Chemical potential dependence of the endpoint of the first-order phase transition in the heavy-quark region of finite-temperature lattice QCD

Shinji Ejiri (Niigata University)
Kazuyuki Kanaya (Univ. Tsukuba)
Masakiyo Kitazawa (YITP, Kyoto Univ.)

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QCD phase transition in heavy quark region

- The critical mass at which the first-order phase transition turns into a crossover
- Light quark regime
  - chiral symmetry breaking
- Heavy quark region
  - Confinement phase transition
  - Center symmetry breaking
  - Critical line at finite density
  - We study the heavy region
- It is important to calculate thermodynamic quantities as continuous functions
  - Reweighting method
  - Hopping parameter expansion

WHOT-QCD Collab.
Phys.Rev.D84, 054502(2011)
PTEP 2022, 033B05 (2022)
Efficient theory by hopping parameter expansion

- Expectation value of physical quantity $O$
  \[ \langle O \rangle(\beta, \kappa) = \frac{1}{Z} \int DU \, O[U] (\det M(\kappa))^N f e^{-S_g} = \frac{1}{Z} \int DU \, O[U] \, e^{-S_{\text{eff}}} \]

- Hopping parameter expansion ($\kappa \sim 1/(\text{mass})$)

\[
\ln(\det M(\kappa)) = 288 N_{\text{site}} \kappa^4 P + [768 N_{\text{site}} \kappa^6 (3 \text{ plaquette} + 6 \text{6-step Wilson loop})] + \ldots
\]

+ $12 \times 2^{N_t} N_s^3 [\kappa^{N_t} \Re \Omega + 6N_t \kappa^{N_t+2} + 6N_t \kappa^{N_t+2} + 3N_t \kappa^{N_t+2}]$

- Near the critical point of $N_t = 4$, $\det M$ can be well approximated by the lowest order terms.

- Effective action:
  \[ S_{\text{eff}} \approx 6N_{\text{site}}(\beta + 48N_f \kappa^4)P + 12N_f 2^{N_t} N_s^3 \kappa^{N_t} \Re \Omega \]

- Monte Carlo simulation with the Polyakov loop term
  \[ S_{\text{eff}} \approx 6N_{\text{site}} \beta'P + N_s^3 \lambda \Re \Omega \quad \text{with} \quad \lambda = 12N_f 2^{N_t} \kappa^{N_t} \]

- In this talk, we discuss the correct calculation method when $N_t$ is large.
End point of the first-order phase transition

Quenched QCD with Polyakov loop term, simulation + reweighting

Binder cumulant

$$B_4 = \frac{\langle (\Omega - \langle \Omega \rangle)^4 \rangle}{\langle (\Omega - \langle \Omega \rangle)^2 \rangle^2}$$

$B_4$ is volume independent at the critical point.

$N_t = 4$

$LT = N_s / N_t$

$B_4^\Omega$

$\lambda_c$ critical point

$\lambda = 192N_f\kappa^4$

$[Phys. Rev. D104, 114509(2021)]$

$\lambda_{c,NLO} = 0.00503(14)$

$\kappa_{c,NLO} = 0.0602(4)$

$N_t = 6$

$LT = N_s / N_t$

$B_4$

$\lambda_c$ critical point

$\lambda = 768N_f\kappa^6$

Talk by Masakiyo Kitazawa (Tue, 13:50)

$\lambda_{c,NLO} = 0.0008144(67)$

$\kappa_{c,NLO} = 0.08997(12)$

preliminary
Correlation among expansion terms in HPE

- **Expansion terms:** \( \ln \det M(\kappa) = \sum_{n=1}^{\infty} \frac{1}{n!} \frac{\partial^n \ln \det M}{\partial \kappa^n} \kappa^n \equiv N_{\text{site}} \sum_{n=1}^{\infty} D_n \kappa^n \)

- \( D_n = \frac{1}{N_{\text{site}}} \frac{(-1)^{n-1}}{n} \text{tr} \left[ \left( \frac{\partial M}{\partial \kappa} \right)^n \right] = W(n) + L(N_t, n) \)

- A matrix trace is computed by the noise method at each gauge configuration.

