Study of QCD Phase Transition at Finite Density by a Histogram Method

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WHOT-QCD collaboration

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Fluctuations, Correlations and RHIC Low Energy Runs,

BNL, October 3-5, 2011

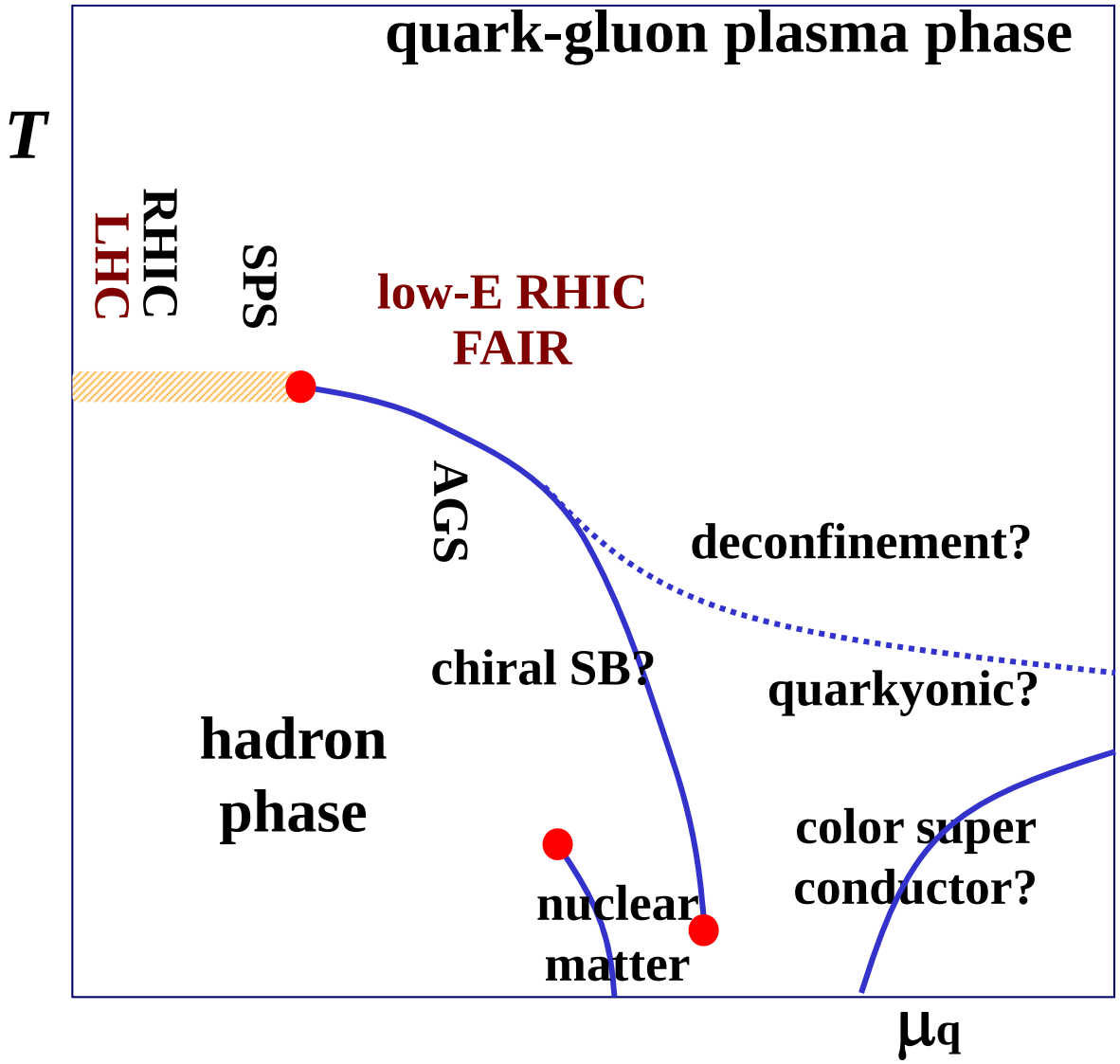
Phase structure of QCD at high temperature and density

Lattice QCD

- Phase transition lines
- Equation of state

- Direct simulation:

  Impossible at $\mu \neq 0$.



Problems in simulations at μ≠0

- Problem of Complex Determinant at μ≠0
  - Boltzmann weight: complex at μ≠0
    - Monte-Carlo method is not applicable.
    - Configurations cannot be generated.

- Density of state method (Histogram method)

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

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

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

- Expectation values

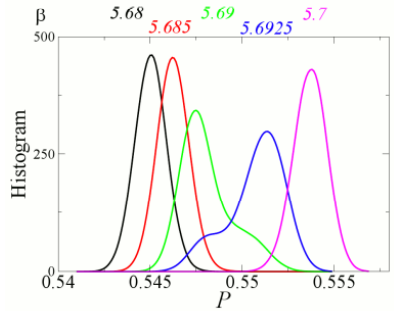
$$\langle O[X]\rangle_{(m,T,\mu)}=\frac{1}{Z}\int dX\ O[X]W(X,m,T,\mu)$$

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

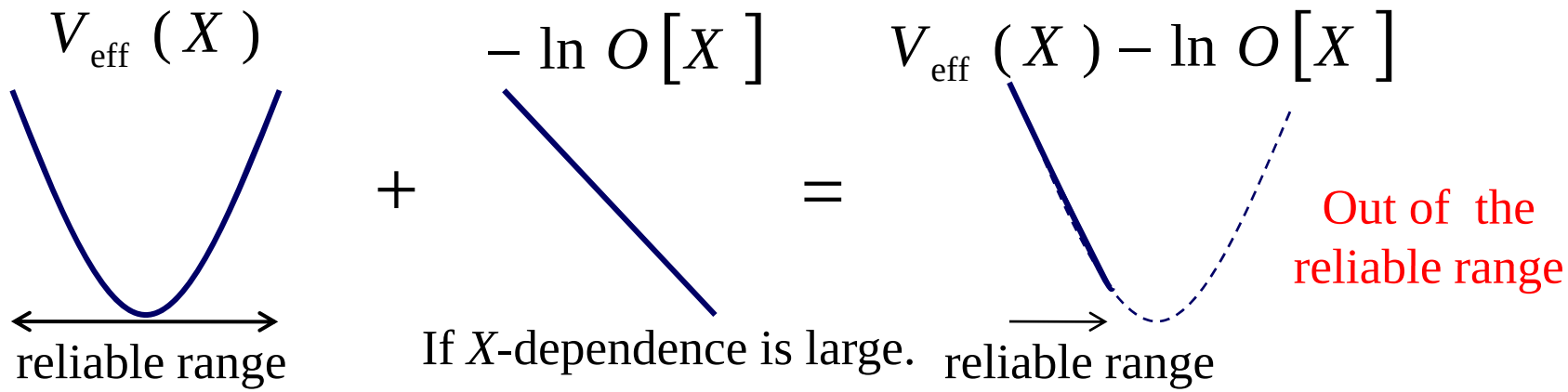
Overlap problem

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

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



- W is computed from the histogram.
- Distribution function around X where $V_{\mathrm{eff}}(X) - \ln O[X]$ 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 $\langle P \rangle$ and chiral condensate $\langle \bar{\psi}\psi \rangle$
  - Pressure at μ=0 $$\frac{p}{T^4} = \frac{1}{VT^3}\ln Z$$
    - Integral $$\left.\frac{p}{T^4}\right|_a - \left.\frac{p}{T^4}\right|_{a_0} = -\int_{a_0}^{a} \frac{\varepsilon' - 3p'}{T'^4} d(\ln a')$$

      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

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

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

$$F\equiv N_f\ \ln\left|\det M(\mu)/\det M(0)\right|,\quad Z(m,T,\mu)=\int dPdF\ W(P,F,m,T,\mu)$$

$$\langle P\rangle_{(m,T,\mu)}=\frac{1}{Z(m,T,\mu)}\int dPdF\ P\,W(P,F,m,T,\mu)$$

$$\left\langle\frac{\det M(\mu)}{\det M(0)}\right\rangle_{(m,T,0)}=\frac{1}{Z(m,T,0)}\int dPdF\ e^{F}\left\langle e^{i\theta}\right\rangle_{P,F}W(P,F,m,T,0)$$

