Numerical Study of QCD Phase Diagram at High Temperature and Density by a Histogram Method

Shinji Ejiri

Niigata University

WHOT-QCD collaboration

S. Ejiri[1], S. Aoki[2], T. Hatsuda[3,4], K. Kanaya[2], Y. Maezawa[5],
Y. Nakagawa[1], H. Ohno[2,6], H. Saito[2], and T. Umeda[7]

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

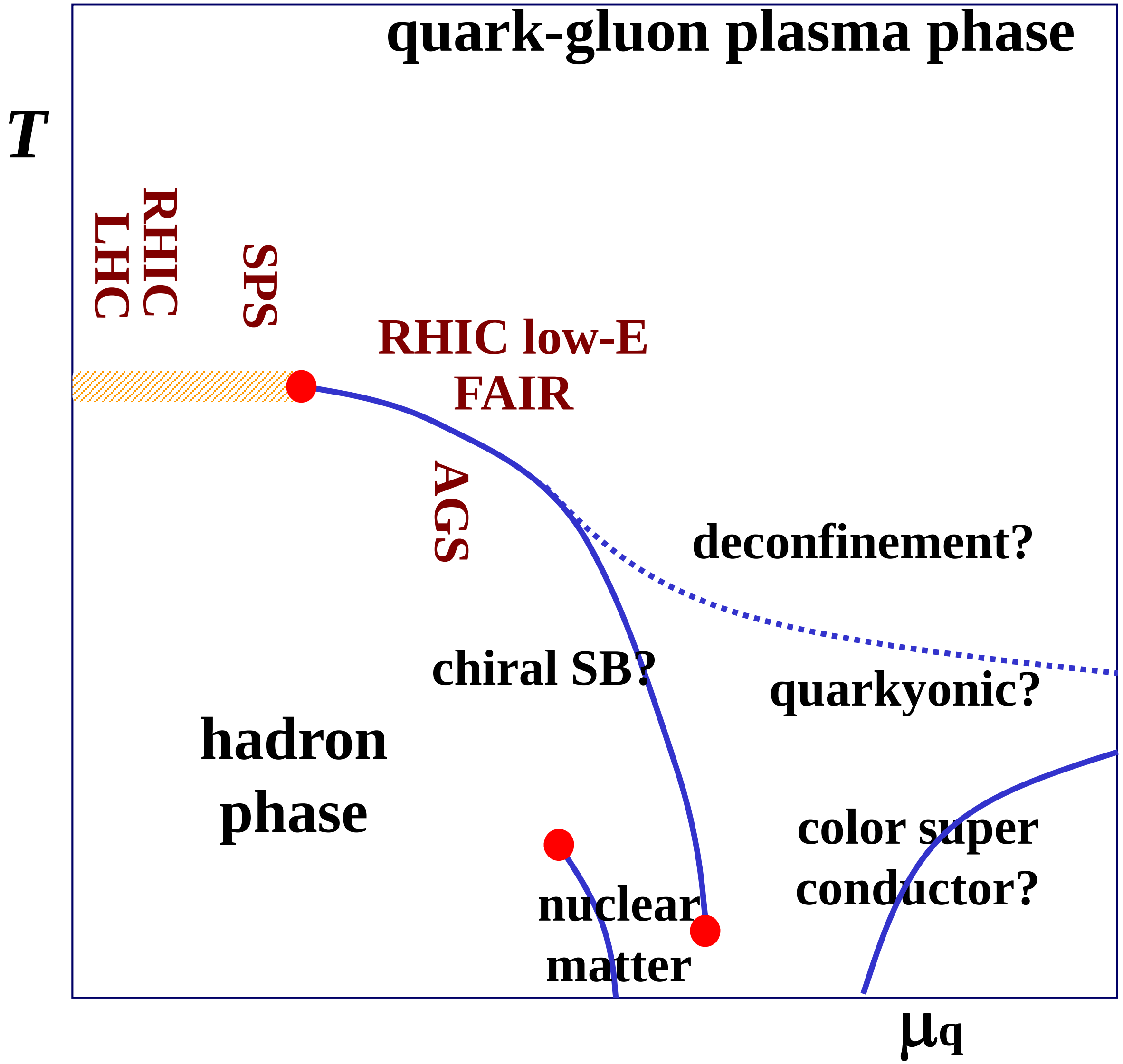
CPOD 2011, Wuhan, November 7-11, 2011

Phase structure of QCD at high temperature and density

Lattice QCD Simulations

- Phase transition lines
- Equation of state

- Direct simulation:
  Impossible at $\mu \neq 0$.



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.

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

histogram

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

- Expectation values

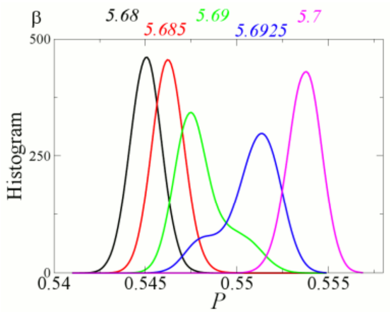
$$\langle O[X] \rangle_{(m,T,\mu)} = \frac{1}{Z} \int dX\, O[X] W(X,m,T,\mu)$$

- Sign problem: det*M* changes its sign $\rightarrow$ the error of *W*: large.

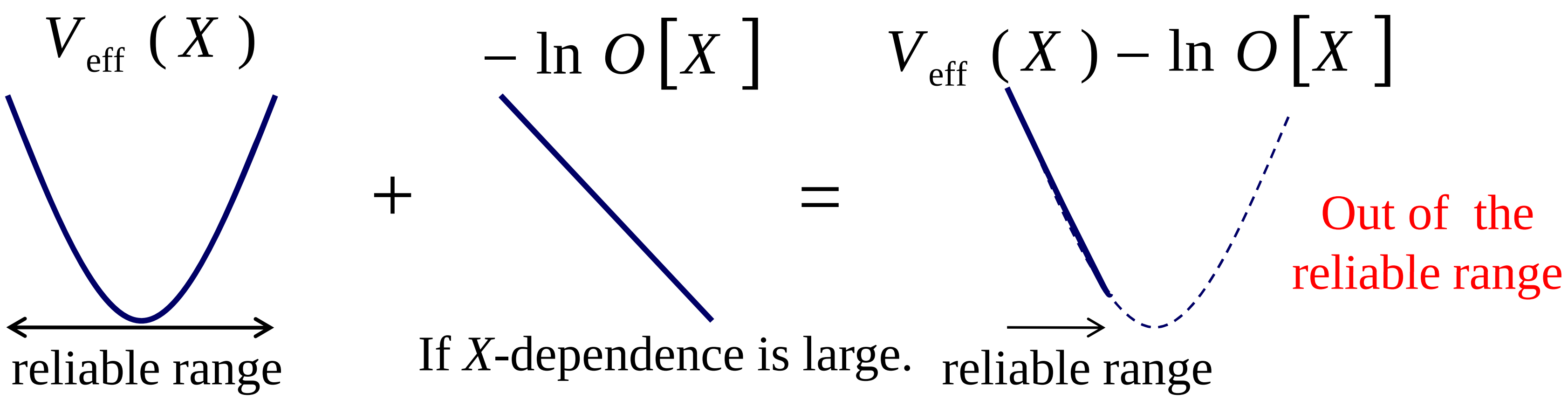
Overlap problem

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

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



- 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 μ=0 $$\frac{p}{T^4} = \frac{1}{VT^3}\ln Z$$
    - Integral $$\left.\frac{p}{T^4}\right|_a - \left.\frac{p}{T^4}\right|_{a_0} = -\int_{a_0}^{a}\frac{\varepsilon' - 3p'}{T'^4}\,d(\ln a')$$

      a0: 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 $$W(P', T, m, \mu) = \int DU \ \delta(P - P')(\det M(m, \mu))^{N_f} \ e^{-S_g}$$