- Separate \( W(n) \) and \( L(N_t, n) \) by changing the boundary conditions.

- \( W^0(n) \) and \( L^0(N_t, n) \) are these terms when all \( U_\mu(x) \) are set to 1.

- The correlation between \( L(N_t, n) \) and \( \text{Re}\, \Omega \) is very strong.

- Approximation:

  \[
  L(N_t, n) = L^0(N_t, n) c_n \text{Re} \, \Omega
  \]

- The values of \( c_n \) is found to be independent of \( \beta \) and \( \kappa \).

- \( W(n) \) terms are improvement terms for the gauge action.
  - As an improvement term, the value is very small.
  - Omitted in this talk.
Determination of critical $\kappa$

\[
\ln \det M(\kappa) \over N_{\text{site}} \quad \text{-(Wilson loops)} = \sum_{n=1}^{n_{\text{max}}} L(N_t, n) \kappa^n \approx \text{Re} \Omega \sum_{n=1}^{n_{\text{max}}} L^0(N_t, n) c_n \kappa^n
\]

- The same as determining the critical point by the first order term only.

\[
\sum_{n=N_t}^{n_{\text{max}}} L^0(N_t, n) c_n \kappa_{c,\text{eff}}^n = L^0(N_t, N_t) \kappa_{c,\text{LO}}^{N_t}
\]

- Solving this equation gives us the critical $\kappa$ considering the higher order terms.

- Determination of effective critical points ($N_t = 6, N_f = 2$)

**Convergence value:** $\kappa_c = 0.08775(11)$

$\kappa_c = 0.0877(9)$ by a full QCD simulation

[Cuteri et al., Phys.Rev.D103(2021), 014513]
Critical Line of 2+1 Flavor QCD Incorporating Higher Order Effects

\[
\ln \left[ \prod_f \det M(\kappa_f) \right] = N_{\text{site}} \text{Re} \Omega \sum_f \sum_{n=N_t}^{n_{\text{max}}} L^0(N_t, n) c_n \kappa_f^n + \text{(Wilson loops)}
\]

\[
2 \sum_{n=N_t}^{n_{\text{max}}} L^0(N_t, n) c_n \kappa_{c,ud}^n + \sum_{n=N_t}^{n_{\text{max}}} L^0(N_t, n) c_n \kappa_{c,s}^n = 2L^0(N_t, N_t) \kappa_{c,2f,\text{LO}}^{N_t}
\]

Solve this equation.

Once one \( \kappa_c \) is determined, the critical line can be obtained for any number of flavors by using \( c_n \).

The critical line converges at \( n_{\text{max}} \geq 12 \).

\( N_t = 8 \) simulations are in progress. Kitazawa’s talk
Critical point in finite density QCD

\[ U_4(x) \Rightarrow e^{\mu a} U_4(x), \quad U_4^\dagger(x) \Rightarrow e^{-\mu a} U_4^\dagger(x) \]

\[ \text{in det} M \]

\[ \Omega \Rightarrow e^{\mu/T} \Omega, \quad \Omega^* \Rightarrow e^{-\mu/T} \Omega^* \]

\[
\ln \det M (\kappa, \mu) = 288N_{\text{site}}\kappa^4 P + 6 \cdot 2^{N_t} N_s^3 \kappa^{N_t} \left( e^{\frac{\mu}{T} \Omega} + e^{\frac{-\mu}{T} \Omega^*} \right) + \cdots
\]

\[
= 288N_{\text{site}}\kappa^4 P + 12 \cdot 2^{N_t} N_s^3 \kappa^{N_t} \left( \cosh(\mu/T) \text{ Re} \Omega + i \sinh(\mu/T) \text{ Im} \Omega \right) + \cdots
\]

Determination with \( N_t = 4 \)

- First order term is dominant in HPE.
- Critical point: Solve \( \kappa_c^{N_t}(\mu) \cosh(\mu/T) = \kappa_c^{N_t}(0) \)
- The contribution from the complex phase is small.

