Study of finite density lattice QCD by a histogram method

Shinji Ejiri

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.

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Histogram method

- Problem of Complex Determinant at $\mu \neq 0$
 - Boltzmann weight: complex at $\mu \neq 0$
 - Monte-Carlo method is not applicable.

$$\langle O \rangle_{(m,T,\mu)} = \frac{1}{Z} \int DU \ O \left(\frac{\det M(m,\mu)}{\operatorname{complex}} \right)^{N_{\mathrm{f}}} e^{-S_{g}}$$

• Distribution function in Density of state method (Histogram method) X: order parameters, total quark number, average plaquette etc. $\det M = |\det M|e^{i\theta}$

$$W(X;m,T,\mu) \equiv \int DU \,\delta(X-\hat{X}) (\det M(m,\mu))^{N_{\rm f}} e^{-S_g} = W_0 \times \left\langle e^{i\theta} \right\rangle_{X:\text{fixed}}$$
$$W_0(X;T,m,\mu) = \int DU \,\delta(X-\hat{X}) |\det M(m,\mu)|^{N_{\rm f}} e^{-S_g} \qquad \begin{array}{c} \text{Complex phase} \\ \text{factor} \end{array}$$

histogram in phase-quenched simulations

• Expectation values

$$\langle O[X] \rangle_{(m,T,\mu)} = \frac{1}{Z} \int dX \ O[X] W(X,m,T,\mu) \qquad Z(m,T,\mu) = \int dX \ W(X,m,T,\mu)$$

(β, m, μ) -dependence of the Distribution function

• Distributions of plaquette P (1x1 Wilson loop for the standard action) $W(P',\beta,m,\mu) \equiv \int DU\delta(\hat{P}-P') (\det M(m,\mu))^{N_{\rm f}} e^{6N_{\rm site}\hat{P}}$

$$R(P,\beta,\beta_{0}m,m_{0},\mu) \equiv W(P,\beta,m,\mu)/W(P,\beta_{0},m_{0},0) \quad \text{(Reweight factor)}$$

$$R(P') = e^{6N_{\text{site}}(\beta-\beta_{0})P'} \frac{\left\langle \delta(\hat{P}-P') \left(\frac{\det M(m,\mu)}{\det M(m_{0},0)} \right)^{N_{\text{f}}} \right\rangle_{(\beta_{0},\mu=0)}}{\left\langle \delta(\hat{P}-P') \right\rangle_{(\beta_{0},\mu=0)}} \equiv e^{6N_{\text{site}}(\beta-\beta_{0})P'} \left\langle \left(\frac{\det M(m,\mu)}{\det M(m_{0},0)} \right)^{N_{\text{f}}} \right\rangle_{P}$$

Effective potential:

$$V_{\text{eff}}(P,\beta,m,\mu) = -\ln[W(P,\beta m,\mu)] = V_{\text{eff}}(P,\beta_0,m_0,0) - \ln R(P,\beta,\beta_0 m,m_0,\mu)$$
$$\ln R(P) = \frac{6N_{\text{site}}(\beta-\beta_0)P}{4} + \ln\left\langle \left(\frac{\det M(m,\mu)}{\det M(m_0,0)}\right)^{N_{\text{f}}}\right\rangle_P$$

$$\langle OR \rangle = \frac{1}{Z} \int ORW(X) dX = \frac{1}{Z} \int \exp(-V_{\text{eff}}(X) + \ln(OR)) dX$$

$$V_{\text{eff}}(X) = -\ln W(X)$$

- *W* is computed from the histogram.
- Distribution function around X where $V_{\text{eff}}(X) - \ln(OR)$ is minimized: important.



• V_{eff} must be computed in a wide range.



Distribution function in quenched simulations

Effective potential in a wide range of *P*: required.