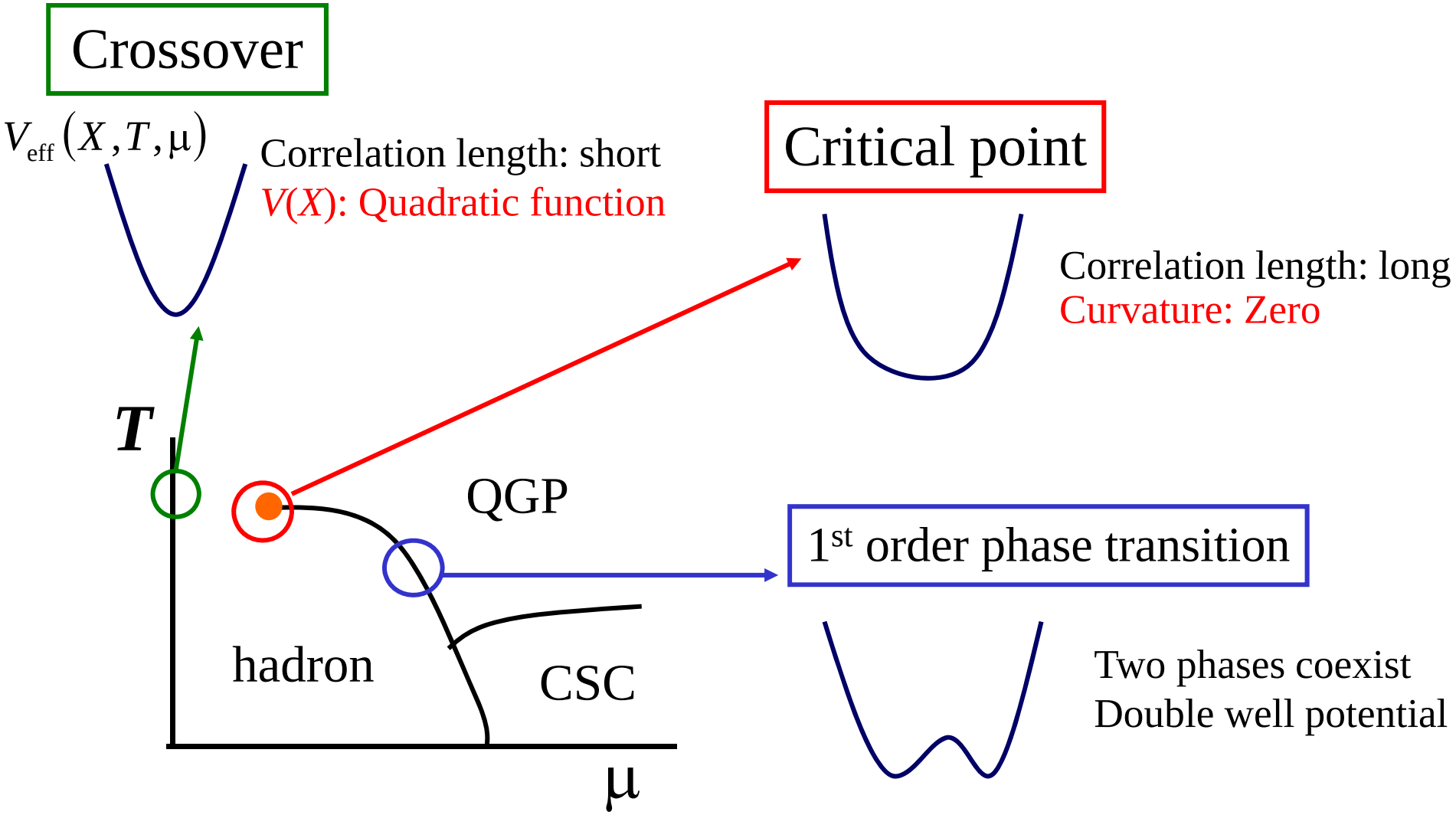
θ : complex phase of $(\det M(\mu))^{N_f}$

- We must calculate *W* in a wide range of *P* and *F*.
- The sign problem must be solved to obtain *W*.
  - We propose a method for the calculation of *W*.

μ-dependence of the effective potential

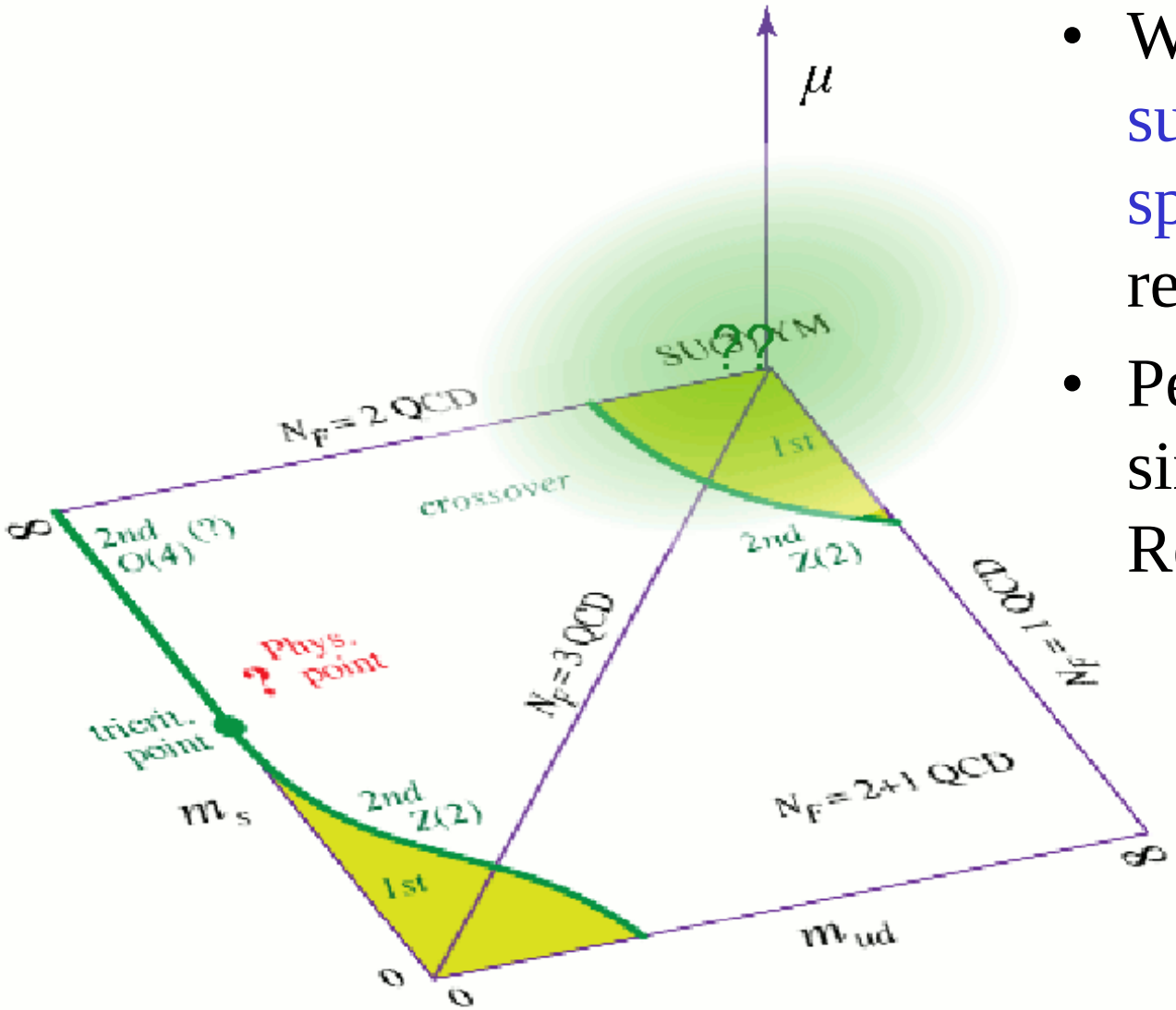
$$Z(T,\mu)=\int dX\, W(X,T,\mu), \qquad V_{\mathrm{eff}}(X) = -\ln W(X)$$

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



Distribution function in the heavy quark region

WHOT-QCD, 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-dependence of the distribution function

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

Change: $\beta_1(T)$ ➡ $\beta_2(T)$ $\qquad$ P: Average plaquette (1x1 Wilson loop)

Weight: $W(\beta_1)\Rightarrow W(\beta_2)=e^{6N_{\rm site}(\beta_2-\beta_1)P}W(\beta_1)$ $\qquad$ $(\beta=6/g^2)$

