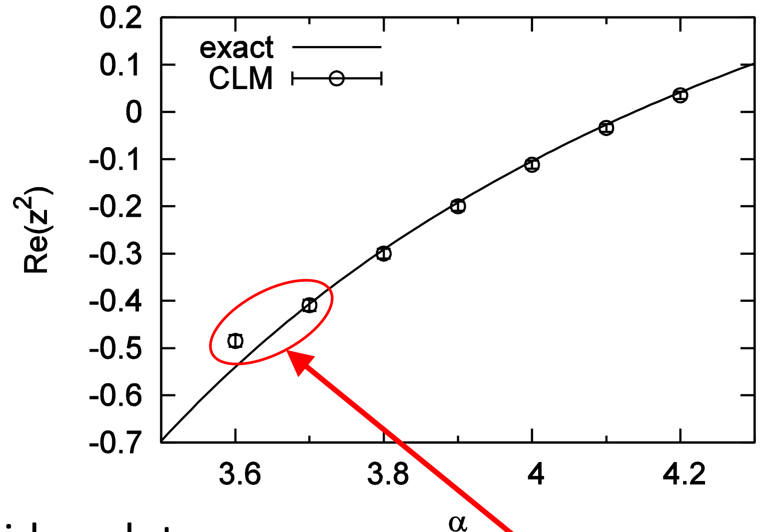
Refinement of this argument led to the criterion:
the probability of the drift term should be suppressed exponentially at large magnitude.

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

Note:

- This provides a clear and practical criterion for correct convergence.
- No additional cost needed. (Drift term has to be calculated anyway !)
- In the case of real Langevin simulation, this criterion need not be satisfied.

Demonstration of our condition

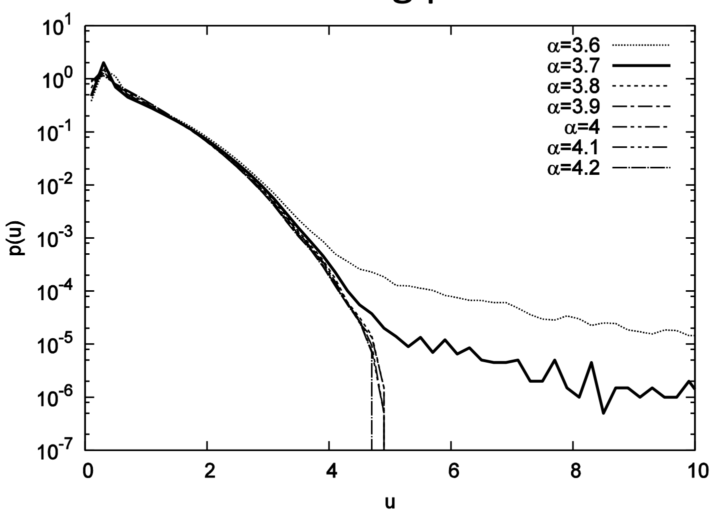


$$Z = \int dx\, w(x)$$

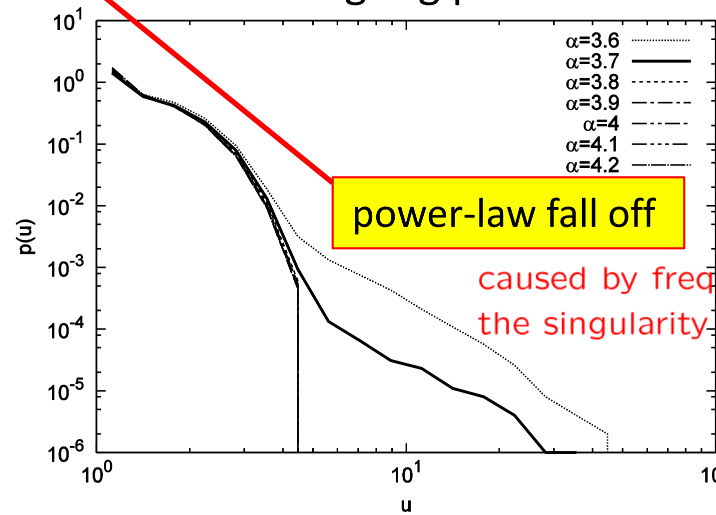
$$w(x) = (x + i\alpha)^p \, \mathrm{e}^{-x^2/2}$$

$$p = 4$$

semi-log plot



log-log plot



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. Application to lattice QCD at finite density

complex Langevin method for finite densiy QCD

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

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

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

t_a: generators of SU(3)

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”

Seiler-Sexty-Stamatescu, PLB 723 (2013) 213

Nagata-J.N.-Shimasaki, Phys.Rev. D94 (2016) no.11, 114515

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

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

Mollgaard-Splittorff, Phys.Rev. D88 (2013) no.11, 116007

J.N.-Shimasaki, Phys.Rev. D92 (2015) no.1, 011501

3.1 Can we see the deconfining transition ?

Ref.) Tsutsui, Ito, Matsufuru, J.N., Shimasaki, Tsuchiya, PoS LATTICE2018 (2018) 144, arXiv:1811.07647 [hep-lat]

Simulation setup

Tsutsui, Ito, Matsufuru, J.N., Shimasaki, Tsuchiya, PoS LATTICE2018 (2018) 144,
arXiv:1811.07647 [hep-lat]

