New developments in finite density QCD calculations by the complex Langevin method

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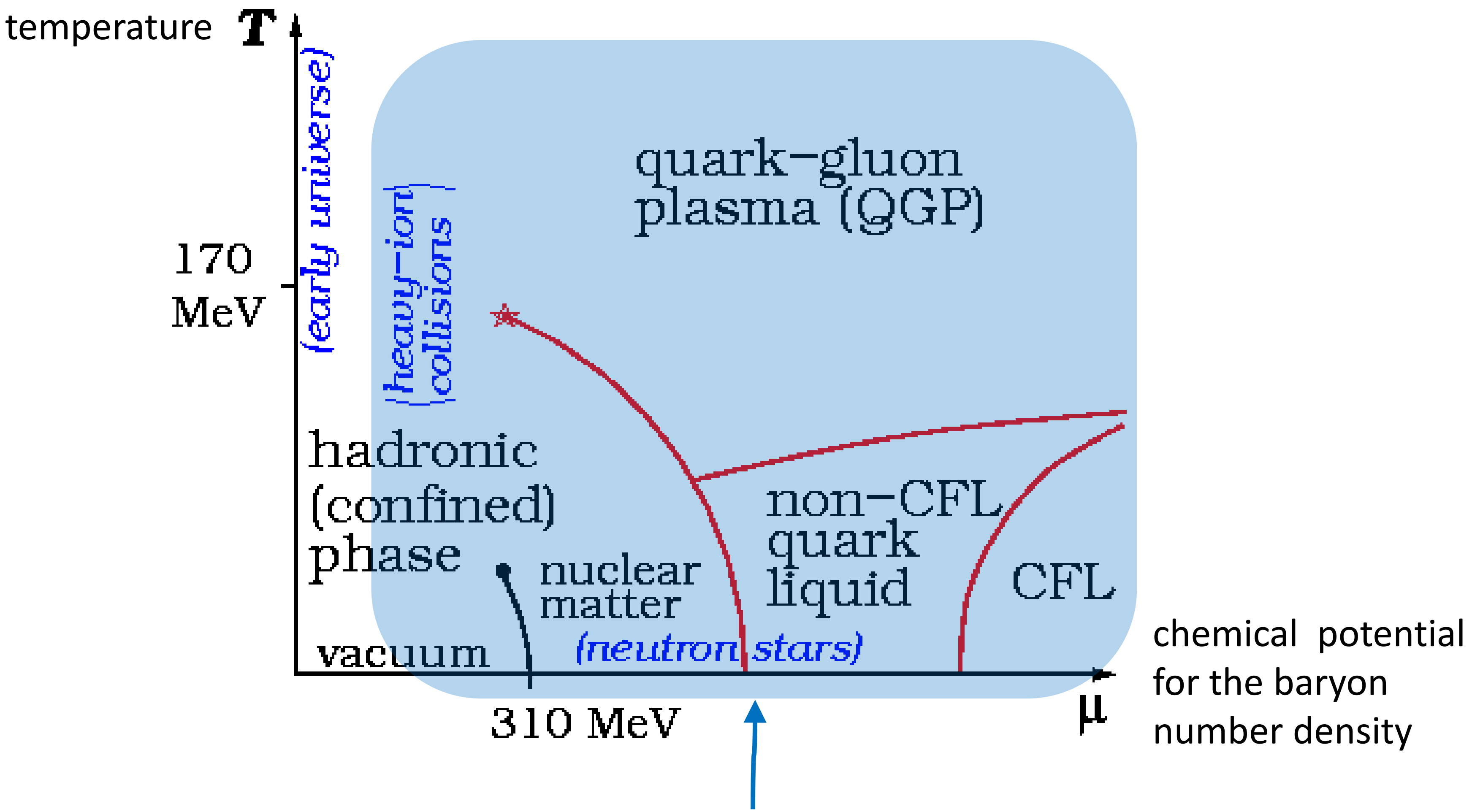
International workshop on "Discrete Approaches to the Dynamics of Fields and Space-Time"
APCTP, Korea, Sept.19-23, 2017

Ref.) Nagata-J.N.-Shimasaki, PRD 94 (2016) no.11, 114515, [arXiv:1606.07627 [hep-lat]]
Nagata-J.N.-Shimasaki, in preparation
Ito-Matsufuru-Moritake-J.N.-Shimasaki-Tsuchiya-Tsutsui, work in progress
Ito-J.N.: JHEP 1612 (2016) 009 [arXiv/1609.04501 [hep-lat]]
Anagnostopoulos-Azuma-Ito-J.N.-Papadoudis, work in progress

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 ($\mu \neq 0$),

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

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 $\mathrm{e}^{-S_{\mathrm{g}}[U]}\, |\det\mathcal{M}[U]|$
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"

It also occurs in the IKKT matrix model for superstring theory.

$$S = -\frac{1}{g^2}\mathrm{tr}\left(\frac{1}{4}[A_\mu, A_\nu]^2 + \frac{1}{2}\psi\Gamma^\mu[A_\mu, \psi]\right)$$

Ishibashi-Kawai-Kitazawa-Tsuchiya 1997

- a nonperturbative formulation of superstring theory
- SSB of SO(10) → SO(4) speculated to occur

$$S_{\mathrm{F}} = \frac{1}{2g^2}(\Gamma_\mu)_{\alpha\beta}\,\mathrm{tr}\left\{\psi_\alpha[A_\mu, \psi_\beta]\right\} \sim \Psi_i \mathcal{M}_{ij} \Psi_j$$

$$Z = \int dA\, \mathrm{e}^{-S_{\mathrm{B}}[A]}\, \mathrm{Pf}\mathcal{M}[A]$$

→ complex in general
phase Γ

The phase of the Pfaffian is expected to play a crucial role in the speculated SSB.

