Lattice QCD at finite temperature and density

Shinji Ejiri
(Niigata University)

YITP workshop "New Frontiers in QCD 2010"
(Kyoto YITP, March 11, 2010)
QCD thermodynamics at $\mu \neq 0$

- Phase structure of QCD at $\mu \neq 0$
  Critical point at finite density
- Lattice simulations: important.
- Methods for the high density region: required

In this talk
- We study nature of transitions by an effective potential approach.
- Avoiding the sign problem.
- Discussion about the phase structure of QCD at finite density using the effective potential.
Effective potential $V_{\text{eff}}(P)$

Distribution function (histogram)

- First order phase transition
  Two phases coexists at $T_c$
  e.g. SU(3) Pure gauge theory

- Average plaquette (1x1 Wilson loop): $P$

- Partition function
  $$Z(T) = \int dP \, W(P, T)$$

- Effective potential
  $$V_{\text{eff}}(P) \equiv -\ln(W(P))$$
μ-dependence of the effective potential

\[ Z(T, \mu) = \int dX \ W(X, T, \mu), \quad V_{\text{eff}}(X) = -\ln W(X) \]

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

Crossover

Correlation length: short
\( W(X) \): Gaussian distribution
\( V(X) \): Quadratic function

Critical point

Correlation length: long
Curvature: Zero

1st order phase transition

Two phases coexist
Double well potential
Curvature: Negative
Problem of complex quark determinant at $\mu \neq 0$

- Problem of Complex Determinant at $\mu \neq 0$

\[
\left(M(\mu)\right)^\dagger = \gamma_5 M(-\mu) \gamma_5 \quad (\gamma_5\text{-conjugate})
\]

\[
\Rightarrow \quad \left(\det M(\mu)\right)^* = \det M(-\mu) \neq \det M(\mu)
\]

- Boltzmann weight: complex at $\mu \neq 0$
  - Monte-Carlo method is not applicable.
  - Configurations cannot be generated.
Distribution function and Effective potential at $\mu \neq 0$
(S.E., Phys.Rev.D77, 014508(2008))

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

\[
Z(\mu) = \int dP \frac{R(P, \mu) W(P, \beta)}{W(\bar{P}, \beta)}
\]

\[
S_g = -6N_{\text{site}} \beta P
\]

\[
W(\bar{P}, \beta) = \int DU \delta(\bar{P}-\bar{P})(\det M(0))^{N_f} e^{-S_g}
\]

(Weight factor at $\mu=0$)

\[
R(\bar{P}, \mu) = \frac{\int DU \delta(\bar{P}-\bar{P})(\det M(\mu))^{N_f}}{\int DU \delta(\bar{P}-\bar{P})(\det M(0))^{N_f}}
\]

\[
= \frac{\left\langle \delta(\bar{P}-\bar{P}) \left( \frac{\det M(\mu)}{\det M(0)} \right)^{N_f} \right\rangle_{(\beta, \mu=0)}}{\left\langle \delta(\bar{P}-\bar{P}) \right\rangle_{(\beta, \mu=0)}} \equiv \left\langle \left( \frac{\det M(\mu)}{\det M(0)} \right)^{N_f} \right\rangle_P
\]

\[R(P, \mu): \text{independent of } \beta, \quad \rightarrow \quad R(P, \mu) \text{ can be measured at any } \beta.
\]

Effective potential:

\[
V_{\text{eff}}(P) = -\ln[R(P, \mu) W(P, \beta)] = \mu=0 \text{ crossover}
\]

\[\text{non-singular} \quad 1^{\text{st}} \text{ order phase transition?}
\]

\[-\ln[W(P, \beta)] - \ln[R(P, \mu)] \]
The $\mu$-dependence of the effective potential is given by:

$$Z(\beta, \mu) = \int dP \, R(P, \mu) W(P, \beta), \quad V_{\text{eff}}(P) = -\ln[R(P, \mu) W(P, \beta)]$$

Critical point:
$$-\ln[W(P, \beta)] - \ln[R(P, \mu)]$$

Curvature: Zero
- $\mu=0$ reweighting

Crossover:
$$-\ln[W(P, \beta)]$$

Curvature: Negative
- $\mu=0$ reweighting

1st order phase transition:
$$-\ln[W(P, \beta)] - \ln[R(P, \mu)]$$

Curvature: Negative
- $\mu=0$ reweighting
Avoiding the sign problem
(SE, Phys.Rev.D77,014508(2008))