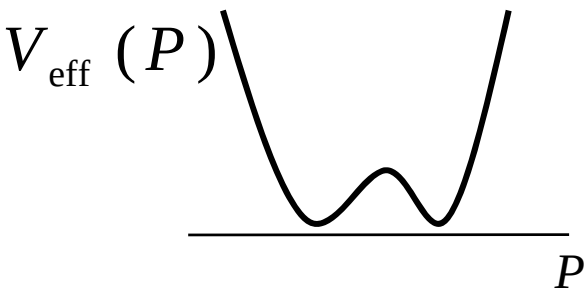
Potential: $V_{\rm eff}(P)\equiv-\ln(W(P))$ ➡ $V_{\rm eff}(\beta_2)=V_{\rm eff}(\beta_1)-6N_{\rm site}(\beta_2-\beta_1)P$

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

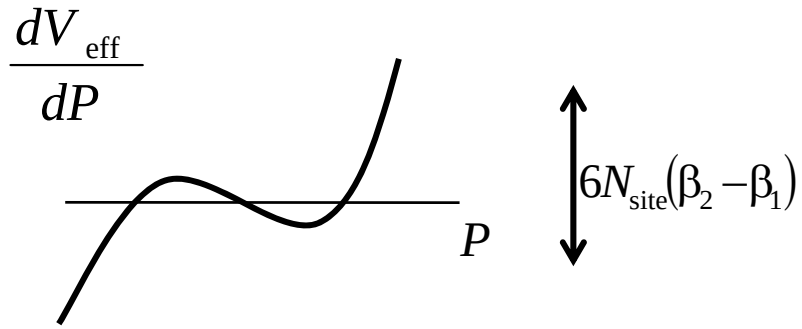
$$\frac{d^2V_{\rm eff}}{dP^2}(\beta_2)=\frac{d^2V_{\rm eff}}{dP^2}(\beta_1)$$

Curvature of $V_{\rm eff}$: independent of β.

1st order phase transition



➡

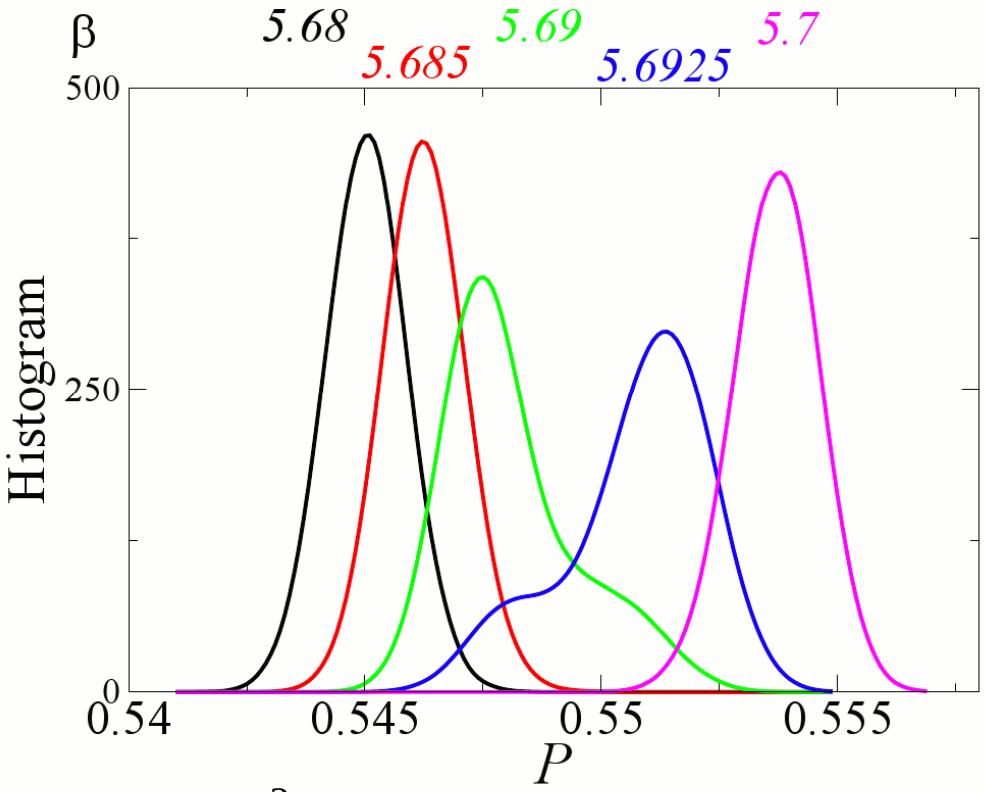


Shape of $dV_{\rm eff}/dP$: independent of β. ➡ Easy to identify 1st order phase transition.

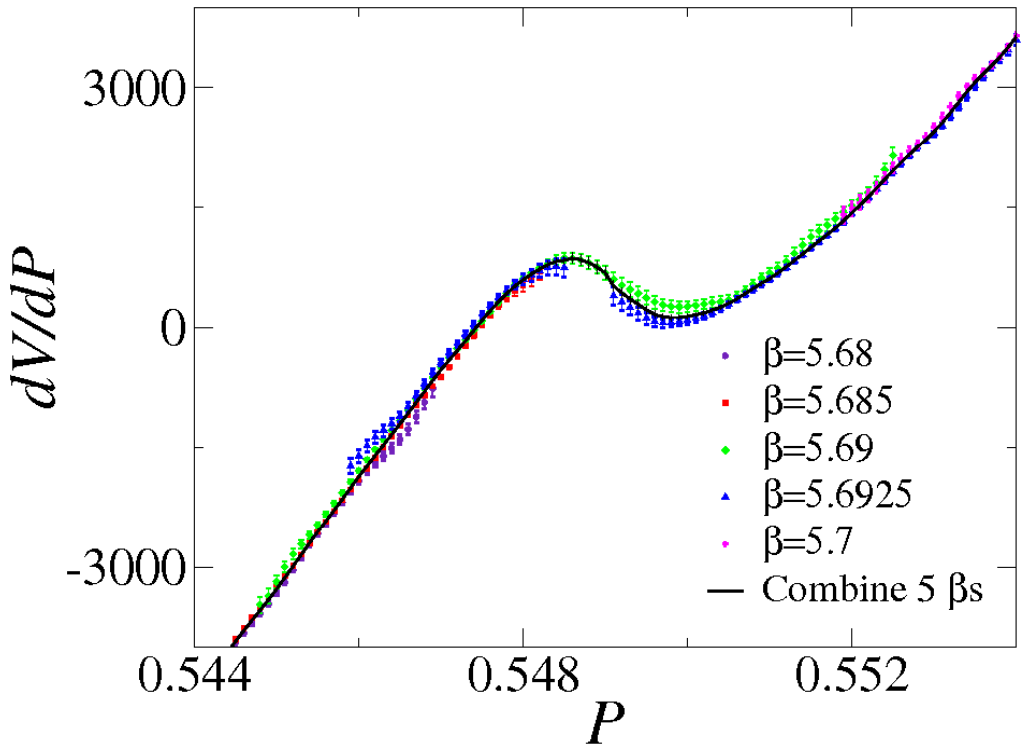
Solving the overlap problem

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.

