Phase structure of finite density lattice QCD by a histogram method

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WHOT-QCD collaboration

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YIPQS-HPCI international molecule-type workshop on New-type of Fermions on the Lattice (YITP, Kyoto, Feb.9-24, 2012)

Phase structure of QCD at high temperature and density



Probability distribution function

• Distribution function (Histogram)

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

$$Z(m,T,\mu) = \int dX \ W(X,m,T,\mu)$$
 histogram

• In the Matsubara formalism,

$$Z(m,T,\mu) \equiv \int DU (\det M(m,\mu))^{N_{\rm f}} e^{-S_g}$$
$$W(X',m,T,\mu) \equiv \int DU \delta(X-X') (\det M(m,\mu))^{N_{\rm f}} e^{-S_g}$$

- where detM: quark determinant, S_g : gauge action.
- Useful to identify the nature of phase transitions
 - e.g. At a first order transition, two peaks are expected in W(X).



Quark mass dependence of the critical point



- Where is the physical point?
- Extrapolation to finite density
 - investigating the quark mass dependence near μ =0
- Critical point at finite density?

Equation of State

• Integral method

- Interaction measure
$$\frac{\varepsilon - 3p}{T^4} = -\frac{1}{VT^3} \frac{\partial \ln Z}{\partial \ln a},$$

computed by plaquette (1x1 Wilson loop) $\langle P \rangle$ and the derivative of det*M*.

- Pressure at $\mu=0$ $\frac{p}{T^4} = \frac{1}{VT^3} \ln Z$

• Integral

$$\frac{p}{T^4}\Big|_a - \frac{p}{T^4}\Big|_{a_0} = -\int_{a_0}^a \frac{\varepsilon' - 3p'}{T'^4} d\left(\ln a'\right)$$

$$a_0: \text{ start point } p=0$$
Pressure at $\mu \neq 0$, $\frac{p}{T^4}(\mu) - \frac{p}{T^4}(0) = \frac{1}{VT^3} \ln\left(\frac{Z(\mu)}{Z(0)}\right) = \left(\frac{N_t}{N_s}\right)^3 \ln\left(\frac{\det M(\mu)}{\det M(0)}\right)_{\mu=0}$

•
$$\langle X \rangle_{(m,T,\mu)} = \frac{1}{Z} \int dX \ X \ W(X,m,T,\mu)$$
 with $X = P$ or $\det M(\mu) / \det M(0)$

Plan of this talk

- Test in the heavy quark region
 - H. Saito et al. (WHOT-QCD Collab.), Phys.Rev.D84, 054502(2011)
 - WHOT-QCD Collaboration, in preparation
- Application to the light quark region at finite density

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

– WHOT-QCD Collaboration, in preparation

(Lattice 2011 proc.: Y. Nakagawa et al., arXiv:1111.2116)

Distribution function in the heavy quark region WHOT-QCD Collab., Phys.Rev.D84, 054502(2011)



- We study the critical surface in the (*m*_{ud}, *m*_s, μ) space in the heavy quark region.
- Performing quenched simulations + Reweighting.

ð

plaquette gauge action +
 Wilson quark action

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

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

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

Effective potential:

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

Distribution function in quenched simulations

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



Effective potential near the quenched limit

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



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

Endpoint of 1st order transition in 2+1 flavor QCD



The critical line is described by

$$2K_{ud}^{N_t} + K_s^{N_t} = 2K_{cp(Nf=2)}^{N_t}$$

Finite density QCD in the heavy quark region

Phase quenched simulations, Isospin chemical potential $(N_{\rm f}=2), \ \mu_{\rm u}=-\mu_{\rm d}.$ $\det M(K,-\mu) = [\det M(K,\mu)]^*$ $\det M(K,\mu)^2 = \det M(K,\mu)\det M(K,-\mu)$