- **Sign problem:** If \( e^{i\theta} \) changes its sign,

\[
R(P, \mu) = \left\langle \left( \frac{\det M(\mu)}{\det M(0)} \right)^{N_f} \right\rangle_{P \text{ fixed}} \equiv \left\langle e^{i\theta} \right\rangle_P \ll \text{(statistical error)}
\]

- **Cumulant expansion**

\[
\left\langle e^{i\theta} \right\rangle_P = \int F \left\langle e^{i\theta} \right\rangle_{F,P} dF
\]

\[
\approx \int F \exp \left[ i\langle \theta \rangle_C - \frac{1}{2} \langle \theta^2 \rangle_C - \frac{i}{3!} \langle \theta^3 \rangle_C + \frac{1}{4!} \langle \theta^4 \rangle_C + \cdots \right] dF
\]

cumulants

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

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

Source of the complex phase

If the cumulant expansion converges, \( \text{No sign problem.} \)
Convergence of the cumulant expansion

- Because \( \theta \sim O(\mu) \), \( \langle \theta^n \rangle_C \sim O(\mu^n) \)
  - The cumulant expansion is a power expansion of \( \mu \).
- Applicable at low density.
  - If one takes into account \( \langle \theta^n \rangle_C \), the truncation error does not affect up to \( O(\mu^n) \).

- Gaussian distribution function
  - The cumulants vanish except for \( \langle \theta^2 \rangle_C \).

\[
\langle F e^{i\theta} \rangle = \int dF \int d\theta \, F e^{i\theta} W(F, \theta) \approx \int dF \, F e^{-1/(4\alpha)} W'(F)
\]

\[
W(F, \theta) \approx \sqrt{\frac{\alpha(F)}{\pi}} e^{-\alpha(F)\theta^2} W'(F)
\]

\[
\frac{1}{2\alpha(F')} = \frac{\int \theta^2 W(F', \theta) d\theta}{\int W(F', \theta) d\theta} \equiv \langle \theta^2 \rangle_F
\]
Gaussian distribution of the complex phase

- **Complex phase of detM**  \( \theta = N_f \, \text{Im} \left[ \ln \det M(\mu) \right] \)
  - Taylor expansion: odd terms of \( \ln \det M \) (Bielefeld-Swansea, PRD66, 014507 (2002))
    \[
    \theta = N_f \text{Im} \left[ \frac{\mu}{T} \frac{\partial \ln \det M}{\partial (\mu/T)} + \frac{1}{3!} \left( \frac{\mu}{T} \right)^3 \frac{\partial^3 \ln \det M}{\partial (\mu/T)^3} + \frac{1}{5!} \left( \frac{\mu}{T} \right)^5 \frac{\partial^5 \ln \det M}{\partial (\mu/T)^5} + \cdots \right]
    \]

- **Gaussian distribution**  \( \theta: \text{NOT in the range of } [-\pi, \pi] \)
  - Results for p4-improved staggered
  - Taylor expansion up to \( O(\mu^5) \)
  - Dashed line: fit by a Gaussian function

- **Binder cumulant**
  \[
  B_4^\theta \equiv \frac{\langle \theta^4 \rangle}{\langle \theta^2 \rangle^2} = \frac{\langle \theta^4 \rangle_C}{\langle \theta^2 \rangle^2_C} + 3 = 3
  \]
  for Gaussian

- Histogram of \( \theta \)
  - \( T \approx T_c \)
  - Dashed line: fit by a Gaussian function

- Well approximated
Convergence in the large volume ($V$) limit

- Because $\theta \sim O(V)$, Naïve expectation: $\langle \theta^n \rangle_C \sim O(V^n)$?
  - If so, the cumulant expansion does not converge.

However, this problem is solved in the following situation.

- The phase is given by $\theta = \sum_{x} \theta_x$
  - No correlation between $\theta_x$.
  - This situation is realized if we define the phase as

$$
\theta = N_f \text{Im} \left[ \frac{\mu}{T} \frac{d \ln \det M}{d(\mu/T)} + \frac{1}{3!} \left( \frac{\mu}{T} \right)^3 \frac{d^3 \ln \det M}{d^3(\mu/T)} + \frac{1}{5!} \left( \frac{\mu}{T} \right)^5 \frac{d^5 \ln \det M}{d^5(\mu/T)} + \ldots \right]
$$

  or

$$
\theta = N_f \int_0^{\mu/T} \text{Im} \left[ \frac{d \ln \det M}{d(\mu/T)} \right] d\left( \frac{\mu'}{T} \right)
$$

- The first derivative is the sum of the local density operator.