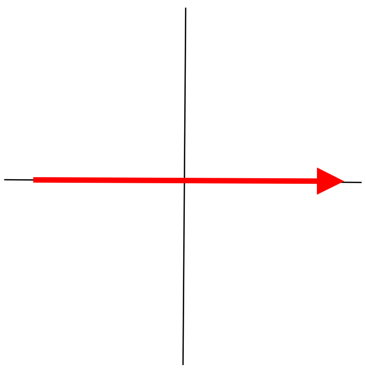
A new development toward solution to the sign problem

2011～

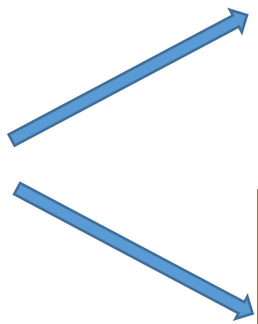
Key : complexification of dynamical variables

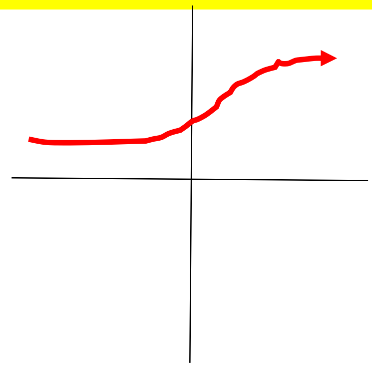
The original path integral

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



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



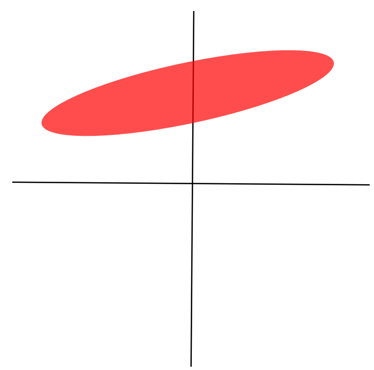


$$Z = \int dz\, w(z)$$

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.

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
4. Application to the IKKT matrix model of
   superstring theory
5. Summary and future prospects

1. Complex Langevin method

The complex Langevin method

Parisi ('83), Klauder ('83)

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

complex

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

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

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

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

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

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.

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

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

where $\rho(x;t) \in \mathbb{C}$ obeys $\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x}\left(\frac{\partial}{\partial x} - \frac{1}{w(x)}\frac{\partial w(x)}{\partial x}\right)\rho$ Fokker-Planck eq.

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

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

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

Previous argument for the key identity

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

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

$$P(x,y;0) = \rho(x;0)\,\delta(y)$$
$$L\,\mathcal{O}(z)|_{y=0} = L_0\,\mathcal{O}(x)$$ 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]

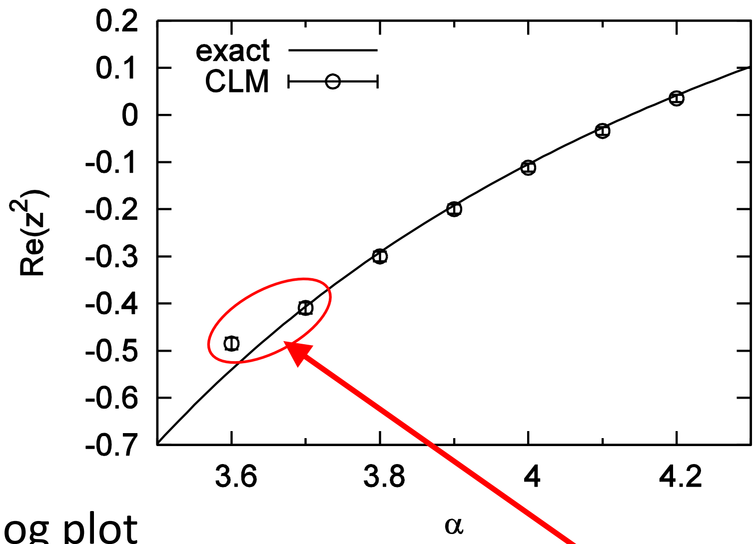
$$\int dxdy\{\mathrm{e}^{\tau L}\mathcal{O}(x+iy)\}P(x,y;t)$$
$$=\sum_{n=0}^{\infty}\frac{\tau^n}{n!}\int dxdy\{L^n\mathcal{O}(x+iy)\}P(x,y;t)$$

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.

