Phase diagram and a sign problem in lattice QCD at strong coupling

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Auxiliary field Monte-Carlo simulation of strong coupling lattice QCD for QCD phase diagram

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We study the QCD phase diagram in the strong coupling limit by using the auxiliary field Monte-Carlo method, which includes field fluctuation effects. We apply the chiral angle fixing technique in order to obtain finite chiral condensate in the chiral limit in finite volume. The behavior of order parameters suggests that chiral phase transition is the second order or crossover at low chemical potential and the first order at high chemical potential. Compared with the mean field results, a hadron phase is suppressed at low chemical potential, and is extended at high chemical potential as already suggested in the monomer-dimer-polymer simulations. We find that the sign problem originating from the bosonization procedure is weakened by the phase cancellation mechanism; a complex phase from one site is tend to be canceled by the nearest neighbor site phase as long as low momentum auxiliary field contributions dominate.

I. INTRODUCTION

Quantum Chromodynamics (QCD) phase diagram is attracting much attention in recent years. At high temperature ($T$), there is a transition from quark-gluon plasma (QGP) to hadronic matter via the crossover transition, which was realized in the early universe and is now extensively studied in high-energy heavy-ion collision experiments at RHIC and LHC. At high quark chemical potential ($\mu$), we also expect the transition from baryonic to quark matter, which may be realized in cold dense matter such as the neutron star core. Provided that the high density transition is the first order, the QCD critical point (CP) should exist as the end point of the first order phase boundary. Large fluctuations of the order parameters around CP may be observed in the beam energy scan program at RHIC.

The Monte-Carlo simulation of the lattice QCD (MCLQCD) is one of the first principle non-perturbative methods to investigate the phase transition. We can obtain various properties of QCD: hadron masses and interactions, color confinement, chiral and deconfinement transitions, equation of state, and so on. We can apply these methods for different applications.
How can we investigate QCD phase diagram?

- Non-pert. & ab initio approach
  = Monte-Carlo simulation of lattice QCD
    but lattice QCD at finite \( \mu \) has the sign problem.
Sign Problem

Monte-Carlo integral of oscillating function

\[ Z = \int dx \exp(-x^2 + 2iax) = \sqrt{\pi} \exp(-a^2) \]

\[ \langle O \rangle = \frac{1}{Z} \int dx \, O(x) \exp(-x^2 + 2iax) \]

Easy problem for human is not necessarily easy for computers.
**Sign Problem (cont.)**

- **Generic problem in quantum many-body problems**
- **Example: Euclid action of interacting Fermions**

\[
S = \sum_{x, y} \bar{\psi}_x D_{x, y} \psi_y + g \sum_x (\bar{\psi} \psi)_x (\bar{\psi} \psi)_x
\]

- **Bosonization and MC integral (g>0 → repulsive)**

\[
\exp(-g M_x M_x) = \int d \sigma_x \exp(-g \sigma_x^2 - 2i g \sigma_x M_x) \quad (M_x = (\bar{\psi} \psi)_x)
\]

\[
Z = \int D[\psi, \bar{\psi}, \sigma] \exp\left[-\bar{\psi}(D+2i g \sigma)\psi - g \sum_x \sigma_x^2\right]
\]

\[
= \int D[\sigma] \ Det(D+2i g \sigma) \exp\left[-g \sum_x \sigma_x^2\right]
\]

*complex Fermion det.*

*→ complex stat. weight*

*→ sign problem*
Sign problem in lattice QCD

- Fermion determinant (= stat. weight of MC integral) becomes complex at finite $\mu$ in LQCD.

- $\gamma_5$ Hermiticity

$$Z = \int D[U,q,\bar{q}] \exp(-\bar{q} D(\mu,U)q - S_G(U))$$
$$= \int D[U] \ Det(D(\mu,U)) \ exp(-S_G(U))$$

$$\gamma_5 D(\mu,U) \gamma_5 = [D(-\mu^*,U^+)]^+$$
$$\rightarrow \ Det(D(\mu,U)) = [\ Det(D(-\mu^*,U^+))]^*$$

- Fermion det. ($\det D$) is real for zero $\mu$ (and pure imag. $\mu$)
- Fermion det. is complex for finite real $\mu$.
- Phase quenched weight = Weight at isospin chem. pot.

$$Z_{\text{phase quench}}(T,\mu_u=\mu_d=\mu) = Z_{\text{full}}(T,\mu_u=-\mu_d=\mu)$$
How can we investigate QCD phase diagram?