Reweighting method for quark part

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

$$W(P',\beta,m,0) \equiv \int DU\delta(P\text{-}P')(\det M(m,0))^{N_f}\ \mathrm{e}^{-S_g}$$ (Weight factor at m and μ=0)

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

$$R(P') = \frac{\int DU\ \delta(P\text{-}P')(\det M(m,\mu))^{N_f}}{\int DU\ \delta(P\text{-}P')(\det M(m_0,0))^{N_f}} = \frac{\left\langle \delta(P\text{-}P')\left(\frac{\det M(m,\mu)}{\det M(m_0,0)}\right)^{N_f}\right\rangle_{(\beta,\mu=0)}}{\langle \delta(P\text{-}P')\rangle_{(\beta,\mu=0)}} \equiv \left\langle \left(\frac{\det M(m,\mu)}{\det M(m_0,0)}\right)^{N_f}\right\rangle_P$$

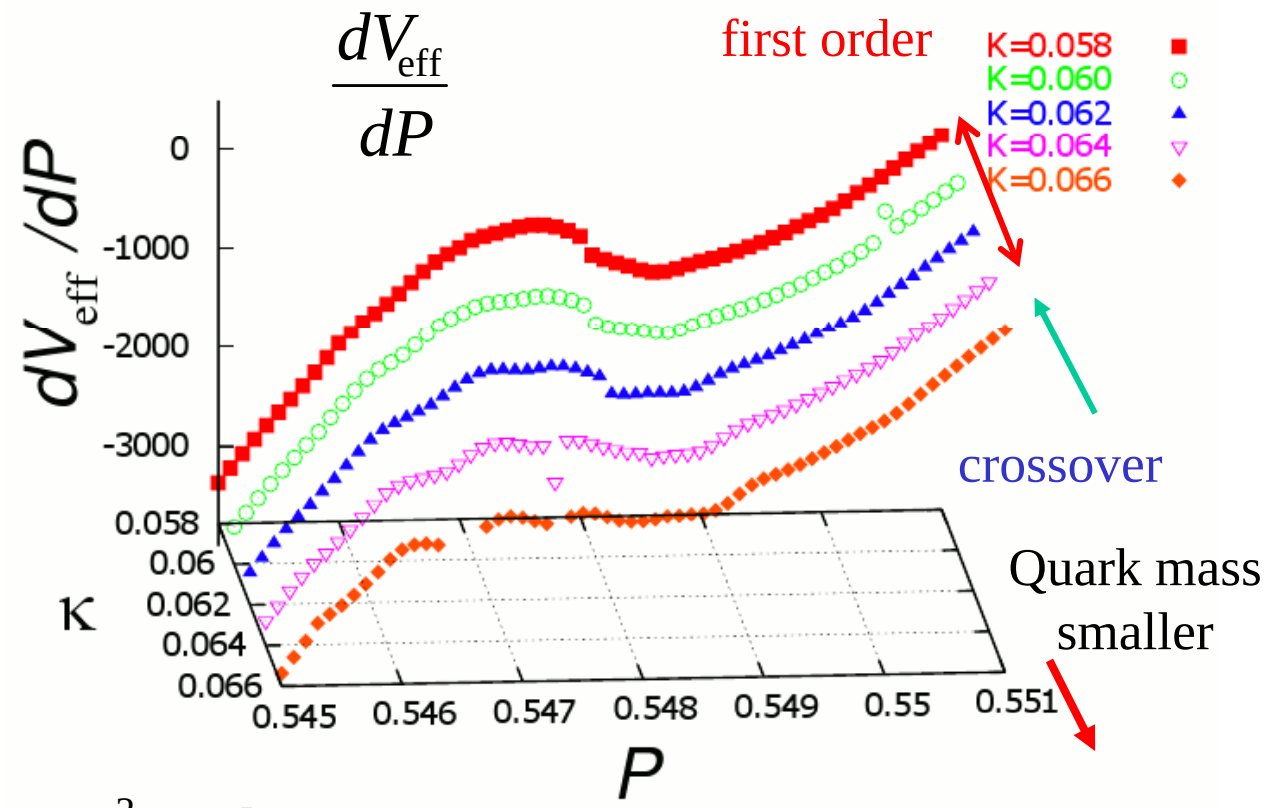
$R(P,m,m_0,\mu)$: independent of β, → $R(P,m,m_0,\mu)$ can be measured at any β.

Effective potential:

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

Effective potential near the quenched limit

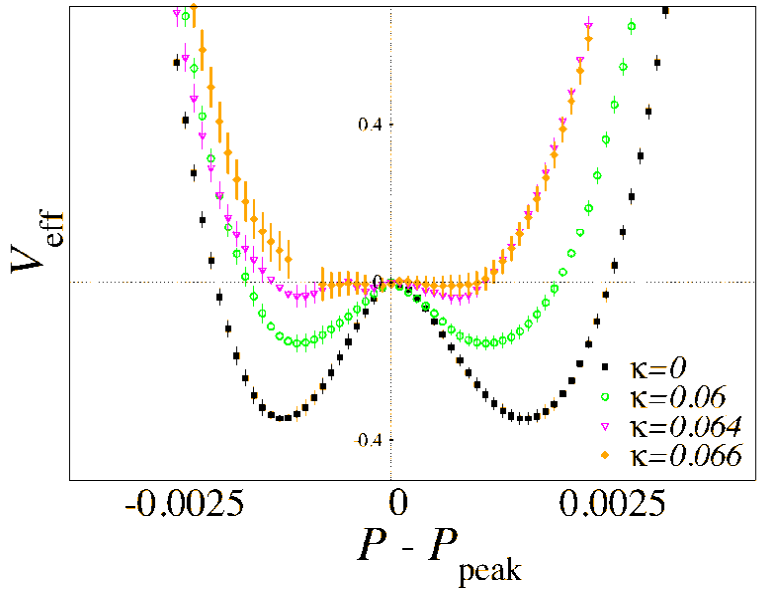
WHOT-QCD, Phys.Rev.D84, 054502(2011)



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

Quenched Simulation (m_q=∞, K=0)

K~1/m_q for large m_q



- detM: Hopping parameter expansion.
- K-dependence is calculated by the reweighting.
- First order transition at K = 0 changes to crossover at K > 0.

Distribution function in the light quark region

WHOT-QCD, in preparation

- We perform phase quenched simulations with the weight:

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

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

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

Distribution function of the phase quenched.

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

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,

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

- Cumulant expansion

<..>$_{P,F}$: expectation values fixed F and P.

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

cumulants

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

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

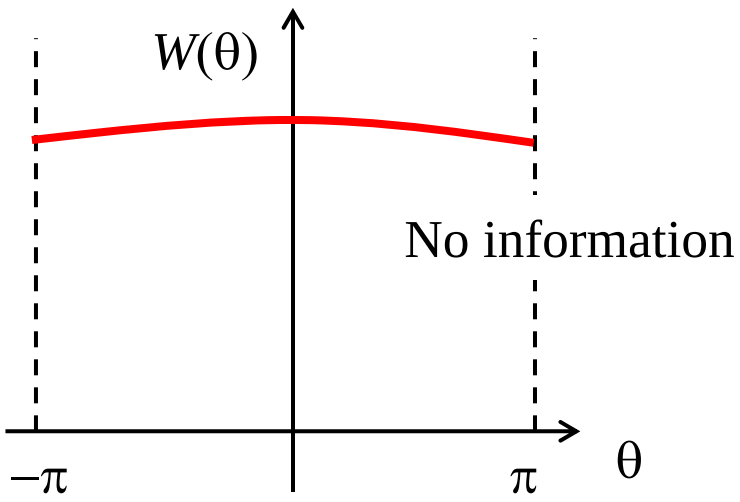
Source of the complex phase

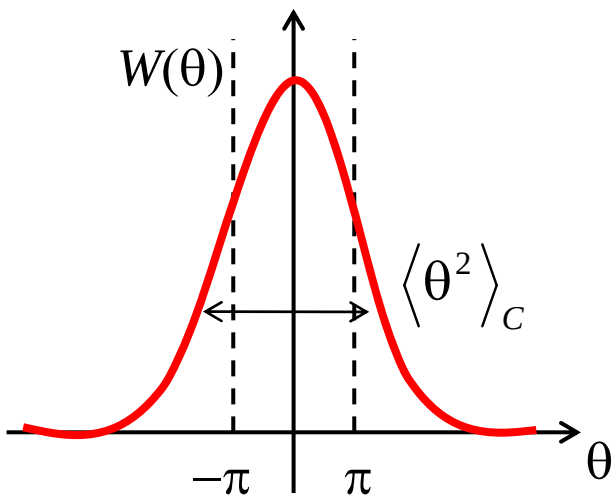
If the cumulant expansion converges, No sign problem.

