Study of finite density lattice QCD by the histogram method

Shinji EJIRI
Niigata University

WHOT-QCD collaboration
S. Ejiri¹, S. Aoki², T. Hatsuda³, K. Kanaya²,
Y. Nakagawa¹, H. Ohno⁴, H. Saito², and T. Umeda⁵

¹Niigata Univ., ²Univ. of Tsukuba, ³RIKEN, ⁴Bielefeld Univ., ⁵Hiroshima Univ.

Quarks to Universe in Computational Science (QUCS 2012),
Nara, Japan, December 13-16, 2012
Phase structure of QCD at high temperature and density

- Phase transition lines
- Critical point
- Order of the transition

Lattice QCD Simulations

- Direct simulation: Impossible at $\mu \neq 0$. 
Distribution function & the effective potential

\[ W(X; m, T, \mu) \equiv \int DU \delta(X - \hat{X})(\text{det} M(m, \mu))^{N_f} e^{-S_g} \]  
(Histogram)

\( X \): order parameters, total quark number, average plaquette, etc.

Crossover

- \( W(X) \): Gaussian function
- \( V(X) \): Quadratic function

Critical point

- \( W(X) \): Flat
- \( V(X) \): Curvature: Zero

1st order phase transition

- \( W(X) \): Two phases coexist
- \( V(X) \): Double well potential

\[ V_{\text{eff}}(X) = -\ln W(X) \]
Mass-dependence of the effective potential

\[ W(X',m,T,\mu) \equiv \int DUD\delta(X-X') \sum_{f=1}^{N_f} \det M\left(m_f,\mu_f\right)e^{-S_g}, \quad V_{\text{eff}}(X) = -\ln W(X) \]

\( X \): order parameters, total quark number, average plaquette etc.

1st order phase transition

Critical point

Crossover

Curvature: Zero

Quadratic function

Tricritical point

Quenched

Nf=2

Nf=3

\( m_T \)

\( m_s \)

\( \mu=0 \)

Two phases coexist

Double well potential

1st order phase transition
$$(\beta, m, \mu)-dependence\ of\ the\ Distribution\ function$$

$$W(X, \beta, m, \mu) \equiv \int DU \delta(\hat{X} - X) (\det M(m, \mu))^{N_f} e^{6N_{site}\beta\hat{P}}$$

(plaquette $P$ (1x1 Wilson loop for the standard action))

$$R(X, \beta, \beta_0 m, m_0, \mu) \equiv W(X, \beta, m, \mu)/W(X, \beta_0, m_0, 0) \quad (Reweight\ factor)$$

$$R(X) = \frac{\left\langle \delta(\hat{X} - X) e^{6N_{site}(\beta - \beta_0)\hat{P}} \left( \frac{\det M(m, \mu)}{\det M(m_0, 0)} \right)^{N_f} \right\rangle_{\beta = \beta_0, \mu = 0}}{\left\langle \delta(\hat{X} - X) \right\rangle_{\beta = \beta_0, \mu = 0}} \equiv \left\langle e^{6N_{site}(\beta - \beta_0)\hat{P}} \left( \frac{\det M(m, \mu)}{\det M(m_0, 0)} \right)^{N_f} \right\rangle_{X:fixed}$$

Effective potential:

$$V_{eff}(X, \beta, m, \mu) = -\ln[W(X, \beta m, \mu)] = V_{eff}(X, \beta_0, m_0, 0) - \ln R(X, \beta, \beta_0 m, m_0, \mu)$$

$$\ln R(X) = \ln \left\langle \exp\left[6N_{site}(\beta - \beta_0)\hat{P}\right] \left( \frac{\det M(m, \mu)}{\det M(m_0, 0)} \right)^{N_f} \right\rangle_{X:fixed}$$

Performing simulations at various $\beta$, combine the data by multi-$\beta$ reweighting

(Ferrenberg & Swendsen, 89)
Distribution function in the heavy quark region

- We study the properties of $W(X)$ in the heavy quark region.
- Performing quenched simulations + Reweighting.
- Standard Wilson quark action + plaquette gauge action, $S_g = -6N_{\text{site}}\beta P$
- lattice size: $N_s^3 \times N_t = 24^3 \times 4$
- 5 simulation points; $\beta$=5.68-5.70.

