

Finite Density Lattice QCD by a Histogram Method

Shinji Ejiri



Niigata University

WHOT-QCD collaboration

S. Ejiri¹, S. Aoki², T. Hatsuda^{3,4}, K. Kanaya², Y. Maezawa⁵,
Y. Nakagawa¹, H. Ohno^{2,6}, H. Saito², and T. Umeda⁷

¹Niigata Univ., ²Univ. of Tsukuba, ³Univ. of Tokyo, ⁴RIKEN,
⁵BNL, ⁶Bielefeld Univ., ⁷Hiroshima Univ.

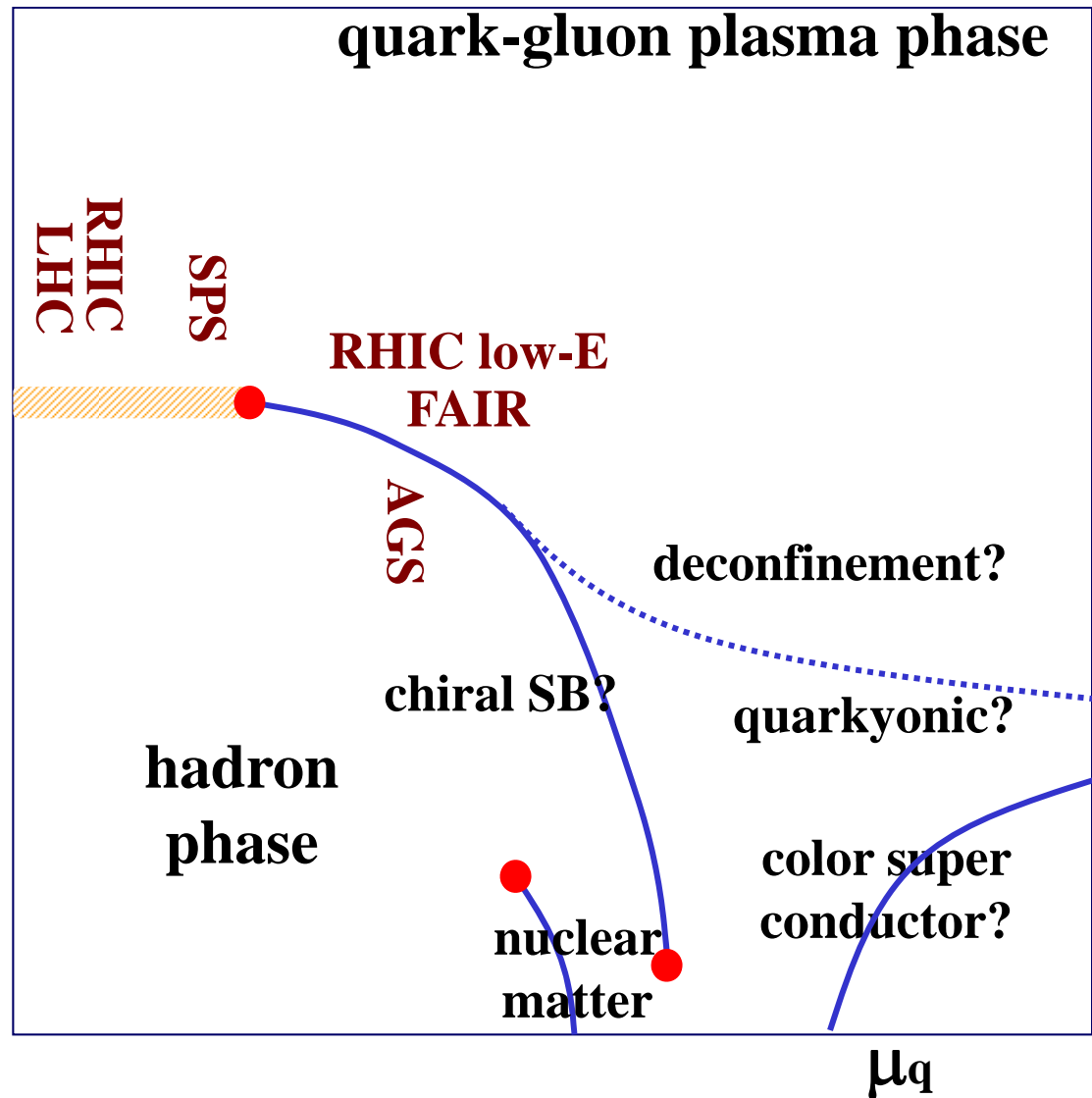
Workshop on Quarks and Hadrons under Extreme Conditions,
Keio, November 17-18, 2011

Phase structure of QCD at high temperature and density

Lattice QCD Simulations

- Phase transition lines
- Equation of state
- **Direct simulation:**
Impossible at $\mu \neq 0$.

T



Problems in simulations at $\mu \neq 0$

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

- Boltzmann weight: complex at $\mu \neq 0$
 - Configurations cannot be generated.
 - Monte-Carlo method is not applicable.

- Density of state method (Histogram method)

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

$$Z(m, T, \mu) = \int dX \underline{W(X, m, T, \mu)} \text{ histogram}$$

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

- Expectation values

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

- $W(X)$ can be defined even when $\det M$ is complex. \longrightarrow Sign problem

Sign problem

$$\begin{aligned} W(X') &= \int DU \delta(X - X') (\det M(m, \mu))^{N_f} e^{-S_g} \\ &= \int DU \delta(X - X') \underbrace{e^{i\theta} |\det M(m, \mu)|^{N_f}} e^{-S_g} \end{aligned}$$

generate the configuration
with this weight

θ : complex phase of $\det M$

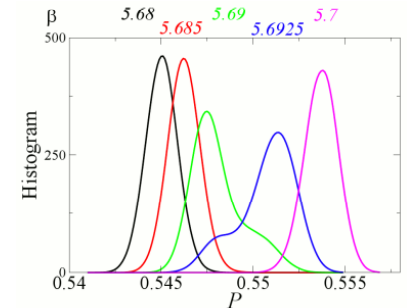
- Sign problem: If $e^{i\theta}$ changes its sign frequently,

$$W(X) \sim \left\langle e^{i\theta} \right\rangle_{X \text{ fixed}} \ll (\text{statistical error})$$

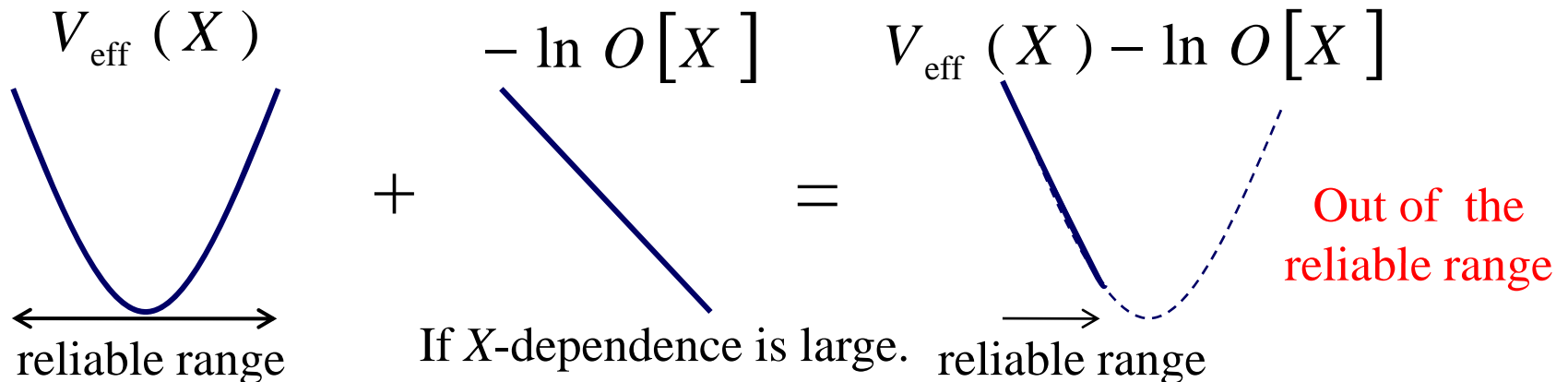
Overlap problem

$$\langle O[X] \rangle = \frac{1}{Z} \int O[X] W(X) dX = \frac{1}{Z} \int \exp(-V_{\text{eff}}(X) + \ln O[X]) dX$$

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



- W is computed from the histogram.
- Distribution function around X where $V_{\text{eff}}(X) - \ln O[X]$ is minimized: important.
- V_{eff} must be computed in a wide range.



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

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

a_0 : start point $p=0$

- Pressure at $\mu \neq 0$ $\frac{p}{T^4}(\mu) - \frac{p}{T^4}(0) = \frac{1}{VT^3} \ln \left(\frac{Z(\mu)}{Z(0)} \right) = \left(\frac{N_t}{N_s} \right)^3 \ln \left\langle \frac{\det M(\mu)}{\det M(0)} \right\rangle_{\mu=0}$

- Calculation of $\langle P \rangle$ and $\langle \det M(\mu) / \det M(0) \rangle$: required.