Distribution of the complex phase

- We should not define the complex phase in the range from $-\pi$ 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

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

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

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

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

- The reweighting factor is also computed,

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

Integral method for the calculation of the quark determinant

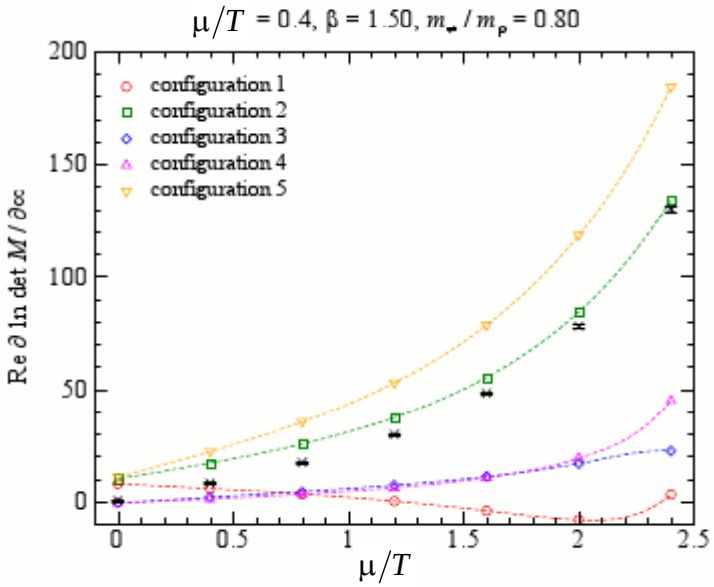
$$\frac{\partial \ln \det M}{\partial(\mu/T)}$$

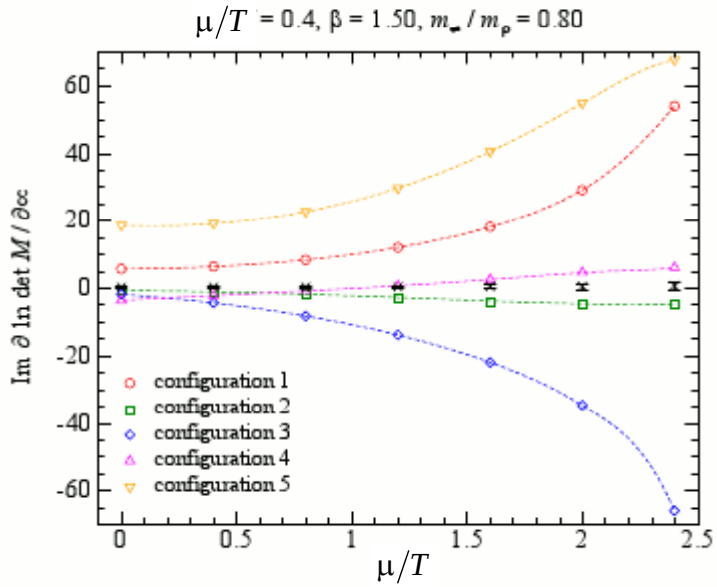
$8^3 \times 4$ lattice

$\beta = 1.50$

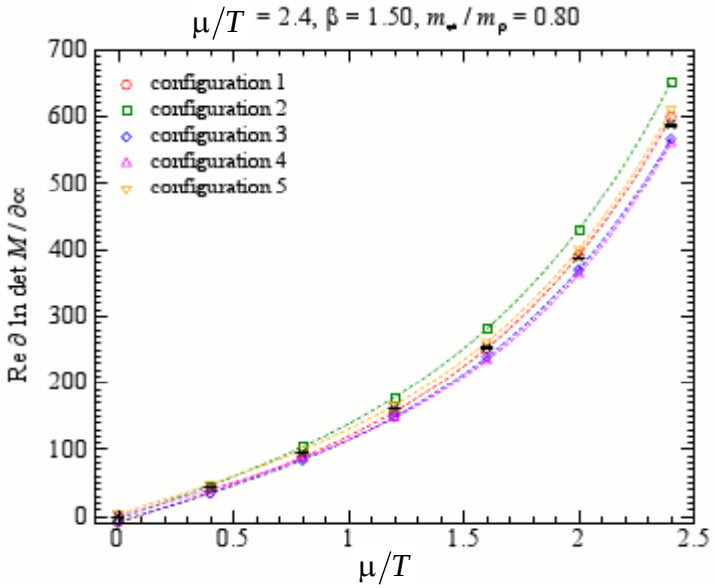
$m_\pi / m_\rho = 0.8$

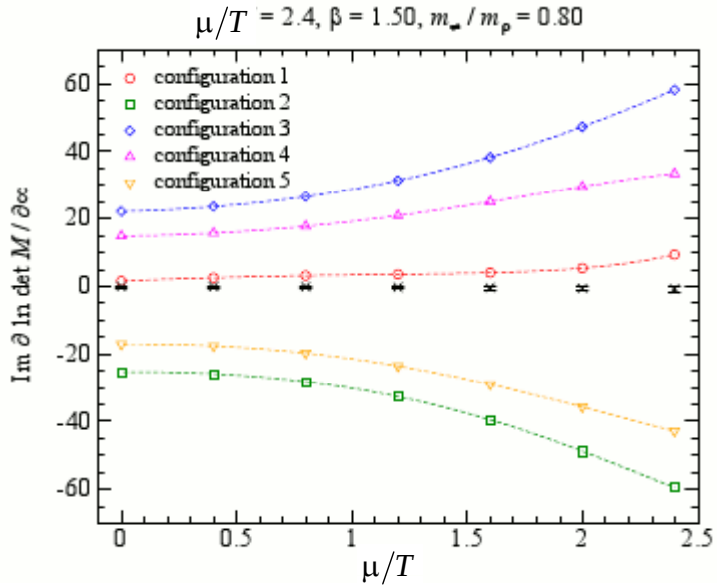
2-flavor QCD
Iwasaki gauge
+ clover Wison
quark action