(WHOT-QCD, Phys.Rev.D84, 054502(2011))

Hopping parameter expansion ($\kappa \sim 1/m$)

$$N_f \ln \left( \frac{\det M(\kappa, \mu)}{\det M(0,0)} \right) = N_f \left( 288N_{\text{site}}\kappa^4 P + 12 \cdot 2^N \kappa^N_s \kappa^N_t \left( \cosh(\mu/T)\Omega_R + i \sinh(\mu/T)\Omega_I \right) + \cdots \right)$$

$P$: plaquette, $\Omega = \Omega_R + i\Omega_I$ : Polyakov loop (order parameter)

The plaquette term can be absorbed into the gauge action by redefining $\beta$. 
Order of the phase transition
Polyakov loop distribution
(order parameter of confinement)

Effective potential of $|\Omega|$ on the pseudo-critical line at $\mu=0$

- The pseudo-critical line is determined by $\chi_\Omega$ peak.

- Double-well at small $\kappa$
  - First order transition

- Single-well at large $\kappa$
  - Crossover

Critical point: $\kappa^4 \approx 2.0 \times 10^{-5}$
Polyakov loop distribution in the complex plane

$\kappa^4 = 0.0 \quad \text{Z(3) symmetric} \quad \kappa^4 = 5.0 \times 10^{-6} \quad \kappa^4 = 1.0 \times 10^{-5}$

$\kappa^4 = 1.5 \times 10^{-5} \quad \kappa^4 = 2.0 \times 10^{-5} \quad \kappa^4 = 2.5 \times 10^{-5}$

critical point

- on $\beta_{pc}$ measured by the Polyakov loop susceptibility.
Distribution function of $\Omega_R$ at finite density

\[
W(\Omega_R; \beta, \kappa, \mu) = \int DU \, \delta(\Omega_R - \hat{\Omega}_R) e^{6N_{\text{site}} \hat{P} \left( \det M(\kappa) \right)}^{N_f} \\
= \int DU \, \delta(\Omega_R - \hat{\Omega}_R) e^{6N_{\text{site}} \hat{P}} \left| \det M(\kappa) \right|^{N_f} e^{i\theta} \\
= W_0(\Omega_R; \beta, \kappa, \mu) \langle e^{i\theta} \rangle_{\Omega_R}
\]

Phase-quenched simulation: \[W_0(\Omega_R) = \int DU \, \delta(\Omega_R - \hat{\Omega}_R) |\det M|^{N_f} e^{6N_{\text{site}} \beta \hat{P}} \left( \theta = 12 \cdot 2^{N_f} N_s^3 N_f \kappa^{N_t} \sinh(\mu/T) \hat{\Omega}_I \right)\]

- Heavy quark region
- Effective potential: \[V_{\text{eff}}(\Omega_R) = -\ln W(\Omega_R), \quad V_0(\Omega_R) = -\ln W_0(\Omega_R)\]
   (Phase-quenched part)
   \[V_{\text{eff}}(\beta, \kappa, \mu) = V_0(\beta, \kappa, \mu) - \ln \langle e^{i\theta} \rangle_{\Omega_R}\]
   Phase average

- $V_0$ is equal to $V_{\text{eff}}(\mu=0)$ when we replace $\kappa^{N_t} \Rightarrow \kappa^{N_t} \cosh(\mu/T)$
- Critical point (phase-quenched)

\[\kappa_{\text{cp}}^{N_t}(0) = \kappa_{\text{cp}}^{N_t}(\mu) \cosh(\mu/T)\]

$N_f=2$ at $\mu=0$: $\kappa_{\text{cp}}=0.0658(3)(8)$
(WHOT-QCD, Phys.Rev.D84, 054502(2011))
Avoiding the sign problem

$\theta$: complex phase  \[ \theta \equiv \text{Im} \ln \det M \approx 12 \cdot 2^n N^3_s N_f \kappa^{N_t} \sinh(\mu/T) \Omega_I \]