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- Effective model and/or Approximations are necessary.
  - Effective models:
    NJL, PNJL, PQM, ...
    Model dependence is large.
  - Approximation / Truncation
    Taylor expansion,
    Imag. $\mu$, Canonical,
    Re-weighting,
    Strong coupling LQCD
  - Alternative method
    Fugacity expansion,
    Histogram method,
    Complex Langevin
Various method work at small $\mu$ ($\mu/T < 1$).

Large $\mu$

- Roberge-Weiss transition
  $\rightarrow$ Conv. $\mu/T < \pi/3$ at $T > T_{RW}$

- No go theorem
  Splittorff ('06), Han, Stephanov ('08), Hanada, Yamamoto ('11), Hidaka, Yamamoto ('11)

Phase quenched sim.
$\sim$ Isospin chem. pot.

$$Z_{\text{phase quench}}(T, \mu_u = \mu_d = \mu) = Z_{\text{full}}(T, \mu_u = -\mu_d = \mu)$$

$\rightarrow$ CP in $\pi$ cond. phase
(Silver Blaze)
Phase diagram in isospin chemical potential space

- Important in Compact Astrophys. phen.
- At vanishing quark chem. pot., there is no sign problem.
- Interesting 3D phase structure.

Kogut, Sinclair ('04); Sakai et al. ('10); AO, Ueda, Nakano, Ruggieri, Sumiyoshi ('11)

FRG: Kamikado, Strodthoff, von Smekal, Wambach ('13)

PQM: Ueda, Nakano, AO, Ruggieri, Sumiyoshi ('13)
“Watson, the dog did not bark at night. This is the evidence that he is the criminal who stole Silver Blaze.”

In physics,
“If $\delta \mu > m_\pi/2$ at low $T$ and you do not have pion condensation, that theory should be wrong.”

Phase quench $D_d(\mu, U) \rightarrow D_d(-\mu^*, U^+)$
$\rightarrow$ We can compose pions from original di-quark configuration.

To do: Directly sample with complex $S$ (CLE), Integrate $U$ first (SC-LQCD), and some other method....
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  - Approximation / Truncation
    - Taylor expansion,
    - Imag. $\mu$, Canonical,
    - Re-weighting,
    - Strong coupling LQCD

  - Alternative method
    - This talk
      - Fugacity expansion, *Nakamura, Nagata*
      - Histogram method, *Ejiri*
      - Complex Langevin, *Stamatescu*
Strong coupling lattice QCD
Strong Coupling Lattice QCD

**Pure YM**

- Wilson ('74), Creutz ('80), Munster ('80, '81), Lottini, Philipsen, Langelage's ('11)

**Phase diagram (mean field)**

- Kawamoto ('80), Kawamoto, Smit ('81), Damgaard, Hochberg, Kawamoto ('85), Bilic, Karsch, Redlich ('92), Fukushima ('03); Nishida ('03), Kawamoto, Miura, AO, Ohnuma ('07).
- Miura, Nakano, AO, Kawamoto ('09)
- Nakano, Miura, AO ('10)

**Fluctuations**

- Mutter, Karsch ('89), de Forcrand, Fromm ('10), de Forcrand, Unger ('11), AO, Ichihara, Nakano ('12), Ichihara, Nakano, AO ('13)
Effective action in SCL ($1/g^0$), NLO ($1/g^2$), NNLO ($1/g^4$) terms and Polyakov loop.

**NLO:** Faldt-Petersson ('86), Bilic-Karsch-Redlich ('92)
Conversion radius > 6 in pure YM ? Osterwalder-Seiler ('78)

**One species of unrooted staggered fermion** ($N_f=4$ @ cont.)

**Moderate $N_f$ deps. of phase boundary:** BKR92, Nishida('04), D'Elia-Lombardo ('03)

Leading order in $1/d$ expansion ($d=3$=space dim.)
→ Min. # of quarks for a given plaquette configurations,
no spatial B hopping term.

