Phase structure of finite density lattice QCD with a histogram method

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for

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— Finite density lattice QCD —

- Various approaches
  ✓ Reweighting method
  ✓ Canonical approach
  ✓ Histogram method
  ✓ Taylor expansion
  ✓ Imaginary chemical potential
  ✓ Langevin approach

We explore the phase diagram by the histogram method
+ phase quenched simulations
+ cumulant expansion for the complex phase of the quark determinant
— Histogram method and phase transition —

✓ Explore the phase diagram by the histogram method

- Label configurations by the value of an operator $\hat{O}$
- Calculate the histogram $w(O)$ of $O$ and the effective potential $V = -\ln w$
- Change the parameter ($\beta$, $\kappa$, $\mu$, ...) and see if the curvature changes

### Crossover

![Crossover Diagram]

### First order

![First order Diagram]

Curvature < 0
Label gauge configurations by $P = - \frac{S_g}{6\beta N_{\text{site}}}$ and $F(\mu) = N_f \ln \left| \frac{\det M(\mu)}{\det M(0)} \right|$

$$\frac{Z(\beta, \mu)}{Z(\beta, 0)} = \frac{1}{Z(\beta, 0)} \int DUE^{i\theta(\mu)} \left| \det M(\mu) \right| e^{N_f e^{6\beta N_{\text{site}}} \delta P} = \int dPdFw(P, F; \beta, \mu) \left\langle e^{i\theta(\mu)} \right\rangle (P, F; \beta, \mu)$$
— Histogram method —

✓ Label gauge configurations by $P = -\frac{S_g}{6\beta N_{\text{site}}}$ and $F(\mu) = N_f \ln \left| \frac{\det M(\mu)}{\det M(0)} \right|$

$$
\frac{Z(\beta, \mu)}{Z(\beta, 0)} = \frac{1}{Z(\beta, 0)} \int DU e^{i\theta(\mu)} |\det M(\mu)|^{N_f} e^{6\beta N_{\text{site}} P} \\
= \int dP dF w(P, F; \beta, \mu) \langle \langle e^{i\theta(\mu)} \rangle \rangle (P, F; \beta, \mu)
$$

✓ Probability distribution function

$$
w(P', F'; \beta, \mu) = \frac{1}{Z(\beta, 0)} \int DU \delta(\hat{P} - P') \delta(\hat{F} - F') |\det M(\mu)|^{N_f} e^{6\beta N_{\text{site}} \hat{P}}
$$

phase quenched measure
— Histogram method —

✓ Label gauge configurations by $P = -\frac{S_g}{6\beta N_{\text{site}}}$ and $F(\mu) = N_f \ln \left| \frac{\det M(\mu)}{\det M(0)} \right|$

\[
\frac{Z(\beta, \mu)}{Z(\beta, 0)} = \frac{1}{Z(\beta, 0)} \int DU e^{i\theta(\mu)} |\det M(\mu)|^{N_f} e^{6\beta N_{\text{site}} \hat{P}}
\]

\[= \int d\hat{P} d\hat{F} w(\hat{P}, \hat{F}; \beta, \mu) \left< e^{i\theta(\mu)} \right>(\hat{P}, \hat{F}; \beta, \mu) \]

✓ Probability distribution function

\[w(P', F'; \beta, \mu) = \frac{1}{Z(\beta, 0)} \int D U \delta(\hat{P} - P') \delta(\hat{F} - F') |\det M(\mu)|^{N_f} e^{6\beta N_{\text{site}} \hat{P}}\]

phase quenched measure

✓ Complex phase of the quark determinant

\[\left< e^{i\theta(\mu)} \right>(P', F'; \beta, \mu) = \frac{\left< \left< e^{i\theta(\mu)} \delta(\hat{P} - P') \delta(\hat{F} - F') \right> \right>_{(\beta, \mu)}}{\left< \left< \delta(\hat{P} - P') \delta(\hat{F} - F') \right> \right>_{(\beta, \mu)}} \]

(\langle \langle \cdots \rangle \rangle_{(\beta, \mu)}: \text{the expectation value with the phase quenched measure})
— Sign problem —

✓ Poor signal to noise ratio if $e^{i\theta}$ changes sign frequently
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✓ Poor signal to noise ratio if $e^{i\theta}$ changes sign frequently