Distribution function for Equation of state

$$W(P', F', T, m, \mu) = \int DU \delta(P - P') \delta(F - F') (\det M(m, \mu))^{N_f} e^{-S_g}$$

or
$$W(P', T, m, \mu) = \int DU \delta(P - P') (\det M(m, \mu))^{N_f} e^{-S_g}$$

$$S_g = -6N_{\text{site}}\beta P, \quad Z(m, T, \mu) = \int dP dF W(P, F, m, T, \mu)$$

$$F \equiv N_f \ln |\det M(\mu) / \det M(0)|,$$

- We propose a method for the calculation of this W .
 - We must calculate W in a wide range of P and F .
 - The sign problem must be solved to obtain W .
- Once we get the pressure, we can calculate

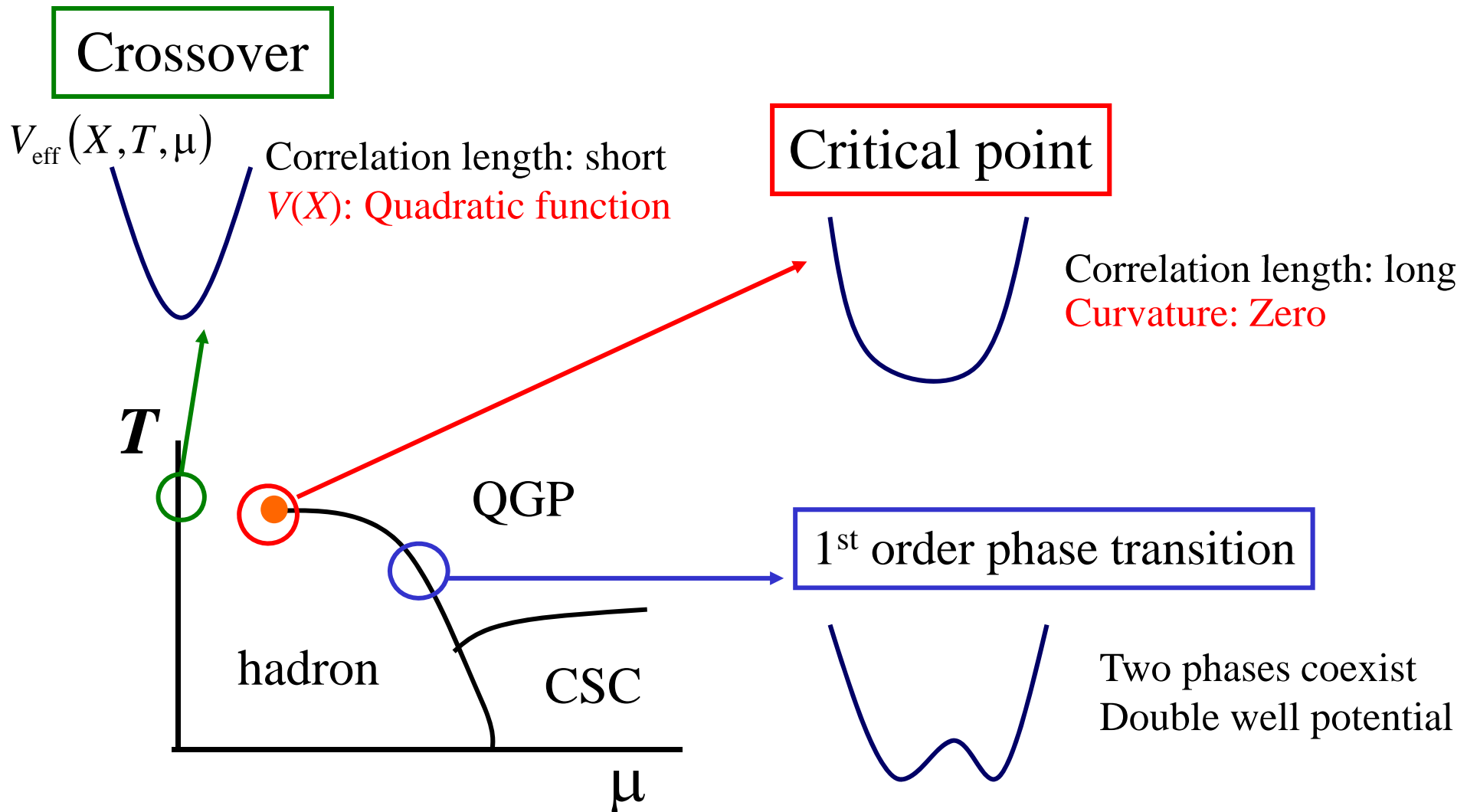
$$\frac{n}{T^3} = \frac{\partial(P/T^4)}{\partial(\mu/T)}, \quad \frac{\chi_q}{T^3} = \frac{\partial^2(P/T^4)}{\partial(\mu/T)^2} \text{ etc.}$$

Critical point search

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, quark determinant etc.

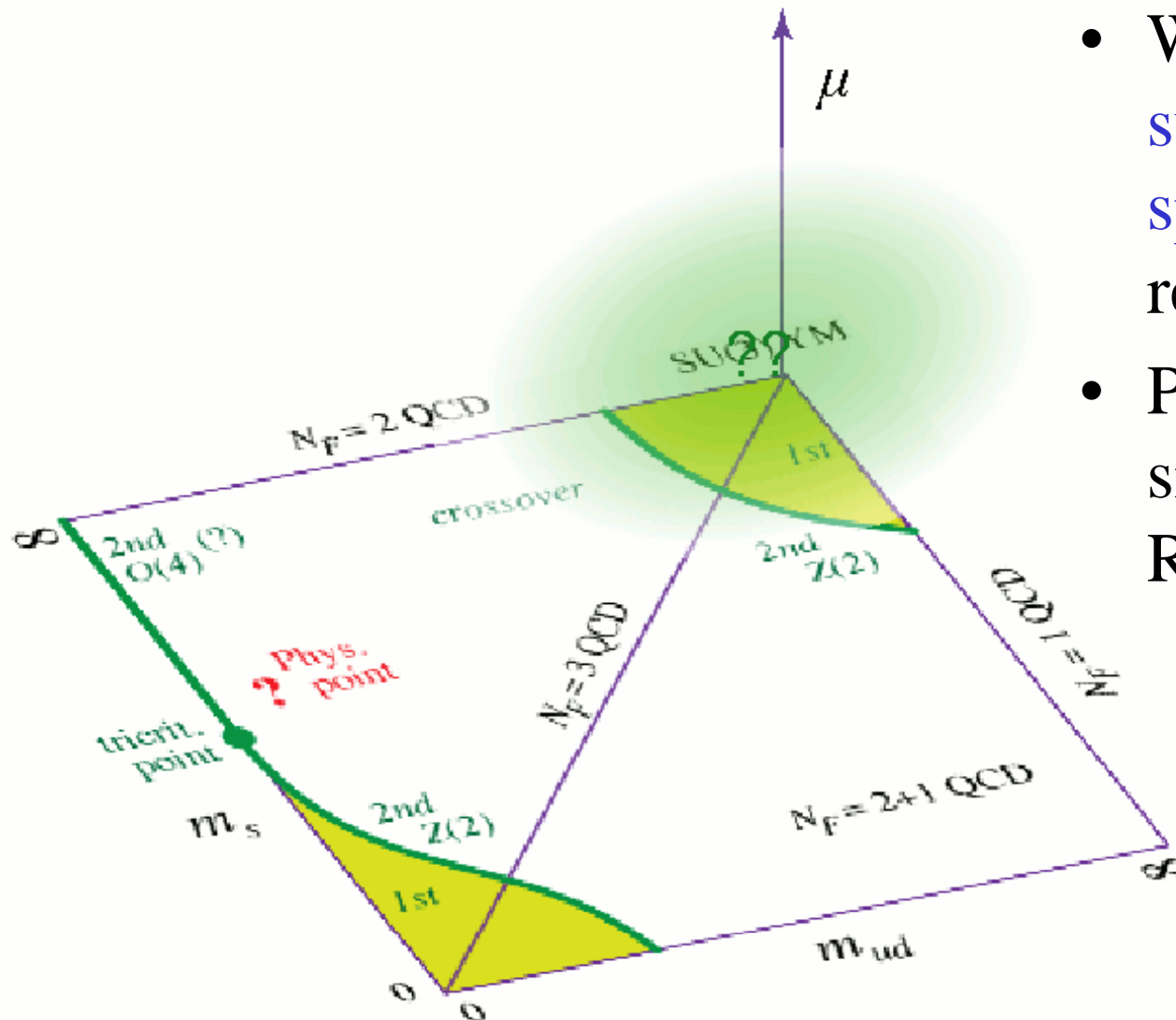


Plan of this talk

- Introduction: Distribution function
- Test in the heavy quark region
- Application to the light quark region at finite density

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.

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

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

$$W(P', \beta, m, \mu) \equiv \int DU \delta(P-P') (\det M(m, \mu))^{N_f} e^{6N_{\text{site}} P}$$

$$R(P, \beta, \beta_0, m, m_0, \mu) \equiv W(P, \beta, m, \mu) / W(P, \beta_0, m_0, 0) \quad \text{(Reweight factor)}$$

$$R(P') = e^{6N_{\text{site}}(\beta - \beta_0)P'} \frac{\left\langle \delta(P-P') \left(\frac{\det M(m, \mu)}{\det M(m_0, 0)} \right)^{N_f} \right\rangle_{(\beta_0, \mu=0)}}{\langle \delta(P-P') \rangle_{(\beta_0, \mu=0)}} \equiv e^{6N_{\text{site}}(\beta - \beta_0)P'} \left\langle \left(\frac{\det M(m, \mu)}{\det M(m_0, 0)} \right)^{N_f} \right\rangle_{P'}$$

Effective potential:

$$V_{\text{eff}}(P, \beta, m, \mu) = -\ln[W(P, \beta, m, \mu)] = V_{\text{eff}}(P, \beta_0, m_0, 0) - \ln R(P, \beta, \beta_0, m, m_0, \mu)$$