Different from “strong coupling” in “large $N_c$”

*Still far from “Realistic”, but SC-LQCD would tell us useful qualitative features of the phase diagram and EOS.*
Lattice QCD action

- **Gluon field → Link variables**  \( U_\mu(x) \approx \exp(i g A_\mu) \)

- **Gluon action → Plaquette action**

  \[
  S_G = \frac{2 N_c}{g^2} \sum_{\text{plaq.}} \left[ 1 - \frac{1}{N_c} \text{Re tr} \ U_{\mu\nu}(n) \right]
  \]

- **Loop → surface integral of “rotation”**  \( F_{\mu\nu} \) in the U(1) case.

- **Quark action (staggered fermion)**

  \[
  S_F = \frac{1}{2} \sum_x \left[ \overline{\chi}_x e^{\mu} U_{0,x} \chi_{x+\hat{0}} - \overline{\chi}_{x+\hat{0}} e^{-\mu} U^+_{0,x} \chi_x \right] \\
  + \frac{1}{2} \sum_{x,j} \eta_j(x) \left[ \overline{\chi}_x U_{x,j} \chi_{x+j} - \overline{\chi}_{x+j} U^+_{x,j} \chi_x \right] + \sum_x m_0 M_x \\
  = S_F^{(t)} + S_F^{(s)} + \sum_x m_0 M_x
  \]
Link integral $\rightarrow$ Area Law

- **One-link integral**
  \[
  \int dU \ U_{ab} U_{cd}^+ = \frac{1}{N_c} \delta_{ad} \delta_{bc}
  \]

- **Wilson loop in pure Yang-Mills theory**
  \[
  \langle W(C = L \times N_\tau) \rangle = \frac{1}{Z} \int D U \ W(C) \exp \left[ \frac{1}{g^2} \sum_P \text{tr}(U_P + U_P^+) \right]
  \]
  \[
  = \exp(-V(L)N_\tau)
  \]

  in the strong coupling limit
  \[
  \langle W(C) \rangle = N \left( \frac{1}{g^2 N} \right)^{LN_\tau}
  \]
  \[
  \rightarrow V(L) = L \log(g^2 N)
  \]

- **Linear potential between heavy-quarks**
  \[
  \rightarrow \text{Confinement (Wilson, 1974)}
  \]
  \[
  = 1/N_c \ g^2
  \]
Effective action in the strong coupling limit (SCL)

- Ignore plaquette action \((1/g^2)\)
  → We can integrate each link independently!

- Integrate out \textit{spatial} link variables of min. quark number diagrams (1/d expansion)

\[
S_{\text{eff}} = S_F^{(t)} - \frac{1}{4N_c} \sum_{x, j} M_x M_{x+j} + m_0 \sum_{x} M_x \left( M_x = \bar{\chi}_x \chi_x \right)
\]

*Damgaard, Kawamoto, Shigemoto ('84)*

\[
\int dU \ U_{ab}^+ U_{cd}^- = \delta_{ad} \delta_{bc} \ / \ N_c
\]

\( \chi \ U_0^+ \ U_0^- \ m_0 \)

\( \chi \ U_0^+ \ U_0^- \ m_0 \)

\( \frac{1}{g^2} \)

\( \chi \ U_0^+ \ U_0^- \ m_0 \)
Phase diagram in SC-LQCD (mean field)

- “Standard” simple procedure in Fermion many-body problem
  - Bosonize interaction term (Hubbard-Stratonovich transformation)
  - Mean field approximation (constant auxiliary field)
  - Fermion & temporal link integral
    - Damgaard, Kawamoto, Shigemoto (’84); Faldt, Petersson (’86); Bilic, Karsch, Redlich (’92); Fukushima (’04); Nishida (’04)