✓ Cumulant expansion of the complex phase

\[
\langle e^{i\theta(\mu)} \rangle_{(P,F,\mu)} = \exp \left[ i \langle \theta \rangle_c - \frac{1}{2} \langle \theta^2 \rangle_c - \frac{i}{3!} \langle \theta^3 \rangle_c + \frac{1}{4!} \langle \theta^4 \rangle_c + \cdots \right]
\]
— Sign problem —

✓ Poor signal to noise ratio if $e^{i\theta}$ changes sign frequently

✓ Cumulant expansion of the complex phase

$$\langle e^{i\theta(\mu)} \rangle_{(P,F,\mu)} = \exp \left[ -i \langle \theta \rangle_c - \frac{1}{2} \langle \theta^2 \rangle_c - \frac{i}{3!} \langle \theta^3 \rangle_c + \frac{1}{4!} \langle \theta^4 \rangle_c + \cdots \right]$$

✓ $\mu \rightarrow -\mu$ corresponds to time reversal

✓ Odd terms vanish if the system is invariant under the time reversal

✓ The phase factor is real and positive
— Sign problem —

✓ Poor signal to noise ratio if $e^{i\theta}$ changes sign frequently

✓ Cumulant expansion of the complex phase

$$
\langle e^{i\theta(\mu)} \rangle_{(P,F,\mu)} = \exp \left[ i \langle \theta \rangle_c - \frac{1}{2} \langle \theta^2 \rangle_c - \frac{i}{3!} \langle \theta^3 \rangle_c + \frac{1}{4!} \langle \theta^4 \rangle_c + \cdots \right]
$$

✓ $\mu \rightarrow -\mu$ corresponds to time reversal

✓ Odd terms vanish if the system is invariant under the time reversal

✓ The phase factor is real and positive

✓ No sign problem if the cumulant expansion converges

✓ Need the definition of $\theta$ (NOT a Taylor expansion), giving nearly a Gaussian distribution (ideal case)
We calculate $\theta$ as follows:

$$F(\mu) = N_f \ln \left| \frac{\det M(\mu)}{\det M(0)} \right| = N_f \int_0^{\mu/T} \Re \left[ \frac{\partial (\ln \det M(\bar{\mu}))}{\partial (\bar{\mu}/T)} \right] d \left( \frac{\bar{\mu}}{T} \right),$$

$$C(\mu, \mu_0) = N_f \ln \left| \frac{\det M(\mu)}{\det M(\mu_0)} \right| = N_f \int_{\mu_0/T}^{\mu/T} \Re \left[ \frac{\partial (\ln \det M(\bar{\mu}))}{\partial (\bar{\mu}/T)} \right] d \left( \frac{\bar{\mu}}{T} \right),$$

$$\theta(\mu) = N_f \Im [\ln \det M(\mu)] = N_f \int_0^{\mu/T} \Im \left[ \frac{\partial (\ln \det M(\bar{\mu}))}{\partial (\bar{\mu}/T)} \right] d \left( \frac{\bar{\mu}}{T} \right).$$

The complex phase, (the absolute value of) the quark determinant, and the reweighting factor can be obtained as continuous functions of $\mu$. 
We calculate $\theta$ as follows:

\[
F(\mu) = \left. N_f \ln \left| \frac{\det M(\mu)}{\det M(0)} \right| \right| = N_f \int_0^{\mu/T} \Re \left[ \frac{\partial (\ln \det M(\bar{\mu}))}{\partial (\bar{\mu}/T)} \right] d \left( \frac{\mu}{T} \right),
\]

\[
C(\mu, \mu_0) = \left. N_f \ln \left| \frac{\det M(\mu)}{\det M(\mu_0)} \right| \right| = N_f \int_{\mu_0/T}^{\mu/T} \Re \left[ \frac{\partial (\ln \det M(\bar{\mu}))}{\partial (\bar{\mu}/T)} \right] d \left( \frac{\mu}{T} \right),
\]

\[
\theta(\mu) = \left. N_f \Im \left[ \ln \det M(\mu) \right] \right| = N_f \int_0^{\mu/T} \Im \left[ \frac{\partial (\ln \det M(\bar{\mu}))}{\partial (\bar{\mu}/T)} \right] d \left( \frac{\mu}{T} \right).
\]
✓ Clover-improved Wilson quark action
✓ RG-improved Iwasaki action
✓ On $8^3 \times 4$ lattice, $N_f = 2$, $\kappa = 0.141139$ ($m_{PS}/m_V = 0.8$ for $\beta = 1.80$)
✓ $\beta = 1.25, 1.30, 1.35, 1.40, ..., 1.90, 1.95, 2.00$
✓ $\mu_0/T = 2.4, 2.8, 3.2, 3.6$
✓ Measurement every 10 trajectories
✓ Random noise method with 50 noises to calculate the derivatives of $\ln \det M$
✓ Statistics is 2900
Curvature of the effective potential