- Sign problem: If $e^{i\theta}$ changes its sign,
  \[ \langle e^{i\theta} \rangle_{\Omega_R} \text{ fixed} \ll \text{(statistical error)} \]

- Cumulant expansion
  \[ \langle e^{i\theta} \rangle_{\Omega_R} = \exp \left[ i \langle \theta \rangle_C - \frac{1}{2} \langle \theta^2 \rangle_C - \frac{i}{3!} \langle \theta^3 \rangle_C + \frac{1}{4!} \langle \theta^4 \rangle_C + \cdots \right] \]
  \[ \rightarrow 0 \]
  \[ \rightarrow 0 \]

  cumulants
  \[ \langle \theta \rangle_C = \langle \theta \rangle_{\Omega_R}, \quad \langle \theta^2 \rangle_C = \langle \theta^2 \rangle_{\Omega_R} - \langle \theta \rangle_{\Omega_R}^2, \quad \langle \theta^3 \rangle_C = \langle \theta^3 \rangle_{\Omega_R} - 3 \langle \theta \rangle_{\Omega_R} \langle \theta \rangle_{\Omega_R}^2 + 2 \langle \theta \rangle_{\Omega_R}^3, \quad \langle \theta^4 \rangle_C = \cdots \]

  - **Odd terms** vanish from a symmetry under $\mu \leftrightarrow -\mu$ ($\theta \leftrightarrow -\theta$)

Source of the complex phase

If the cumulant expansion converges, **No sign problem.**
Effect from the complex phase factor

- Polyakov loop effective potential at various $\kappa^{N_t} \cosh(\mu/T)$ at the transition point.

- Solid lines: $\mu=0$, i.e., $\cosh(\mu/T) = 1$, $\sinh(\mu/T) = 0$
- Dashed lines: $\mu = \infty$, i.e., $\sinh(\mu/T) = \cosh(\mu/T)$

The effect from the complex phase factor is very small except near $\Omega_R=0$. 
Critical surface in 2+1-flavor finite density QCD in the heavy quark region

- The effect from the complex phase is very small for the determination of $\kappa_{cp}$.
- The phase effect is neglected.
Probability distribution function in the light qurk region \(\rightarrow\) Nakagawa’s poster

- We perform phase quenched simulations with the weight:
  \[
  |\det M(m, \mu)|^{N_f} e^{-S_g}
  \]

\[
W(P', F', \beta, m, \mu) = \int DU \delta(\hat{P} - P')\delta(\hat{F} - F')|\det M(m, \mu)|^{N_f} e^{6N_{\text{site}}\beta\hat{P}}
\]

\[
= \int DU \delta(\hat{P} - P')\delta(\hat{F} - F')e^{i\theta}|\det M(m, \mu)|^{N_f} e^{6N_{\text{site}}\beta\hat{P}}
\]

\[
= \langle e^{i\theta} \rangle_{P', F'} \times W_0(P', F', \beta, m, \mu)
\]

expectation value with fixed \(P,F\) histogram

\(P\): plaquette \(F(\mu) = \frac{N_f}{N_{\text{site}}} \ln \left| \frac{\det M(\mu)}{\det M(0)} \right| \theta \equiv N_f \Im \ln \det M\)

Distribution function of the phase quenched.

\[
W_0(P', F') = \int DU \delta(\hat{P} - P')\delta(\hat{F} - F')|\det M|^{N_f} e^{6N_{\text{site}}\beta\hat{P}}
\]
**μ-dependence of the effective potential**

Curvature of the effective potential

- **Crossover**

  \[-\ln[W(P, \beta)]\]

- **Critical point**

  \[-\ln[W_0(P, \beta)] - \ln\langle e^{i\theta} \rangle\]

  + \(\text{phase effect}\)

  \(\text{Curvature: Zero}\)

- **1st order phase transition**

  \[-\ln[W_0(P, \beta)] - \ln\langle e^{i\theta} \rangle\]

  + \(\text{phase effect}\)

  \(\text{Curvature: Negative}\)