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

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

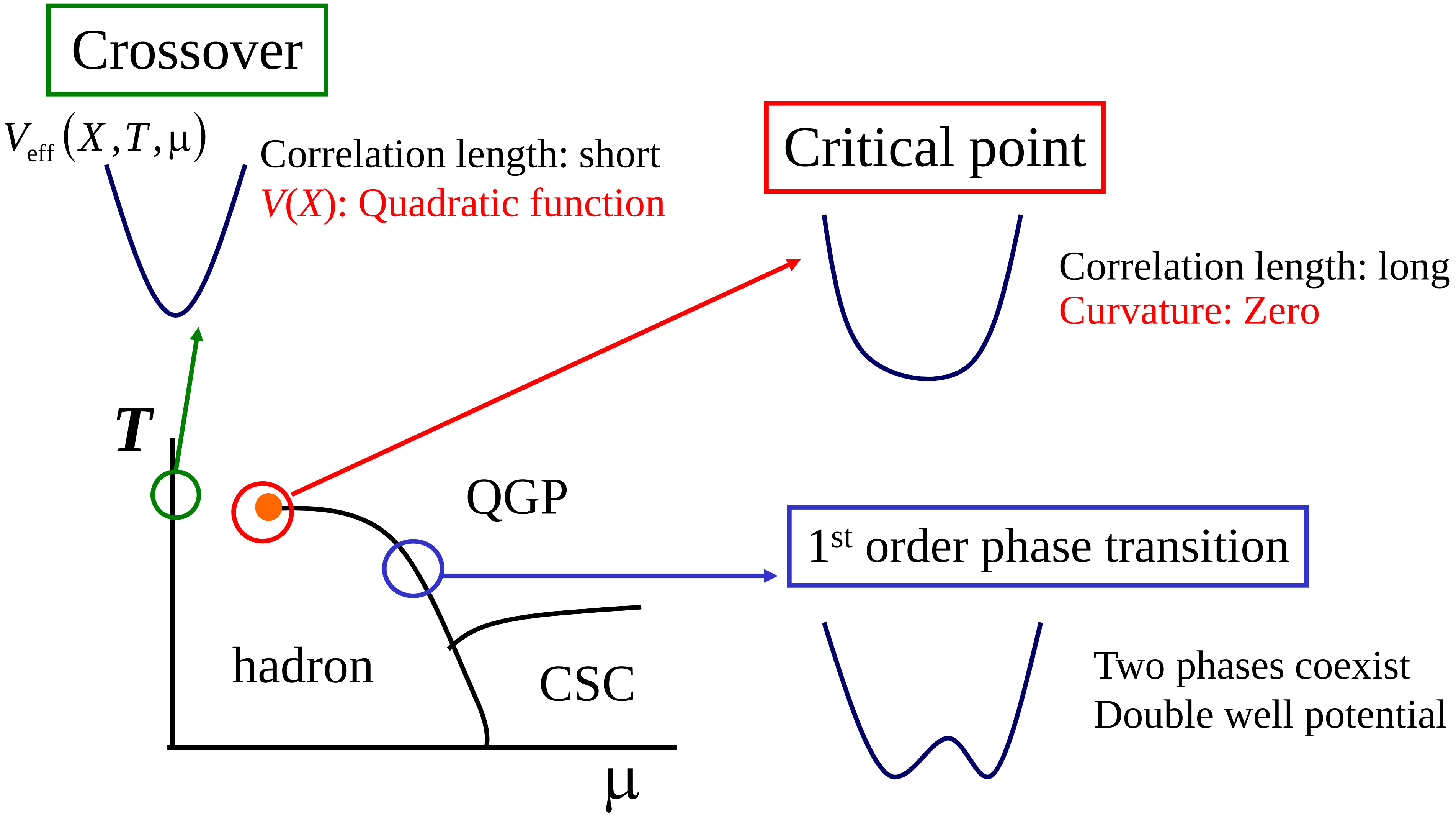
- We propose a method for the calculation of this *W*.
  - We must calculate *W* in a wide range of *P* and *F*.
  - The sign problem must be solved to obtain *W*.
- Once we get the pressure, we can calculate

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

μ-dependence of the effective potential

$$Z(T,\mu)=\int dX\, W(X,T,\mu), \qquad V_{\rm eff}(X) = -\ln W(X)$$

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

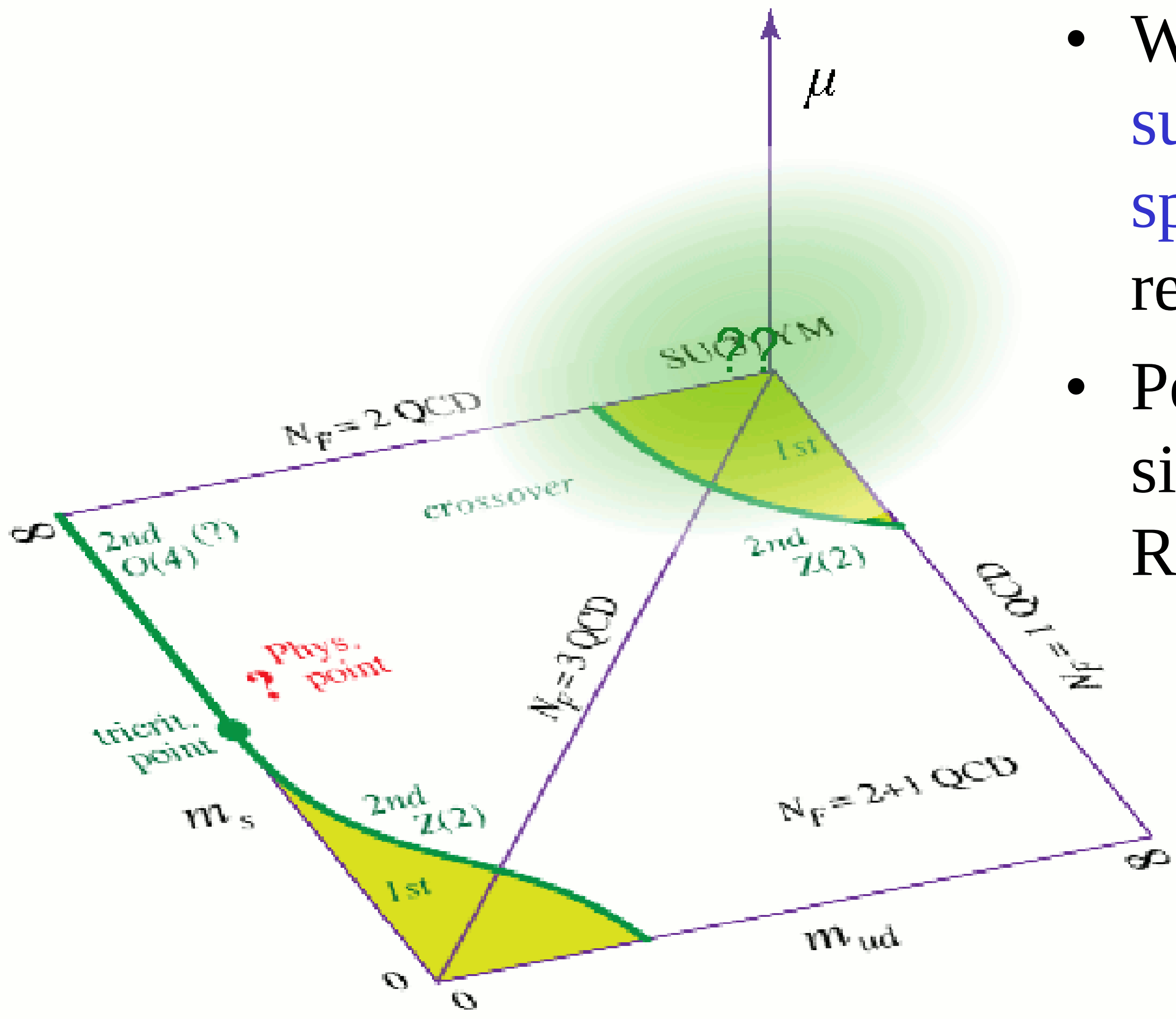


Plan of this talk

- 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)