Ratio of the partition function
\[ \frac{Z(\beta, \mu)}{Z(\beta, 0)} = \int dP dF w(P, F; \beta, \mu_0) \left\langle e^{i\theta(\mu)} \right\rangle (P, F; \beta, \mu) = \int dP dF e^{-V(P, F; \beta, \mu)} \]

Effective potential
\[ V(P, F; \beta, \mu) = -\ln w(P, F; \beta, \mu_0) + \frac{1}{2} \left\langle \theta^2 \right\rangle_c (P, F; \beta, \mu, \mu_0) \]

Curvature of the effective potential
\[ \frac{\partial^2 V}{\partial P^2} = \frac{\partial^2 (- \ln w)}{\partial P^2} + \frac{1}{2} \frac{\partial^2 \left\langle \theta^2 \right\rangle_c}{\partial P^2}, \quad \frac{\partial^2 V}{\partial F^2} = \frac{\partial^2 (- \ln w)}{\partial F^2} + \frac{1}{2} \frac{\partial^2 \left\langle \theta^2 \right\rangle_c}{\partial F^2} \]
— Curvature of the effective potential —

✓ Ratio of the partition function
\[
\frac{\mathcal{Z}(\beta, \mu)}{\mathcal{Z}(\beta, 0)} = \int dPdF w(P, F; \beta, \mu_0) \langle e^{i \theta(\mu)} \rangle (P, F; \beta, \mu) = \int dPdF e^{-V(P, F; \beta, \mu)}
\]

✓ Effective potential
\[
V(P, F; \beta, \mu) = -\ln w(P, F; \beta, \mu_0) + \frac{1}{2} \langle \theta^2 \rangle_c (P, F; \beta, \mu, \mu_0)
\]

✓ Curvature of the effective potential
\[
\frac{\partial^2 V}{\partial P^2} = \frac{\partial^2 (-\ln w)}{\partial P^2} + \frac{1}{2} \frac{\partial^2 \langle \theta^2 \rangle_c}{\partial P^2}, \quad \frac{\partial^2 V}{\partial F^2} = \frac{\partial^2 (-\ln w)}{\partial F^2} + \frac{1}{2} \frac{\partial^2 \langle \theta^2 \rangle_c}{\partial F^2}
\]
Assume a Gaussian distribution for $P$ and $F$ around $\langle P \rangle_{(\beta, \mu)}$ and $\langle F \rangle_{(\beta, \mu)}$,

$$w(P, F) = \frac{1}{\sqrt{2\pi}\chi_P} \frac{1}{\sqrt{2\pi}\chi_F} \exp \left[ -\frac{1}{2\chi_P} (P - \langle P \rangle)^2 - \frac{1}{2\chi_F} (F - \langle F \rangle)^2 \right]$$

$$\chi_P \equiv \langle (P - \langle P \rangle)^2 \rangle, \quad \chi_F \equiv \langle (F - \langle F \rangle)^2 \rangle$$

Curvature of (the log of) the histogram

$$\frac{\partial^2 (-\ln w)}{\partial P^2} = \frac{1}{\chi_P} = \frac{1}{\langle (P - \langle P \rangle)^2 \rangle}, \quad \frac{\partial^2 (-\ln w)}{\partial F^2} = \frac{1}{\chi_F} = \frac{1}{\langle (F - \langle F \rangle)^2 \rangle}$$
— Curvature of the distribution function —

\[
\frac{\partial^2 (-\ln w)}{\partial P^2} = \frac{1}{\chi_P} = \frac{1}{\langle (P - \langle P \rangle)^2 \rangle}
\]

\[
\frac{\partial^2 (-\ln w)}{\partial F^2} = \frac{1}{\chi_F} = \frac{1}{\langle (F - \langle F \rangle)^2 \rangle}
\]
— Second order cumulant of the complex phase —

\[ \beta_0 < \theta^2 > c / 2 \mu_0 / T = 2.4 \]
\[ \mu_0 / T = 2.8 \]
\[ \mu_0 / T = 3.2 \]
\[ \mu_0 / T = 3.6 \]
\[ \kappa = 0.141139, \mu / T = \mu_0 / T \]
χ_P, χ_F, and ⟨θ²⟩_c in T-µ plane