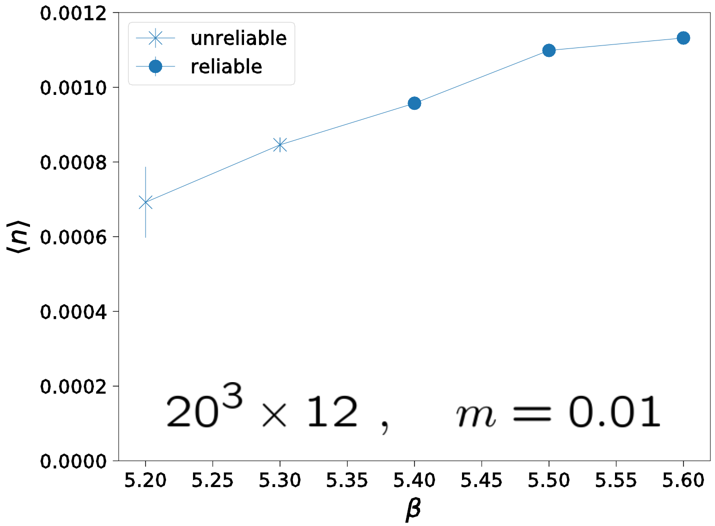
- lattice size : $20^3 \times 12$, $24^3 \times 12$ $\quad a \sim 0.07$fm
- plaquette action with $\beta = 5.2 \sim 5.6$
- staggered fermion (4 quark flavors)
- quark chemical pot.: $\mu a = 0.1$
  corresponding to $\mu/T = 1.2$
- quark mass : $ma = 0.01 \sim 0.5$
- Langevin stepsize : $\epsilon = 5 \times 10^{-5}$

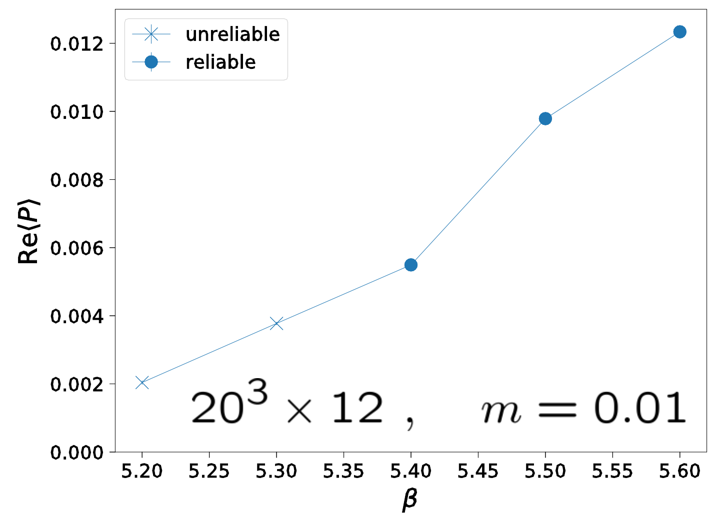
Earlier attempts by Z. Fodor, S.D. Katz, D. Sexty, C. Török, Phys.Rev. D92 (2015) no.9, 094516

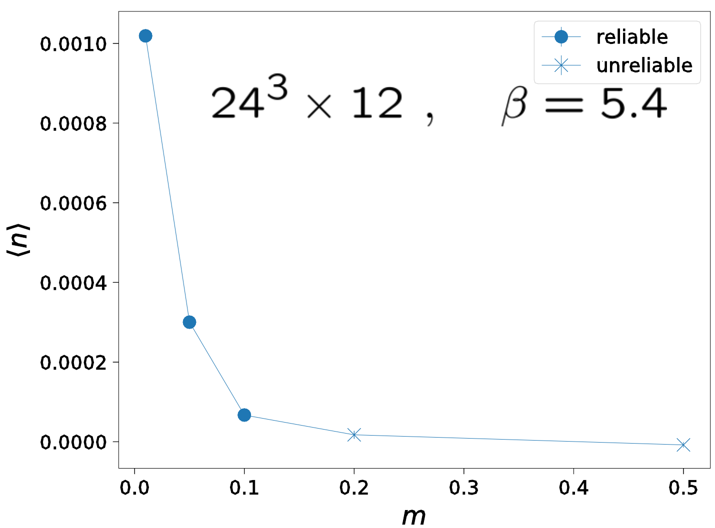
N_t = 8, CL simulation becomes unstable at $\beta < 5.2$.

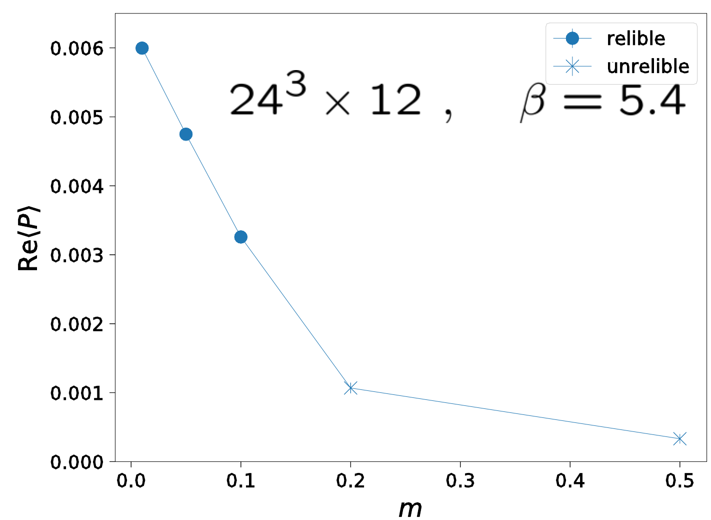
baryon number density

Polyakov loop









Singular-drift problem seems to occur in the confined phase in general.