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

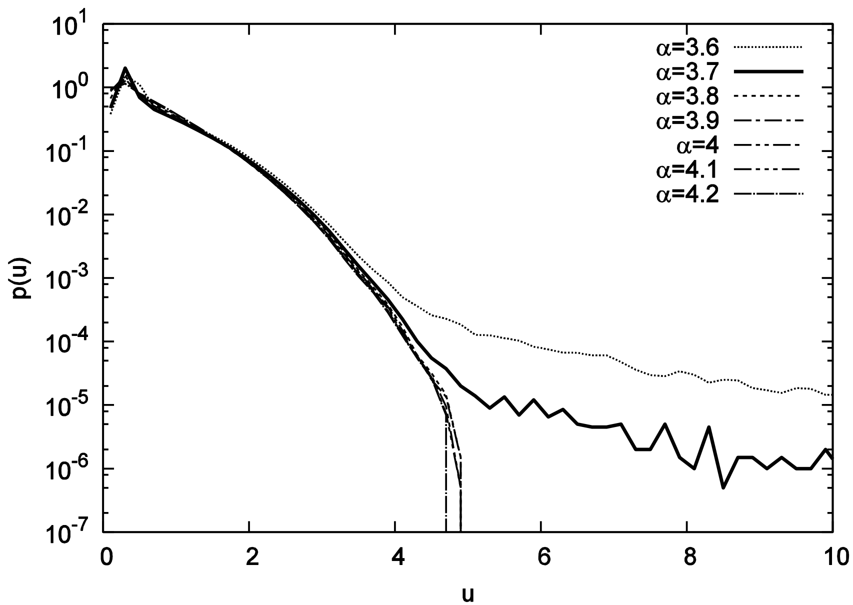
Demonstration of our condition



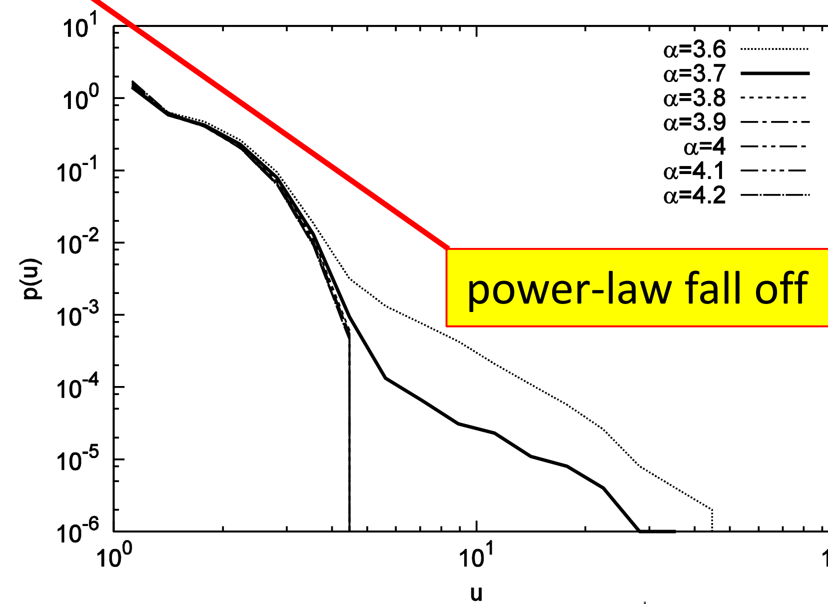
$$
\begin{aligned}
Z &= \int dx\, w(x) \\
w(x) &= (x+i\alpha)^p \, \mathrm{e}^{-x^2/2}
\end{aligned}
$$

$$p = 4$$

semi-log plot



log-log plot



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

3. Application to lattice QCD at finite density

Ref.) Nagata-J.N.-Shimasaki, in preparation
Ito-Matsufuru-Moritake-J.N.-Shimasaki-Tsuchiya-Tsutsui, work in progress

Applications to QCD at finite density

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

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

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)

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

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

"Gauge cooling" can be used to avoid the these problems.

"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 :

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

"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 !

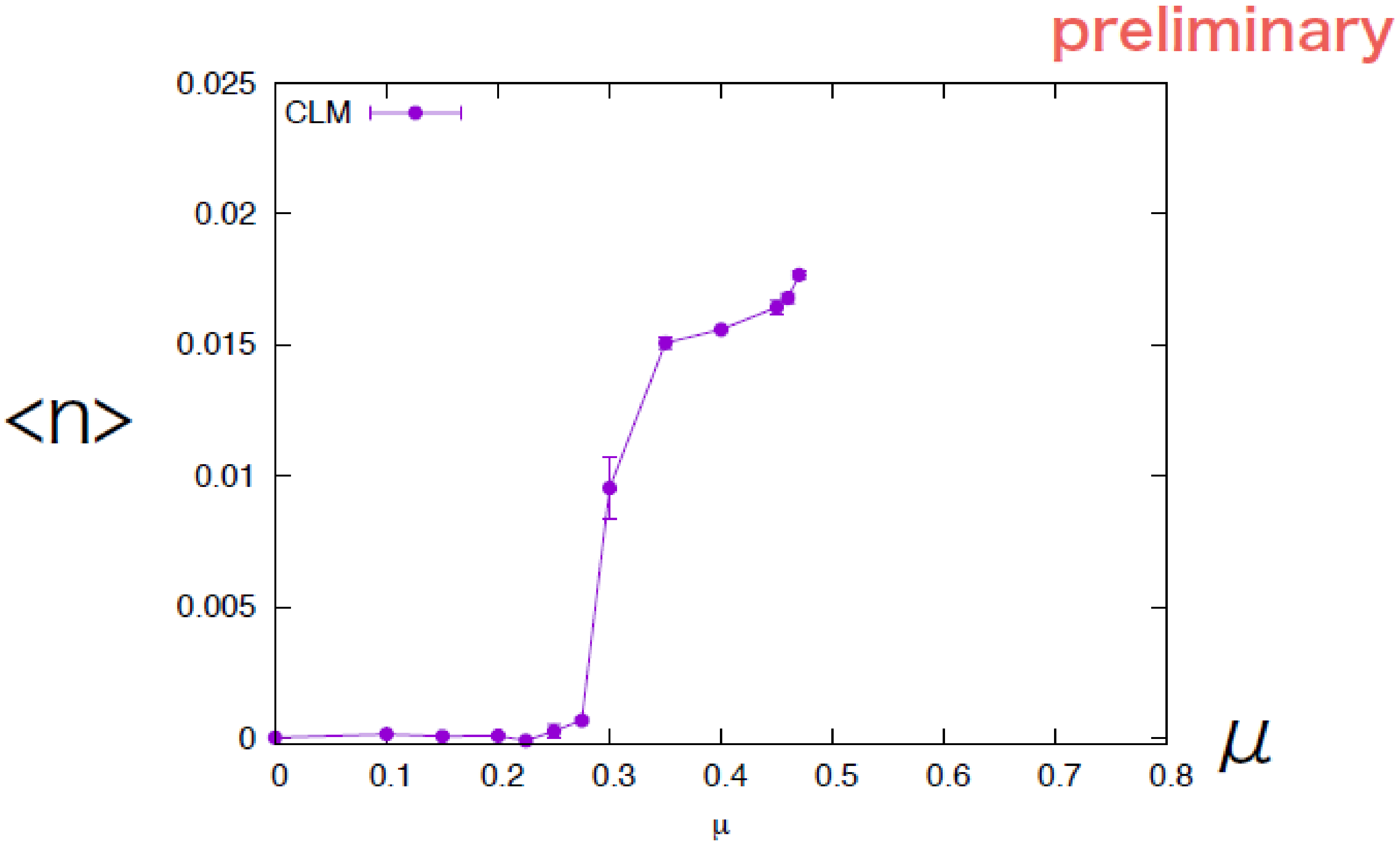
$\mathcal{O}(z)$ and $\tilde{L} = \left(v_k(z) + \frac{\partial}{\partial z_k} \right) \frac{\partial}{\partial z_k}$ are invariant under complexified symmetry transformations.