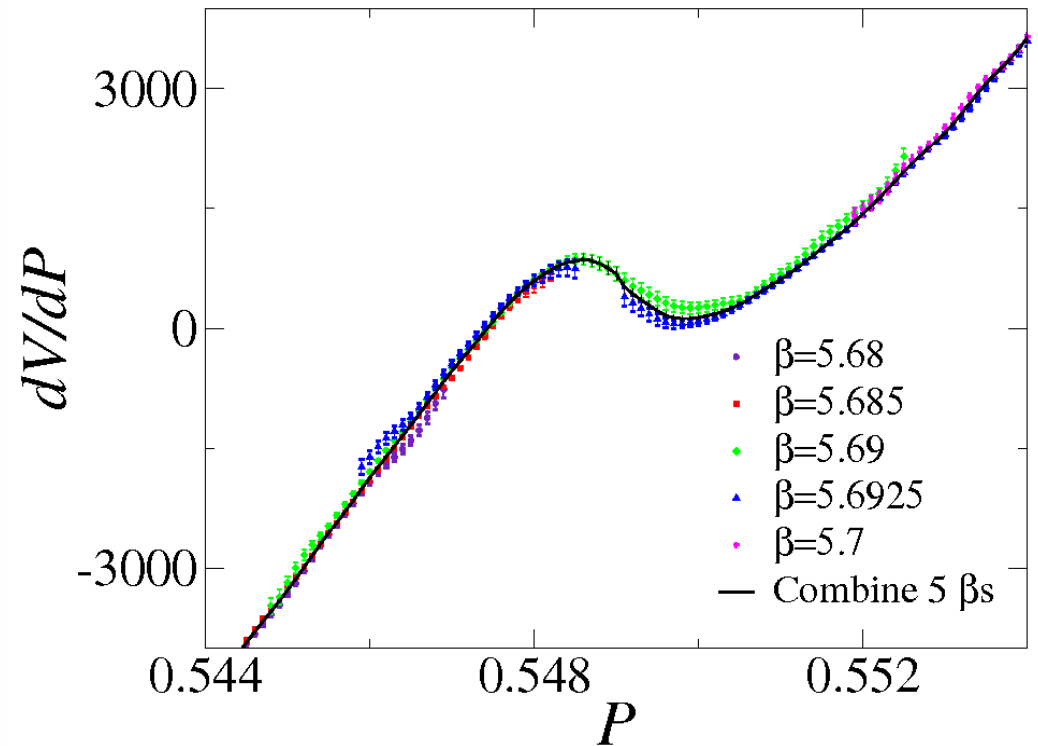
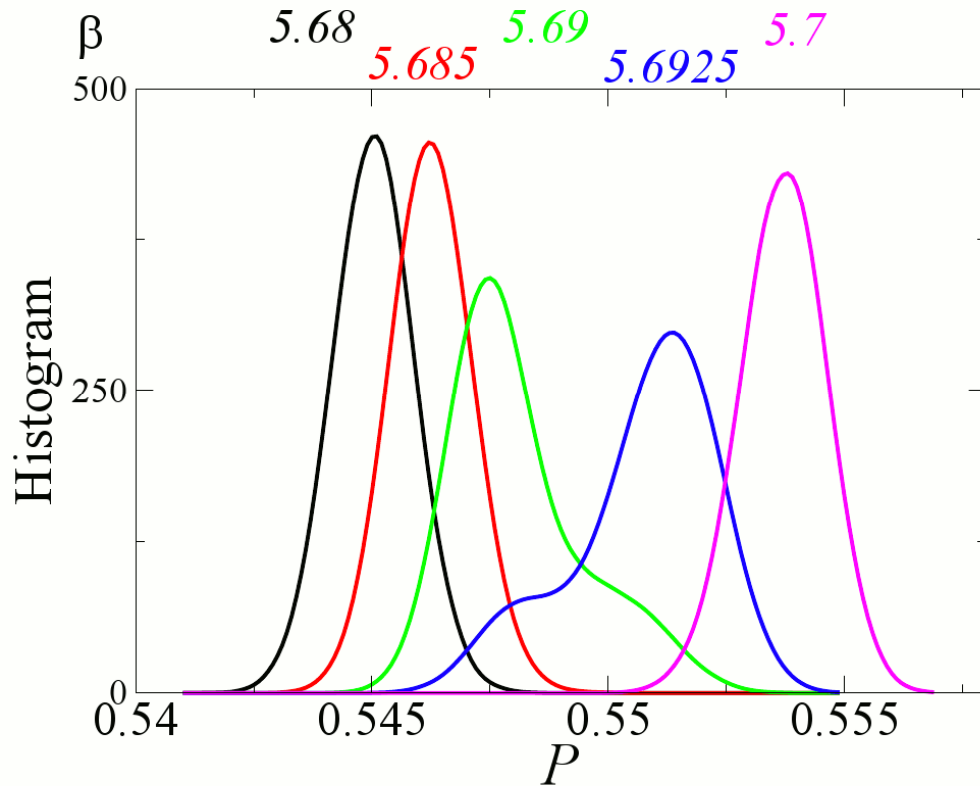
$$\ln R(P) = \underline{6N_{\text{site}}(\beta - \beta_0)P} + \ln \left\langle \left(\frac{\det M(m, \mu)}{\det M(m_0, 0)} \right)^{N_f} \right\rangle_P$$

Solving the overlap problem

Effective potential in a wide range of P : required.

Plaquette histogram at $K=1/m_q=0$.

Derivative of V_{eff} at $\beta=5.69$



$N_{\text{site}} = 24^3 \times 4$, 5 β points, quenched.

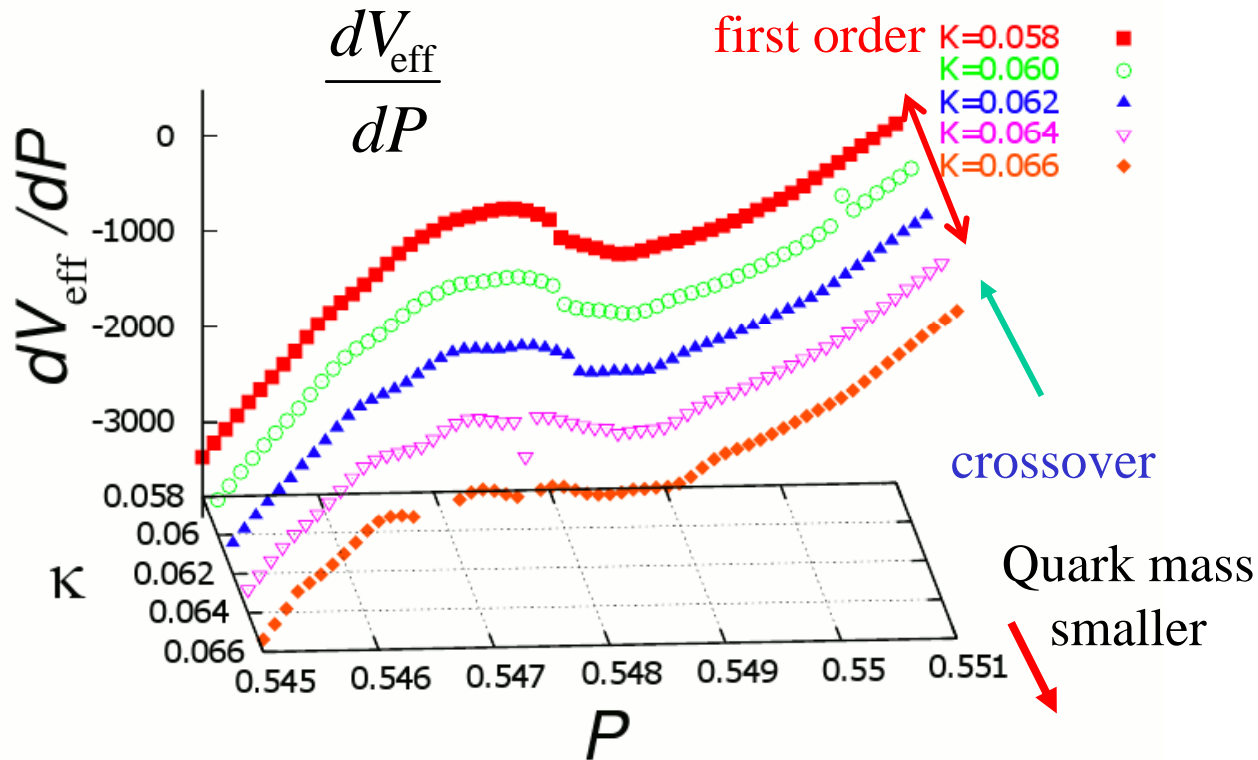
dV_{eff}/dP is adjusted to $\beta=5.69$, using

$$\frac{dV_{\text{eff}}}{dP}(\beta_2) = \frac{dV_{\text{eff}}}{dP}(\beta_1) - 6N_{\text{site}}(\beta_2 - \beta_1)$$

These data are combined by taking the average.