the generalized Banks-Casher relation

Splittorff, Phys.Rev. D91 (2015) no.3, 034507, arXiv:1412.0502 [hep-lat]
Nagata-J.N.-Shimasaki, JHEP 1607 (2016) 073, arXiv:1604.07717 [hep-lat]

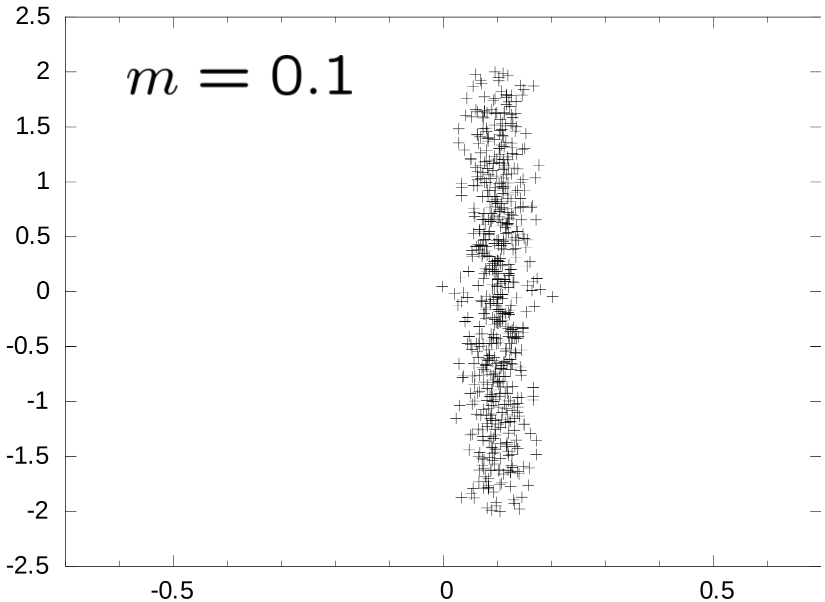
$$\lim_{m\to 0} \Sigma = \pi i \lim_{r\to +0} r \int_0^{\pi} d\theta \lim_{m\to 0} \tilde{\rho}_{\mathrm{CL}}(r,\theta)$$

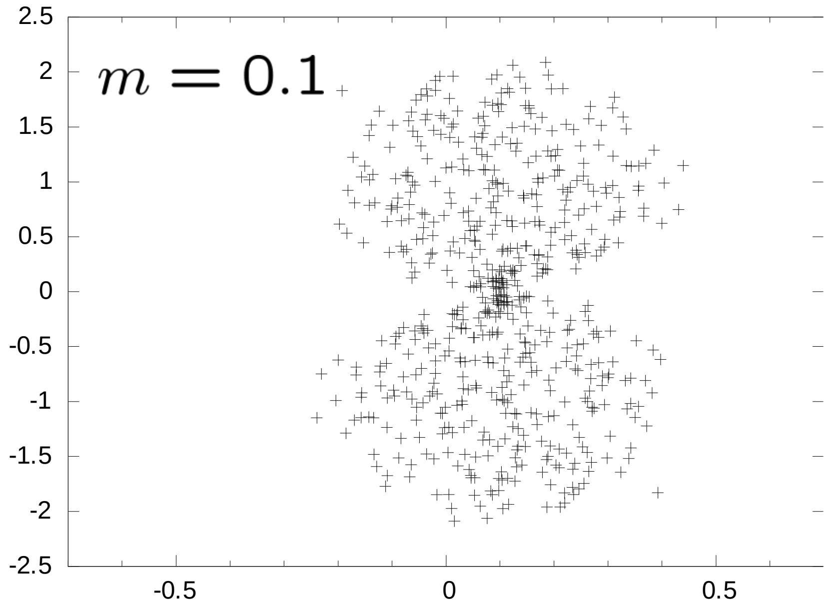
chiral condensate

eigenvalue distribution of the Dirac op.

Result for chiral Random Matrix Theory

Distribution depends on how one applies the gauge cooling,
but the quantity on the r.h.s. is universal.





Our claim based on simulation results

c.f.) poster presentation by S. Tsutsui, this evening

- Singular-drift problem occurs *in general* in the confined phase, where the chiral condensate becomes non-zero. (assuming light quarks and large volume)

- This conclusion is understandable from the viewpoint of the generalized Banks-Casher relation.

- One can actually investigate the high density region in which the chiral condensate vanishes!
  (One has to use sufficiently large β in order to avoid the excursion problem, though.)

- The "confined" phase can be investigated by using small spatial volume, which causes a gap in the eigenvalue distribution of the Dirac op. (next section.)