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

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

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

Effective potential:

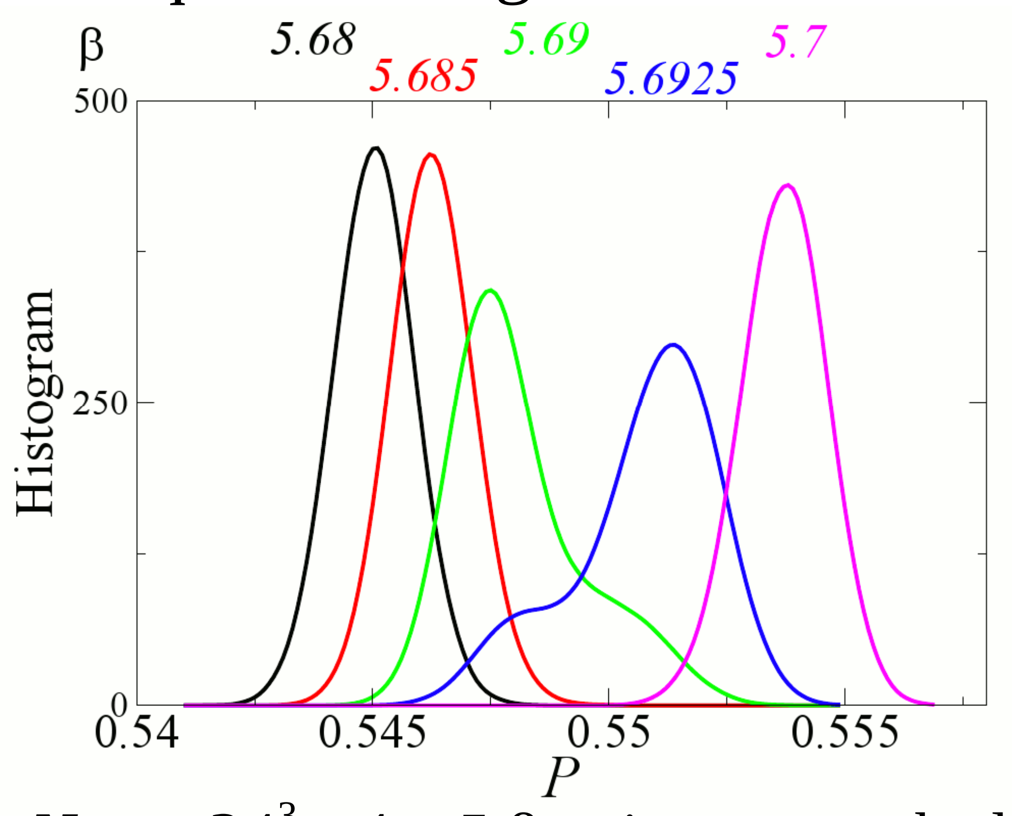
$$V_{\rm eff}(P,\beta,m,\mu) = -\ln[W(P,\beta m,\mu)] = V_{\rm eff}(P,\beta_0,m_0,0) - \ln R(P,\beta,\beta_0 m,m_0,\mu)$$

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

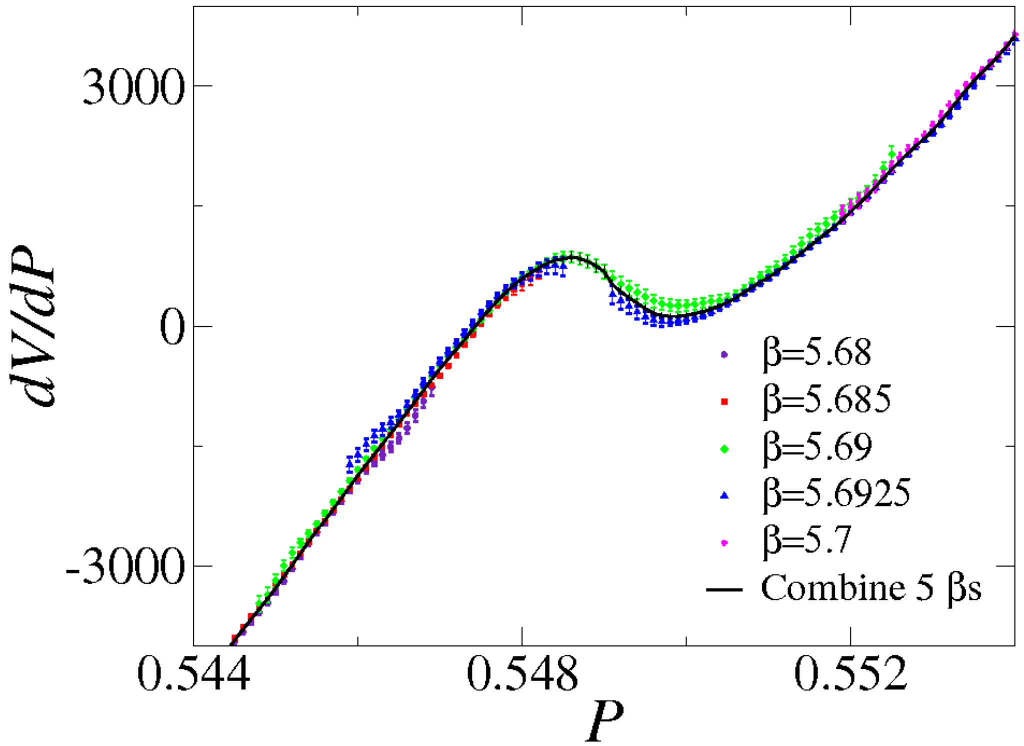
Solving the overlap problem

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

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



Derivative of V_{eff} at β=5.69



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

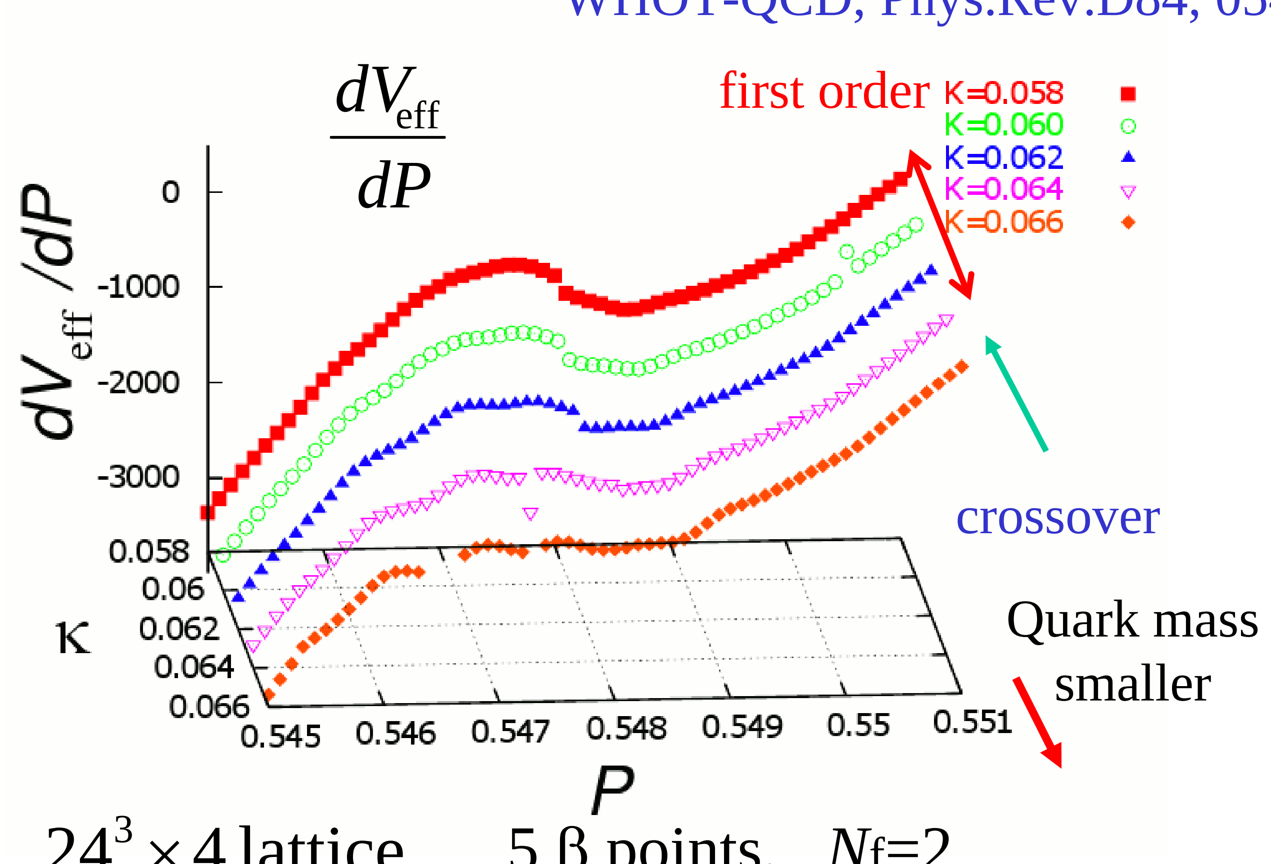
dV_{eff}/dP is adjusted to β=5.69, using

