

# Study of finite density lattice QCD by the histogram method

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WHOT-QCD collaboration

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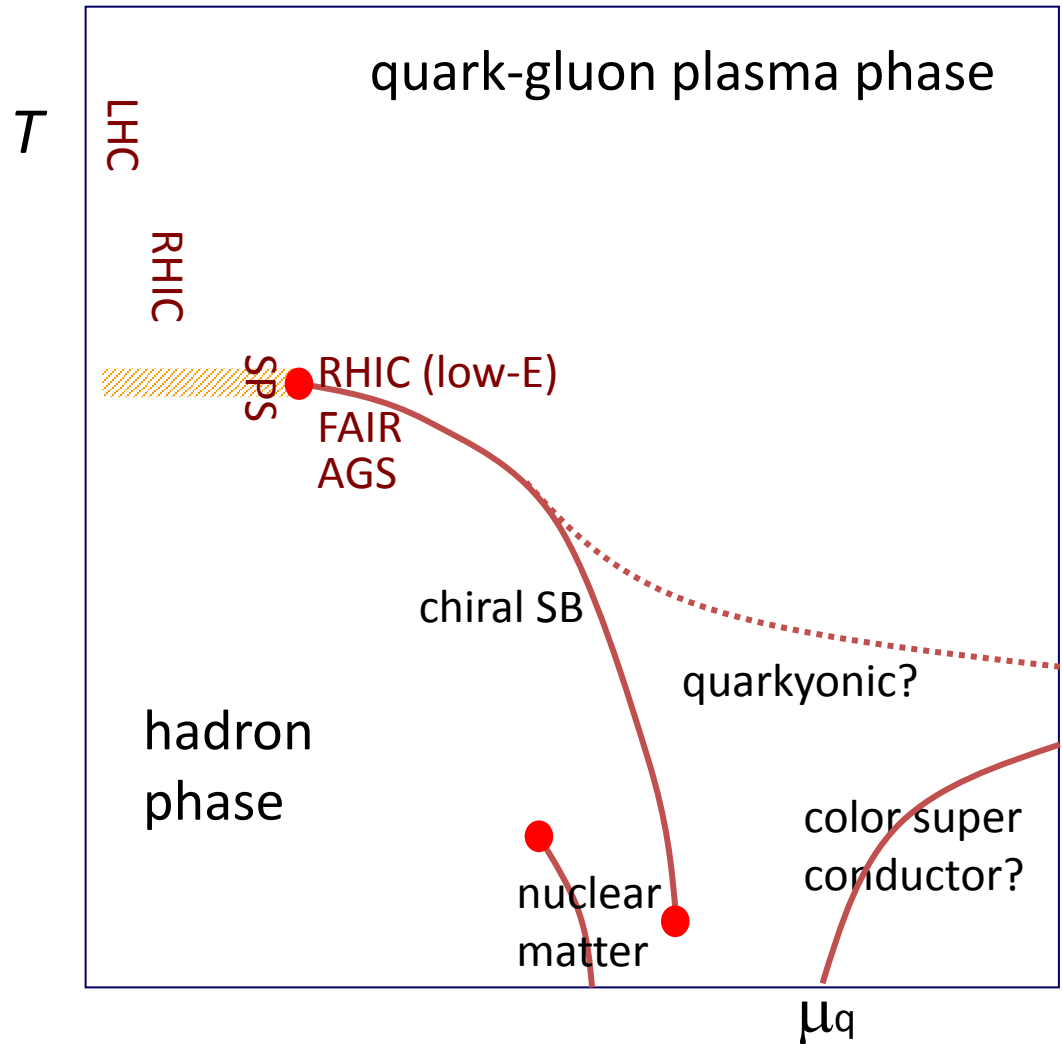
Quarks to Universe in Computational Science (QUCS 2012),  
Nara, Japan, December 13-16, 2012