3.2 Studies of the low-T high density region

Ref.) Ito, Matsufuru, J.N., Shimasaki, Tsuchiya, Tsutsui, PoS LATTICE2018 (2018) 146, arXiv:1811.12688 [hep-lat]

Simulation setup

Ito, Matsufuru, J.N., Shimasaki, Tsuchiya, Tsutsui, PoS LATTICE2018 (2018) 146,
arXiv:1811.12688 [hep-lat]

- lattice size : $8^3 \times 16$ $\qquad a \sim 0.045\text{fm}$
- plaquette action with $\beta = 5.7$
- staggered fermion (4 quark flavors)
- quark chemical pot.: $0 \leq \mu a \leq 0.5$
  corresponding to $0 \leq \mu/T \leq 8$
- quark mass : $ma = 0.01$
- total Langevin time $= 50 \sim 150$
  with stepsize $\epsilon = 10^{-4}$

Note : the spatial extent of our lattice : 0.045fm × 8 = 0.36 fm

c.f.) previous study on a $4^3 \times 8$ lattice
Nagata, JN, Shimasaki, Phys.Rev. D98 (2018) no.11, 114513, arXiv:1805.03964 [hep-lat]

Histogram of the drift term

$8^3 \times 16, \quad N_f = 4$

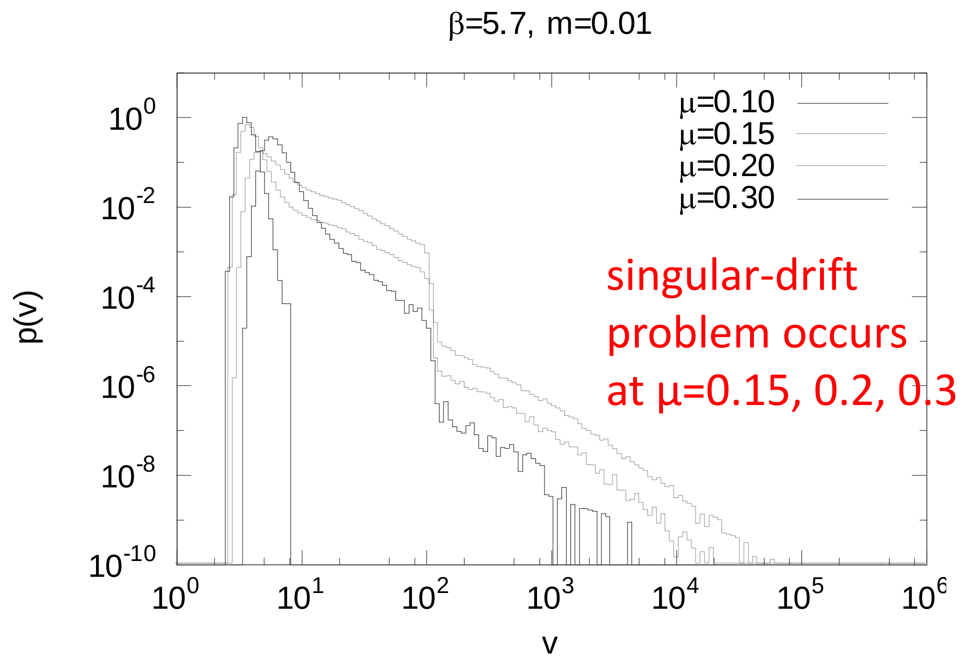
$\beta = 5.7$

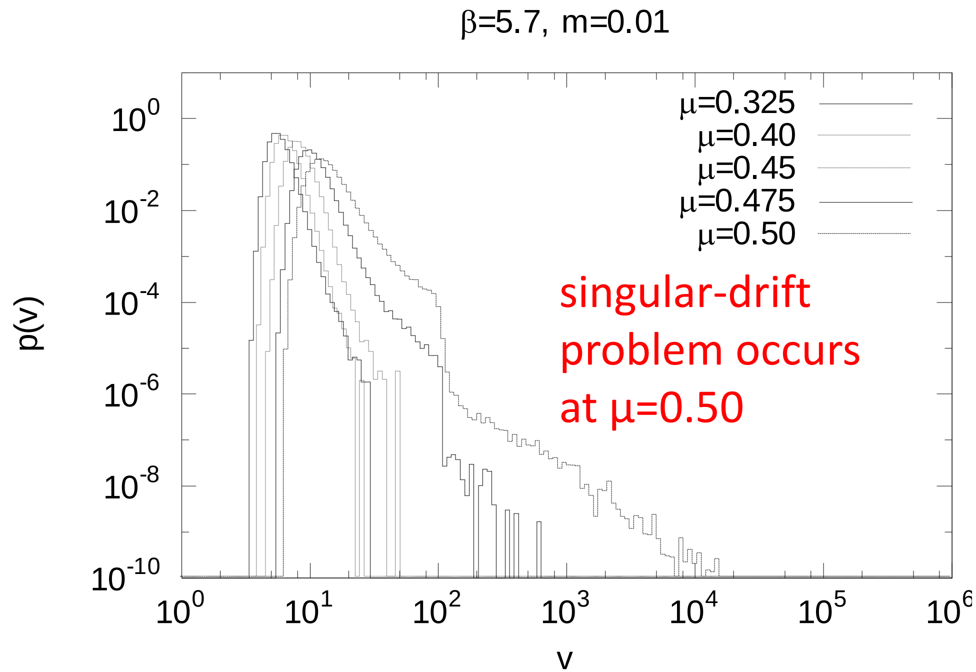