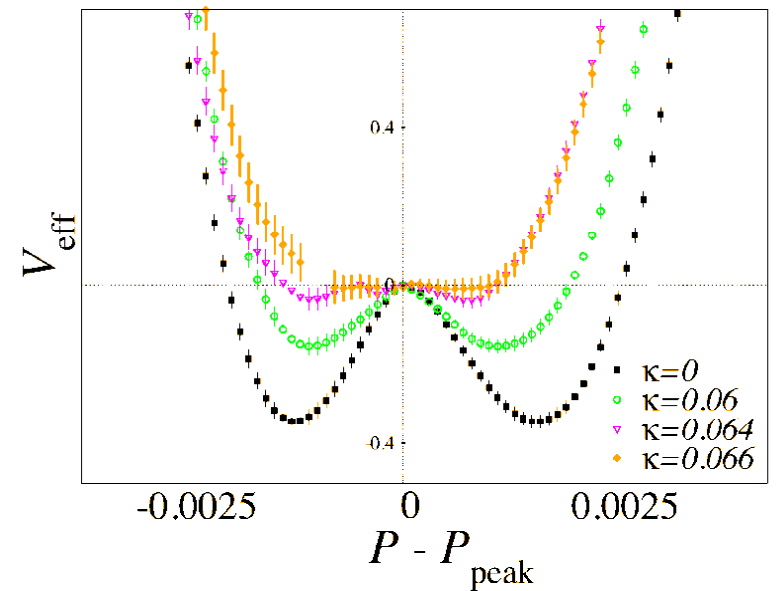
Effective potential near the quenched limit

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



Quenched Simulation
($m_q = \infty$, $K=0$)

$K \sim 1/m_q$ for large m_q



$24^3 \times 4$ lattice, 5 β points, $N_f=2$

- detM: Hopping parameter expansion,

$$N_f \ln \left(\frac{\det M(K)}{\det M(0)} \right) = N_f \left(288 N_{\text{site}} K^4 P + 12 \times 2^{N_t} N_s^3 K^{N_t} \underline{\Omega_R} + \dots \right)$$

real part of Polyakov loop

$$N_f=2: K_{cp}=0.0658(3)(8)$$

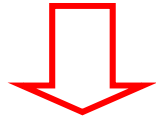
$$\frac{T_c}{m_\pi} \approx 0.02$$

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

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

$$N_f=2: K_{cp}=0.0658(3)(8)$$

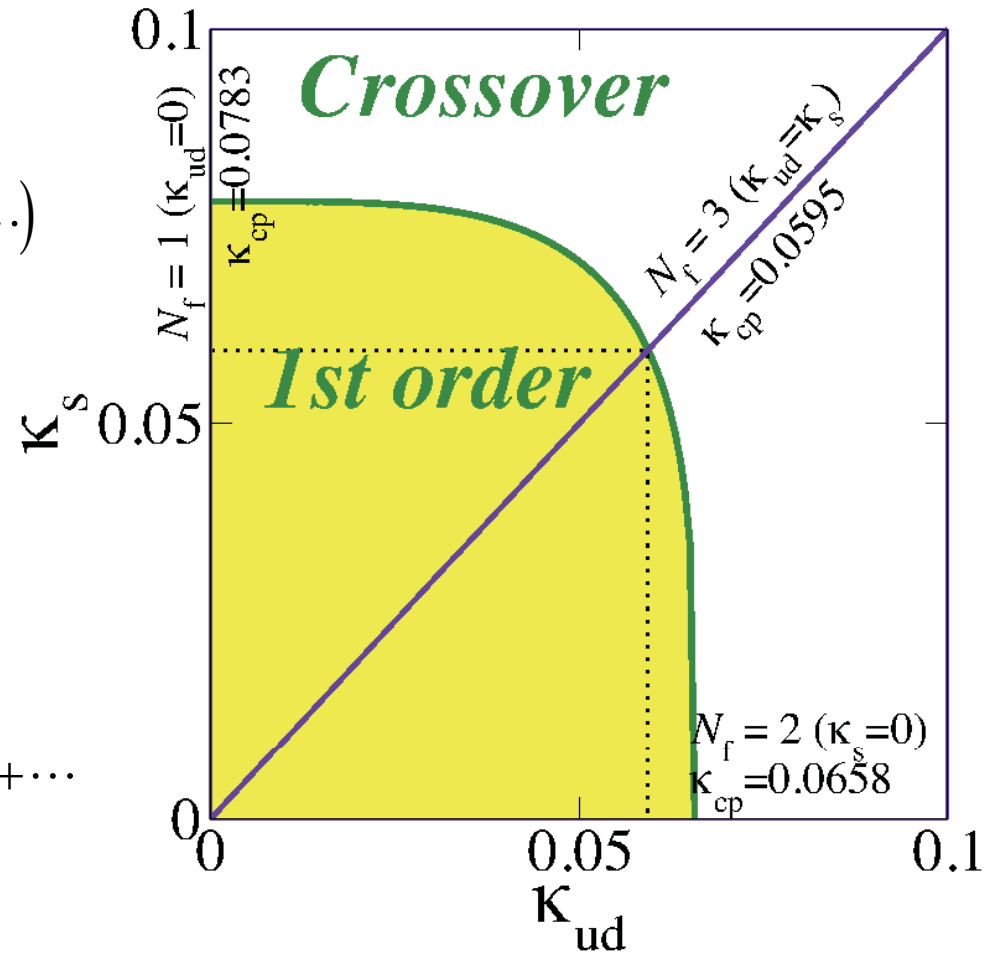
$$2\ln\left(\frac{\det M(K)}{\det M(0)}\right) = 2\left(288N_{site}K^4P + 12 \times 2^{N_t} N_s^3 K^{N_t} \Omega_R + \dots\right)$$



$$N_f=2+1$$

$$\ln\left[\frac{(\det M(K_{ud}))^2 \det M(K_s)}{(\det M(0))^3}\right]$$

$$= 288N_{site} \left(2K_{ud}^4 + K_s^4\right)P + 12 \times 2^{N_t} N_s^3 \left(2K_{ud}^{N_t} + K_s^{N_t}\right)\Omega_R + \dots$$



The critical line is described by

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

Finite density QCD in the heavy quark region

$$U_4(x) \Rightarrow e^{\mu_q a} U_4(x), \quad U_4^\dagger(x) \Rightarrow e^{-\mu_q a} U_4^\dagger(x) \quad \text{in } \det M$$



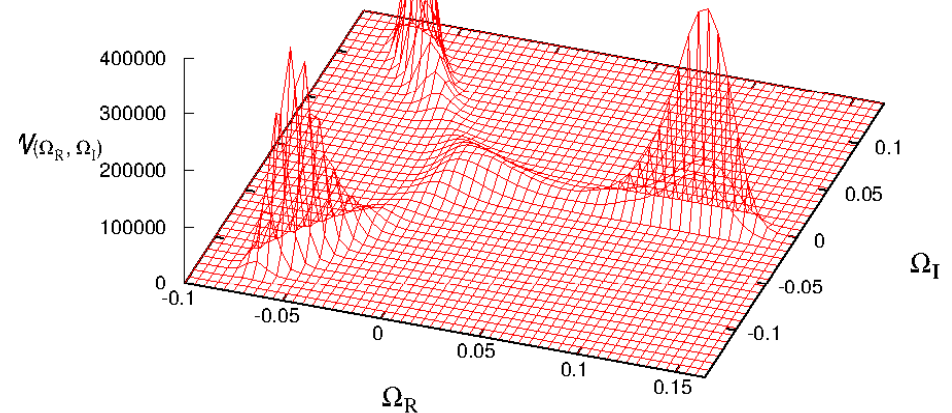
$$\Omega \Rightarrow e^{\mu_q/T} \Omega, \quad \Omega^* \Rightarrow e^{-\mu_q/T} \Omega^* \quad \text{Polyakov loop}$$

$$\begin{aligned} N_f \ln \left(\frac{\det M(K, \mu)}{\det M(0, 0)} \right) &= N_f \left(288 N_{\text{site}} K^4 P + 6 \cdot 2^{N_t} N_s^3 K^{N_t} \left(e^{\mu/T} \Omega + e^{-\mu/T} \Omega^* \right) + \dots \right) \\ &= N_f \left(288 N_{\text{site}} K^4 P + 12 \cdot 2^{N_t} N_s^3 K^{N_t} \left(\cosh(\mu/T) \Omega_R + \underline{i \sinh(\mu/T) \Omega_I} \right) + \dots \right) \end{aligned}$$

phase

Polyakov loop
distribution

$$\Omega = \Omega_R + i\Omega_I$$



- We can extend this discussion to finite density QCD.

Phase quenched simulations, Isospin chemical potential

$$(N_f=2), \mu_u = -\mu_d.$$

$$\det M(K, -\mu) = [\det M(K, \mu)]^*$$

$$|\det M(K, \mu)|^2 = \det M(K, \mu) \det M(K, -\mu)$$

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

- If the complex phase is neglected,

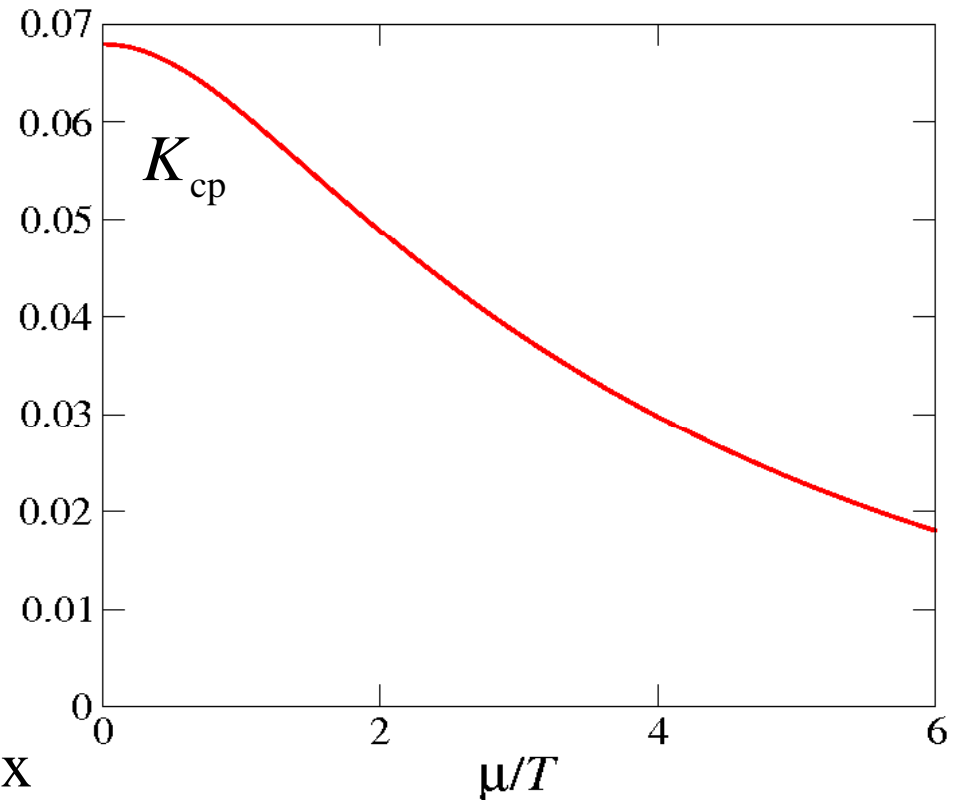
$$K^{N_t} \Rightarrow K^{N_t} \cosh(\mu/T)$$