  The spatial density correlation length is short at a non-singular point.

$$
\text{Im} \left[ \frac{d \ln \det M}{d(\mu/T)} \right] = \text{Im} \left[ Tr \left( M^{-1} \frac{\partial M}{\partial(\mu/T)} \right) \right]
$$

Diagonal element: local density operator
Convergence in the large volume ($V$) limit

This problem is solved in the following situation.

• The phase is given by $\theta = \sum_x \theta_x$
  
  – No correlation between $\theta_x$.

\[
\left\langle e^{i\theta} \right\rangle_{F,P} = \left\langle e^{i\sum_x \theta_x} \right\rangle_{F,P} \approx \prod_x \left\langle e^{i\theta_x} \right\rangle_{F,P} = \exp \left[ \sum_x \sum_n \frac{i^n}{n!} \left\langle \theta^n_x \right\rangle_C \right]
\]

\[
\left\langle e^{i\theta} \right\rangle_{F,P} = \exp \left[ \sum_n \frac{i^n}{n!} \left\langle \theta^n \right\rangle_C \right] \quad \Rightarrow \quad \left\langle \theta^n \right\rangle_C \approx \sum_x \left\langle \theta^n_x \right\rangle_C \sim O(V)
\]

– Ratios of cumulants do not change in the large $V$ limit.

– Convergence property is independent of $V$
  
  although the phase fluctuation becomes larger as $V$ increases

– The application range of $\mu$ can be measured on a small lattice.
Gaussian approximation (S.E., Phys.Rev.D77, 014508(2008))

If Gaussian distribution,

\[ \text{Higher order cumulants vanish.} \]

- If the second term is dominated, the calculation: much easier.

\[ \langle e^F e^{i\theta} \rangle_P \approx \left( e^F e^{-\langle \theta^2 \rangle_{F,P}} \right)_P \]

- Configurations with large fluctuations of \( \theta \): not important.
  - Such a configuration is suppressed as
    \[ W(P) \sim \exp \left[ -\frac{1}{2} \langle \theta^2 \rangle_{F,P} \right] \]
  - If configurations with small \( \theta \) are important, the cumulant expansion must be good.
Effective potential and First order phase transition


• Simulations:
  – 2-flavor p4-improved staggered quarks with $m_\pi \approx 770\text{MeV}$
  – $16^3 \times 4$ lattice
  – $\ln \det M$: Taylor expansion up to $O(\mu^6)$
\[ Z(\beta, \mu) = \int dP \, R(P, \mu) W(P, \beta) \quad \text{and} \quad V_{\text{eff}}(P) = -\ln[R(P, \mu) W(P, \beta)] \]

### Diagram

- **Crossover**
  - \(-\ln[W(P, \beta)]\)
- **Critical point**
  - \(-\ln[W(P, \beta)]\) \(-\ln[R(P, \mu)]\)
- **Curvature of \(V_{\text{eff}}\) or \(W\): independent of \(\beta\)**
  - Curvature: Zero
  - Curvature: Negative

- **1st order phase transition**
  - \(-\ln[W(P, \beta)]\) \(-\ln[R(P, \mu)]\)
  - \(\mu=0\) reweighting
  - Curvature: Negative

- **Temperature (T)**
- **Hadron**
- **Quark-Gluon Plasma (QGP)**
- **Conformal Symmetry Limit (CSC)**

- **\(\mu\)-dependence of the effective potential**
Effective potential at $\mu \neq 0$

(S.E., Phys.Rev.D77, 014508(2008))

Results of $N_f=2$ p4-staggared, $m_\pi/m_\rho \approx 0.7$
[data in PRD71,054508(2005)]

- $\det M$: Taylor expansion up to $O(\mu^6)$

- The peak position of $W(P)$ moves left as $\beta$ increases at $\mu=0$.

$V_{\text{eff}}(P,\beta,\mu) = -\ln W(P,\beta) - \ln R(P,\mu)$

$-\ln W$ at $\mu=0$

Solid lines: reweighting factor at finite $\mu/T$, $R(P,\mu)$

Dashed lines: reweighting factor without complex phase factor.
Curvature of the effective potential

Critical point:
\[ \frac{d^2 V_{\text{eff}}(P, \beta, \mu)}{dP^2} = \frac{d^2 \ln W(P, \beta)}{dP^2} + \frac{d^2 \ln R(P, \mu)}{dP^2} = 0 \]

- First order transition for \( \mu_q/T \geq 2.5 \)
- Existence of the critical point: suggested
Canonical approach
Quark number effective potential