$m = 0.01$

reliable regions

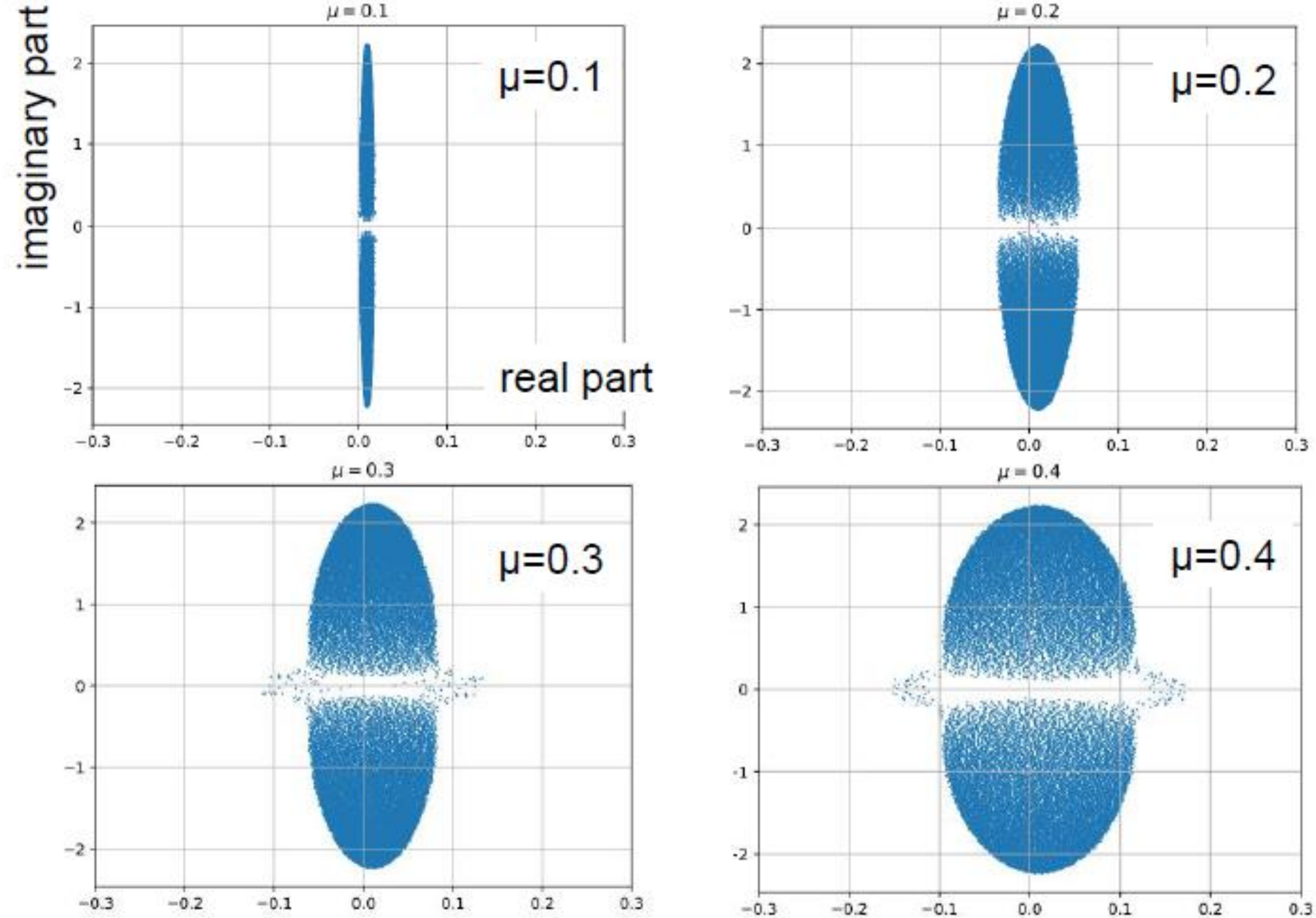
$\mu \le 0.1$

$0.325 \le \mu \le 0.475$

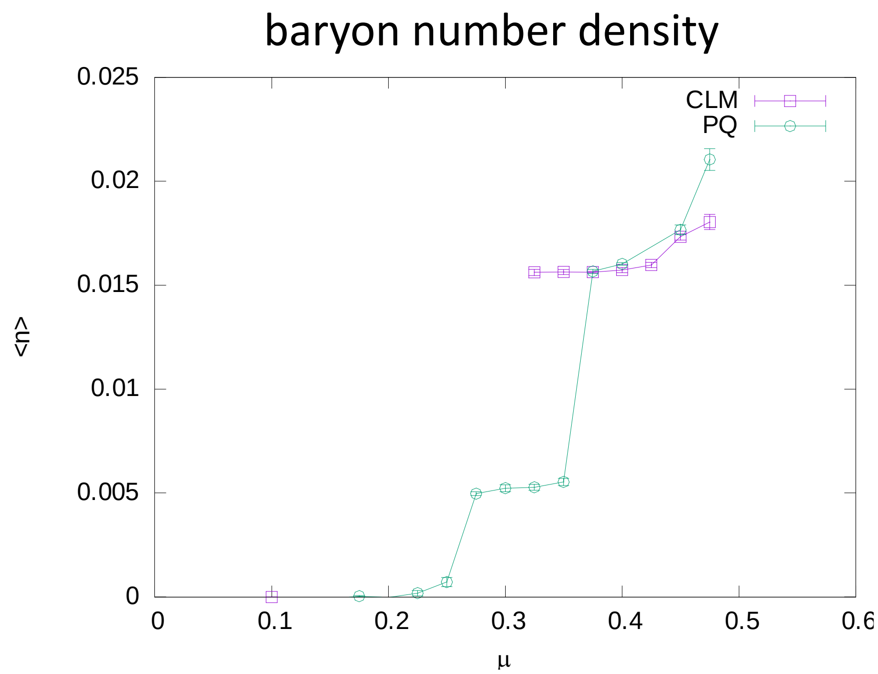


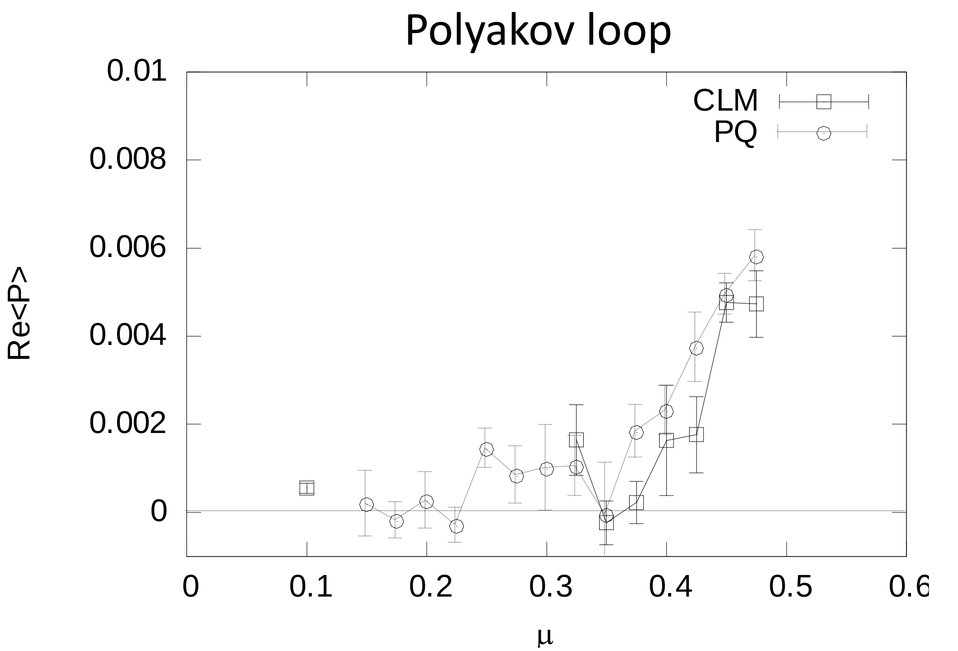


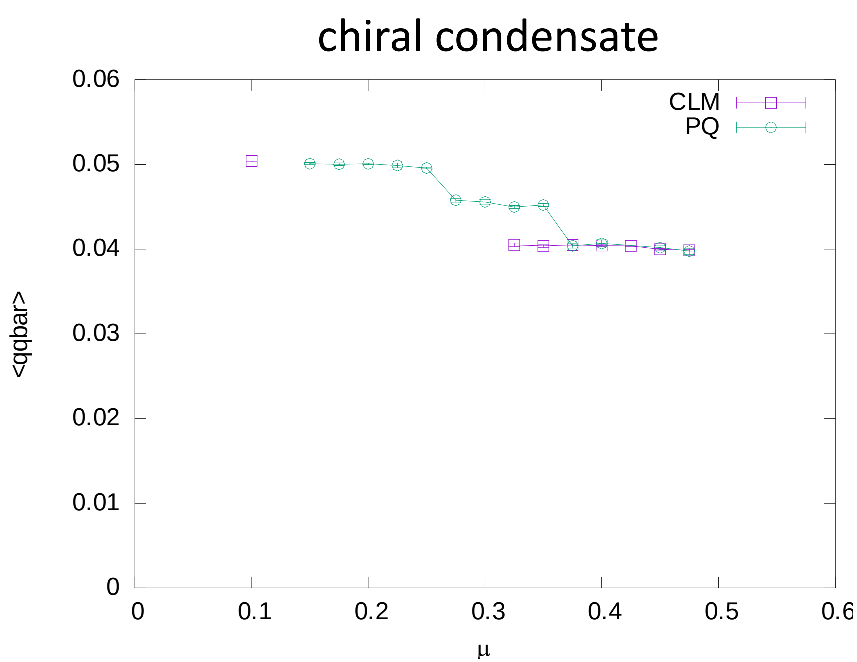
Eigenvalue distribution of (D+m)



We always have a gap due to finite spatial volume effects, but still the singular-drift problem occurs at $\mu = 0.2$ and $\mu = 0.3$ possibly due to large fluctuation associated with the phase transition.