- Critical point:

$$\underline{K_{\text{cp}}^{N_t}(\mu) \cosh(\mu/T) = K_{\text{cp}}^{N_t}(0)}$$

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

- Even if we add the effect from the complex phase, it is small for the determination of K_{cp} . (WHOT-QCD Collab., in preparation, 11)



$$\leftarrow \theta \propto K^{N_t} \sinh(\mu/T)$$

Distribution function in the light quark region

WHOT-QCD Collaboration, in preparation, (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:

$$|\det M(m, \mu)|^{N_f} e^{-S_g}$$

$$\begin{aligned} W(P', F', \beta, m, \mu) &= \int DU \delta(P - P') \delta(F - F') (\det M(m, \mu))^{N_f} e^{-S_g} \\ &= \int DU \delta(P - P') \delta(F - F') e^{i\theta} |\det M(m, \mu)|^{N_f} e^{-S_g} \\ &= \underbrace{\langle e^{i\theta} \rangle}_{P', F'} \times \underbrace{W_0(P', F', \beta, m, \mu)} \end{aligned}$$

expectation value with fixed P, F histogram

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

Distribution function
of the phase quenched.

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

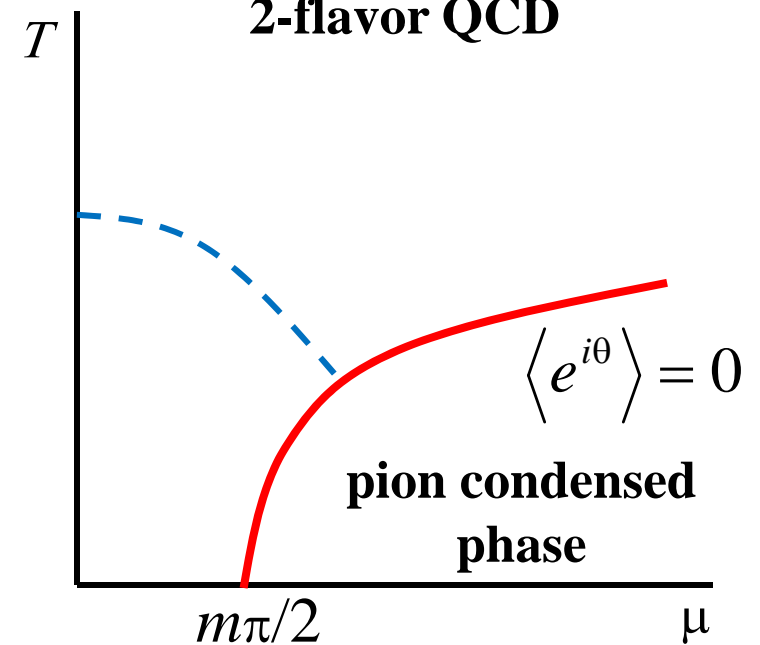
Phase quenched simulation

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

$$|\det M(K, \mu)|^2 = \det M(K, \mu) \det M(K, -\mu)$$

- When $\mu_u = -\mu_d$, pion condensation occurs.
- $\langle e^{i\theta} \rangle = 0$ is suggested in the pion condensed phase by phenomenological studies. [Han-Stephanov '08, Sakai et al. '10]
- **→ No overlap between $W(\mu)$ and $W_0(\mu)$.**
- Tail of the distribution W_0 is important.
 - Computed by simulations **out of the pion condensed phase.**
- The calculations of W_0 in a wide range of (P, F) is very important.

Phase structure of the phase quenched 2-flavor QCD



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,

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

- Cumulant expansion $\langle \dots \rangle_{P,F}$: expectation values fixed F and P .

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

cumulants

$$\langle \theta \rangle_C = \langle \theta \rangle_{P,F}, \quad \langle \theta^2 \rangle_C = \langle \theta^2 \rangle_{P,F} - \langle \theta \rangle_{P,F}^2, \quad \langle \theta^3 \rangle_C = \langle \theta^3 \rangle_{P,F} - 3 \langle \theta^2 \rangle_{P,F} \langle \theta \rangle_{P,F} + 2 \langle \theta \rangle_{P,F}^3, \quad \langle \theta^4 \rangle_C = \dots$$

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

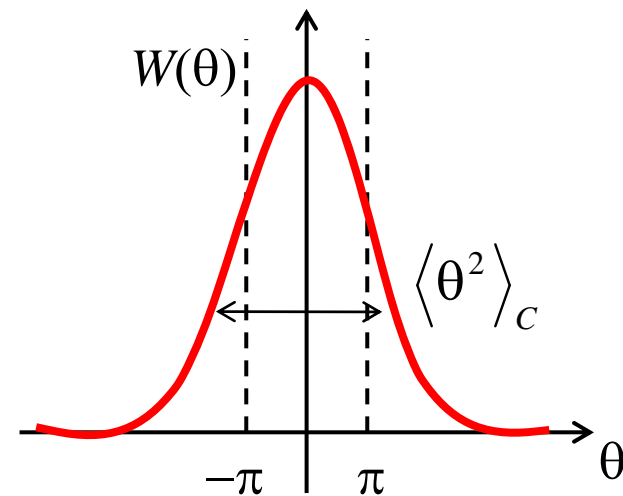
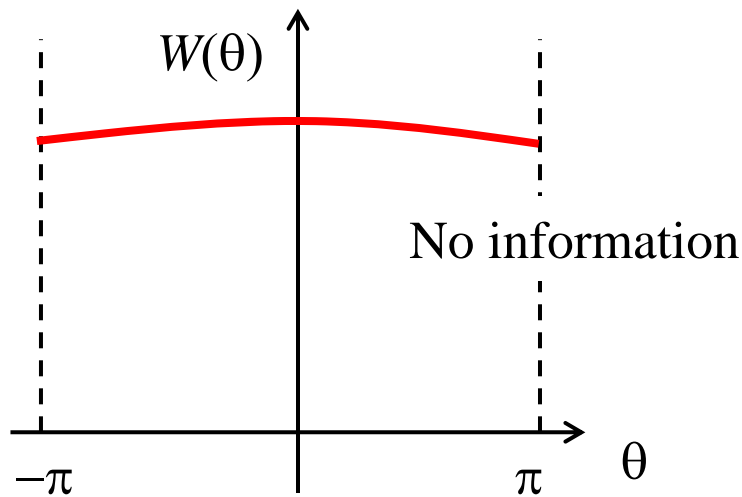
Source of the complex phase

If the cumulant expansion converges, No sign problem.

Distribution of the complex phase

- 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),

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



Complex phase

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

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

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

- At the same time, we calculate F as a function of μ ,

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

- The reweighting factor is also computed,

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

$$R(P, F) = \frac{W_0(P, F, \mu)}{W_0(P, F, \mu_0)} = \left\langle \left| \frac{\det M(\mu)}{\det M(\mu_0)} \right|^{N_f} \right\rangle_{P, F \text{ fixed}}$$

F and C are strongly correlated. $\rightarrow R$: small error

Integral method for the calculation of the quark determinant

$$\frac{\partial \ln \det M}{\partial(\mu/T)}$$

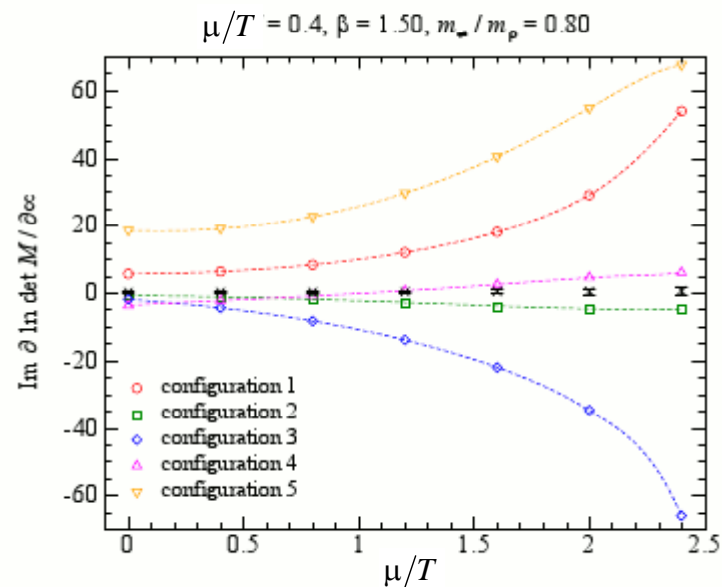
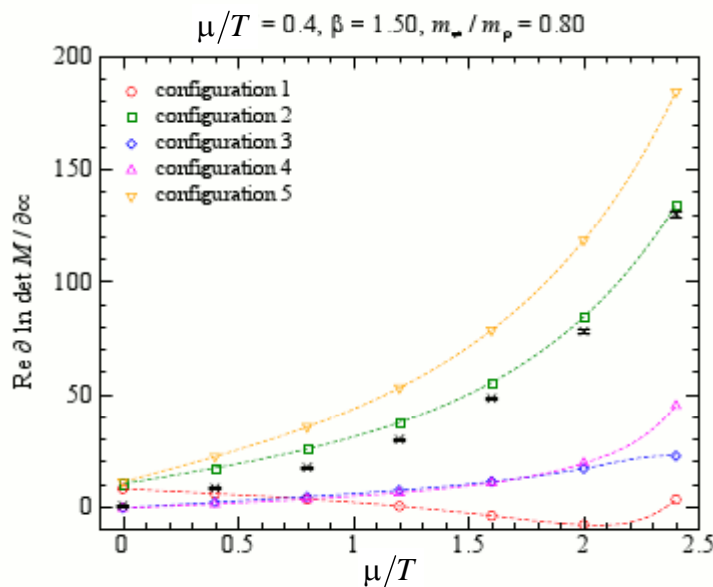
$8^3 \times 4$ lattice