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

These data are combined by taking the average.

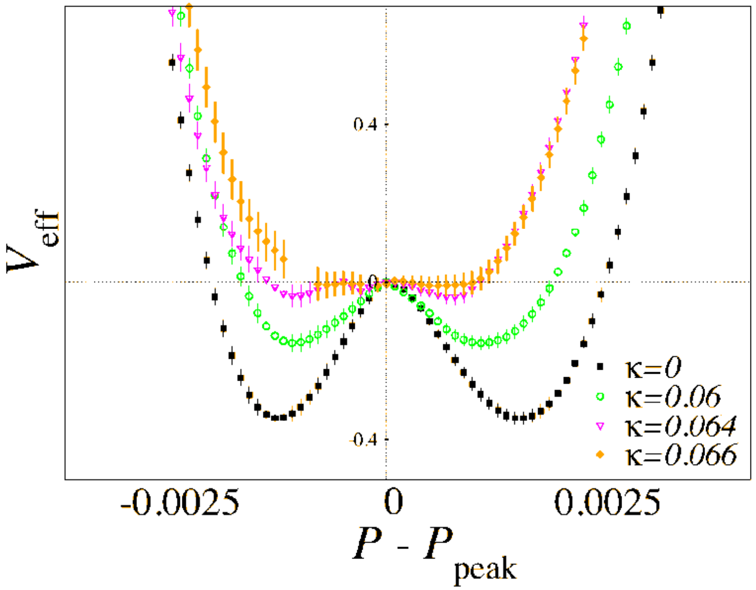
Effective potential near the quenched limit

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



Quenched Simulation
(mq=∞, K=0)

K~1/mq for large mq



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

- detM: Hopping parameter expansion,

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

real part of Polyakov loop

Nf=2: Kcp=0.0658(3)(8)

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

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

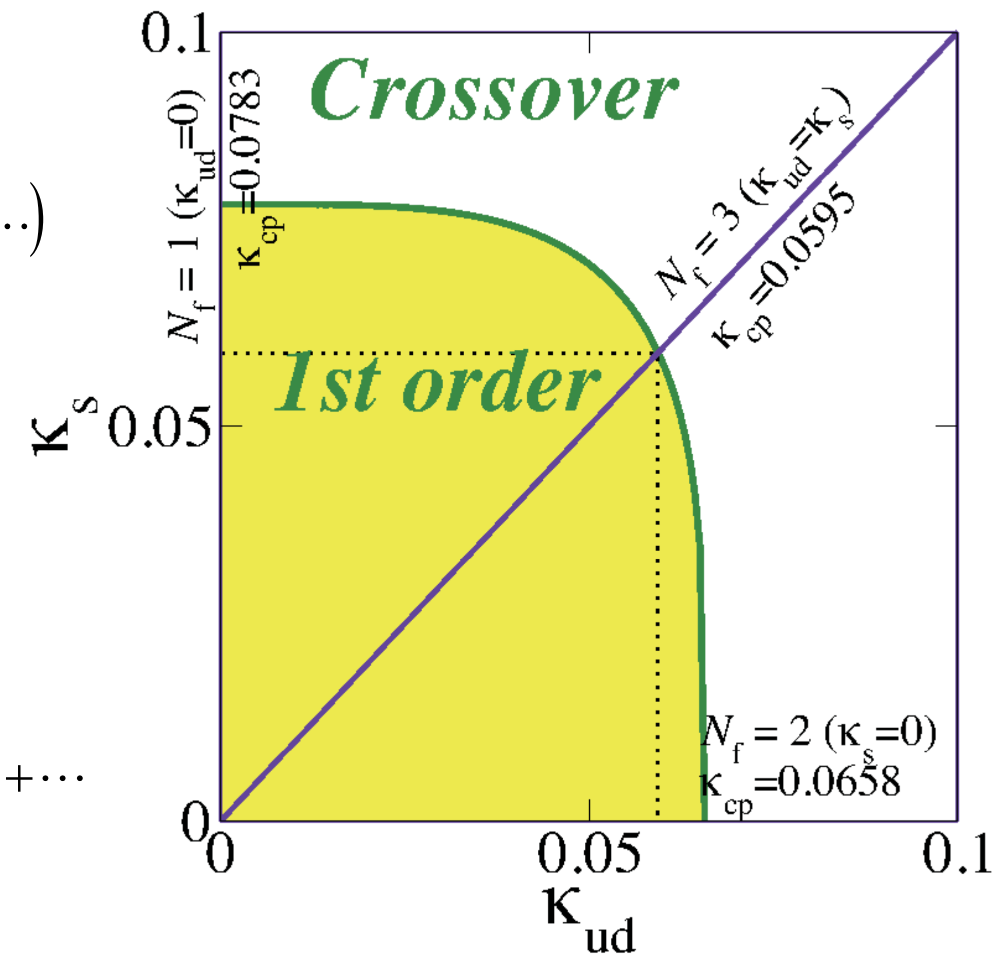
Endpoint of 1st order transition in 2+1 flavor QCD

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

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

N_f=2+1

$$\ln\left[\frac{(\det M(K_{ud}))^2 \det M(K_s)}{(\det M(0))^3}\right]$$
$$= 288 N_{site}\left(2K_{ud}^4 + K_s^4\right)P + 12\times 2^{N_t} N_s^3 \left(2K_{ud}^{N_t} + K_s^{N_t}\right)\Omega_R + \cdots$$



The critical line is described by

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

Finite density QCD in the heavy quark region

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

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

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

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

phase

- We can extend this discussion to finite density QCD.