Complex phase of \( (\det M)^{N_f} \) \( \theta = 12 \cdot 2^{N_t} N_s^3 N_f \kappa_c^{N_t}(0) \tanh(\mu/T) \text{ Im} \Omega \)

The sign problem is not serious (because \( \tanh(\mu/T) < 1 \))

When incorporating higher-order terms for \( N_t = 6 \)

\[
\cosh \left( \frac{\mu}{T} \right) \sum_{n=N_t}^{n_{\text{max}}} L^0(N_t, n) c_n \kappa_c^n(\mu) = L^0(N_t, N_t) \kappa_c^{N_t}\text{LO}(0)
\]
Finite density hopping parameter expansion

\[ \ln \det M(\kappa) = N_{\text{site}} \sum_{n=1}^{\infty} D_n \kappa^n \]

\[ L_m(N_t, n) = L^+_m(N_t, n) + L^-_m(N_t, n) \]

\[ L^+_m(N_t, n) = (L^-_m(N_t, n))^*, \quad 2i \ \text{Im}L^+_m(N_t, n) = L^+_m(N_t, n) - L^-_m(N_t, n) \]

We ignore the phase and \( m \geq 2 \) terms, since \( m \geq 2 \) terms are very small for \( N_t = 6 \).

\[ L(N_t, n) \approx L^0(N_t, n)c_n \ \text{Re} \ \Omega \]

at \( \mu = 0 \)

\[ \cosh \left( \frac{\mu}{T} \right) L(N_t, n) \approx \cosh \left( \frac{\mu}{T} \right) L^0(N_t, n)c_n \ \text{Re} \ \Omega \]
Critical point at finite density (ignoring complex phase)

\[
cosh\left(\frac{\mu}{T}\right) \sum_{n=N_t}^{n_{\text{max}}} L^0(N_t, n) c_n \kappa_{c,\text{eff}}^n(\mu) = L^0(N_t, N_t) \kappa_{c,\text{LO}}^{N_t}(0)
\]

- Solve this equation

\[N_t = 6, \quad N_f = 2 \quad \text{case}\]

\[\kappa_{c,\text{NLO}} = 0.08997(12) \quad \text{preliminary}\]

\[\kappa_c = 0.08775(11) \quad (n_{\text{max}} = 22)\]

The higher the density, the smaller the first-order phase transition region.

\[N_t = 6, \quad N_f = 2 + 1 \quad \text{case}\]

The higher the density, the smaller the first-order phase transition region.
Complex phase in the hopping parameter expansion

$$\ln \det M (\kappa)$$

$$= N_{\text{site}} \sum_{n=1}^{\infty} \left( W(n) + \sum_{m=1}^{\infty} \cosh \left( \frac{m\mu}{T} \right) L_m(N_t, n) + \sum_{m=1}^{\infty} i \sinh \left( \frac{m\mu}{T} \right) 2 \text{Im} L_m^+(N_t, n) \right) \kappa^n$$

In the lowest order

$$2i \text{Im} L_1^+(N_t, N_t) = L_1^+(N_t, N_t) - L_1^-(N_t, N_t) = L^0(N_t, N_t) i \text{Im} \Omega$$

**Strong correlation between**

\( \text{Arg} \ L_1^+(N_t, n) \) and \( \text{Arg} \ \Omega \)

\[ \text{Arg} \ L_1^+(N_t, n) \approx \text{Arg} \ \Omega \]

\[ \frac{\text{Im} L_1^+(N_t, n)}{\text{Re} L_1^+(N_t, n)} \approx \frac{\text{Im} \Omega}{\text{Re} \ \Omega} \]

We can approximate as

\[ 2L^+(N_t, n) \approx L^0(N_t, n)c_n \Omega \]

\[ (2 \text{Im} L^+(N_t, n) = L^0(N_t, n)c_n \text{Im} \Omega) \]

For \( m \geq 2 \), there was no appreciable correlation within error.
Reweighting method at finite density