- small χ_P^{-1}
- large χ_F^{-1}
- complex phase gives negative curvature
- confinement phase
- large χ_P^{-1}
- small χ_F^{-1}
- pion condensation phase in phase quenched
- large ⟨θ²⟩_c
- small ⟨θ²⟩_c

deconfinement phase

1.2 1.4 1.6 1.8 2
β
10000 20000
1/(<(P-<P>)^2>)
µ_0/T = 2.4
µ_0/T = 2.8
µ_0/T = 3.2
µ_0/T = 3.6
κ =0.141139, µ/T=µ_0/T
— Average of $P$ and $F(\mu)$ —

\[ \kappa = 0.141139, \mu / T = 3.2 \]
Average of $P$ and $F(\mu)$

$\kappa = 0.141139, \mu/T = 3.6$

$\beta$

$\mu_0/T = 2.4$
$\mu_0/T = 2.8$
$\mu_0/T = 3.2$
$\mu_0/T = 3.6$
— Average of $P$ and $F(\mu)$ —

\[ \mu_0/T = 2.4, \mu_0/T = 2.8, \mu_0/T = 3.2, \mu_0/T = 3.6 \]

\[ \kappa = 0.141139, \mu/T = 4.0 \]
Reweighting technique

✓ Ratio of the partition function

\[
\frac{Z(\beta, \mu)}{Z(\beta, 0)} = \int dPdF \, w(P, F; \beta, \mu) \langle e^{i\theta(\mu)} \rangle (P, F; \beta, \mu)
\]

\[\Rightarrow \text{We need } w(P, F) \text{ and } \langle e^{i\theta} \rangle (P, F) \text{ in a wide range of } P \text{ and } F\]
Reweighting technique

✓ Ratio of the partition function

\[
\frac{Z(\beta, \mu)}{Z(\beta, 0)} = \int dP dF w(P, F; \beta, \mu) \langle e^{i\theta(\mu)} \rangle (P, F; \beta, \mu)
\]

⇒ We need \( w(P, F) \) and \( \langle e^{i\theta} \rangle (P, F) \) in a wide range of \( P \) and \( F \)

✓ Overlap problem → simulations at various simulation points

\[
w(F; \beta, \mu) = R(P, F; \beta, \mu, \mu_0) w(P, F; \beta, \mu_0)
\]

\[
R(F; \beta, \mu, \mu_0) = \frac{\left\langle \left\langle \left| \frac{\det M(\mu)}{\det M(\mu_0)} \right|^{N_f} \delta(\hat{P} - P') \delta(\hat{F} - F') \right\rangle \right\rangle_{(\beta, \mu_0)}}{\left\langle \left\langle \delta(\hat{P} - P') \delta(\hat{F} - F') \right\rangle \right\rangle_{(\beta, \mu_0)}}
\]

\[
\langle e^{i\theta(\mu)} \rangle (P', F'; \mu, \mu_0) = \frac{\left\langle \left\langle \left| \frac{\det M(\mu)}{\det M(\mu_0)} \right|^{N_f} e^{i\theta(\mu)} \delta(\hat{P} - P') \delta(\hat{F} - F') \right\rangle \right\rangle_{(\beta, \mu_0)}}{\left\langle \left\langle \left| \frac{\det M(\mu)}{\det M(\mu_0)} \right|^{N_f} \delta(\hat{P} - P') \delta(\hat{F} - F') \right\rangle \right\rangle_{(\beta, \mu_0)}}
\]
✓ Complex phase of the quark determinant

\[
\left\langle e^{i\theta(\mu)} \right\rangle (P', F'; \mu, \mu_0) = \frac{\left\langle \left\langle e^{i\theta(\mu)} \left| \frac{\det M(\mu)}{\det M(\mu_0)} \right|^N_f \delta(\hat{P} - P')\delta(\hat{F} - F') \right\rangle \right\rangle_{(\beta, \mu_0)}}{\left\langle \left\langle \left| \frac{\det M(\mu)}{\det M(\mu_0)} \right|^N_f \delta(\hat{P} - P')\delta(\hat{F} - F') \right\rangle \right\rangle_{(\beta, \mu_0)}}
\]