Phase quenched simulations, Isospin chemical potential

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

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

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

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

phase

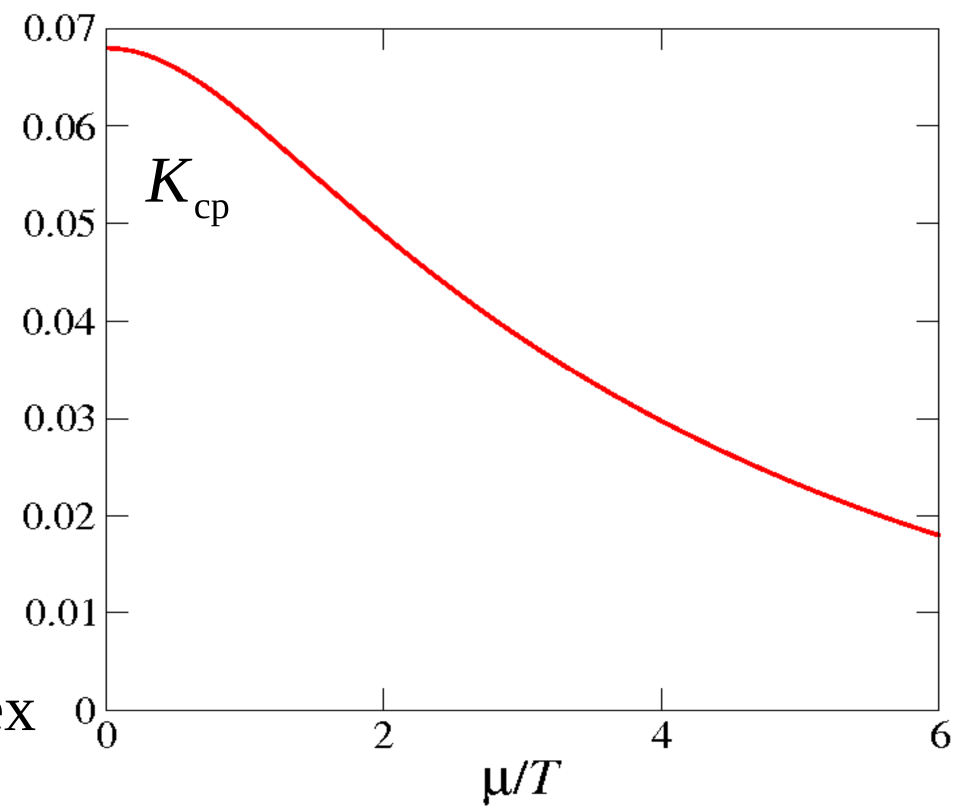
- If the complex phase is neglected,

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

  – Critical point:

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

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



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

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:

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

$$W(P',F',\beta,m,\mu) = \int DU\ \delta(P-P')\delta(F-F')(\det M(m,\mu))^{N_f} e^{-S_g}$$

$$= \int DU\ \delta(P-P')\delta(F-F') e^{i\theta}\left|\det M(m,\mu)\right|^{N_f} e^{-S_g}$$

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

expectation value with fixed *P,F* histogram

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

Distribution function of the phase quenched.

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

Phase quenched simulation

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

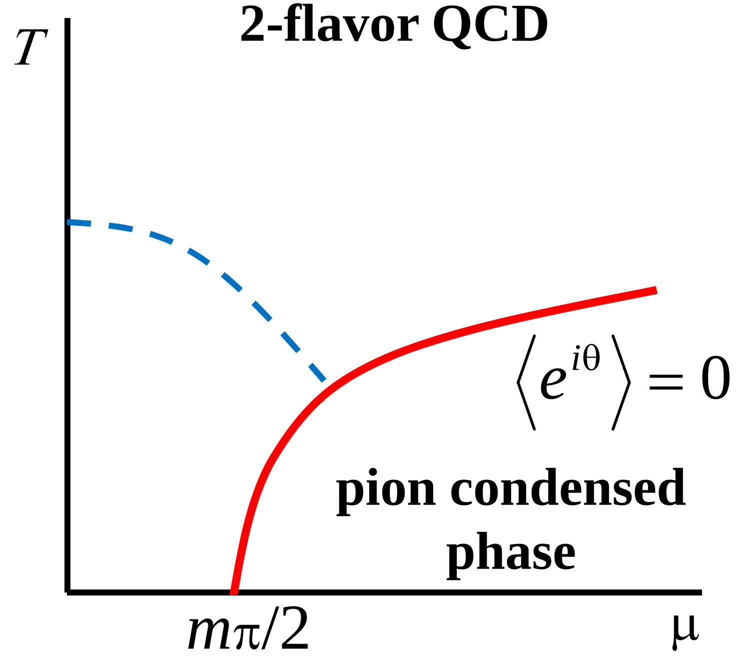
$$\left|\det M(K,\mu)\right|^2 = \det M(K,\mu) \det M(K,-\mu)$$

- When $\mu_u = -\mu_d$, pion condensation occurs.
- $\left\langle e^{i\theta} \right\rangle = 0$ 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 $\theta \equiv \mathrm{Im} \ln \det M$

- 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.

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

$\to 0$ $\to 0$

cumulants

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

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

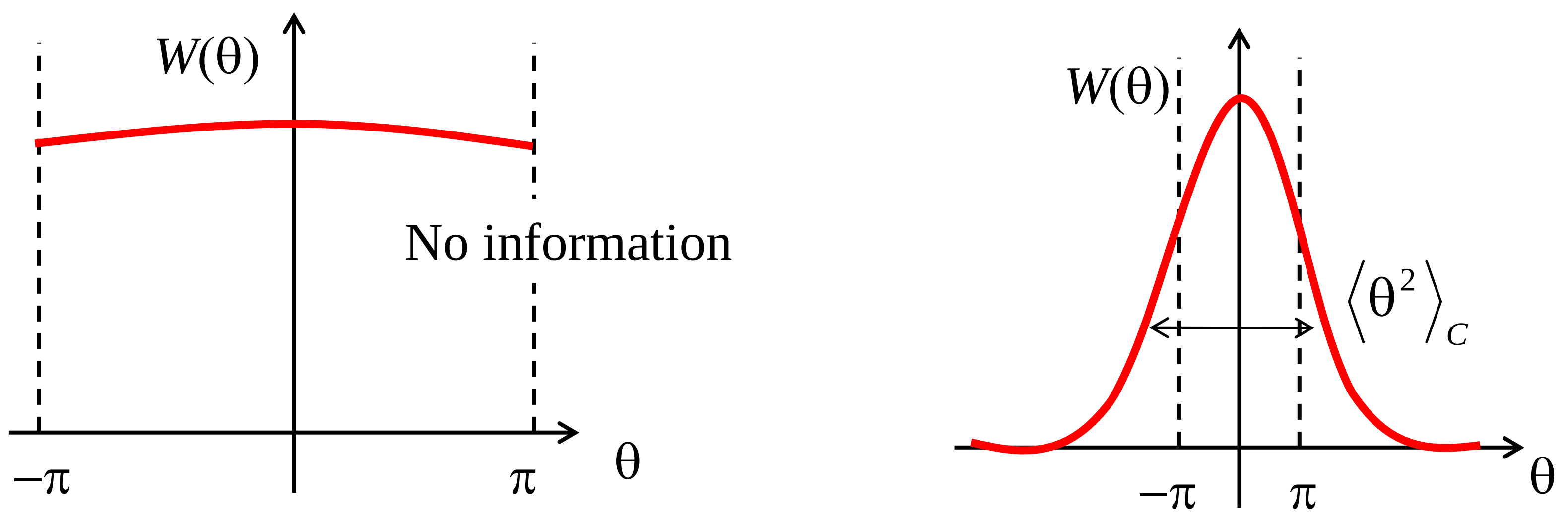
Source of the complex phase

If the cumulant expansion converges, No sign problem.

Distribution of the complex phase

- We should not define the complex phase in the range from –π to π.
- When the distribution of θ is perfectly Gaussian, the average of the complex phase is give by the second order (variance),

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



Complex phase

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

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

  – The range of θ is from -∞ to ∞.