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



Distribution function for *P* and Ω_R at $\mu=0$

$$W(P', \Omega_{R}', \beta, \kappa) = \int DU \,\delta(P - P') \delta(\Omega_{R} - \Omega_{R}') (\det M(\kappa))^{N_{f}} e^{-S_{g}}$$

$$\frac{W(\beta,\kappa)}{W(\beta_0,0)} = \left\langle \exp\left(6(\beta-\beta_0)N_{\text{site}}P + 288N_fN_{\text{site}}K^4P + 12 \times 2^{N_t}N_fN_s^3K^{N_t}\Omega_R + \cdots\right)\right\rangle_{P,\Omega_R \text{ fixed}}$$

$$\approx \exp\left(\left(6(\beta-\beta_0) + 288N_fK^4\right)N_{\text{site}}P + 12 \times 2^{N_t}N_fN_s^3K^{N_t}\Omega_R\right)$$

$$\implies V_{\text{eff}}(\beta,\kappa) - V_{\text{eff}}(\beta_0,0) = -\left(6(\beta-\beta_0) + 288N_fK^4\right)N_{\text{site}}P - 12 \times 2^{N_t}N_fN_s^3K^{N_t}\Omega_R$$

• Peak position of *W*:



crossover 1 intersection



3 intersections





Lines of constant derivatives obtained by quenched simulations



• The number of the intersection changes around κ =0.658

Finite density QCD in the heavy quark region

$$U_{4}(x) \Rightarrow e^{\mu_{q}a}U_{4}(x), \quad U_{4}^{\dagger}(x) \Rightarrow e^{-\mu_{q}a}U_{4}^{\dagger}(x)$$

$$\square \Rightarrow e^{\mu_{q}/T}\Omega, \quad \Omega^{*} \Rightarrow e^{-\mu_{q}/T}\Omega^{*}$$

$$N_{f} \ln\left(\frac{\det M(K,\mu)}{\det M(0,0)}\right) = N_{f}\left(288N_{site}K^{4}P + 6\cdot 2^{N_{t}}N_{s}^{3}K^{N_{t}}\left(e^{\mu/T}\Omega + e^{-\mu/T}\Omega^{*}\right) + \cdots\right)$$

$$= N_{f}\left(288N_{site}K^{4}P + 12\cdot 2^{N_{t}}N_{s}^{3}K^{N_{t}}\left(\cosh(\mu/T)\Omega_{R} + \underline{i\sinh(\mu/T)\Omega_{I}}\right) + \cdots\right)$$
phase

• We can extend this discussion to finite density QCD.

Finite density QCD

$$N_{\rm f} \ln \left(\frac{\det M(K)}{\det M(0)}\right) = N_{\rm f} \left(288N_{\rm site}K^4P + 6 \cdot 2^{N_t}N_s^3K^{N_t} \left(e^{\mu/T}\Omega + e^{-\mu/T}\Omega^*\right) + \cdots\right)$$
$$= N_{\rm f} \left(288N_{\rm site}K^4P + 12 \cdot 2^{N_t}N_s^3K^{N_t} \left(\cosh(\mu/T)\Omega_R + i\sinh(\mu/T)\Omega_I\right) + \cdots\right)$$
phase

$$\frac{W(\beta,\kappa)}{W(\beta_{0},0)} = \left\langle \exp\left(6(\beta-\beta_{0})N_{\text{site}}P + 288N_{\text{f}}N_{\text{site}}K^{4}P + 12 \times 2^{N_{t}}N_{\text{f}}N_{s}^{3}K^{N_{t}}\left(\cosh(\mu/T)\Omega_{R} + i\sinh(\mu/T)\Omega_{I}\right) + \cdots\right)\right\rangle_{P,\Omega_{R}\text{ fixed}}$$

$$\approx \exp\left(\left(6(\beta-\beta_{0}) + 288N_{\text{f}}K^{4}\right)N_{\text{site}}P + 12 \times 2^{N_{t}}N_{\text{f}}N_{s}^{3}K^{N_{t}}\cosh(\mu/T)\Omega_{R}\right) \times \left\langle e^{i\theta}\right\rangle_{P,\Omega_{R}\text{ fixed}}$$

$$\theta = 12 \cdot 2^{N_{t}}N_{\text{f}}N_{s}^{3}K^{N_{t}}\sinh(\mu/T)\Omega_{I}$$

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

• Reweighting: $\ln \langle e^{i\theta} \rangle_{P,\Omega_R \text{ fixed}}$ is a non-linear term in $V_{\text{eff}}(\beta,\kappa) - V_{\text{eff}}(\beta_0,0)$. Sign problem.