Fukushima, 2004
**Finite Coupling Effects**

Effective Action with finite coupling corrections

Integral of $\exp(-S_G)$ over spatial links with $\exp(-S_F)$ weight $\rightarrow S_{\text{eff}}$

\[
S_{\text{eff}} = S_{\text{SCL}} - \log \langle \exp(-S_G) \rangle = S_{\text{SCL}} - \sum_{n=1} \frac{(-1)^n}{n!} \langle S_G^n \rangle_c
\]

$\langle S_G^n \rangle_c = \text{Cumulant (connected diagram contr.)}$ c.f. R.Kubo('62)

\[
S_{\text{eff}} = \frac{1}{2} \sum_x (V_x^+ - V_x^-) - \frac{b_0}{2d} \sum_{x,j>0} [MM]_{j,x}
\]

\[
+ \frac{1}{2} \frac{\beta_x}{2d} \sum_{x,j>0} [V^+V^- + V^-V^+]_{j,x} - \frac{1}{2} \frac{\beta_x}{d(d-1)} \sum_{x,j>0,k>0,k\neq j} [MMMM]_{j,x,k}
\]

\[
- \beta_{FF} \sum_{x,j>0} [W^+W^- + W^-W^+]_{j,x} - \frac{\beta_{ss}}{4d(d-1)(d-2)} \sum_{x,j>0,k>0,|k|>0,|j|>0} [MMMM]_{j,x,k}[MM]_{j,x+|l|
\]

\[
+ \frac{\beta_{ss}}{8d(d-1)} \sum_{x,j>0,|k|\neq j} [V^+V^- + V^-V^+]_{j,x} ([MM]_{j,x+k} + [MM]_{j,x+k+0})
\]

\[- \left( \frac{1}{g^2 N_c} \right)^{N_T} \sum_{x,j>0} \left( \bar{P}_x P_{x+j} + h.c. \right)\]

SCL (Kawamoto-Smit, '81)

NLO (Faldt-Petersson, '86)

NNLO (Nakano, Miura, AO, '09)

Polyakov loop (Gocksch, Ogilvie ('85), Fukushima ('04)
Nakano, Miura, AO ('11))

Ohnishi @ Lattice QCD at Finite T and $\rho$, KEK, Jan.20-22, 2014
P-SC-LQCD reproduces MC results of $T_c(\mu=0)$ ($\beta = 2N_c/g^2 \leq 4$)
MC data: SCL (Karsch et al. (MDP), de Forcrand, Fromm (MDP)), $N_\tau = 2$ (de Forcrand, private), $N_\tau = 4$ (Gottlieb et al. ('87), Fodor-Katz ('02)), $N_\tau = 8$ (Gavai et al. ('90))
Beyond the mean field approximation

Constant auxiliary field $\rightarrow$ Fluctuating auxiliary field

$$S_{\text{eff}} = S_F^{(i)} + \sum_x m_x M_x + \frac{L^3}{4N_c} \sum k, \tau f(k) \left[ |\sigma_{k,\tau}|^2 + |\pi_{k,\tau}|^2 \right]$$

$$m_x = m_0 + \frac{1}{4N_c} \sum_j \left( (\sigma + i \varepsilon \pi)_{x+\hat{j}} + (\sigma + i \varepsilon \pi)_{x-\hat{j}} \right)$$

$$f(k) = \sum_j \cos k_j <, \quad \varepsilon = (-1)^{x_0 + x_1 + x_2 + x_3}$$

Auxiliary Field Monte-Carlo (AFMC) integral

Another method: Monomer-Dimer-Polymer simulation

*Mutter, Karsch ('89), de Forcrand, Fromm ('10), de Forcrand, Unger ('11)*

Bosonization of “repulsive” mode: Extended HS transf.

$\rightarrow$ Introducing “$i$” leads to the complex Fermion determinant.

*Miura, Nakano, AO (09), Miura, Nakano, AO, Kawamoto (09)*
Origin of the sign problem in AFMC

**Extended Hubbard-Stratonovich transformation**

Miura, Nakano, AO ('09), Miura, Nakano, AO, Kawamoto ('09)

\[ e^{\alpha A B} = \int d\phi \, d\varphi \, e^{-\alpha \left[ (\phi + (A+B)/2)^2 + (\varphi + i (A-B)/2)^2 - AB \right]} \]

\[ = \int d\phi \, d\varphi \, e^{-\alpha \left[ \varphi^2 + \varphi^2 + \phi (A+B) + i \varphi (A-B) \right]} \]

Complex

We need “i” to bosonize product of different kind.
→ Fermion determinant becomes complex.