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

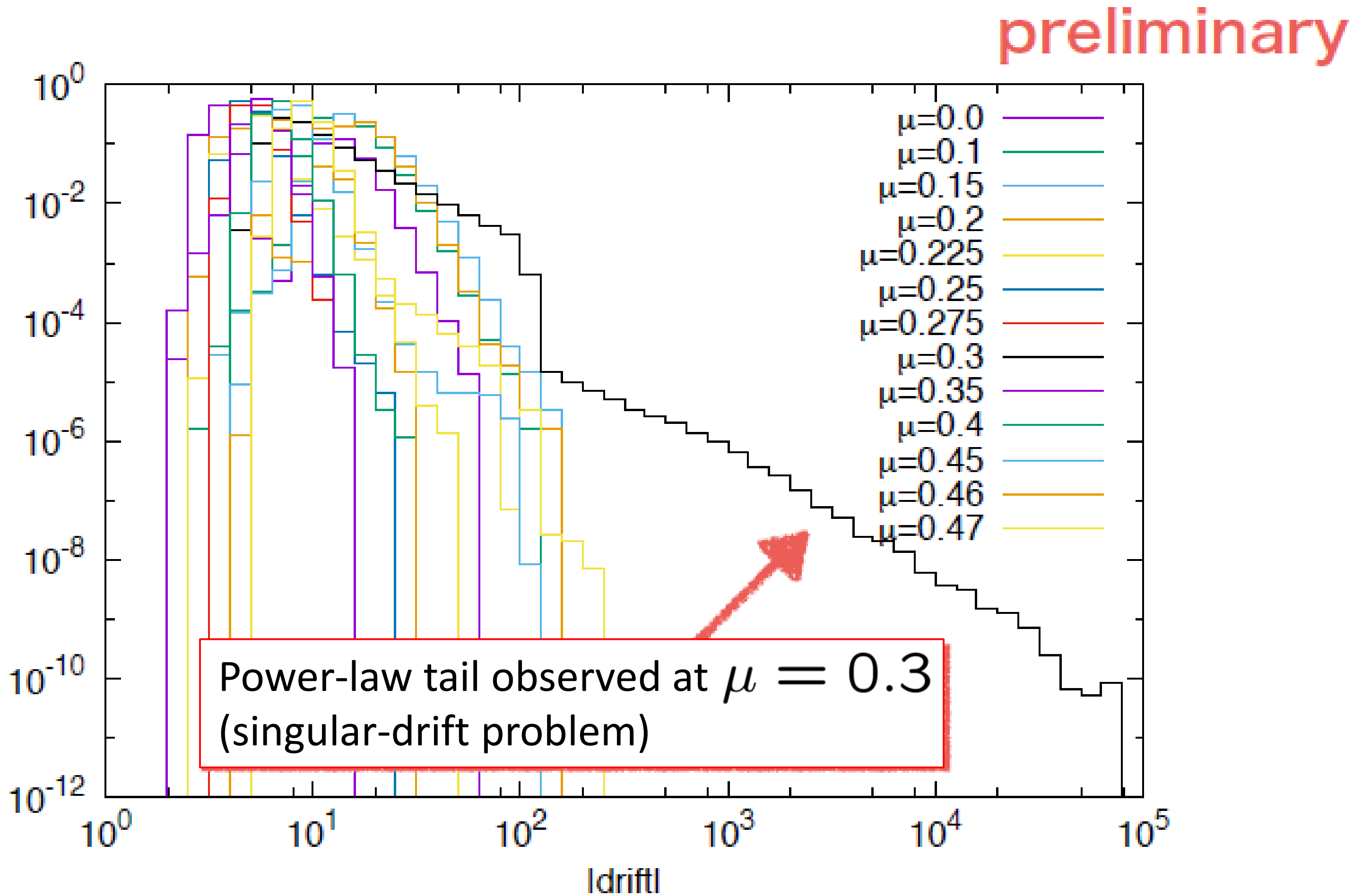
One can use this freedom to satisfy the condition for correct convergence !

Results for full QCD at finite density

$8^3 \times 16$, β=5.7
staggered fermion (4 flavors), m=0.05
Dt=10^{-4}, T=50-150
Gauge cooling used to control the unitarity norm