$\mu/T = 0.4$



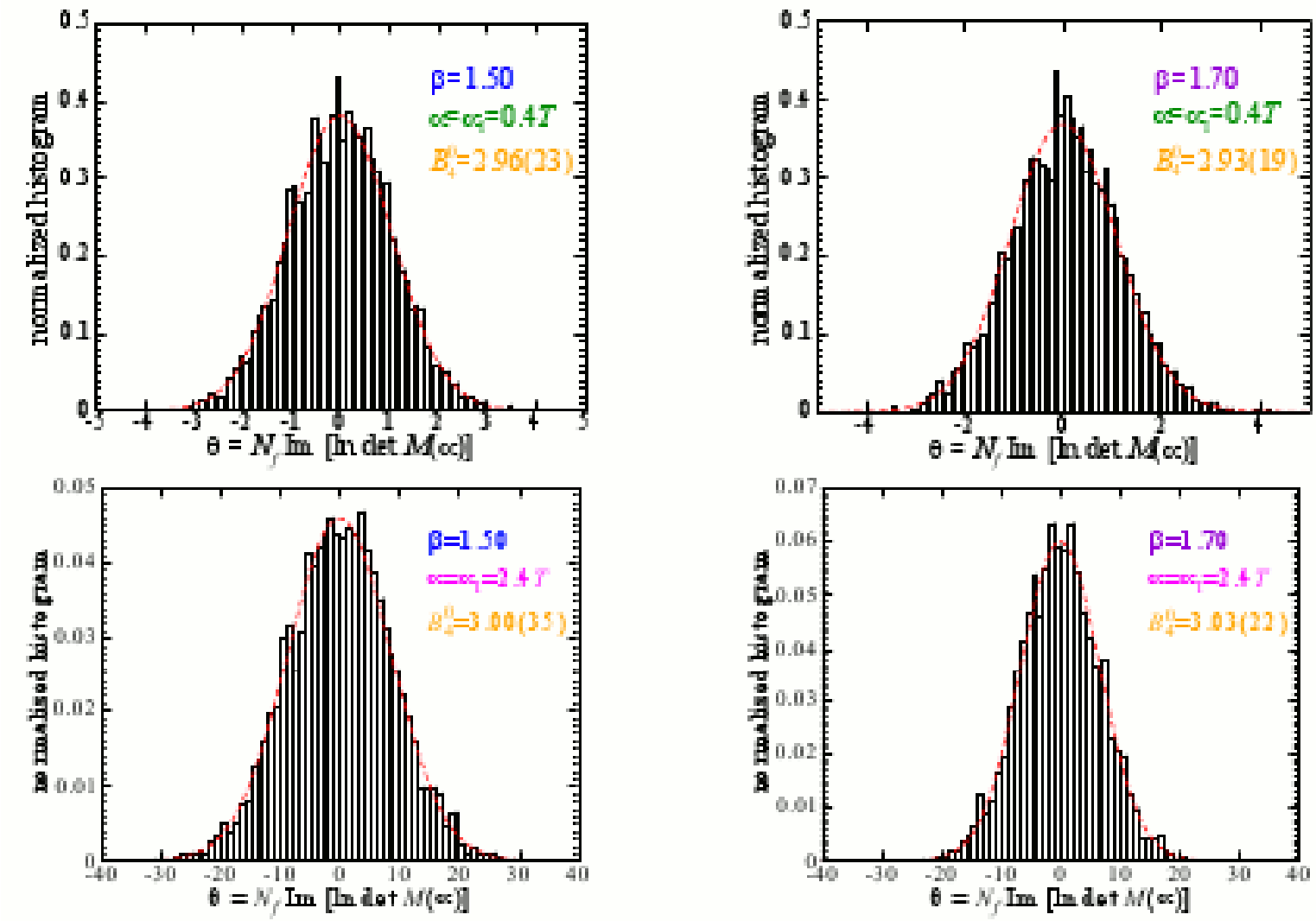


$\mu/T = 2.4$

Real part

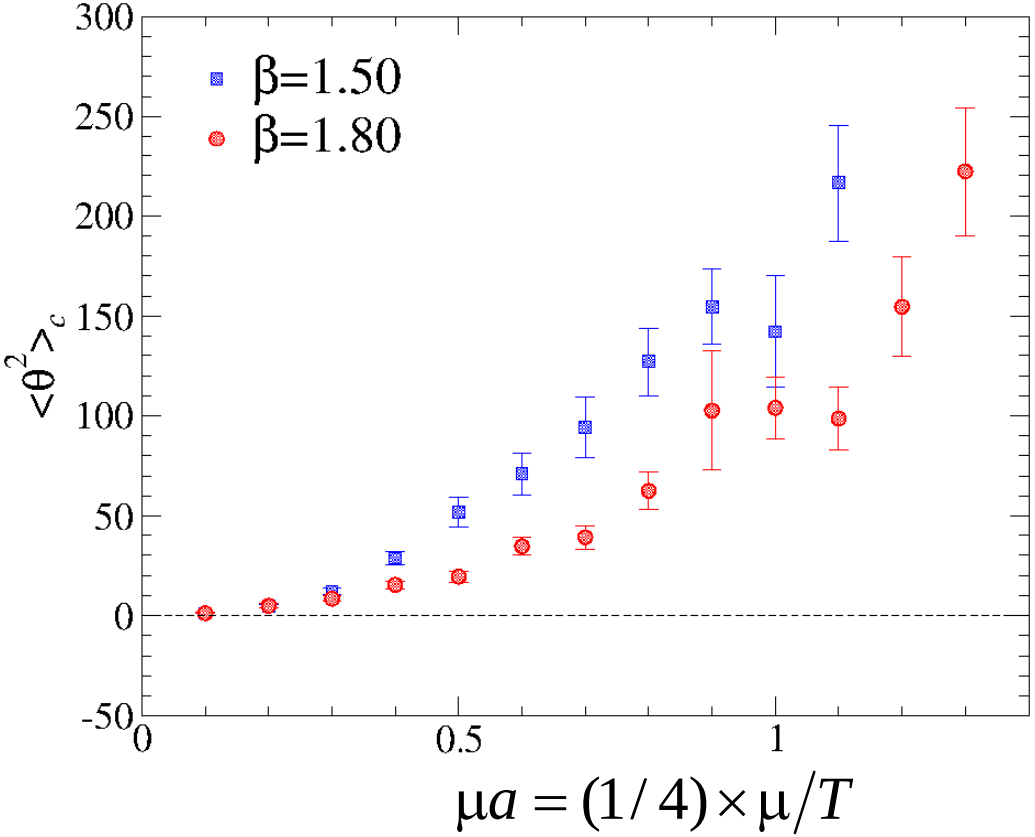
Imaginary part

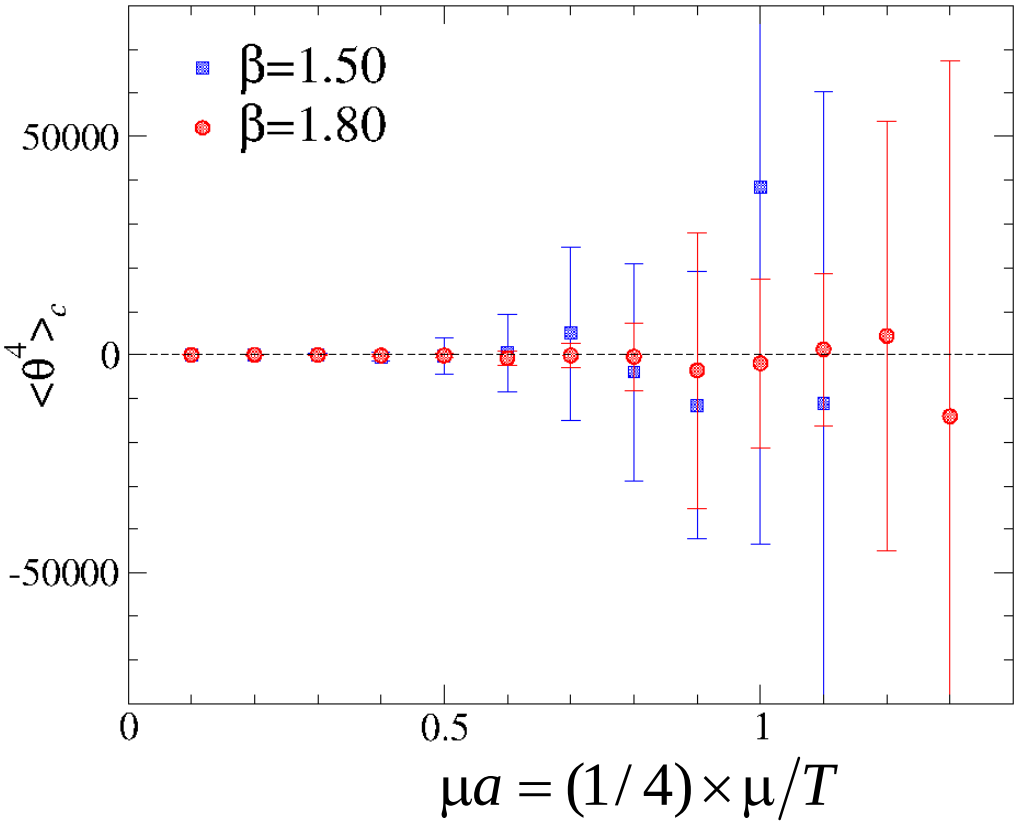
Distribution of the complex phase



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

2nd and 4th cumulants





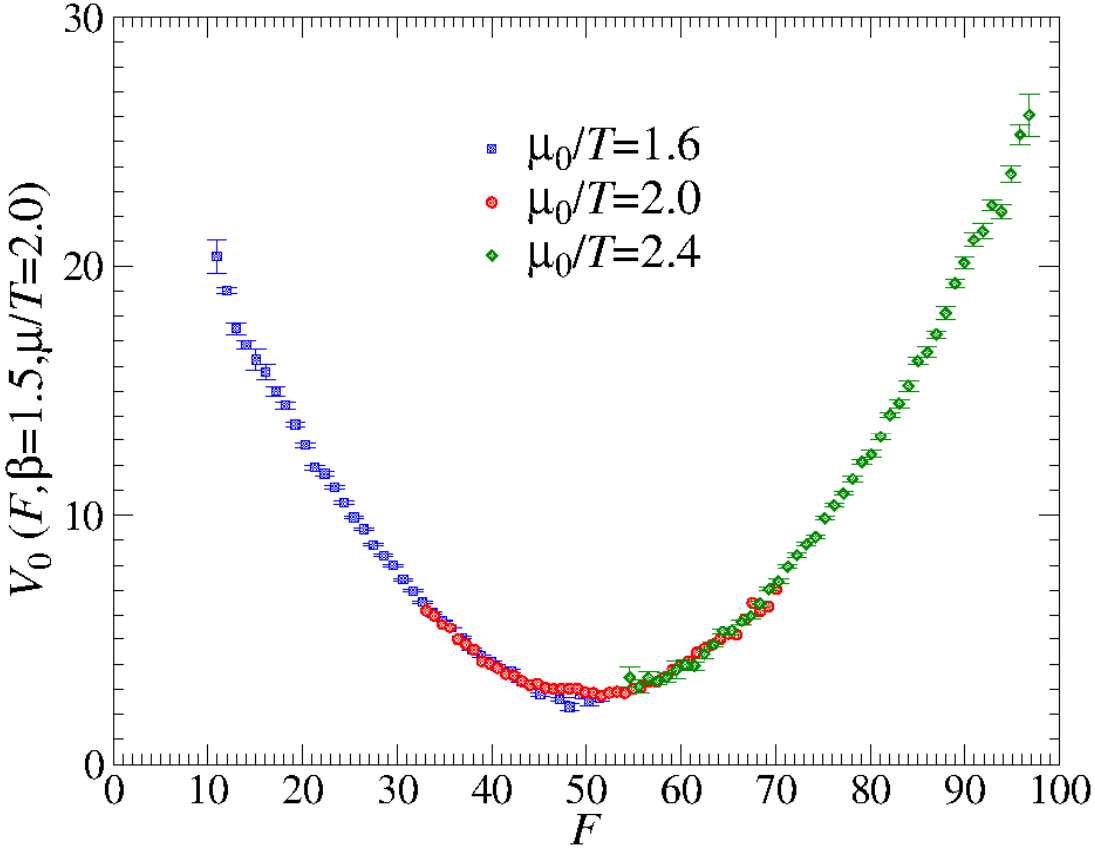
- Large μ and β dependence
- courses the Overlap problem

- 4th cumulant is zero.
- Good convergence.