Distribution function in the heavy quark region



Hopping parameter expansion

- We study the properties of *W*(*X*) in the heavy quark region.
- Performing quenched simulations + Reweighting.
- We find the critical surface.
- Standard Wilson quark action + plaquette gauge action, $S_g = -6N_{site}\beta P$
- lattice size: $24^3 \times 4$
- 5 simulation points; β=5.68-5.70.
 (WHOT-QCD, Phys.Rev.D84, 054502(2011))

 $N_{\rm f} \ln \left(\frac{\det M(K,\mu)}{\det M(0,0)} \right) = N_{\rm f} \left(288N_{\rm site} K^4 P + 12 \cdot 2^{N_t} N_s^3 K^{N_t} \left(\cosh(\mu/T) \Omega_R + i \sinh(\mu/T) \Omega_I \right) + \cdots \right)$ phase

P: plaquette, $\Omega = \Omega R + i \Omega I$: Polyakov loop

 $\det M(0,0) = 1$

Distribution function for P and Ω_{R}

$$W(P,\Omega_R,\beta,\kappa) = \int DU \,\delta\!\left(P - \hat{P}\right) \delta\!\left(\Omega_R - \hat{\Omega}_R\right) \left(\det M(\kappa)\right)^{N_{\rm f}} e^{-6N_{\rm site}\hat{P}}$$

$$\frac{W(\beta, K, \mu)}{W(\beta_0, 0, 0)} = \frac{\left\langle \delta\left(P - \hat{P}\right) \delta\left(\Omega_R - \hat{\Omega}_R\right) e^{6N_{\text{site}}(\beta - \beta_0)P} \left(\frac{\det M(K, \mu)}{\det M(0, 0)}\right)^{N_f} \right\rangle_{(\beta_0, K = \mu = 0)}}{\left\langle \delta\left(P - \hat{P}\right) \delta\left(\Omega_R - \hat{\Omega}_R\right) \right\rangle_{(\beta_0, K = \mu = 0)}} \equiv \left\langle e^{6N_{\text{site}}(\beta - \beta_0)\hat{P}} \left(\frac{\det M(K, \mu)}{\det M(0, 0)}\right)^{N_f} \right\rangle_{P, \Omega_R}$$

- Effective potential $V_{eff}(P,\Omega_R;\beta,\kappa) = -\ln W(P,\Omega_R;\beta,\kappa)$
- Hopping parameter expansion

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 $V_{\rm eff}(\beta,\kappa) - V_{\rm eff}(\beta_0,0) = -\left(6(\beta - \beta_0) + 288N_{\rm f}K^4\right)N_{\rm site}P - 12 \times 2^{N_t}N_{\rm f}N_s^3K^{N_t}\cosh(\mu/T)\Omega_R - \ln\langle e^{i\theta}\rangle_{P,\Omega_R}$

$$= V_{0}(\beta, \kappa) - \ln \langle e^{i\theta} \rangle_{P,\Omega_{R}} \qquad (\theta = 12 \cdot 2^{N_{t}} N_{s}^{3} N_{f} K^{N_{t}} \sinh(\mu/T) \hat{\Omega}_{I})$$
Phase-quenched part
$$P \text{ parameters in } V_{0}: \qquad \beta + 48N_{f} K^{4} \equiv \beta^{*}, \qquad K^{N_{t}} \cosh(\mu/T)$$

$$- V_{0} \text{ is the same as } V_{\text{eff}}(\mu=0) \text{ when } K^{N_{t}} \Rightarrow K^{N_{t}} \cosh(\mu/T)$$
parameter in $\theta: \qquad K^{N_{t}} \sinh(\mu/T) = K^{N_{t}} \cosh(\mu/T) \tanh(\mu/T) < K^{N_{t}} \cosh(\mu/T)$

Distribution function for P and Ω_{R}

Expectation value of Polyakov loop and its susceptibility by the reweightuing method at $\mu=0$. $24^3 \times 4$ lattice



χΩ

Ω

- If $W(P,\Omega)$ is a Gaussian distribution,
 - The peak position of $W(P,\Omega) \implies (\langle P \rangle, \langle \Omega \rangle)$
 - The width of $W(P,\Omega)$ \implies susceptibilities χ_P, χ_Ω
- If $W(P,\Omega)$ have two peaks, \implies first order transition

Effective potential near the quenched limit(μ =0)

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



• First order transition at K = 0 changes to crossover at K > 0.