✓ \( F = N_f \ln \left| \frac{\det M(\mu)}{\det M(0)} \right|^N_f \) and \( C = N_f \ln \left| \frac{\det M(\mu)}{\det M(\mu_0)} \right|^N_f \) are strongly correlated, and assume \( C \propto F \)

\[
\left\langle e^{i\theta(\mu)} \right\rangle (P', F'; \mu, \mu_0) \approx \frac{\left\langle \left\langle e^{i\theta(\mu)} \delta(\hat{P} - P')\delta(\hat{F} - F') \right\rangle \right\rangle_{(\beta, \mu_0)}}{\left\langle \left\langle \delta(\hat{P} - P')\delta(F - F') \right\rangle \right\rangle_{(\beta, \mu_0)}}
\]
Curvature of the distribution function in $F$ direction decreases with increasing $\mu/T$. 

$$\frac{\partial^2 (- \ln w)}{\partial F^2}$$
The second order cumulant of the complex phase takes large values in small $P$ and $F$ region while small in large $P$ and $F$ region.
Curvature of the effective potential in $F$ direction

\[
\frac{\partial^2 V}{\partial F^2} = \frac{\partial^2 (-\ln w)}{\partial F^2} + \frac{1}{2} \frac{\partial^2 \langle \theta^2 \rangle_c}{\partial F^2}
\]

✓ The curvature of the effective potential is small in the confinement phase and decreases with increasing $\mu/T$. 

$k=0.144139, \mu/T=3.2$

$k=0.144139, \mu/T=3.6$

$k=0.144139, \mu/T=4.0$
Summary and outlook

✓ We investigated the phase structure of finite density QCD by the histogram method

✓ We adopted the cumulant expansion for the complex phase

✓ The complex phase is calculated by the $\mu$-integration of $\partial \ln \det M(\mu)/\partial \mu$

✓ The curvature of the distribution function in $F$ direction decreases with increasing $\mu/T$

✓ The curvature of the complex phase in $P-F$ plane has a negative region

✓ The first order phase transition at $\mu/T \approx 4.0$?
— Noise error in \((\text{Tr} \theta)^2\) —

\[
(\text{Tr} \theta)^2 = \lim_{N_{\text{noise}} \to \infty} \left[ \left( \frac{1}{N_{\text{noise}}} \sum_{i=1}^{N_{\text{noise}}} \eta_i^\dagger \theta \eta_i \right)^2 - \epsilon^2(\theta) \right]
\]

\[
\epsilon^2(\theta) = \frac{1}{N_{\text{noise}} - 1} \left[ \frac{1}{N_{\text{noise}}} \sum_{i=1}^{N_{\text{noise}}} (\eta_i^\dagger \theta \eta_i)^2 - \left( \frac{1}{N_{\text{noise}}} \sum_{i=1}^{N_{\text{noise}}} \eta_i^\dagger \theta \eta_i \right)^2 \right]
\]

\[\beta = 1.40, \quad \kappa = 0.141139, \quad \mu = \mu_0 = 2.8T\]

\[\beta = 1.60, \quad \kappa = 0.141139, \quad \mu = \mu_0 = 2.8T\]
— Noise error in \((\text{Tr } \theta)^2\) —

\[ \kappa = 0.141139, \frac{\mu_0}{T} = \frac{\mu}{T} = 2.8 \]

\[
\begin{align*}
\langle \theta^2 \rangle_c / 2 & \quad \text{w/o subtraction (50 noises)} \\
& \quad \text{w/o sub. + noise ave. } \theta \text{ (50 noises)} \\
& \quad \text{w/o subtraction (100 noises)} \\
& \quad \text{with subtraction (50 noises)}
\end{align*}
\]
Curvature of the distribution function in $P$ direction

$$\frac{\partial^2 (- \ln w)}{\partial P^2}$$

$k=0.144139, \mu/T=2.4$

$k=0.144139, \mu/T=2.8$

$k=0.144139, \mu/T=3.2$