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.

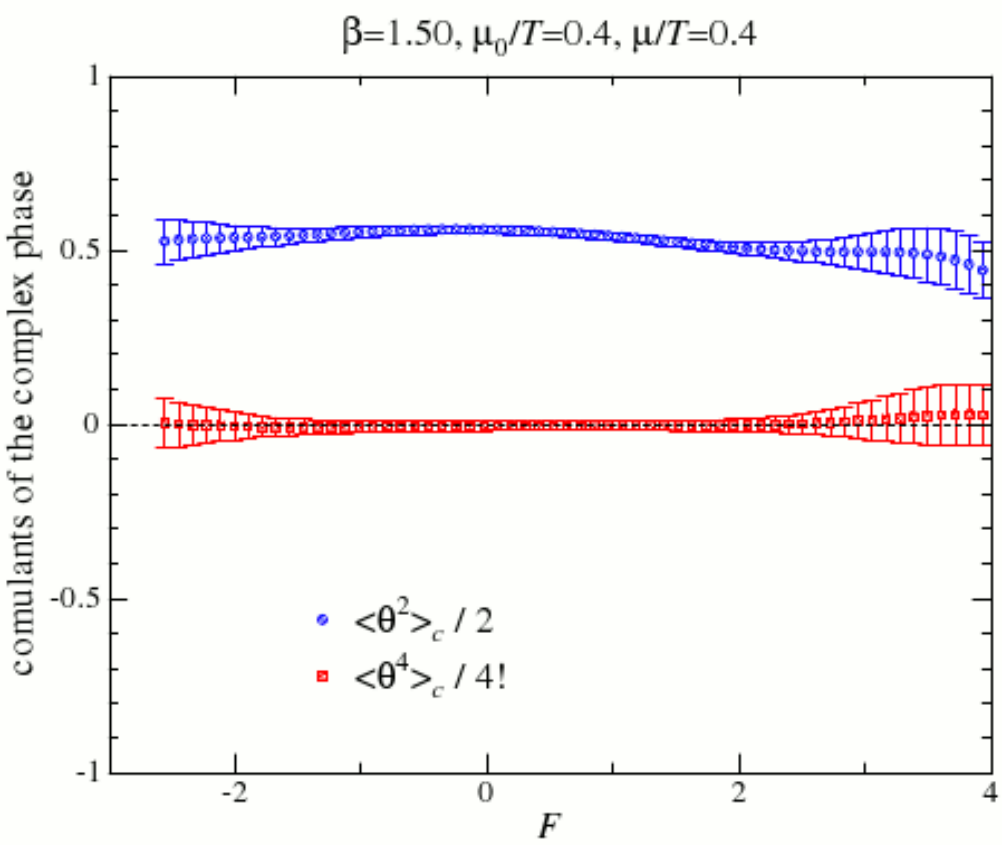
- The error of R is small because F is fixed.

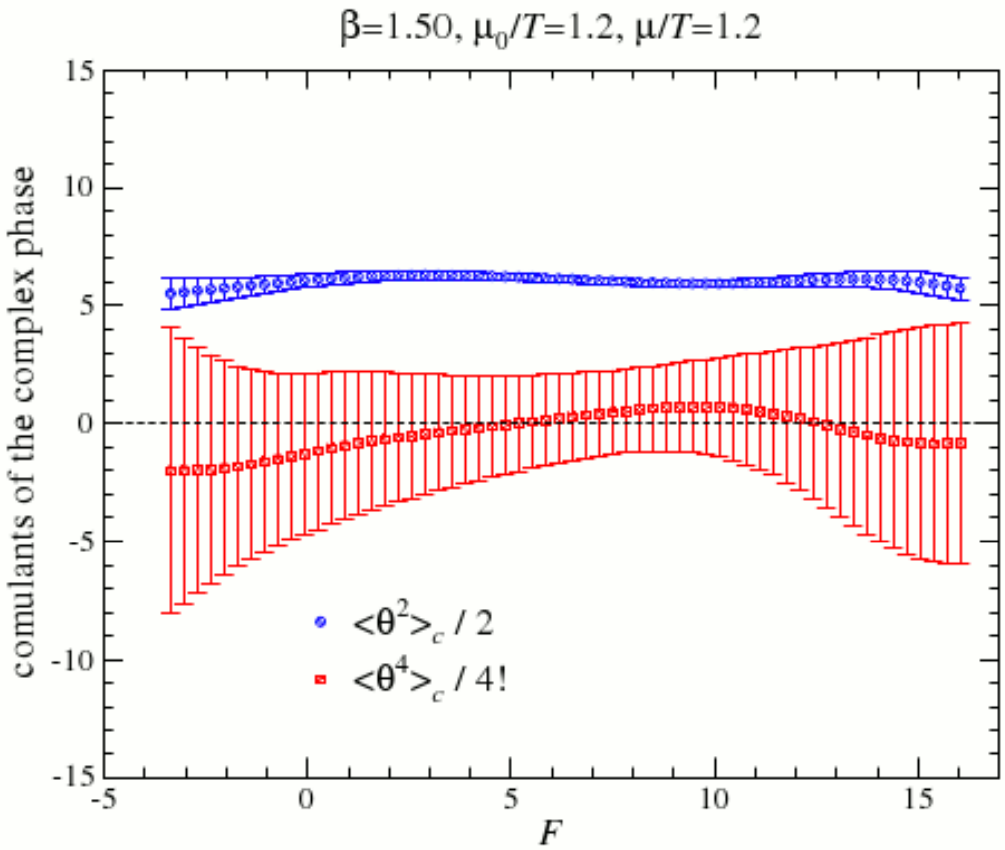
$$-\ln W_0(P,F,\mu_0)-\ln R(P,F,\mu,\mu_0)=-\ln W_0(P,F,\mu)$$