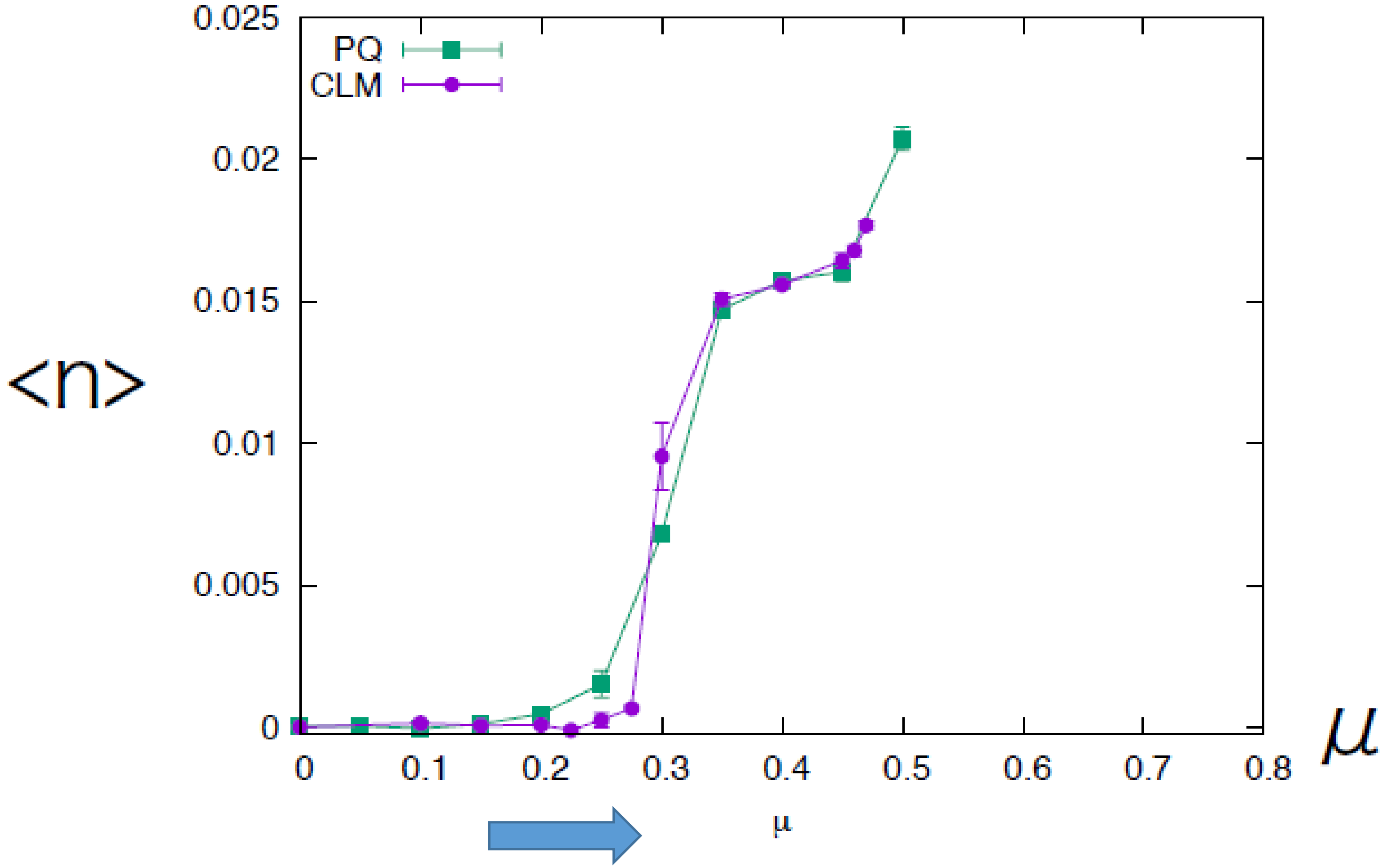
The histogram of the drift term



We can trust all the data within $0 \le \mu \le 0.47$ except for $\mu = 0.3$.

Comparison with the phase-quenched model

preliminary

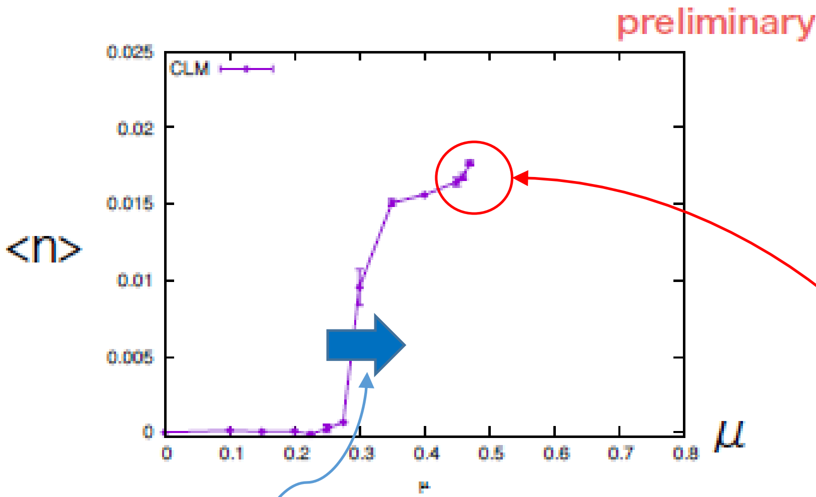


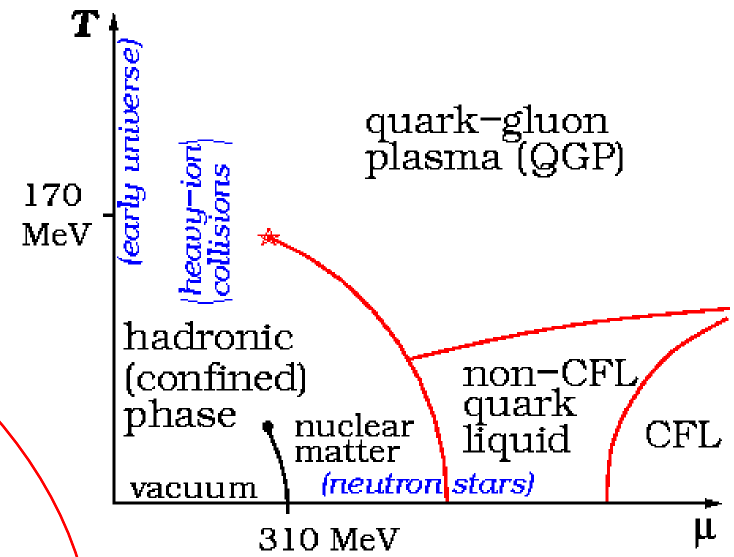
<u>Expected delay of the onset of <n></u> observed for the first time!

("Silver Blaze phenomenon")

Interpretation of the phase transitions

<n> vs μ





phase transition to
the nuclear-matter phase

phase transition to
the quark-matter phase (?)

The singular-drift problem occurs at larger μ.

The deformation technique may be useful.
(See next Chapter.)

4. Application to the IKKT matrix model of superstring theory

Ito-J.N.: JHEP 1612 (2016) 009 [arXiv/1609.04501 [hep-lat]]
Anagnostopoulos-Azuma-Ito-J.N.-Papadoudis, work in progress

Models with similar properties

(SSB of SO(D) expected due to complex fermion det.)

10d IKKT model

$$\begin{cases} A_\mu & (\mu = 1, \cdots, 10) \\ \psi_\alpha & (\alpha = 1, \cdots, 16) \end{cases}$$ 10d Majorana-Weyl

6d IKKT model

$$\begin{cases} A_\mu & (\mu = 1, \cdots, 6) \\ \psi_\alpha & (\alpha = 1, \cdots, 4) \end{cases}$$ 6d Weyl

adjoint

4d toy model (non SUSY) J.N. ('01)

$$\begin{cases} A_\mu & (\mu = 1, 2, 3, 4) \\ \psi_\alpha & (\alpha = 1, 2) \end{cases}$$ 4d Weyl

Gaussian action

N_f fundamental

a simplified IKKT-type matrix model

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

c.f.) Yuta Ito's talk on Sept. 19

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

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

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

$$f = 1, \cdots, N_\mathrm{f}$$

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

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

order parameters of the SSB of SO(4) symmetry

$$T_{\mu\nu} = \frac{1}{N}\mathrm{tr}\,(A_\mu A_\nu)$$ 4×4 real symmetrix matrix

eigenvalues : $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$

If $\langle \lambda_i \rangle$ are different in the $N \to \infty$ limit

→ SSB of SO(4) symmetry

Note : $$\sum_{i=1}^{4} \langle \lambda_i \rangle = \sum_{\mu=1}^{4} \left\langle \frac{1}{N}\mathrm{tr}\,(A_\mu)^2 \right\rangle = 4\left(1 - \frac{1}{N^2}\right) + 2\,r$$