Order of the phase transition Polyakov loop distribution



The pseudo-critical line is determined by χ_Ω peak.



- Double-well at small *K*
 - First order transition
- Single-well at large *K*
 - Crossover

Polyakov loop distribution in the complex plane $_{(\mu=0)}$



• on β_{PC} measured by the Polyakov loop susceptibility.

Avoiding the sign problem (SE, Phys.Rev.D77,014508(2008), WHOT-QCD, Phys.Rev.D82, 014508(2010))

- θ : complex phase $\theta \equiv \text{Im} \ln \det M \approx 12 \cdot 2^{N_t} N_s^3 N_f K^{N_t} \sinh(\mu/T) \Omega_I$
- Sign problem: If $e^{i\theta}$ changes its sign,

 $\langle e^{i\theta} \rangle_{P,\Omega_{p} \text{ fixed}} \ll \text{(statistical error)}$

Cumulant expansion $\langle ... \rangle P, \Omega_R$: expectation values fixed P and Ω_R .

$$\left\langle e^{i\theta} \right\rangle_{P,\Omega_R} = \exp\left[i\left\langle \theta \right\rangle_C - \frac{1}{2}\left\langle \theta^2 \right\rangle_C - \frac{i}{3!}\left\langle \theta^3 \right\rangle_C + \frac{1}{4!}\left\langle \theta^4 \right\rangle_C + \cdots\right]$$

cumulants

 $\langle \theta \rangle_{C} = \langle \theta \rangle_{P,\Omega_{P}}, \quad \langle \theta^{2} \rangle_{C} = \langle \theta^{2} \rangle_{P,\Omega_{P}}, \quad \langle \theta^{3} \rangle_{C} = \langle \theta^{3} \rangle_{P,\Omega_{P}}, \quad \langle \theta^{2} \rangle_{P,\Omega_{P}} + 2 \langle \theta \rangle_{P,\Omega_{P}}^{3}, \quad \langle \theta^{4} \rangle_{C} = \cdots$

- <u>Odd terms</u> vanish from a symmetry under $\mu \leftrightarrow -\mu (\theta \leftrightarrow -\theta)$ Source of the complex phase
- If the cumulant expansion converges, No sign problem.

Convergence in the large volume (V) limit

The cumulant expansion is good in the following situations.

• If the phase is given by $\theta = \sum \theta_x$

– No correlation between θ_x .

$$\left\langle e^{i\theta} \right\rangle_{P,\Omega_{R}} = \left\langle e^{i\sum_{x}\theta_{x}} \right\rangle_{P,\Omega_{R}} \approx \prod_{x} \left\langle e^{i\theta_{x}} \right\rangle_{P,\Omega_{R}} = \exp\left[\sum_{x} \sum_{n} \frac{i^{n}}{n!} \left\langle \theta_{x}^{n} \right\rangle_{C}\right]$$
$$\left\langle e^{i\theta} \right\rangle_{P,\Omega_{R}} = \exp\left[\sum_{n} \frac{i^{n}}{n!} \left\langle \theta^{n} \right\rangle_{C}\right] \implies \left\langle \theta^{n} \right\rangle_{C} \approx \sum_{x} \left\langle \theta_{x}^{n} \right\rangle_{C} \sim O(V)$$

- 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 µ can be measured on a small lattice.
- When the distribution function of θ is perfectly Gaussian, the average of the phase is give by the second order, $\langle e^{i\theta} \rangle_{P,\Omega_R} = \exp\left[-\frac{1}{2} \langle \theta^2 \rangle_C\right]$



-10

0

0.02

0.04

0.06

0.08

 Ω_{p}

0.1

0.12

0.14

0.16

$$K_{\rm cp}^{N_t}(0) = K_{\rm cp}^{N_t}(\mu) \cosh(\mu/T) > K_{\rm cp}^{N_t}(\mu) \sinh(\mu/T)$$

- Phase fluctuations
 - large in the confinement phase
 - small in the deconfinement phase