• Simulations:
  – 2-flavor p4-improved staggered quarks with $m_{\pi}\approx 770\text{MeV}$
  – $16^3\times 4$ lattice
  – $\ln \det M$: Taylor expansion up to $O(\mu^6)$
Canonical approach

- Canonical partition function (Laplace transformation)

\[ Z_{GC}(T, \mu) = \sum_{N} Z_{C}(T, N) \exp(N\mu/T) \equiv \sum_{N} W(N) \]

- Effective potential as a function of the quark number \( N \).

\[ V_{\text{eff}}(N) = -\ln W(N) = -\ln Z_{C}(T, N) - N \frac{\mu}{T} \]

- At the minimum,

\[ \frac{\partial V_{\text{eff}}(N)}{\partial N} = - \frac{\partial \ln W(N)}{\partial N} = - \frac{\partial \ln Z_{C}(T, N)}{\partial N} - \frac{\mu}{T} = 0 \]

- First order phase transition: Two phases coexist.
First order phase transition line

\[ \frac{\mu^*}{T} \equiv -\frac{\partial \ln Z_c(T, N)}{\partial N} \]

\[ \frac{\mu^*}{T} \rightarrow \frac{\mu}{T} \left( N_s^3 \rightarrow \infty \right) \]

- Mixed state \rightarrow First order transition

Diagram:
- Hot phase
- Critical point
- Cold phase
- Mixed state

Graph:
- A
- B
- $T_{cp}$
- $T < T_{cp}$
- $T > T_{cp}$

$\rho_1, \rho_2, \rho, \rho_1/T^3, \rho_2/T^3, \rho/T^3$
Inverse Laplace transformation with a saddle point approximation (S.E., arXiv:0804.3227)

• Approximations:
  – Taylor expansion: \( \ln \det M \) up to \( O(\mu^6) \)
  – Gaussian distribution: \( \theta \)
  – Saddle point approximation

  Much easier calculations

• Two states at the same \( \mu_q/T \)
  First order transition at \( T/T_c < 0.83 \)

• Study near the physical point important

Solid line: multi-\( \beta \) reweighting
Dashed line: spline interpolation
Dot-dashed line: the free gas limit

\( N_f=2 \) p4-staggered, \( m_\pi/m_\rho \approx 0.7 \), \( 16^3 \times 4 \) lattice
Equation of state by Wilson quark action

WHOT-QCD Collab., arXiv:0909.2121

• Simulations with Wilson quarks are more difficult than by Staggered quarks.

• RG gauge + 2-flavor Clover quark actions
• $16^3 \times 4$ lattice, $m_\pi/m_\rho = 0.65$
• Taylor expansion method up to $O(\mu_q^4)$
Quark number density and Quark number susceptibility by Wilson quark action (WHOT-QCD Collab., 2009)

Taylor expansion method up to $O(\mu_q^4)$

\[
\frac{n_q}{T^2}(\mu_q) = 2c_2\left(\frac{\mu_q}{T}\right) + 4c_4\left(\frac{\mu_q}{T}\right)^3 + \cdots
\]

\[
\frac{\chi_q}{T^2}(\mu) = 2c_2 + 12c_4\left(\frac{\mu_q}{T}\right)^2 + \cdots
\]

\[
c_2 = \frac{N_t}{2!N_s^3} \frac{\partial^2 \ln Z}{\partial \mu^2}, \quad c_4 = \frac{1}{4!N_s^3N_t} \frac{\partial^4 \ln Z}{\partial \mu^4}
\]

- Large statistical errors at high density.
Equation of state by the Hybrid method
WHOT-QCD Collab., arXiv:0909.2121

Hybrid method of Reweighting and Taylor expansion up to \(O(\mu_q^4)\) with Gaussian approximation

- Large enhancement in the quark number fluctuations at high density.
- Temperature-dependence: natural.
Summary

- To avoid the sign problem, we propose a method based on a cumulant expansion of $\theta$. (Gaussian approximation: only the leading term)
- Complex phase distribution: well approximated by a Gaussian function.
- Applying the Gaussian approximation, we studied the effective potentials as functions of the plaquette and the quark number for 2-flavor p4-improved staggered quarks with $m_{\pi}/m_{\rho} \approx 0.7$ on $16^3 \times 4$ lattice.
  - These results suggest existence of the critical point at $\mu \neq 0$.
- The Gaussian approximation improves the results of the equation of state calculated with Wilson quarks.
- The method based on the cumulant expansion is useful for the study at high density.
- Studies of the critical point with the physical quark mass: important.