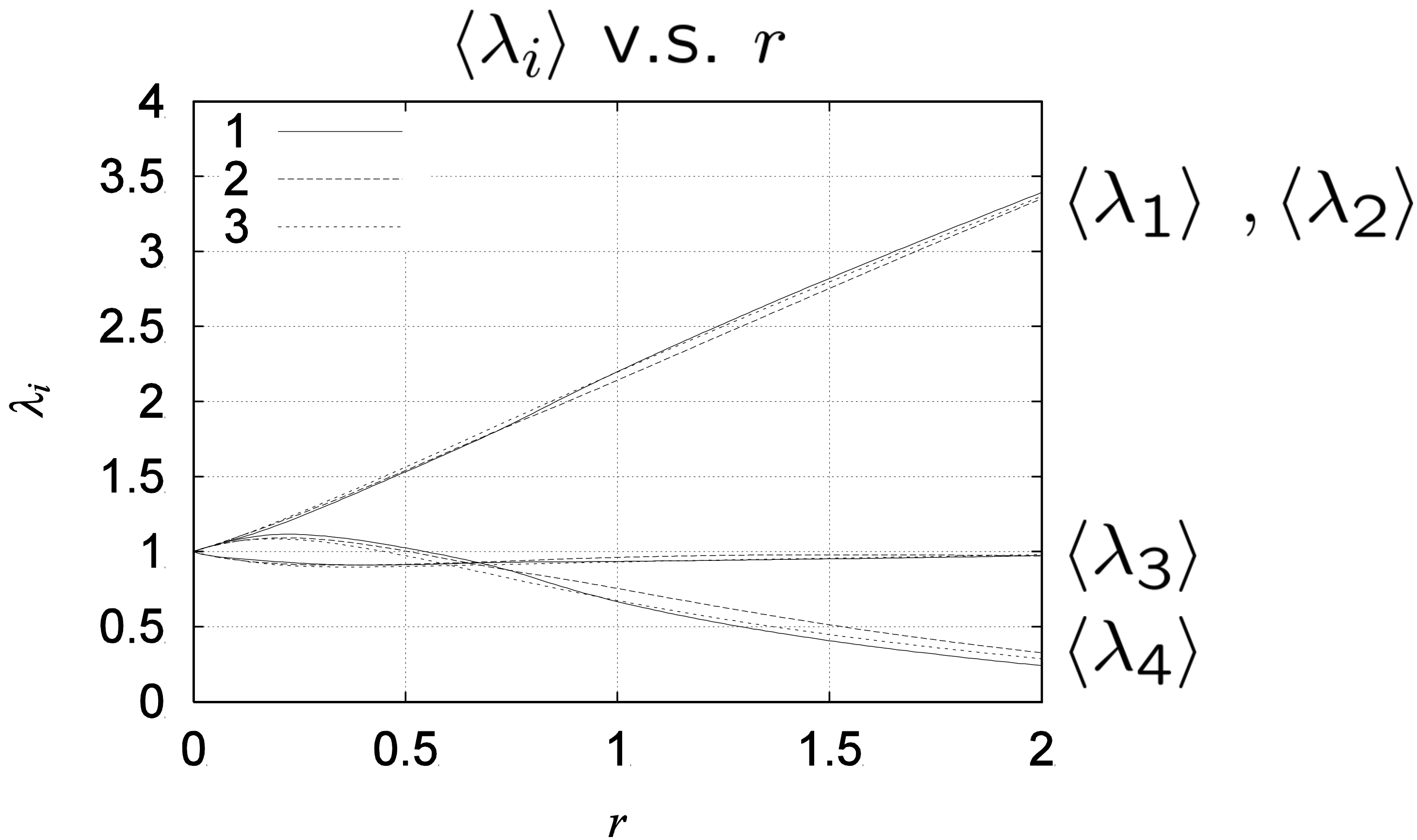
$$\langle \lambda_1 \rangle = \langle \lambda_2 \rangle = \langle \lambda_3 \rangle = \langle \lambda_4 \rangle$$

for the phase-quenched model $|\mathrm{det}D|$ instead of $\mathrm{det}D$

The phase of $\mathrm{det}D$ induces SSB.

Results of the Gaussian expansion method

J.N., Okubo, Sugino: JHEP 0210 (2002) 043 [hep-th/0205253]



SSB SO(4) $\mapsto$ SO(2) occurs !!!

E.g.) $\langle\lambda_1\rangle = \langle\lambda_2\rangle = 2.1 \,, \langle\lambda_3\rangle = 1.0 \,, \langle\lambda_4\rangle = 0.8$ at $r = 1$

Application of the complex Langevin method

Ito-J.N., JHEP 1612 (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 :

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

$$m_1 < m_2 < m_3 < m_4$$

and calculate :