Effect from the complex phase factor

- Polyakov loop effective potential for each $K^{N_t} \cosh(\mu/T)$ at the pseudo-critical (β , K).
 - Solid lines: complex phase omitted, i.e., $tanh(\mu/T)=0$
 - Dashed lines: complex phase is estimated from $\langle \theta^2 \rangle_c / 2$



with $tanh(\mu/T) = 1$

$$V_{\text{eff}}(\Omega_R) = V_0(\Omega_R) - \ln \left\langle e^{i\theta} \right\rangle_{\Omega_R:\text{fixed}}$$
$$\approx V_0(\Omega_R) + \frac{1}{2} \left\langle \theta^2 \right\rangle_{\Omega_R:\text{fixed}}$$

The effect from the complex phase factor is very small except near $\Omega_R=0$.

Critical line in 2+1-flavor finite density QCD

• The effect from the complex phase is very small for the determination of $K_{cp.}$

$$Nf=2 \text{ at } \mu=0: \ Kcp=0.0658(3)(8) \\ (WHOT-QCD, Phys.Rev.D84, 054502(2011)) \\ Nf=2+1 \\ ln\left[\frac{(\det M(K_{ud}))^{2} \det M(K_{s})}{(\det M(0))^{3}}\right] = 288N_{site}(2K_{ud}^{4} + K_{s}^{4})P + 12 \times 2^{N_{t}}N_{s}^{3}\left(2K_{ud}^{N_{t}}\cosh\left(\frac{\mu_{ud}}{T}\right) + K_{s}^{N_{t}}\cosh\left(\frac{\mu_{s}}{T}\right)\right)\Omega_{k} + \cdots$$

The critical line is described by $2K_{ud}^{N_{t}}\cosh\left(\frac{\mu_{ud}}{T}\right) + K_{s}^{N_{t}}\cosh\left(\frac{\mu_{s}}{T}\right) = 2K_{cp(Nf=2)}^{N_{t}}$
Critical line for $\mu u=\mu d=\mu s=\mu$
 $Critical line for $\mu u=\mu d=\mu s=\mu$
 $M_{ud}^{\frac{n}{4}} = \frac{10}{0.02} = 0.06} \int_{0.04}^{0} \int_{0$$

Χ_α

0.08

Distribution function in the light quark region WHOT-QCD Collaboration, in preparation, (Nakagawa et al., arXiv:1111.2116)

- Perform phase quenched simulations
- Add the effect of the complex phase by the reweighting.
- Calculate the probability distribution function.
- Goal
 - The critical point
 - The equation of state

Pressure, Energy density, Quark number density, Quark number susceptibility, Speed of sound, etc.

Probability distribution function by phase quenched simulation

• We perform phase quenched simulations with the weight: $|\det M(m,\mu)|^{N_{\rm f}} e^{-S_g}$

$$W(P', F', \beta, m, \mu) = \int DU \,\delta(\hat{P} - P')\delta(\hat{F} - F')(\det M(m, \mu))^{N_{\rm f}} e^{-S_g}$$
$$= \int DU \,\delta(\hat{P} - P')\delta(\hat{F} - F')e^{i\theta}|\det M(m, \mu)|^{N_{\rm f}} e^{-S_g}$$
$$= \left\langle e^{i\theta} \right\rangle_{P',F'} \times W_0(P', F', \beta, m, \mu)$$

expectation value with fixed *P*,*F* histo

$$F(\mu) = \frac{N_{\rm f}}{N_{\rm site}} \ln \left| \frac{\det M(\mu)}{\det M(0)} \right| \qquad \Theta \equiv N_{\rm f} \, \operatorname{Im} \ln \det M$$

Distribution function of the phase quenched.

$$W_0(P',F') = \int DU \,\delta(\hat{P} - P') \delta(\hat{F} - F') \det M \Big|_{F}^{N_f} e^{6N_{\text{site}}\beta\hat{P}}$$