- **QGP**

- **hadron**

- **CSC**

- **T**

- **μ**
Curvature of the effective potential

• Assuming the distribution is Gaussian,

\[
W_0(P, F) \approx \sqrt{\frac{6N_{\text{site}}}{2\pi\chi_P}} \exp \left[ -\frac{6N_{\text{site}}}{2\chi_P} (P - \langle P \rangle)^2 \right] \times \sqrt{\frac{N_{\text{site}}}{2\pi\chi_F}} \exp \left[ -\frac{N_{\text{site}}}{2\chi_F} (F - \langle F \rangle)^2 \right]
\]

\[
\chi_P = 6N_{\text{site}} \langle (P - \langle P \rangle)^2 \rangle \quad \chi_F = N_{\text{site}} \langle (F - \langle F \rangle)^2 \rangle
\]

\[
\frac{\partial^2}{\partial P^2} \left( -\ln W_0 \right) (\langle P \rangle, \langle F \rangle) = \frac{6N_{\text{site}}}{\chi_P}
\]

\[
\frac{\partial^2}{\partial F^2} \left( -\ln W_0 \right) (\langle P \rangle, \langle F \rangle) \approx \frac{N_{\text{site}}}{\chi_F}
\]

Cumulant expansion

\[
W(P, F) = W_0(P, F) \langle e^{i\theta} \rangle_{P,F: \text{fixed}} \approx W_0(P, F) \exp \left[ \frac{1}{2} \langle \theta^2 \rangle_{P,F: \text{fixed}} \right]
\]

\[
\langle \theta^2 \rangle_{P,F: \text{fixed}} \approx \langle \theta^2 \rangle (\langle P \rangle, \langle F \rangle)
\]

Curvature of \( \langle \theta^2 \rangle \) at the peak of the distribution.
Simulations

$8^3 \times 4$ lattice $\frac{m_\pi}{m_\rho} \approx 0.8$

- Simulation points in the $(\beta, \mu_0/T)$

- Peak of $W_0(P,F)$ for each $\mu$

2-flavor QCD Iwasaki gauge + clover Wilson quark action
Random noise method is used.
Effect from the complex phase

- Rapidly changes around the pseudo-critical point.
- Strong curvature in $\left\langle \theta^2 \right\rangle_c / 2$

\[ -\ln[W_0(P,\beta)] + \frac{1}{2} \left\langle \theta^2 \right\rangle_c \]
Curvature of the effective potential for $F$-direction

• Appearance of the critical point: suggested at $\mu/T=4.0$
  
  (The quark mass is much heavier than the physical mass.)
Curvature of the critical surface

- Usual expectation
- Critical point: exists

\[
\frac{\partial^2 m_C}{\partial \mu^2} > 0
\]

- de Forcrand - Philipsen,
  JHEP01(2007)077; PoS(LAT2007)178
  - Curvature: slightly negative.
  (3-flavor staggered, 8^3x4 lattice)

**New approach**  
2+\(N_f\)-flavor QCD (large \(N_f\))  
Yamada’s talk  
(2 light quarks + \(N_f\) heavy quarks)  
\[\rightarrow\] Curvature: positive.
2+\(N_f\)-flavor QCD (\(N_f \geq 10\))

(Ejiri, Yamada, 2012, in preparation)

\[
h = 2N_f(2\kappa_h)^{N_t}
\]

for Wilson quarks

\[
h = \frac{N_f}{4(2m_h)^{N_t}}
\]

for staggered quarks

2-flavor dynamical simulation
with p4-implemented staggered quarks
and reweighting for the heavy quarks.

\[m_\pi/m_\rho \approx 0.7\]

- The critical mass: larger with \(N_f\).
- For large \(N_f\), the critical mass is in the heavy quark region.
- First order transition region: wider as increasing \(\mu\).
Summary

• We studied the quark mass and chemical potential dependence of the nature of QCD phase transition.

• Heavy quark region: The shape of the probability distribution function changes as a function of the quark mass and chemical potential.

• To avoid the sign problem, the method based on the cumulant expansion of $\theta$ is useful.

• Phase quenched simulations: The effective potential at large $\mu$ suggests the the existence of the critical point.

• $2+N_f$-flavor QCD: First order transition region: wider with $\mu$.

• To find the critical point at finite density, further studies in light quark region are important applying this method.