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

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

Results of the CLM

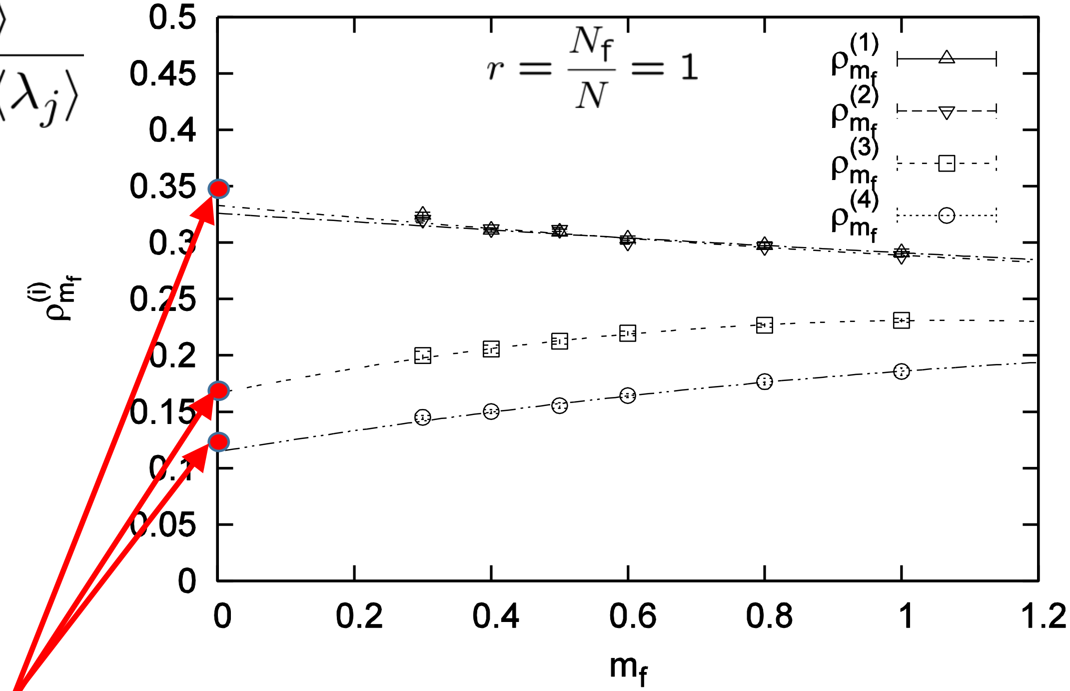
Ito-J.N., JHEP 1612 (2016) 009

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

$$S_{\mathsf{f}} = \bar{\psi}^f_\alpha \, (\Gamma_\mu)_{\alpha\beta} \, A_\mu \, \psi^f_\beta \boxed{+ \, m_4 \, \bar{\psi}^f_\alpha \, (\Gamma_4)_{\alpha\beta} \, \psi^f_\beta}$$

Explicitly breaks $\mathrm{SO}(4) \mapsto \mathrm{SO}(3)$

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



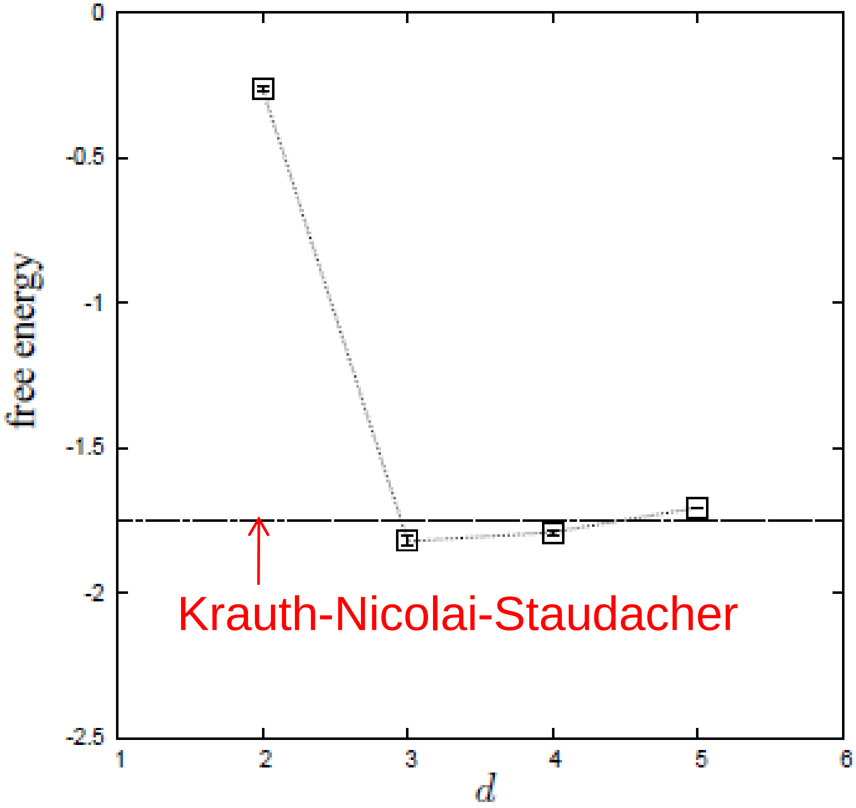
GEM result : $\rho_1 = \rho_2 = 0.35$, $\rho_3 = 0.17$, $\rho_4 = 0.13$

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

CLM reproduces the SSB of SO(4) induced by complex fermion determinant !

GEM results for 6d IKKT model

Aoyama-J.N.-Okubo, Prog.Theor.Phys. 125 (2011)



Free energy becomes minimum at d=3.

SO(6) $\xrightarrow{\text{SSB}}$ SO(3)

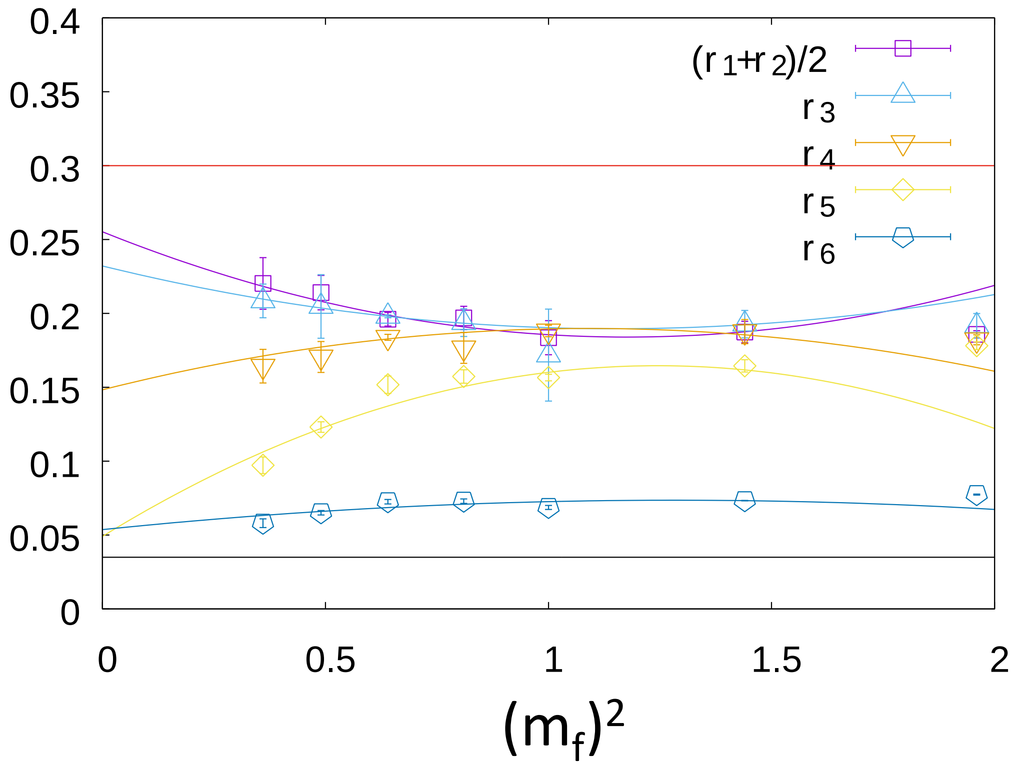
Complex Langevin analysis of 6d IKKT model