µ-dependence of the effective potential Curvature of the effective potential



Curvature of the effective potential

• If the distribution is Gaussian,

$$W_{0}(P,F) \approx \sqrt{\frac{6N_{\text{site}}}{2\pi\chi_{P}}} \exp\left[-\frac{6N_{\text{site}}}{2\chi_{P}} \left(P - \langle P \rangle\right)^{2}\right] \times \sqrt{\frac{N_{\text{site}}}{2\pi\chi_{F}}} \exp\left[-\frac{N_{\text{site}}}{2\chi_{F}} \left(F - \langle F \rangle\right)^{2}\right]$$
$$\chi_{P} = 6N_{\text{site}} \left\langle \left(P - \langle P \rangle\right)^{2} \right\rangle \qquad \chi_{F} = N_{\text{site}} \left\langle \left(F - \langle F \rangle\right)^{2} \right\rangle$$

$$\frac{\partial^2 (-\ln W_0)}{\partial P^2} (\langle P \rangle, \langle F \rangle) = \frac{6N_{\text{site}}}{\chi_P} \qquad \frac{\partial^2 (-\ln W_0)}{\partial F^2} (\langle P \rangle, \langle F \rangle) \approx \frac{N_{\text{site}}}{\chi_F}$$

at the peak of the distribution

Complex phase distribution

- We should not define the complex phase in the range from $-\pi$ to π .
- When the distribution of q is perfectly Gaussian, the average of the complex phase is give by the second order (variance), $\left\langle e^{i\theta} \right\rangle_{P,F} = \exp\left[-\frac{1}{2}\left\langle \theta^2 \right\rangle_C\right]$



- Gaussian distribution \rightarrow The cumulant expansion is good.
- We define the phase

$$\theta(\mu) = N_{\rm f} \operatorname{Im}\left(\ln\frac{\det M(\mu)}{\det M(0)}\right) = N_{\rm f} \int_0^{\mu/T} \operatorname{Im}\left[\frac{\partial \ln \det M}{\partial(\mu/T)}\right]_{\overline{\mu}} d\left(\frac{\overline{\mu}}{T}\right)$$

- The range of q is from $-\infty$ to ∞ .

Distribution of the complex phase



- Well approximated by a Gaussian function.
- Convergence of the cumulant expansion: good.

$$\left\langle e^{i\theta} \right\rangle_{P,F} \approx \exp\left[-\frac{1}{2}\left\langle \theta^2 \right\rangle\right]$$

$$\frac{1}{2} \left\langle \theta^2 \right\rangle_{\langle P \rangle, \langle F \rangle} \approx \frac{1}{2} \left\langle \theta^2 \right\rangle_{\beta_0, \mu_0}$$

at the peak of W₀ in each simulation

Simulations

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

- Simulation point in the (β , μ_0/T)
- Peak of $W_0(P,F)$ for each μ

2-flavor QCD Iwasaki gauge+ clover Wilson quark actionRandom noise method is used.





Curvature of the effective potential -lnWo



• The curvature for F decreases as μ increases.

Effect from the complex phase



• Rapidly changes around the pseudo-critical point.

Critical point at finite µ



• zero curvature: expected at a large μ .

Curvature of the effective potential

• Without the complex phase effect



$$\chi_F = N_{\rm site} \left\langle \left(F - \left\langle F \right\rangle \right)^2 \right\rangle$$



Phase average

• 2nd order cumulant

$$\ln \left\langle e^{i\theta} \right\rangle_{P,F} \approx -\frac{1}{2} \left\langle \theta^2 \right\rangle_{P,F}$$

$$\frac{1}{2} \left\langle \theta^2 \right\rangle_{\langle P \rangle, \langle F \rangle} \approx \frac{1}{2} \left\langle \theta^2 \right\rangle_{\beta_0, \mu_0}$$



Curvature of the effective potential

• The effect of the phase incruded.



QCD phase diagram

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

phase-quenched QCD





Summary

- We studied the quark mass and chemical potential dependence of the nature of QCD phase transition.
- 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 θ is useful.
- To find the critical point at finite density, further studies in light quark region are important applying this method.