Convergence of the cumulant expansion

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

Preliminary



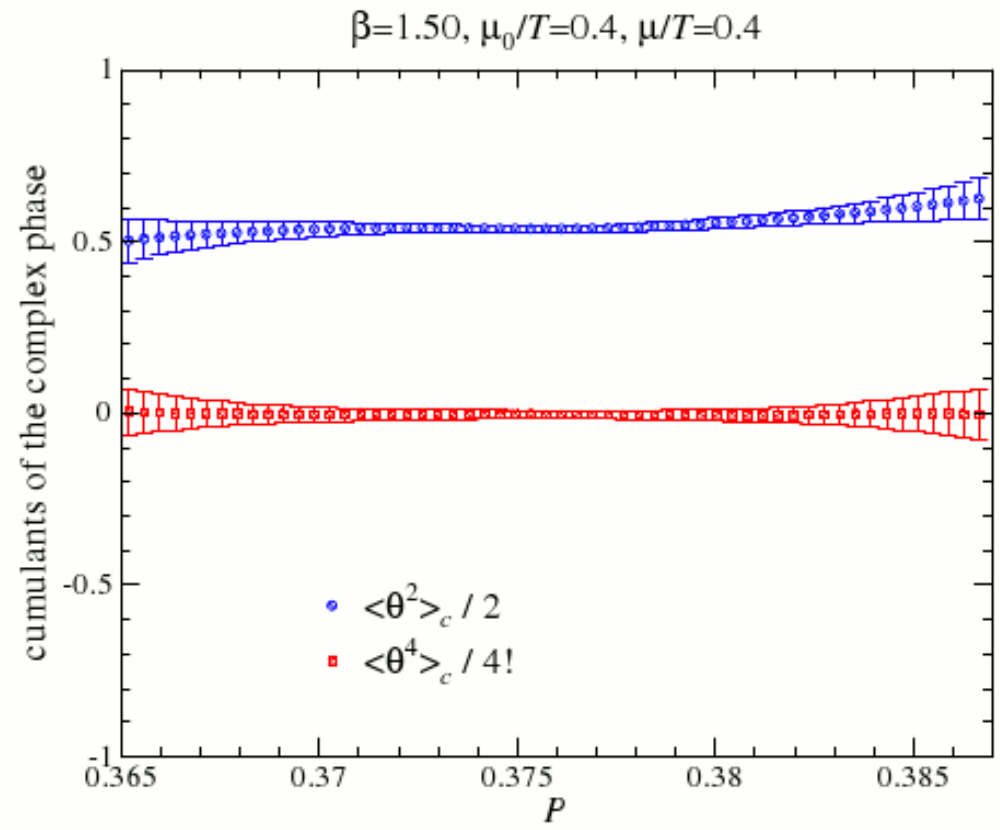


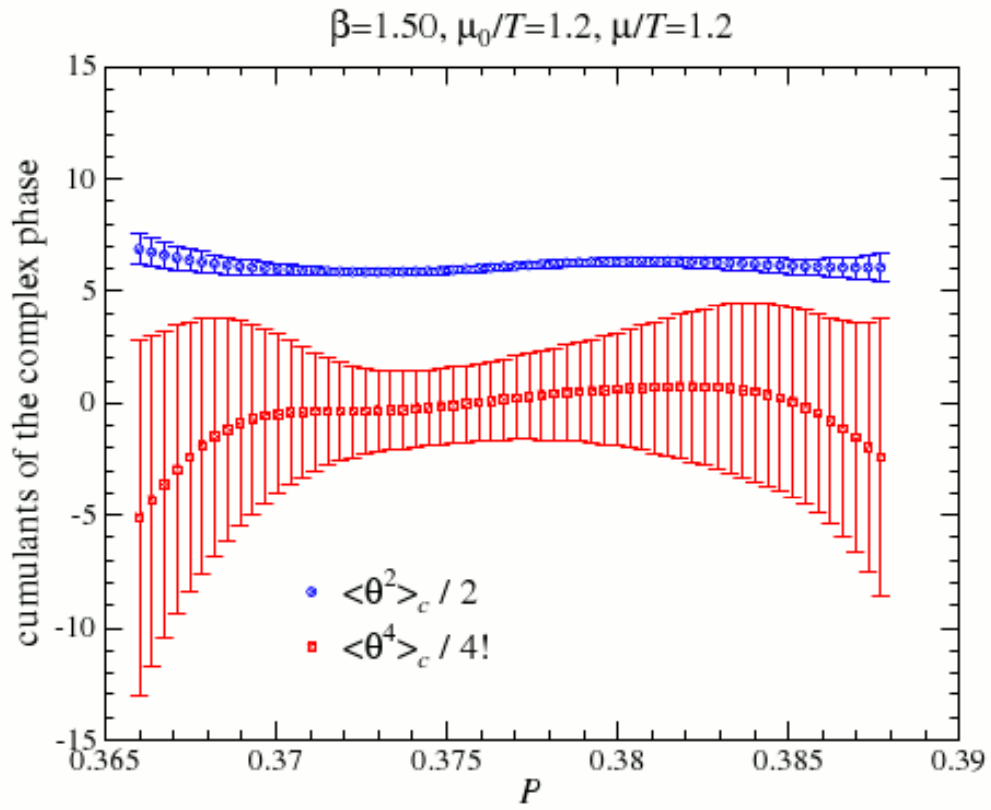
Preliminary

- 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





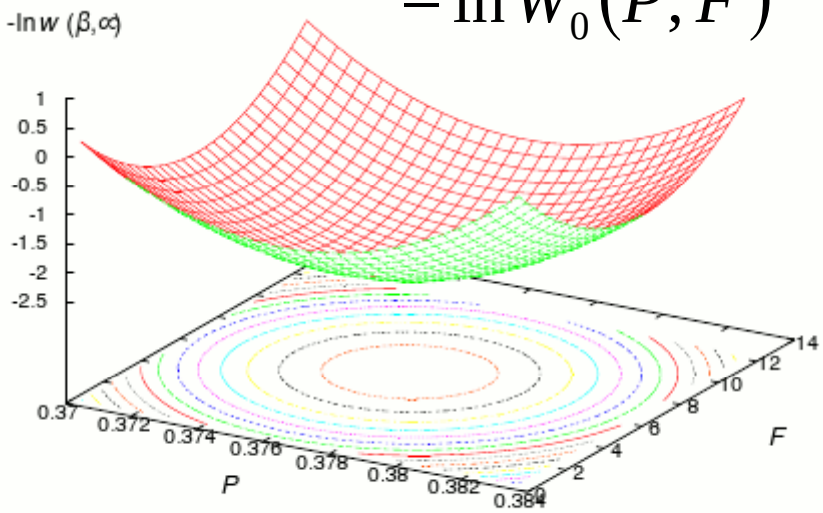
Preliminary

- 4th order cumulant is consistent with zero.

Effective potential at finite μ

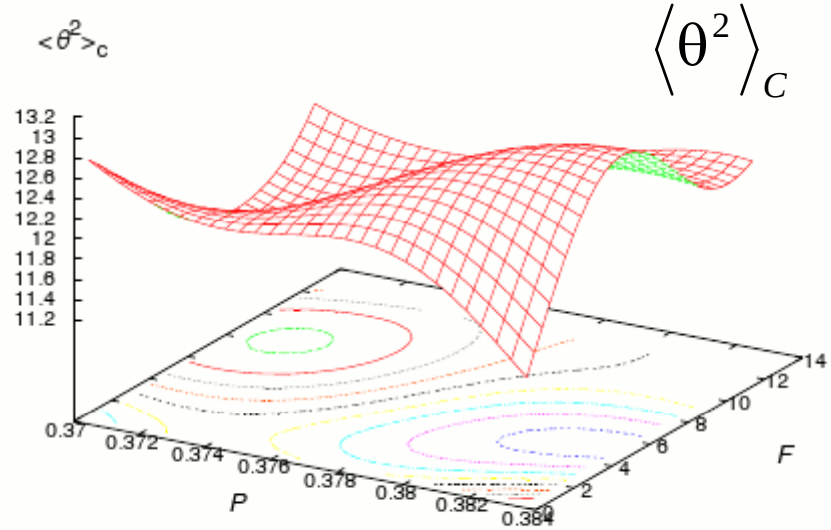
- Combine V_0 and the phase factor. Preliminary

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



+

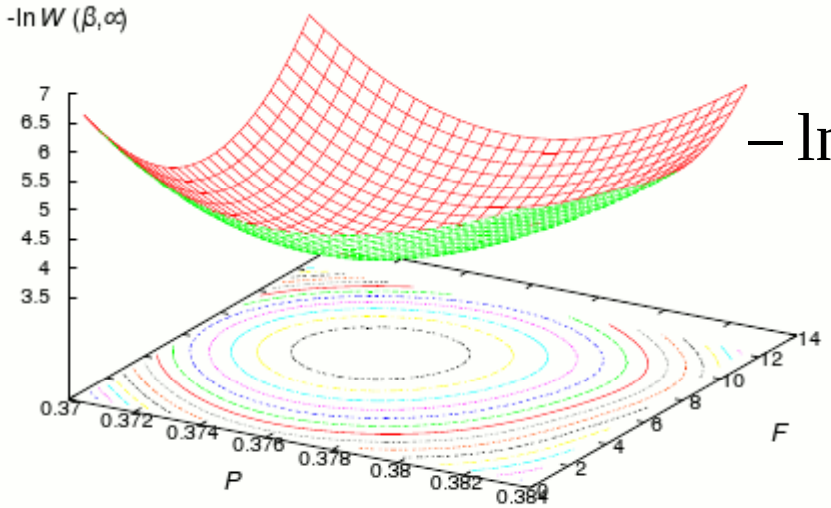
$$\langle \theta^2 \rangle_C$$



$\times 0.5$

=

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



Summary

- We studied the quark mass and chemical potential dependence of QCD phase transition in the heavy quark region and the light 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.