- Quark determinant: \( (\det M (\kappa, \mu))^Nf = |\det M (\kappa, \mu)|^{Nf} e^{i\theta} \)

- If \( 2 \text{Im} L^+_m(N_t, n) = L^0(N_t, n)c_n \text{Im} \Omega \), then the complex phase is

\[
\theta = N_f N_{\text{site}} \sum_{n,m} \sinh \left( \frac{m\mu}{T} \right) 2 \text{Im} L^+_m(N_t, n) \kappa^n \approx N_f N_{\text{site}} \sum_n \sinh \left( \frac{\mu}{T} \right) L^0(N_t, n)c_n\kappa^n \text{Im} \Omega
\]

- Expectation value of \( F(x) \) with \( x = \text{Re}\Omega \) by the reweighting method

\[
\langle F(x) \rangle_{(\beta, \kappa, \mu)} = \frac{1}{Z} \int DU F \left( \det M (\kappa, \mu) \right)^{Nf} e^{-S_g} = \frac{\int DU F \cos \theta |\det M (\kappa, \mu)|^{Nf} e^{-S_g}}{\int DU \cos \theta |\det M (\kappa, \mu)|^{Nf} e^{-S_g}}
\]

\[
= \frac{\int F(x) \langle \cos \theta \rangle_{x=\text{Re}\Omega} W(x) dx}{\int \langle \cos \theta \rangle_{x=\text{Re}\Omega} W(x) dx}
\]

- \( \langle \cos \theta \rangle_{x=\text{Re}\Omega} \) is the expectation value calculated by classifying the value of \( \text{Re}\Omega \),

- \( W(x) \) with \( x = \text{Re}\Omega \) is the probability distribution of \( \text{Re}\Omega \) when configurations are generated by \( |\det M (\kappa, \mu)|^{Nf} \) (phase quench simulation).

- We estimate the shift from the Phase-ignoring critical line by the effect of \( \langle \cos \theta \rangle_x \).
- We calculate \( \langle \cos \theta \rangle_x \) on the critical line and discuss the shift by \( \langle \cos \theta \rangle_x \).
Complex phase along the critical line $\kappa_c$

- Because $\cosh \left( \frac{\mu}{T} \right) \sum_n L^0 (N_t, n) c_n \kappa^n (\mu) = L^0 (N_t, N_t) \kappa_{c,LO}^{N_t}$ on the line of $\kappa_c$.

- $\theta \approx N_f N_{\text{site}} \sum_n \sinh \left( \frac{\mu}{T} \right) L^0 (N_t, n) c_n \kappa^n (\mu) \text{ Im } \Omega \approx N_f N_{\text{site}} L^0 (N_t, N_t) \kappa_{c,LO}^{N_t} (0) \tanh \left( \frac{\mu}{T} \right) \text{ Im } \Omega$

- $\theta = N_s^3 \lambda_{c,LO} \tanh \left( \frac{\mu}{T} \right) \text{ Im } \Omega$ (with $\lambda = N_t N_f L^0 (N_t, N_t) \kappa^{N_t} = 12 N_f 2^{N_t} \kappa^{N_t}$)

- Because $\lambda_{c,LO}$ is small and $\tanh \left( \frac{\mu}{T} \right) < 1$, $\ln \langle \cos \theta \rangle$ is computable without sign problem.

- If the volume is very large, $\ln \langle \cos \theta \rangle$ cannot be calculated, so in that case we use the cumulant expansion
  $$\ln \langle \cos \theta \rangle \approx -\frac{1}{2!} \langle \theta^2 \rangle_c + \frac{1}{4!} \langle \theta^4 \rangle_c - \frac{1}{6!} \langle \theta^6 \rangle_c + \cdots$$

  $\langle \theta^2 \rangle_c = \langle \theta^2 \rangle$, $\langle \theta^4 \rangle_c = \langle \theta^4 \rangle - 3 \langle \theta^2 \rangle^2$, $\langle \theta^6 \rangle_c = \langle \theta^6 \rangle - 15 \langle \theta^4 \rangle \langle \theta^2 \rangle + 30 \langle \theta^2 \rangle^3, \cdots$
Complex phase fluctuation at the critical point

- $\langle \theta^n \rangle_c = \left[ N_s^3 \lambda_{c,LO} \tanh(\mu/T) \right]^n \langle \text{Im}\Omega^n \rangle_c$ on the critical line for $\tanh(\mu/T) = 1$

- Even with $N_s = 90$, the phase fluctuation is small. $\langle \cos \theta \rangle$ can be easily calculated.