Backup

Peak position of W(P,F) $-\ln W(P,F)$ at $\frac{\partial \ln W}{\partial P} = 0, \quad \frac{\partial \ln W}{\partial F} = 0$ • The slopes are zero at the peak of W(P,F). $\frac{\partial \ln W}{\partial P}(P,F,\beta,\mu) = \frac{\partial \ln W_0}{\partial P}(P,F,\beta,\mu) + \frac{\partial \ln \langle e^{i\theta} \rangle_{P,F}}{\partial P} \qquad \left(R(P,F,\mu,\mu_0) = \frac{W_0(P,F,\beta,\mu)}{W_0(P,F,\beta,\mu_0)} \right)$ $=\frac{\partial \ln W_0}{\partial P}(P,F,\beta_0,\mu_0)+6N_{site}(\beta-\beta_0)+\frac{\partial \ln R}{\partial P}(P,F,\mu,\mu_0)+\frac{\partial \ln \langle e^{i\theta} \rangle_{P,F}}{\partial P}$ $\frac{\partial \ln W}{\partial F}(P,F,\beta,\mu) = \frac{\partial \ln W_0}{\partial F}(P,F,\beta,\mu) + \frac{\partial \ln \langle e^{i\theta} \rangle_{P,F}}{\partial F}$ If these terms are canceled, $=\frac{\partial \ln W_0}{\partial F}(P,F,\beta_0,\mu_0)+\frac{\partial \ln R}{\partial F}(P,F,\mu,\mu_0)+\frac{\partial \ln \langle e^{i\theta} \rangle_{P,F}}{\partial F}$ $W(P, F, \beta, \mu) \approx W_0(P, F, \beta_0, \mu_0) \times (\text{const.})$

• $W(\beta, \mu)$ can be computed by simulations around ($\beta_{0,\mu_{0}}$).

Complex phase

- Gaussian distribution \rightarrow The cumulant expansion is good.
- We define the phase

$$\theta(\mu) = N_{\rm f} \operatorname{Im} \ln \frac{\det M(\mu)}{\det M(0)} = N_{\rm f} \int_0^{\mu/T} \operatorname{Im} \left[\frac{\partial \ln \det M}{\partial (\mu/T)} \right]_{\overline{\mu}} d\left(\frac{\overline{\mu}}{T} \right)$$

- The range of θ is from - ∞ to ∞ .
- At the same time, we calculate F as a function of μ ,

$$F(\mu) = N_{\rm f} \ln \left| \frac{\det M(\mu)}{\det M(0)} \right| = N_{\rm f} \int_0^{\mu/T} \operatorname{Re} \left[\frac{\partial \ln \det M}{\partial (\mu/T)} \right]_{\overline{\mu}} d\left(\frac{\overline{\mu}}{T} \right)$$

• The reweighting factor is also computed,

$$C(\mu) = N_{\rm f} \ln \left| \frac{\det M(\mu)}{\det M(\mu_0)} \right| = N_{\rm f} \int_{\mu_0/T}^{\mu/T} \operatorname{Re} \left[\frac{\partial \ln \det M}{\partial (\mu/T)} \right]_{\overline{\mu}} d\left(\frac{\overline{\mu}}{T} \right)$$

Order of phase transitions and Distribution function

$$W(P,\Omega_R,\beta,\kappa) = \int DU \,\delta(P-\hat{P})\delta(\Omega_R-\hat{\Omega}_R)(\det M(\kappa))^{N_f} e^{-6N_{\rm site}P}$$
$$V_{\rm eff}(P,\Omega_R;\beta,\kappa) = -\ln W(P,\Omega_R;\beta,\kappa)$$

• Peak position of *W*:



crossover 1 intersection

 $\frac{dV_{\rm eff}}{dP} = \frac{dV_{\rm eff}}{d\Omega_R} = 0$



first order transition 3 intersections

Lines of zero derivatives for first order





the lines of the zero derivatives at (β,κ) .



- Small K: lines of $\frac{dV_{\text{eff}}}{d\Omega_R} = 0$: S-shape \implies first order
- Large K: lines of $\frac{dV_{\text{eff}}}{d\Omega_R} = 0$: straight line \Rightarrow crossover