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

 θ : complex phase $\theta \equiv \text{Im ln det } M = 12 \cdot 2^{N_t} N_f N_s^3 K^{N_t} \sinh(\mu/T) \Omega_I$

• Sign problem: If $e^{i\theta}$ changes its sign,

 $\left\langle e^{i\theta} \right\rangle_{P,\Omega_R \text{ fixed}} << \text{(statistical error)}$

• Cumulant expansion

<...>F,P: expectation values fixed F and P.

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

cumulants

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

 $- \underbrace{Odd \ terms}_{Source \ of \ the \ complex \ phase} roma \ symmetry \ under \ \mu \leftrightarrow -\mu \ (\theta \leftrightarrow -\theta)$

If the cumulant expansion converges, No sign problem.

Cumulant expansion of the complex phase

• When the distribution of θ is perfectly Gaussian, the average of the complex phase is give by the second order (variance),

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

 $\theta = 12 \cdot 2^{N_t} N_f N_s^3 K^{N_t} \sinh\left(\frac{\mu}{T}\right) \Omega_I$

• Because $W(\mu)$ is enhanced by the factor, $W(\beta,\kappa) \sim \exp(12 \times 2^{N_t} N_f N_s^3 K^{N_t} \cosh(\mu/T) \Omega_R)$

the region of large Ω_R is important.

- The distribution of Ω_I seems to be of Gaussian at $\Omega_R > 0$.
- The higher order cumulants $\langle \Omega_I^4 \rangle_c$ etc. might be small.



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 $\theta = \sum \theta_x$
 - No correlation between θx .
 - In the heavy quark region, the phase is the imaginary part of the Polyakov loop average, Ω I.

$$\theta = 12 \cdot 2^{N_t} N_f N_s^3 K^{N_t} \sinh\left(\frac{\mu}{T}\right) \Omega_I$$



 If the spatial correlation length is short, the distribution of the imaginary part of the Polyakov loop is expected to be Gaussian by the central limit theorem.

Convergence in the large volume (V) limit

This problem is solved in the following situation.

• The phase is given by $\theta = \sum \theta_x$

– No correlation between θ_x .

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

- 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.

Effect from the complex phase



Critical surface at finite density







- Blue line is the dVeff/d Ω R around the critical point.
- Effect from the complex phase is small on the critical line, $\lambda < 2 \times 10^{-5}$.

$$\frac{dV_{\text{eff}}(\beta,K)}{dP} = \frac{dV_{\text{eff}}(\beta_0,0)}{dP} - \left(6(\beta - \beta_0) + 288N_{\text{f}}K^4\right)N_{\text{site}} + \frac{\left(3 \times 2^{N_t + 2}N_{\text{f}}N_s^3\lambda\right)^2}{2}\frac{\partial\left\langle\Omega_I^2\right\rangle_c}{\partial P}}{\frac{\partial P}{\partial \Omega_R}} - \frac{dV_{\text{eff}}(\beta_0,0)}{d\Omega_R} - 12 \times 2^{N_t}N_{\text{f}}N_s^3K^{N_t}\cosh\left(\frac{\mu}{T}\right) + \frac{\left(3 \times 2^{N_t + 2}N_{\text{f}}N_s^3\lambda\right)^2}{2}\frac{\partial\left\langle\Omega_I^2\right\rangle_c}{\partial\Omega_R}}{\frac{\partial \Omega_R}{\partial \Omega_R}}$$

Critical line in finite density QCD (WHOT-QCD Collab., in preparation, 11)