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

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

- The reweighting factor is also computed,

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

Integral method for the calculation of the quark determinant

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

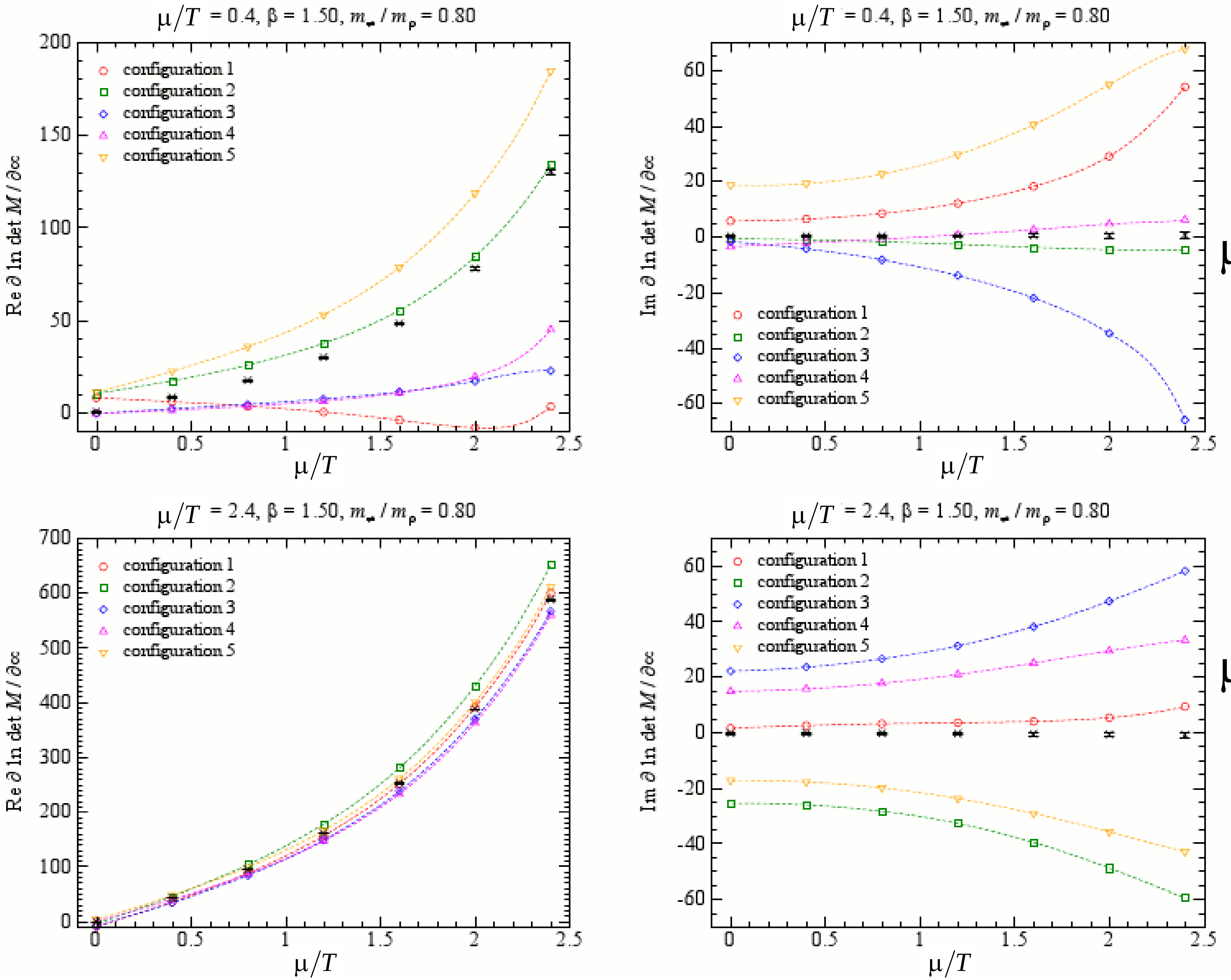
$8^3 \times 4$ lattice

$\beta = 1.50$

$m_\pi / m_\rho = 0.8$

2-flavor QCD
Iwasaki gauge
+ clover Wison
quark action

Random noise
method is used.