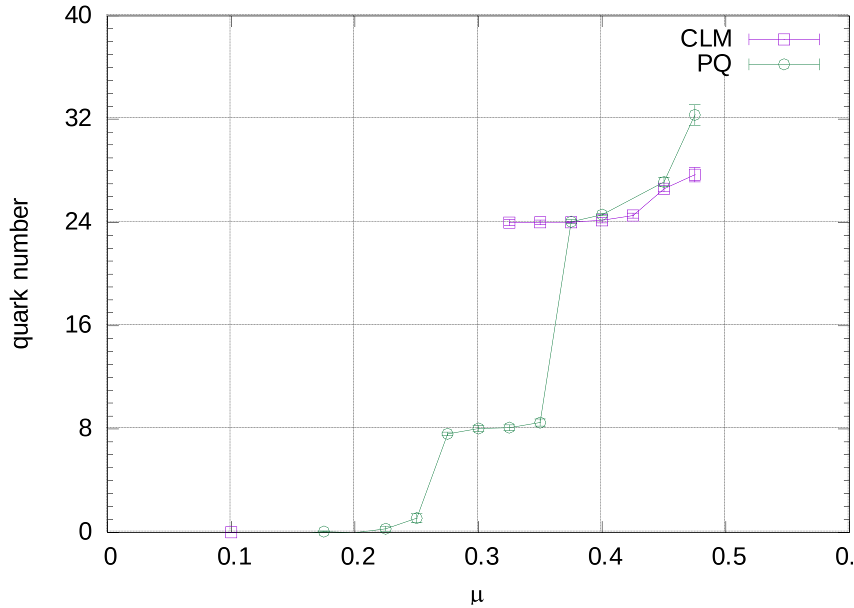




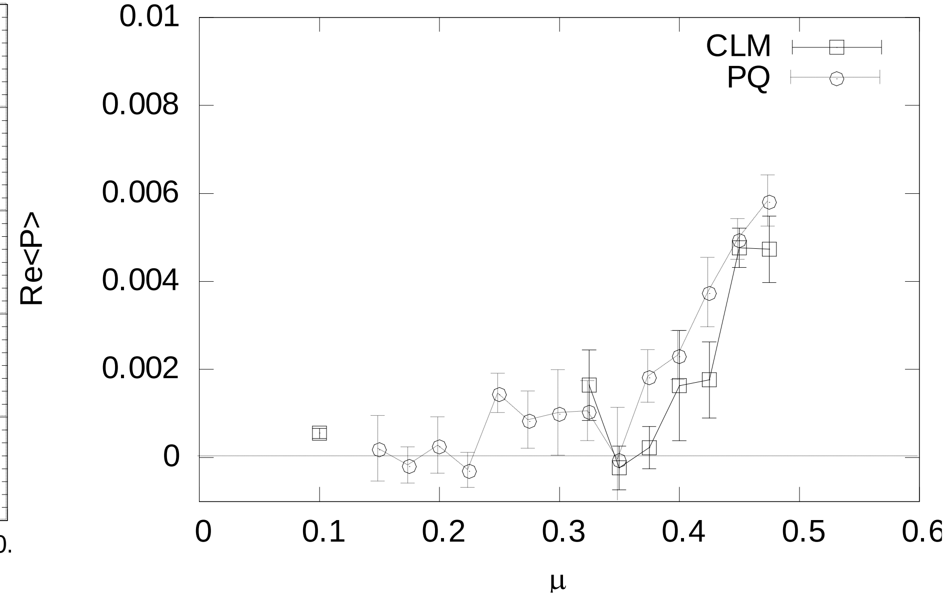


- A clear plateau behavior is observed.
  (formation of 8 baryons)
  a low-T-like behavior (T ～270MeV)
- Polyakov loop is small at the plateau.
  (“confined” phase due to
  finite spatial volume effects)
- Phase-quenched model exhibits another plateau at smaller mu.
  (formation of 4 mesons)