- $\ln \langle \cos \theta \rangle_x \approx -\frac{1}{2} \langle \theta^2 \rangle_c$ This indicates an approximately Gaussian distribution.

- Then, the volume dependence is $\langle \theta^2 \rangle_c \sim N_s^3$.

- The volume dependence of $\ln \langle \cos \theta \rangle_x / (N_s^3 \lambda_{c,LO})$ is small. ($x = \text{Re} \Omega$)

36$^3 \times 6$ lattice

$tanh(\mu/T) = 1$

90$^3 \times 6$ lattice
Effect from the phase fluctuation to $\kappa_C$

\[ \langle F(x) \rangle = \frac{\int F(x) \cos\theta_x \Re \Omega \, W(x) \, dx}{\int \cos\theta_x \Re \Omega \, W(x) \, dx} \]

Approximation: black dashed line

\[ -\ln\langle \cos \theta \rangle_x \left/ \left( N_s^3 \lambda_{c,\text{LO}} \right) \right. = d_0 + d_1 \Re \Omega \]

\[ \approx 0.00075 - 0.015 \Re \Omega \]

Effect from the phase fluctuation is very small.

- On the Phase-ignoring critical line,

\[ N_f \ln |\det M| = - (WL) \approx N_{\text{site}} N_f \cosh \left( \frac{\mu}{T} \right) \sum_n L^0(N_t, n) c_n \kappa^n \Re \Omega = N_s^3 \lambda_{c,\text{LO}} \Re \Omega \]

\[ \theta = N_s^3 \lambda_{c,\text{LO}} \tanh \left( \frac{\mu}{T} \right) \Im \Omega \]

\[ \langle \cos \theta \rangle_{\Re \Omega} |\det M|^{N_f} \approx \exp \left[ \ln \langle \cos \theta \rangle_{\Re \Omega} + N_s^3 \lambda_{c,\text{LO}} \Re \Omega \right] \approx C \exp \left[ N_s^3 \lambda_{c,\text{LO}} (1 - d_1) \Re \Omega \right] \]

- Multiplying $\langle \cos \theta \rangle$ is the same as $\lambda \rightarrow \lambda (1 - d_1)$. For $\tanh \left( \frac{\mu}{T} \right) = 1$, $d_1 \approx -0.015$.

- The phase effect reduces $\lambda_c$ by 1.5%, i.e. $\kappa_c$ is 0.25% smaller. $\lambda = 12 N_f 2^{N_t} \kappa^{N_t}$.  

\[ \lambda = 12 N_f 2^{N_t} \kappa^{N_t} \]
Conclusion and outlook

• We discussed how to efficiently determine the critical point of QCD in the heavy quark region, including the finite density region.

• There is a strong correlation between the expansion terms of the hopping parameter expansion.
  
  • Approximation: \( L(N_t, n) = L^0(N_t, n)c_n \text{ Re } \Omega \)

• We performed numerical simulations with the effective theory.
  
  \[
  S_{\text{eff}} = 6N_{\text{site}}\beta'P + N_s^3\lambda \text{Re } \Omega .
  \]

• Based on this effective theory with the reweighting method, the critical point of the heavy quark region can be determined relatively easily, even if the lattice spacing is small.
  
  • \( N_t = 6 \text{ (Kitazawa’s talk) } \rightarrow N_t = 8 \text{ (in progress) } \rightarrow \text{Continuum limit} \)

• The study at finite density is possible. The critical point decreases exponentially as the chemical potential increases.