- The effect from the complex phase is very small for the determination of K_{cp} because $K_{cp}^{N_t}(0) = K_{cp}^{N_t}(\mu) \cosh(\mu/T)$ is small.
- On the critical line,

$$\theta = 12 \cdot 2^{N_t} N_s^3 N_f K_{cp}^{N_t}(0) \underline{\tanh(\mu/T)}_{<1} \Omega$$

$$\begin{array}{c} 0.08 \\ \kappa_{cp}^{l} \\ 0.06 \\ 0.04 \\ 0.02 \\ 0 \\ 0 \\ 0 \\ 2 \\ 4 \\ \mu/T \end{array}$$

$$\theta = 12 \cdot 2^{N_t} i N_s^3 N_f K^{N_t} \sinh(\mu/T) \Omega_I$$



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

- We perform phase quenched simulations
- The effect of the complex phase is added by the reweighting.
- We 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: $\left|\det M(m,\mu)\right|^{N_{\rm f}} e^{-S_g}$

$$W(P', F', \beta, m, \mu) = \int DU \,\delta(P - P')\delta(F - F')(\det M(m, \mu))^{N_f} e^{-S_g}$$
$$= \int DU \,\delta(P - P')\delta(F - F')e^{i\theta} |\det M(m, \mu)|^{N_f} e^{-S_g}$$
$$= \left\langle e^{i\theta} \right\rangle_{P', F'} \times W_0(P', F', \beta, m, \mu)$$
expectation value with fixed *P,F* histogram

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

Distribution function of the phase quenched.

$$W_0(P',F') = \int DU \,\delta(P-P')\delta(F-F') |\det M|^{N_{\rm f}} e^{6N_{\rm site}\beta P}$$

Phase quenched simulation

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

 $\det M(K,-\mu) = \left[\det M(K,\mu)\right]^*, \quad \left|\det M(K,\mu)\right|^2 = \det M(K,\mu)\det M(K,-\mu)$

- When $\mu_u = -\mu_d$, pion condensation occurs.
- $\langle e^{i\theta} \rangle = 0$ is suggested in the pion condensed phase by phenomenological *T* studies. [Han-Stephanov '08, Sakai et al. '10]

 \longrightarrow No overlap between $W(\mu)$ and $W_0(\mu)$.

- Near the phase boundary,
 - large fluctuations in θ : expected.

$$\left\langle e^{i\theta}\right\rangle_{P,F} \to 0 \quad \left\langle \ln\left\langle e^{i\theta}\right\rangle_{P,F} \to -\infty\right\rangle$$

- W(P,F) and $W_0(P,F)$ are completely different.





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

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

- θ : complex phase $\theta \equiv \text{Im ln det } M$
- Sign problem: If $e^{i\theta}$ changes its sign,

$$\left\langle e^{i\theta} \right\rangle_{P,F \text{ fixed}} << \text{(statistical error)}$$

• Cumulant expansion

<...>P,F: expectation values fixed F and P.

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

cumulants

$$\left\langle \Theta \right\rangle_{C} = \left\langle \Theta \right\rangle_{P,F}, \quad \left\langle \Theta^{2} \right\rangle_{C} = \left\langle \Theta^{2} \right\rangle_{P,F} - \left\langle \Theta \right\rangle_{P,F}^{2}, \quad \left\langle \Theta^{3} \right\rangle_{C} = \left\langle \Theta^{3} \right\rangle_{P,F} - 3\left\langle \Theta^{2} \right\rangle_{P,F} \left\langle \Theta \right\rangle_{P,F} + 2\left\langle \Theta \right\rangle_{P,F}^{3}, \quad \left\langle \Theta^{4} \right\rangle_{C} = \cdots$$

- $\underbrace{Odd \ terms}_{Source \ of \ the \ complex \ phase} roma \ symmetry \ under \ \mu \leftrightarrow -\mu \ (\theta \leftrightarrow -\theta)$
- If the cumulant expansion converges, No sign problem.

Complex phase distribution

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



- 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 θ is from $-\infty$ to ∞ .

Distribution of the complex phase



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

2-flavor QCD Iwasaki gauge + clover Wilson quark action

Random noise method is used.

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

Distribution in a wide range

Reweighting method W_0 : distribution function in phase quenched simulations.



- Perform phase quenched simulations at several points.
 - Range of *F* is different.
- Change μ by reweighting method.
- Combine the data.

Distribution in a wide range: obtained.

The error of *R* is small because F is fixed.

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.