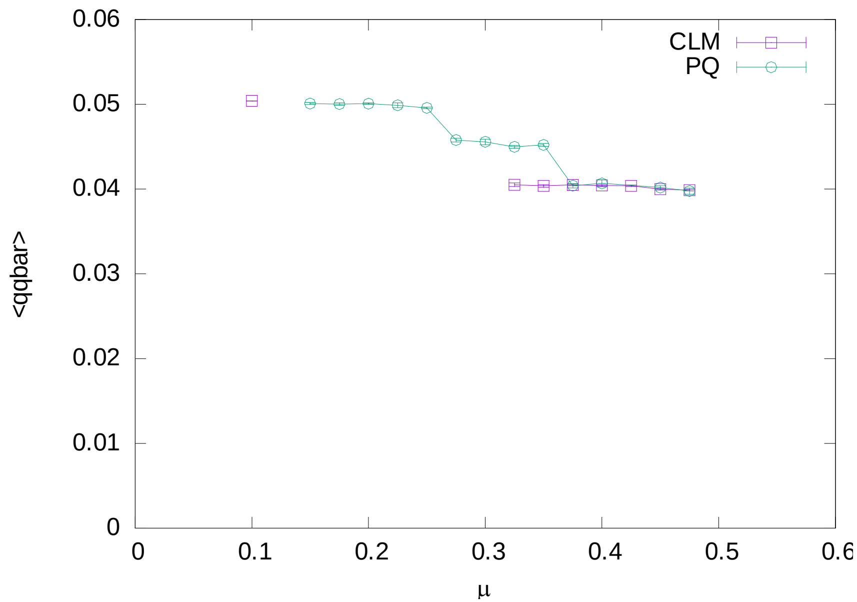
quark number



Polyakov loop



chiral condensate



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  another plateau at smaller mu.
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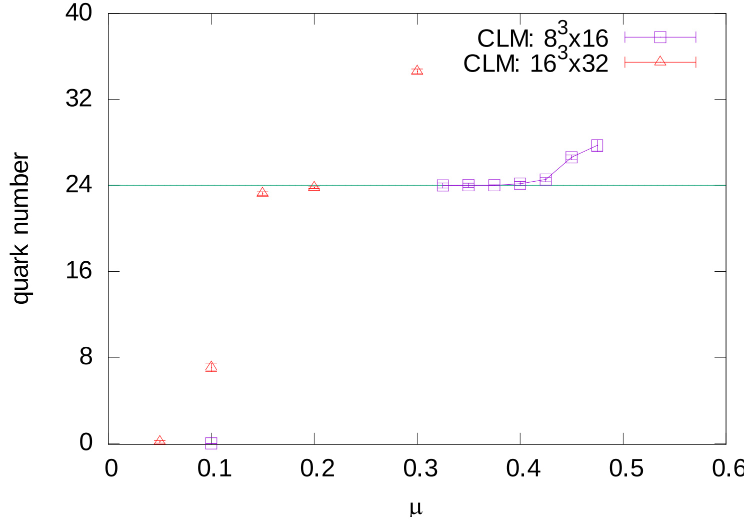
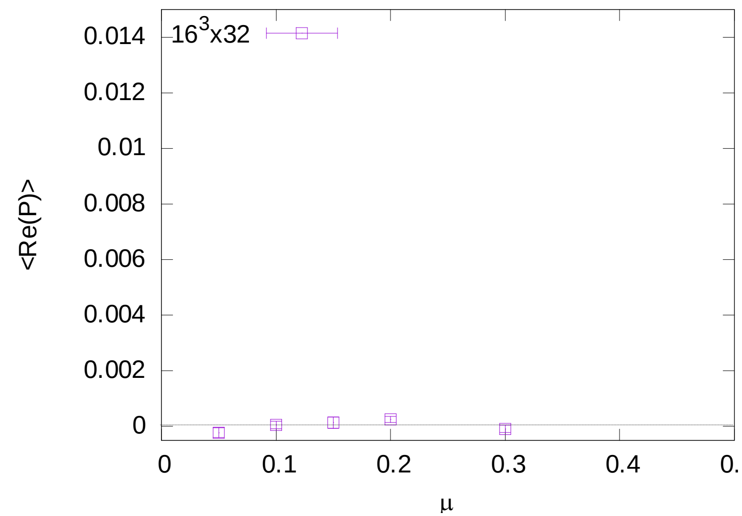
New results for a $16^3 \times 32$ lattice

presented by S. Tsutsui at LATTICE2019

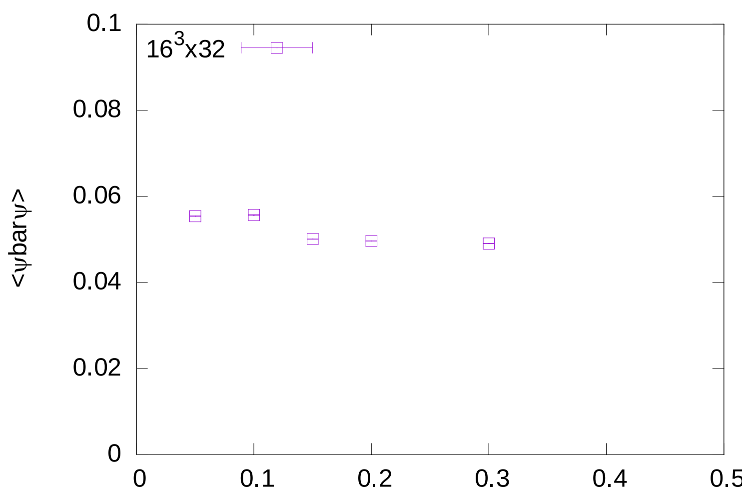
quark number



Polyakov loop



chiral condensate



- The plateau region shifts to smaller μ. (less energy needed to create baryons)
- The height of the plateau remains to be 24 quarks (formation of 8 baryons)
- It may remain the same until we reach the nuclear density 0.17 fm^{-3}. (L_s=80 required to reach that point !)

4. 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 validity region of CLM in finite density QCD
    - The singular-drift problem occurs in general in the confined phase.
    - One can investigate the high density region in which the chiral condensate vanishes.
    - The "confined" phase can be studied on lattices with small spatial extent. The plateau corresponding to 8 baryons observed on $8^3 \times 16$, $16^3 \times 32$ lattices.
- Future directions
    - Larger lattice (important because we use large β to suppress the excursion problem)
    - (Indirect) determination of the phase boundary
    - Investigations of the quark matter using larger β (Can we see the color superconducting phase ?)
    - Extending these studies to 2 quark flavors using Wilson fermions

Backup slides

physical interpretation of the phase quenched model

$$\gamma_5 D(\mu)\gamma_5 = D(-\mu)^\dagger$$

$$\det D(-\mu) = [\det D(\mu)]^*$$

$$|\det D(\mu)^2| = \det D(\mu) \cdot \det D(-\mu)$$

"up" quark "down" quark

full QCD : $w_{\mathrm{B}} = exp\left(-\frac{E-\mu(N_u+N_d)}{T}\right)$

phase quenched model : $w_{\mathrm{B}} = exp\left(-\frac{E-\mu(N_u-N_d)}{T}\right)$

μ in PQ model = isospin chemical potential
$\langle n \rangle$ in PQ model = $\langle n_u - n_d \rangle$

Speculated behaviors at T=0 with large spatial volume