**Bosonization in AFMC in the strong coupling limit**

\[ \exp \left\{ \alpha f(k) \left[ M_{-k,\tau} M_{k,\tau} - M_{-k,\tau} M_{k,\tau} \right] \right\} \]

\[ = \int d\sigma_{k,\tau} \, d\sigma^*_{k,\tau} \, d\pi_{k,\tau} \, d\pi^*_{k,\tau} \exp \left\{ -\alpha f(k) \left[ |\sigma_{k,\tau}|^2 + |\pi_{k,\tau}|^2 \right. \right. \]

\[ + \sigma^*_{k,\tau} M_{k,\tau} + M_{-k,\tau} \sigma_{k,\tau} - i \pi^*_{k,\tau} M_{k,\tau} - i M_{-k,\tau} \pi_{k,\tau} \right\} \]
Mean field treatment of repulsive interaction

\[
e^{-\alpha A^2} = \int d\varphi \exp\left(-\alpha \left[ \varphi^2 - 2i\varphi A \right]\right)
= \int d\varphi \exp\left(-\alpha \left[ (\varphi + i\omega)^2 - 2i(\varphi + i\omega)A \right]\right)
= \int d\varphi \exp\left(-\alpha \left[ \varphi^2 + 2i\varphi(\omega - A) - \omega^2 + 2\omega A \right]\right)
\approx \exp\left(\alpha \left[ \omega^2 - 2\omega A \right] \right) \quad (\varphi = i\omega, \quad \omega = \langle A \rangle)
\]
**Auxiliary Field Effective Action**

- Fermion det. + U0 integral can be done analytically.
  → Auxiliary field effective action

\[
S_{\text{eff}}^{\text{AF}} = \sum_{k, \tau, f(k) > 0} \frac{L^3 f(k)}{4 N_c} \left[ |\sigma_{k, \tau}|^2 + |\pi_{k, \tau}|^2 \right]
- \sum_x \log \left[ X_N(x)^3 - 2 X_N(x) + 2 \cosh \left( \frac{3 \mu}{T} \right) \right]

\[X_N(x) = X_N[m(x, \tau)] \quad \text{(known func.)}\]

\[m_x = m_0 + \frac{1}{4 N_c} \sum_j \left( (\sigma + i \varepsilon \pi)_{x+j} + (\sigma + i \varepsilon \pi)_{x-j} \right)\]

- \(X_N = \text{Known function of } m(x, \tau)\)  
  \text{Faldt, Petersson ('86)}

For constant \(m\), \(X_N = 2 \cosh (N_\tau \text{ arcsinh } (m/\gamma))\)

- Imag. part from \(X_N\) → Relatively smaller at large \(\mu/T\)
- Imag. part from low momentum AF cancels due to \(i\varepsilon\) factor.
Chiral Angle Fixing

How can we simulate correct thermodynamic chiral limit using finite volume simulations?

ichihara, AO, Nakano ('14)

c.f. rms spin is adopted in spin systems Kurt, Dieter ('10)
Order Parameters

- Low $\mu/T$ region
  → 2nd order or crossover
  (would-be second)

- High $\mu/T$ region
  → sudden change
  & hysteresis
  (would-be first)

Ichihara, AO, Nakano ('14)
Error estimate by Jack-knife method

Error
= Jack-knife error after autocorrelation disappears

Ichihara, AO, Nakano ('14)
**Phase boundary**

- **Low μ/T region** (would-be second)
  → Chiral susc. peak

- **High μ/T region** (would-be first)
  → Average eff. action from Wigner/NG init. cond.
  