$\beta = 1.50$

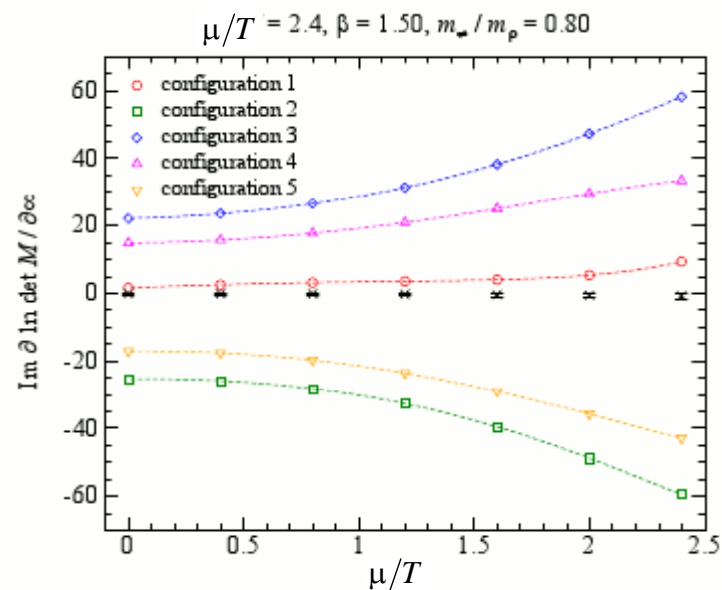
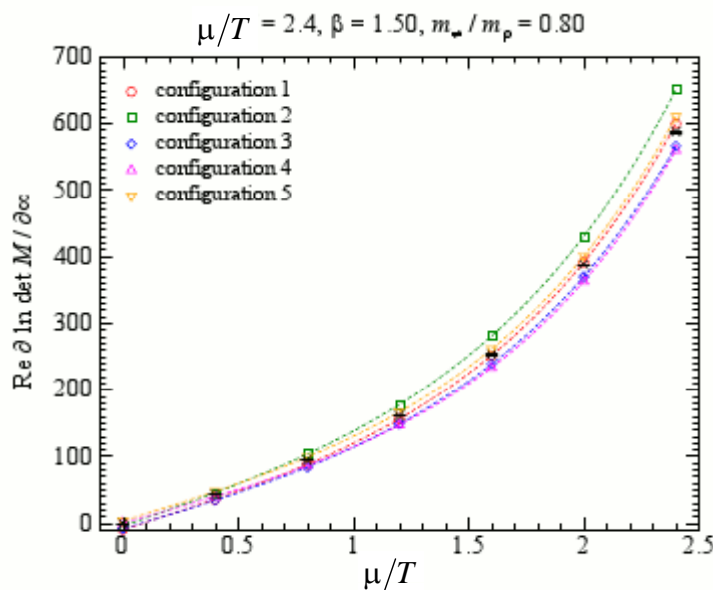
$m_\pi/m_\rho = 0.8$

2-flavor QCD
Iwasaki gauge
+ clover Wilson
quark action

Random noise
method is used.



$\mu/T = 0.4$

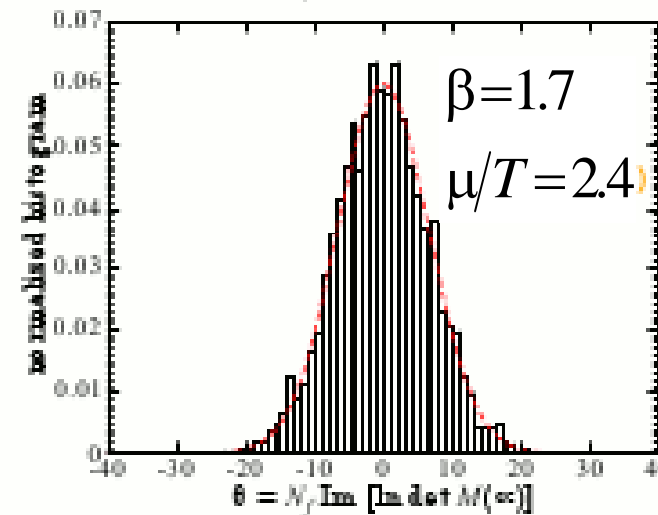
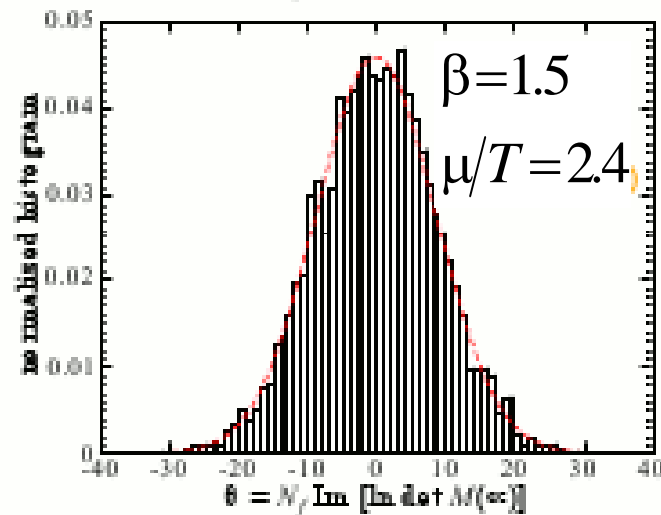
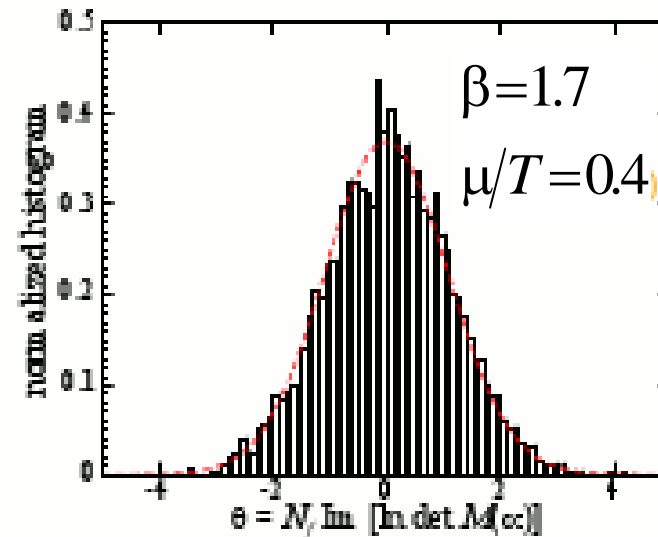
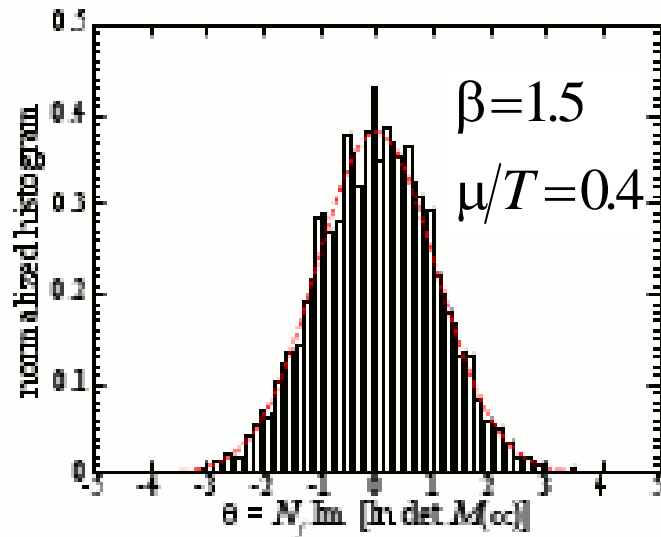