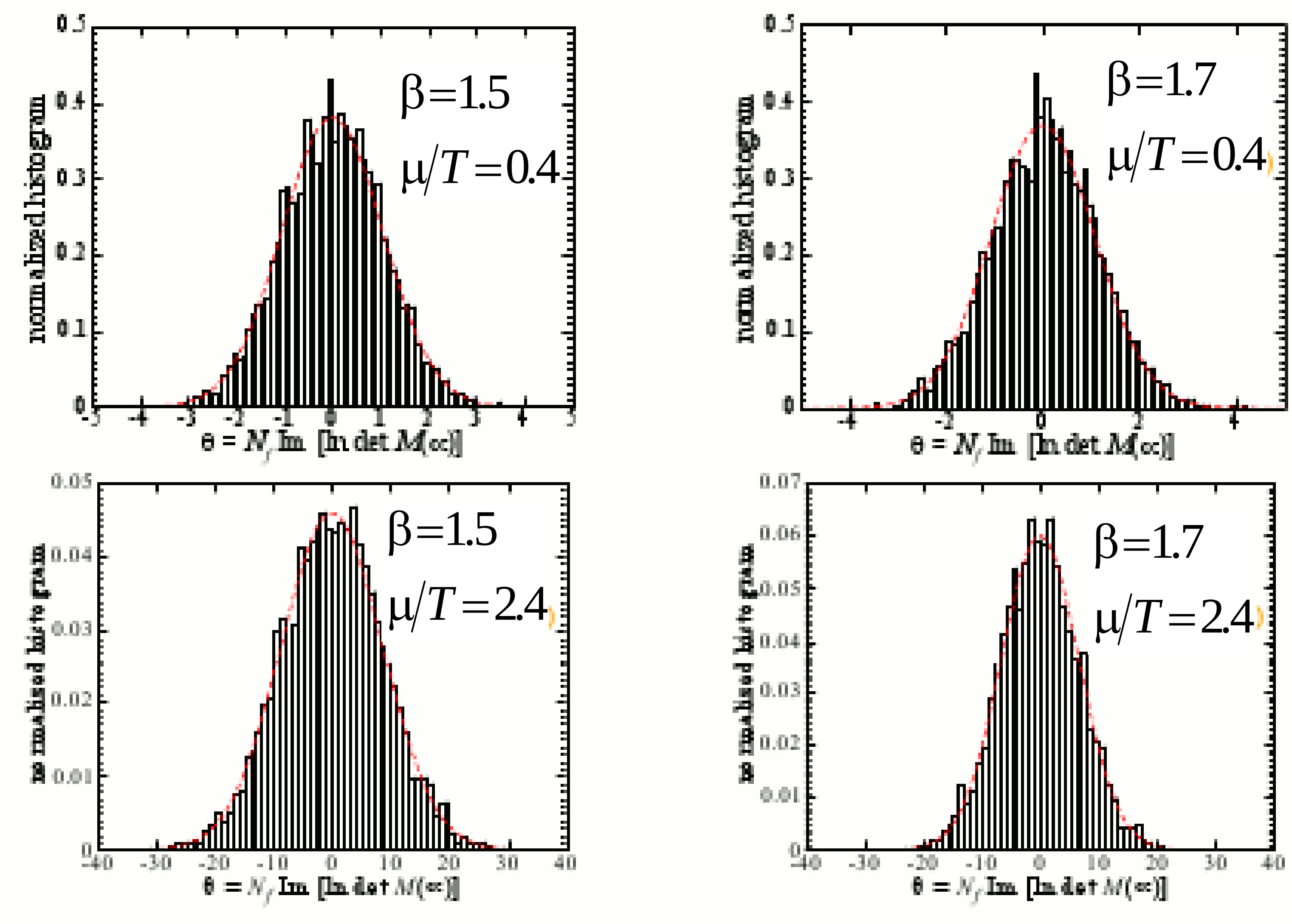
$\mu/T = 0.4$

$\mu/T = 2.4$

Real part

Imaginary part

Distribution of the complex phase

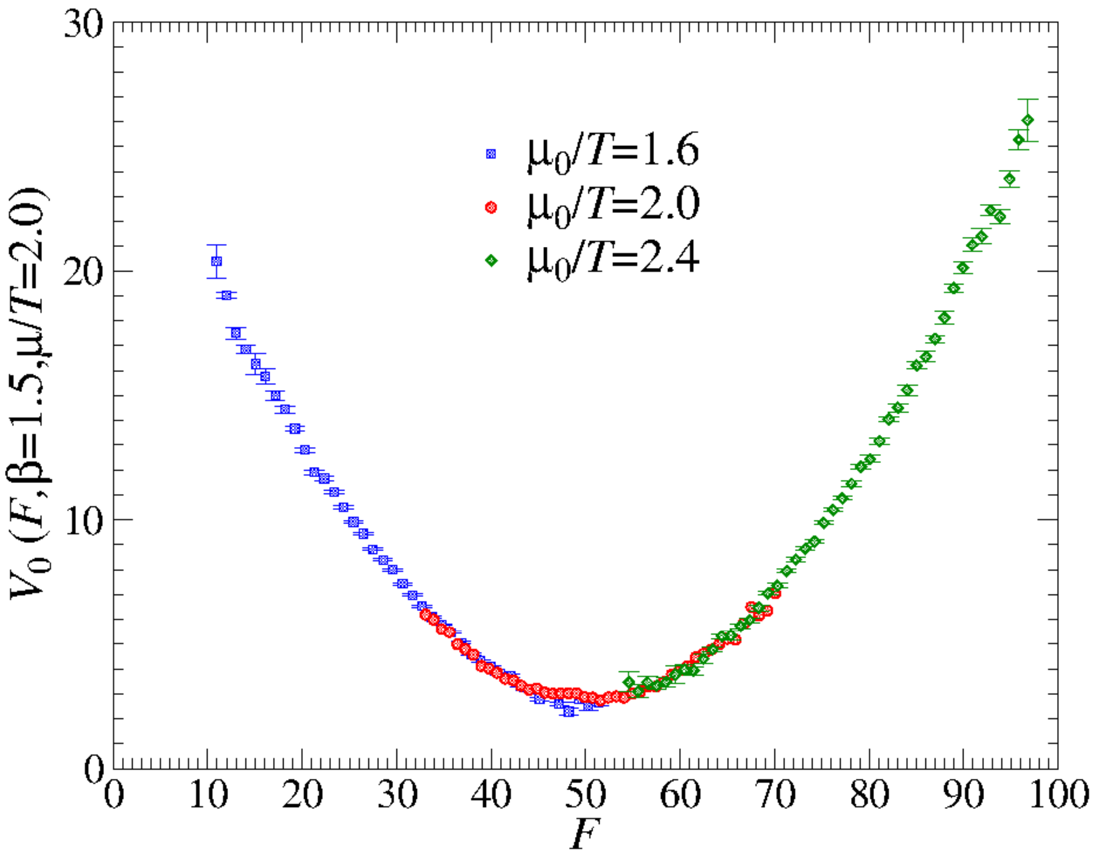


- Well approximated by a Gaussian function.
- Convergence of the cumulant expansion: good.

Overlap problem

Reweighting method W_0: distribution function in phase quenched simulations.

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



- 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.

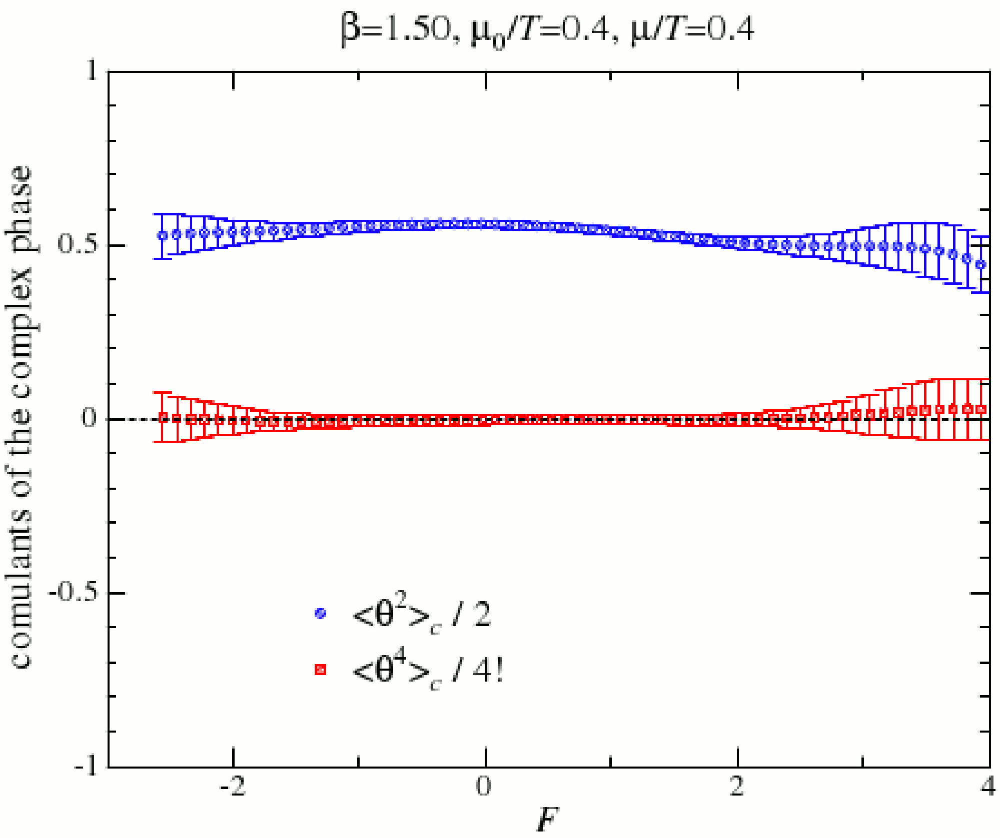
- The error of R is small because F is fixed.

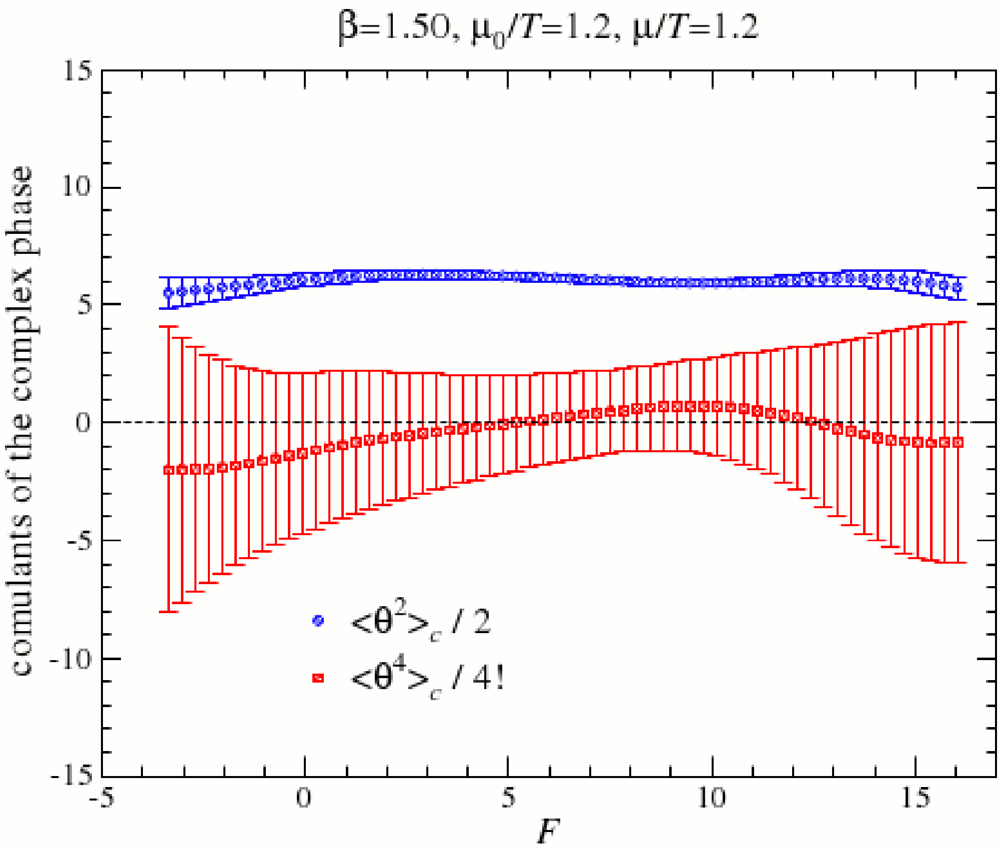
$$-\ln W_0(P,F,\mu_0) - \ln R(P,F,\mu,\mu_0) = -\ln W_0(P,F,\mu)$$