(Anagnostopoulos-Azuma-Ito-J.N.-Papadoudis, work in progress)

$$\Delta S_b = N\frac{\epsilon}{2}\sum_{\mu=1}^{6} m_\mu \mathrm{tr}(A_\mu)^2$$

with $(m_1, m_2, m_3, m_4, m_5, m_6) = (0.5, 0.5, 1, 2, 4, 8)$

mass deformation $\Delta S_b = N m_f \mathrm{tr}(\bar{\psi}\Gamma_6\psi)$
to cure the singular-drift problem

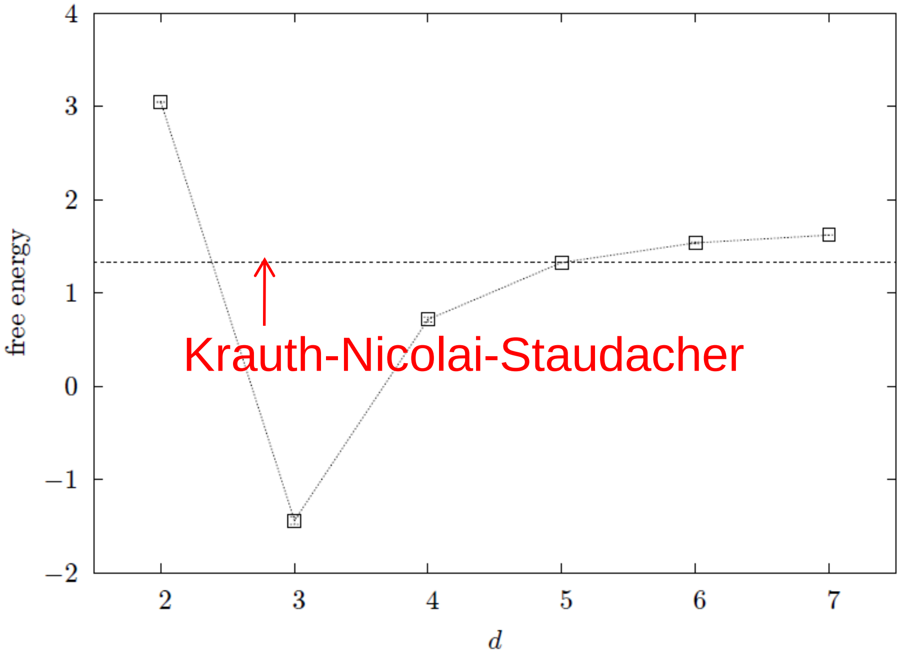


Clear trends toward SSB
SO(6)→SO(3)
is observed as $m_f \to 0$.

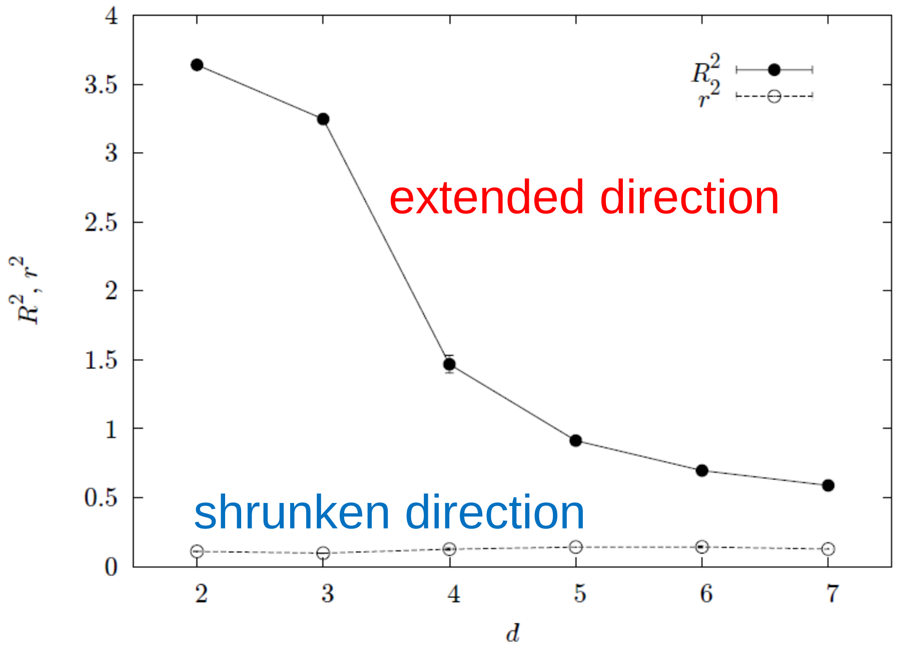
GEM results for 10d IKKT model

J.N.-Sugino ('02), J.N.-Okubo-Sugino,
Kawai, Kawamoto, Kuroki, Matsuo, Shinohara, Aoyama, Shibusa,…

J.N.-Okubo-Sugino, JHEP1110(2011)135



Free energy becomes minimum at d=3.



The extent of space-time is finite in all directions

We are planning to investigate this case also by using the complex Langevin method.

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 gauge cooling was proven to be justified.
  - The singular-drift problem may be avoided by the deformation technique.

- Finite density QCD
  - The delayed onset of the baryon number observed for the first time. (compared with the phase-quenched model)
  - The transition to the quark matter seems to be identified.

    The singular-drift problem has to be cured for even larger mu.

- IKKT matrix model of superstring theory
  - The SSB SO(10) → SO(4) can be investigated using CLM with deformation. (Successful applications in simplified models reported.)