$\mu/T = 2.4$

Real part

Imaginary part

Distribution of the complex phase



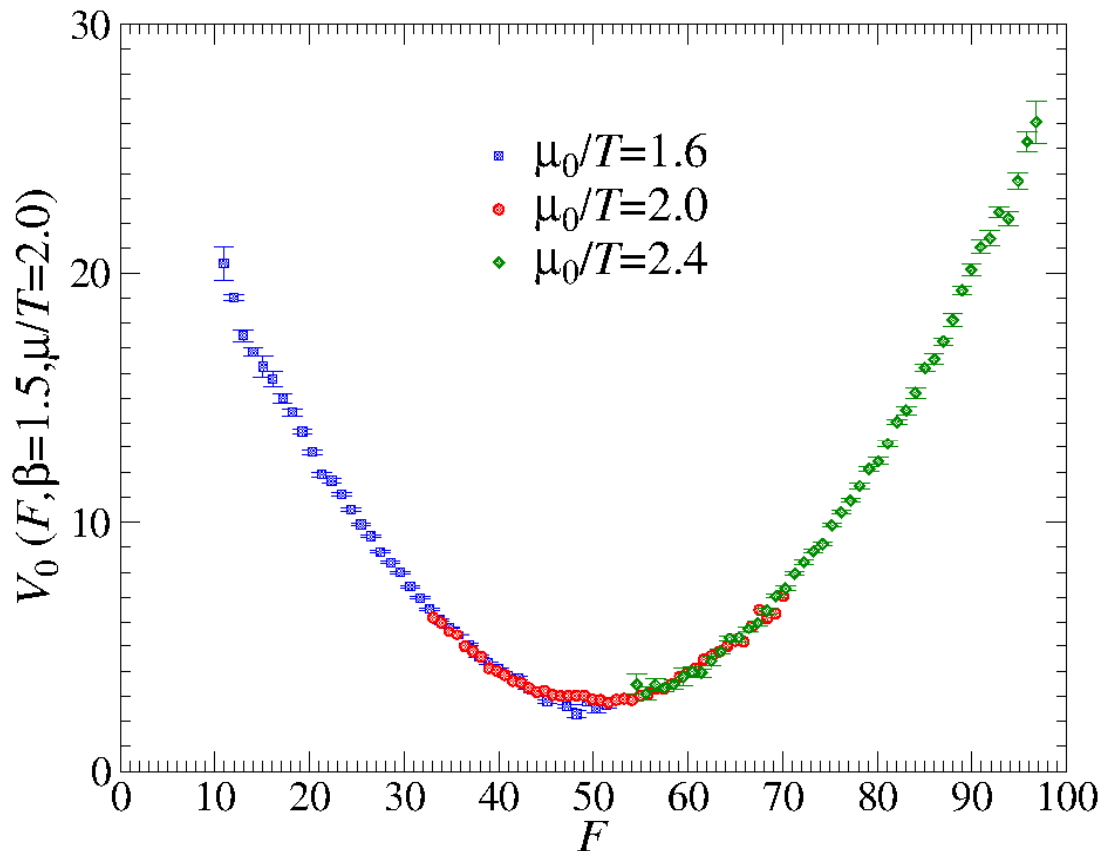
- Well approximated by a Gaussian function.
- Convergence of the cumulant expansion: good.

Overlap problem

Reweighting method

W_0 : distribution function in phase quenched simulations.

$$R(P, F) = \frac{W_0(P, F, \mu)}{W_0(P, F, \mu_0)} = \left\langle \left| \frac{\det M(\mu)}{\det M(\mu_0)} \right|^{N_f} \right\rangle_{P, F \text{ fixed}}$$



$$-\ln W_0(P, F, \mu_0) - \ln R(P, F, \mu, \mu_0) = -\ln W_0(P, F, \mu)$$

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



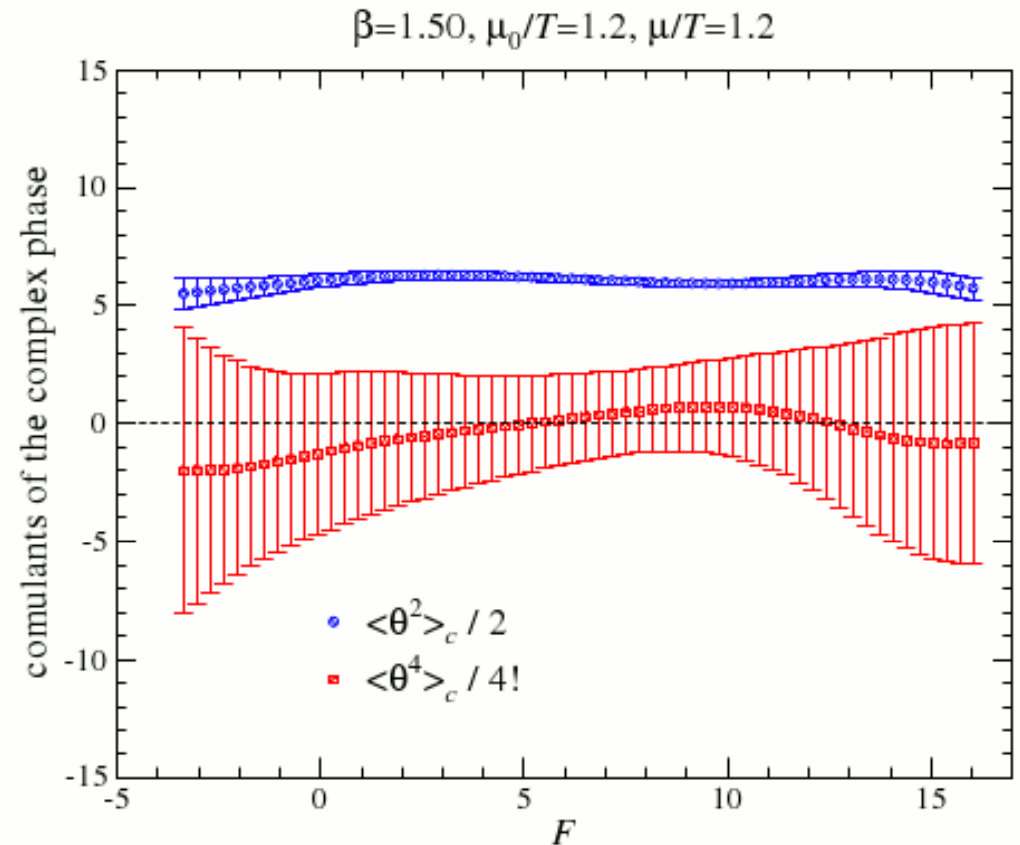
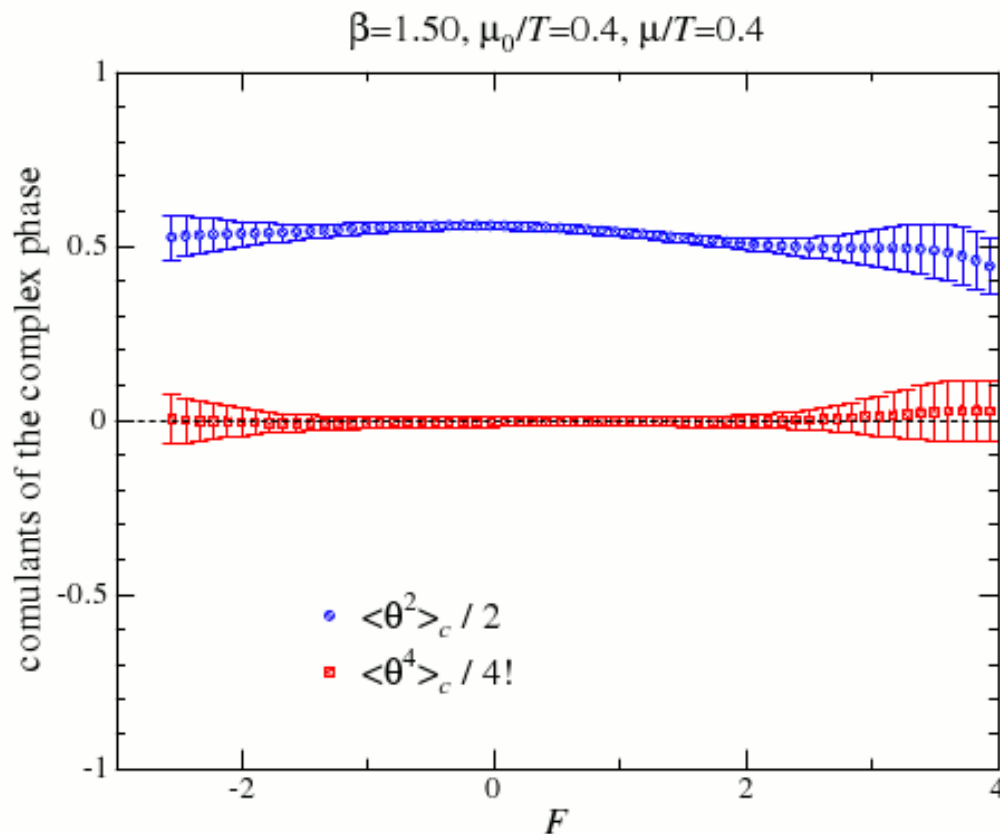
Distribution in a wide range:
obtained.