Convergence of the cumulant expansion

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

Preliminary



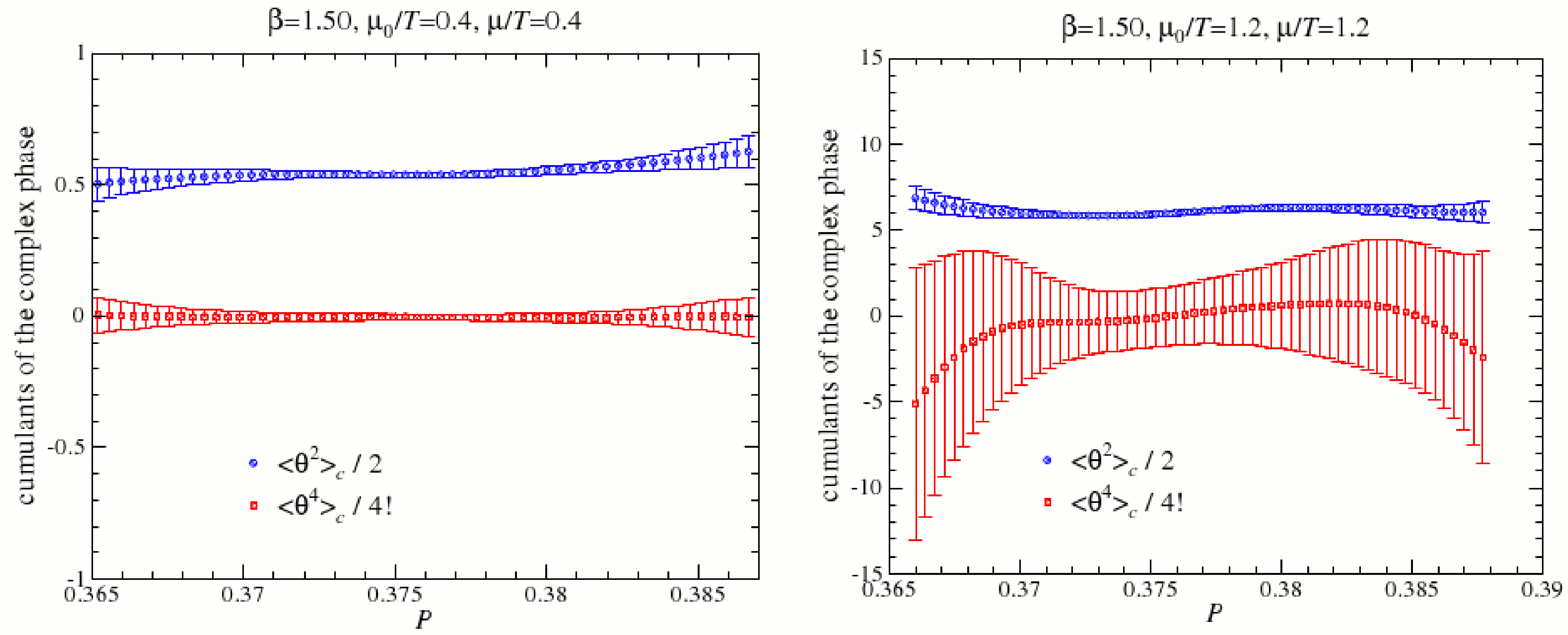


Preliminary

- 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

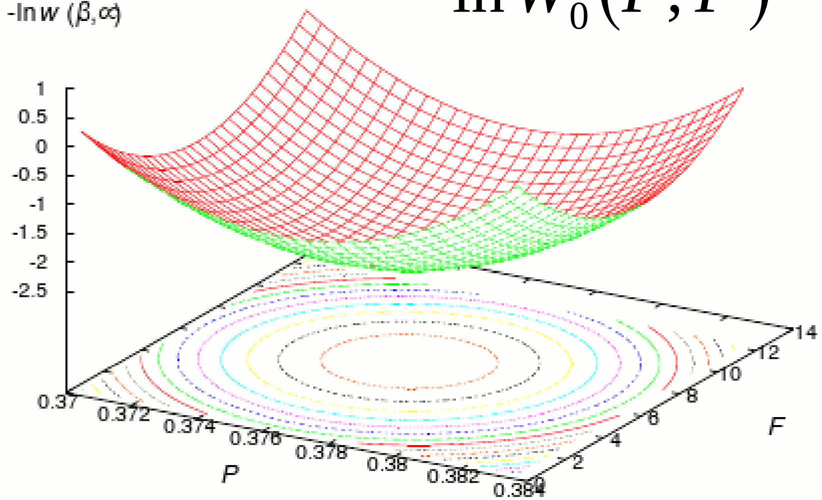
- 4th order cumulant is consistent with zero.

Effective potential at finite μ

- Combine V_0 and the phase factor.

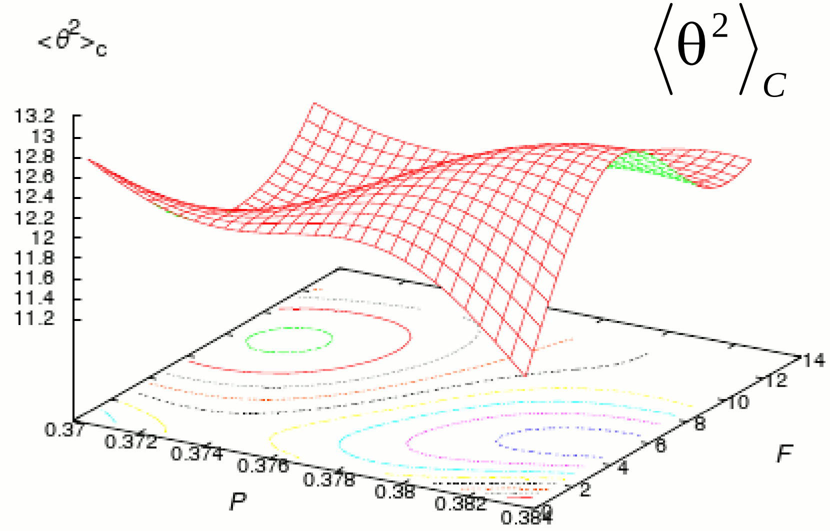
Preliminary

$$-\ln W_0\left(P,F\right)$$



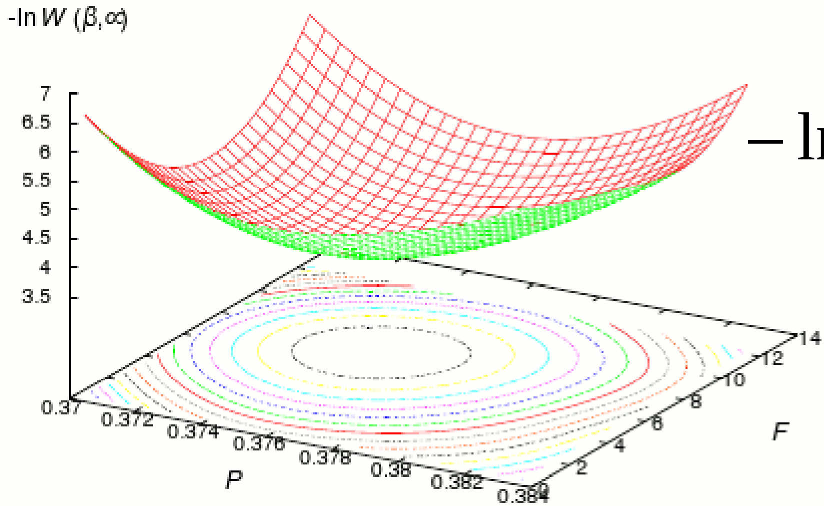
+

$$\left\langle \theta^2 \right\rangle_C$$



× 0.5

=



$$-\ln W\left(P,F\right)$$

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 investigte 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.