  *c.f. Exchange MC (Hukuyama)*

*Ichihara, AO, Nakano ('14)*
Finite Size Scaling of Chiral Susceptibility

Finite size scaling of $\chi_\sigma$ in the $V \to \infty$ limit

- Crossover: Finite
- Second order: $\chi_\sigma \propto V^{(2-\eta)/3}$, $\eta=0.0380(4)$ in 3d O(2) spin
  Campostrini et al. ('01)
- First order: $\chi_\sigma \propto V$

AFMC results: Not First order at low $\mu/T$.

Ichihara, AO, Nakano ('14)
**Phase diagram**

Reduced $T_c$ (low $\mu/T$)
Enhanced $\mu_c$ (high $\mu/T$)

Small spatial size dep.

$Ichihara, AO, Nakano ('14)$
**Monomer-Dimer-Polymer simulation**

The partition function of LQCD can be given as the sum of monomer-dimer-polymer (MDP) configuration weight. The sign problem is mild.

\[ Z(2ma,\mu,r) = \sum_{K} w_K \]

\[ w_K = (2ma)^{N_M} r^{2N_t} (1/3)^{N_1N_2} \prod_x w(x) \prod_C w(C) \]

MDP with worm algorithm is applied to study the phase diagram

\[ \text{de Forcrand, Fromm ('10), de Forcrand, Unger ('11)} \]
Sign problem in SC-LQCD
Average Phase Factor

- Average phase factor
  = Weight cancellation

\[ \langle e^{i\theta} \rangle = \frac{Z_{\text{phase quenched}}}{Z_{\text{full}}} \]

- AFMC results
  - \( \langle e^{i\theta} \rangle > 0.9 \) on 4\(^4\) lattice
  - \( \langle e^{i\theta} \rangle > 0.1 \) on 8\(^4\) lattice

\[ \mu/T = 0.2 \quad \mu/T = 0.6 \quad \mu/T = 1.8 \]

Ichihara, AO, Nakano (’14)
**Comparison with Direct Simulation at finite coupling**

- Lattice MC simulation at finite $\mu$ and **finite $\beta$** with $N_f=4$
  - Takeda et al. ('13)
  - Ave. Phase Factor $\sim 0.3$ at $a\mu_a \sim 0.15$ ($8^3 \times 4$, $a\mu_c = am_\pi/2 \sim 0.7$)

- **AFMC**
  - Ave. Phase Factor $\sim 0.6$ around the transition ($8^4$, SCL)

---

Takeda, Jin, Kuramashi, Y. Nakamura, Ukawa, Lattice 2013  $a\mu_c = am_\pi/2 \sim 0.7$

Ichihara, AO, Nakano ('14)
**Discussion: Comparison with MDP**

- **Free energy difference**
  \[
  \langle \exp(i \theta) \rangle \equiv \exp(-\Omega \Delta f), \quad \Omega = \text{space-time volume}
  \]

- **MDP simulation on anisotropic lattice at finite T and \( \mu \)**
  - de Forcrand, Fromm ('10), de Forcrand, Unger ('11)
  - Strong coupling limit.
  - Higher-order terms in 1/d expansion
  - No sign problem in the continuous time limit (\( N\tau \to \infty \)).

\[
\langle \exp(i \theta) \rangle \equiv \exp(-\Omega \Delta f), \quad \Omega = \text{space-time volume}
\]
**Summary**

- Strong coupling lattice QCD is a promising tool in finite density lattice QCD.
  - Strong coupling limit + finite coupling correction + Polyakov loop → MC results of Tc is roughly reproduced.
  - Fluctuation effects can be included in auxiliary field Monte-Carlo
  - Sign problem could be partially solved in the strong coupling limit. Two independent methods show the same phase boundary, and the spatial size dependence is small. (Monomer-dimer-polymer simulation, AFMC)

**Challenge**

- Finite coupling + Fluctuations
  - Different type of Fermion
    - Minimally doubled fermion, Misumi, Kimura, AO ('12)
    - Higher order terms in 1/d expansion,
    - ....

_Unger et al. ('13)_
Real Challenge: How to live with the sign problem

- Idea 1: Cutoff or Gauss integral of high momentum modes
- Idea 2: Change the integral path
- Idea 3: Combination of Fugacity exp. or Histogram method
Thank you