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

Convergence of the cumulant expansion

F -dependence of the 2nd and 4th order cumulants of the complex phase

Preliminary

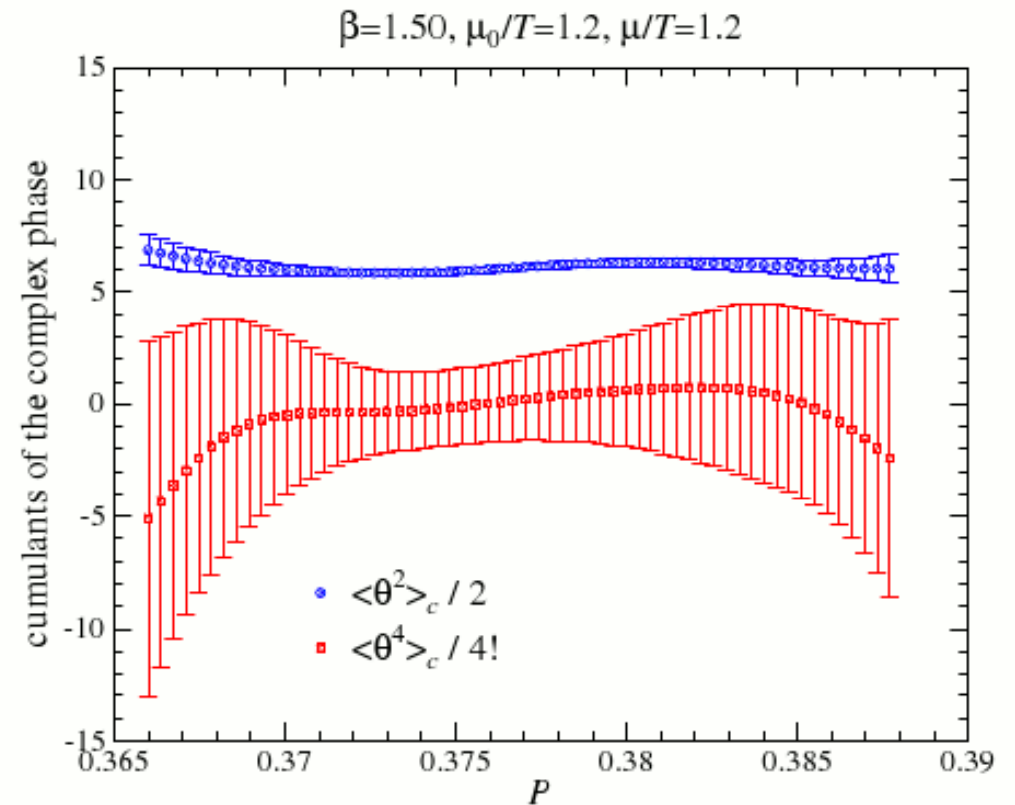
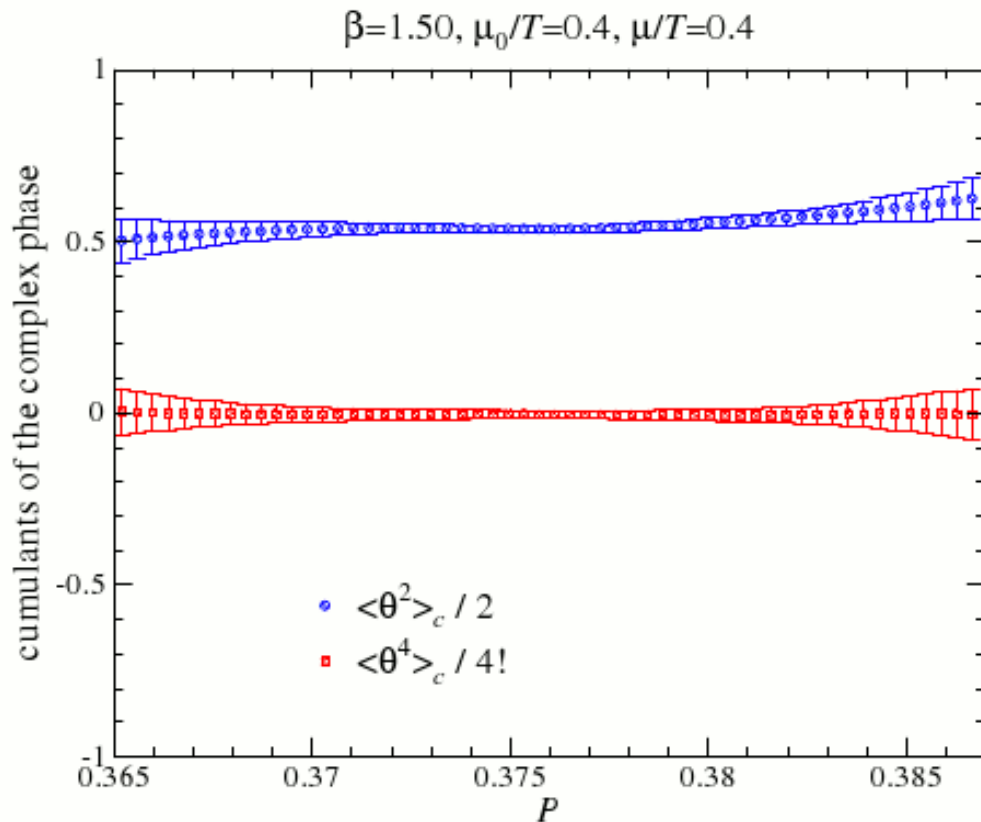


Preliminary

- 4th order cumulant is consistent with zero.

Convergence of the cumulant expansion

P -dependence of the 2nd and 4th order cumulants of the complex phase



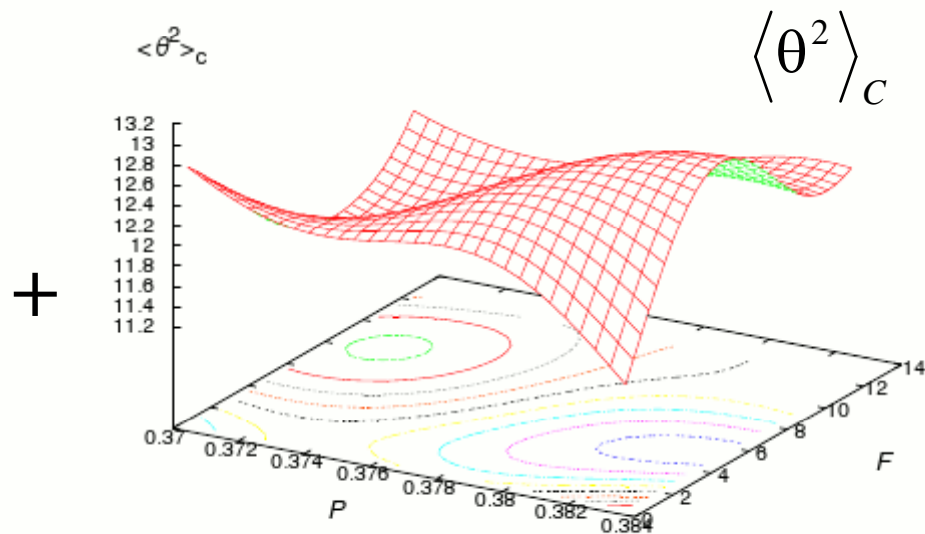
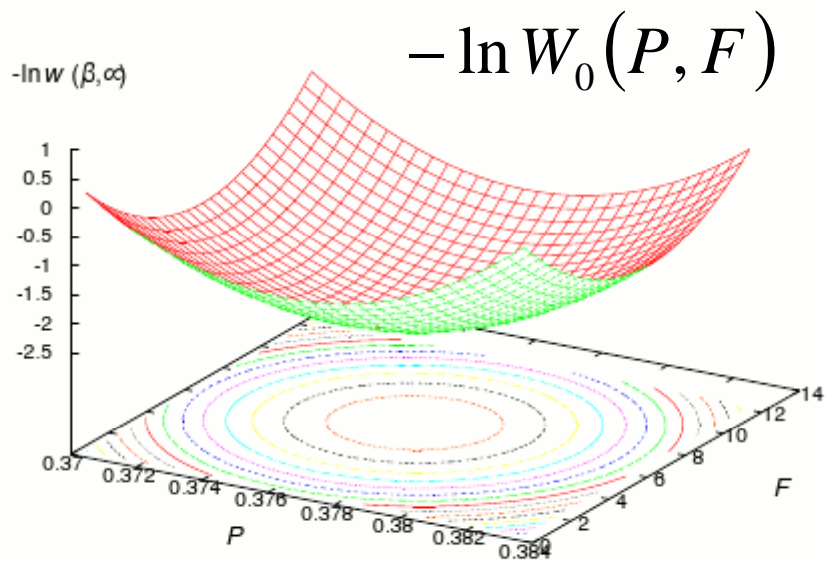
Preliminary

- 4th order cumulant is consistent with zero.

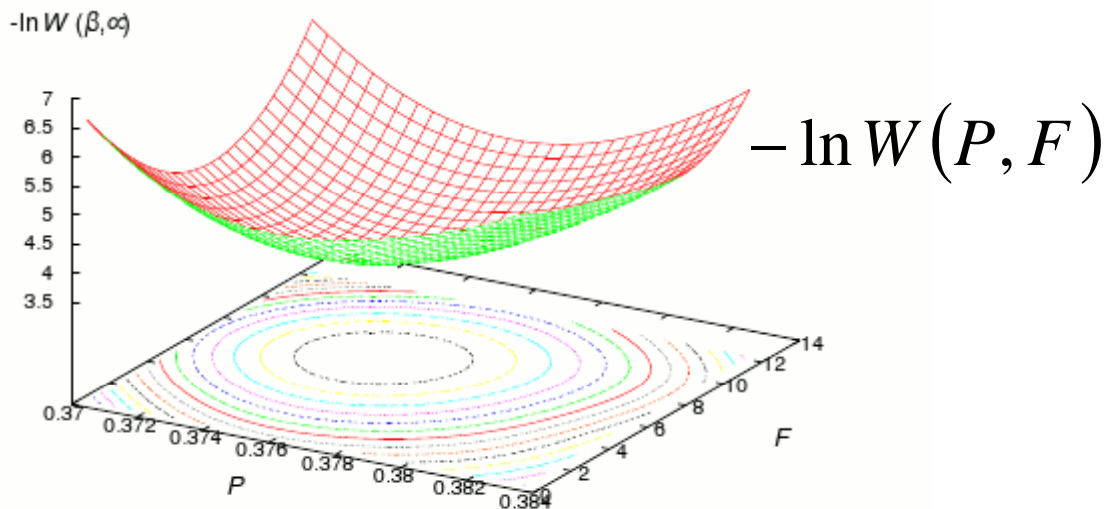
Effective potential at finite μ

- Combine V_0 and the phase factor.

Preliminary



$\times 0.5$



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Summary

- We studied the quark mass and chemical potential dependence of QCD phase transition in the heavy quark region.
- The histogram method is used to investigate the nature of the phase transition.
- To avoid the sign problem, the method based on the cumulant expansion of θ is useful.
- Further studies in light quark region are important applying this method.