# Phase structure of QCD at high temperature and density

- Phase transition lines
- Critical point
- Order of the transition

## Lattice QCD Simulations

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



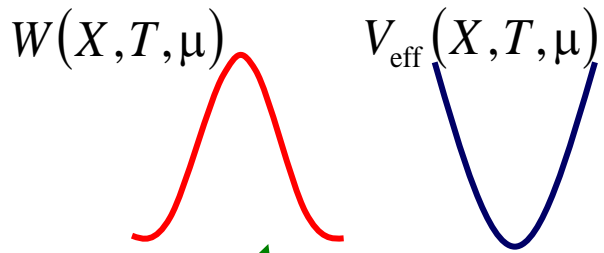
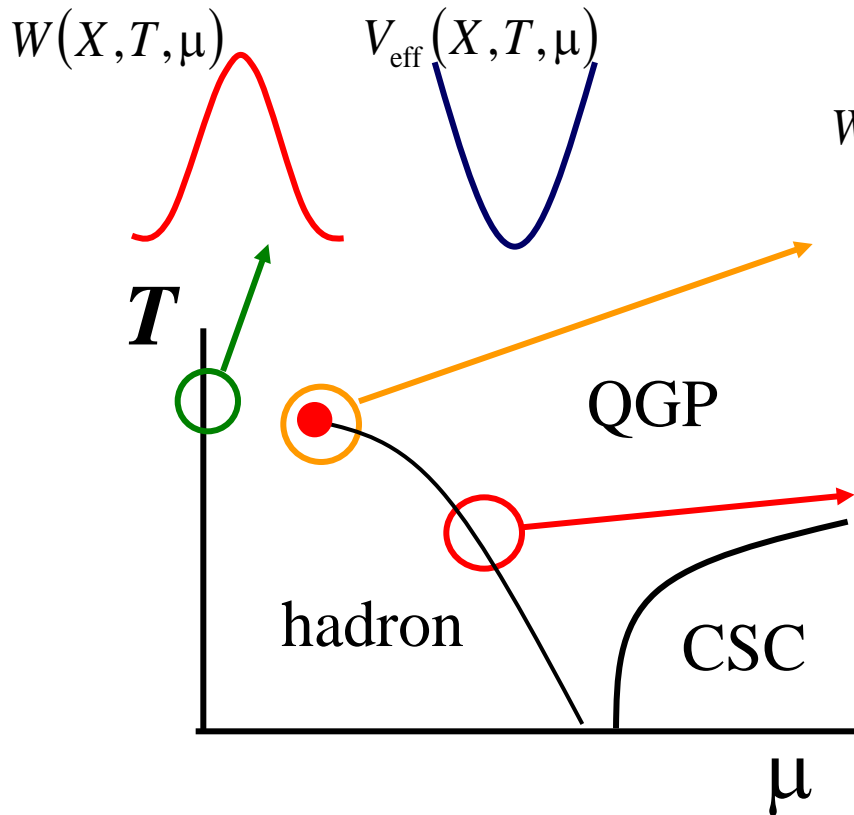
# Distribution function & the effective potential

$$W(X; m, T, \mu) \equiv \int DU \delta(X - \hat{X}) (\det M(m, \mu))^{N_f} e^{-S_g} \quad (\text{Histogram})$$

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

**Crossover**

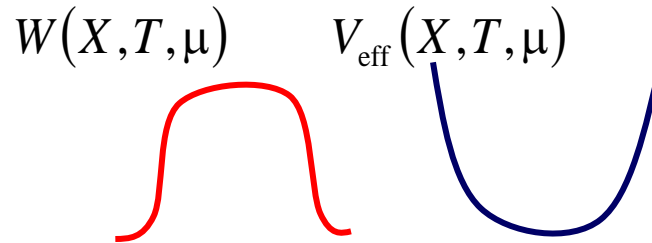
$W(X)$ : Gaussian function  
 $V(X)$ : Quadratic function



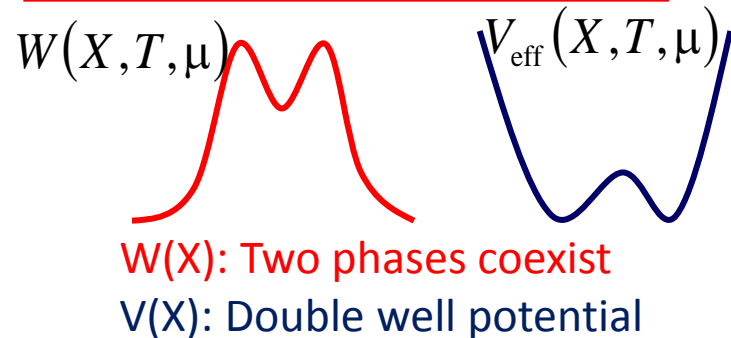
$$V_{\text{eff}}(X) = -\ln W(X)$$

**Critical point**

$W(X)$ : Flat  
 $V(X)$ : Curvature: Zero



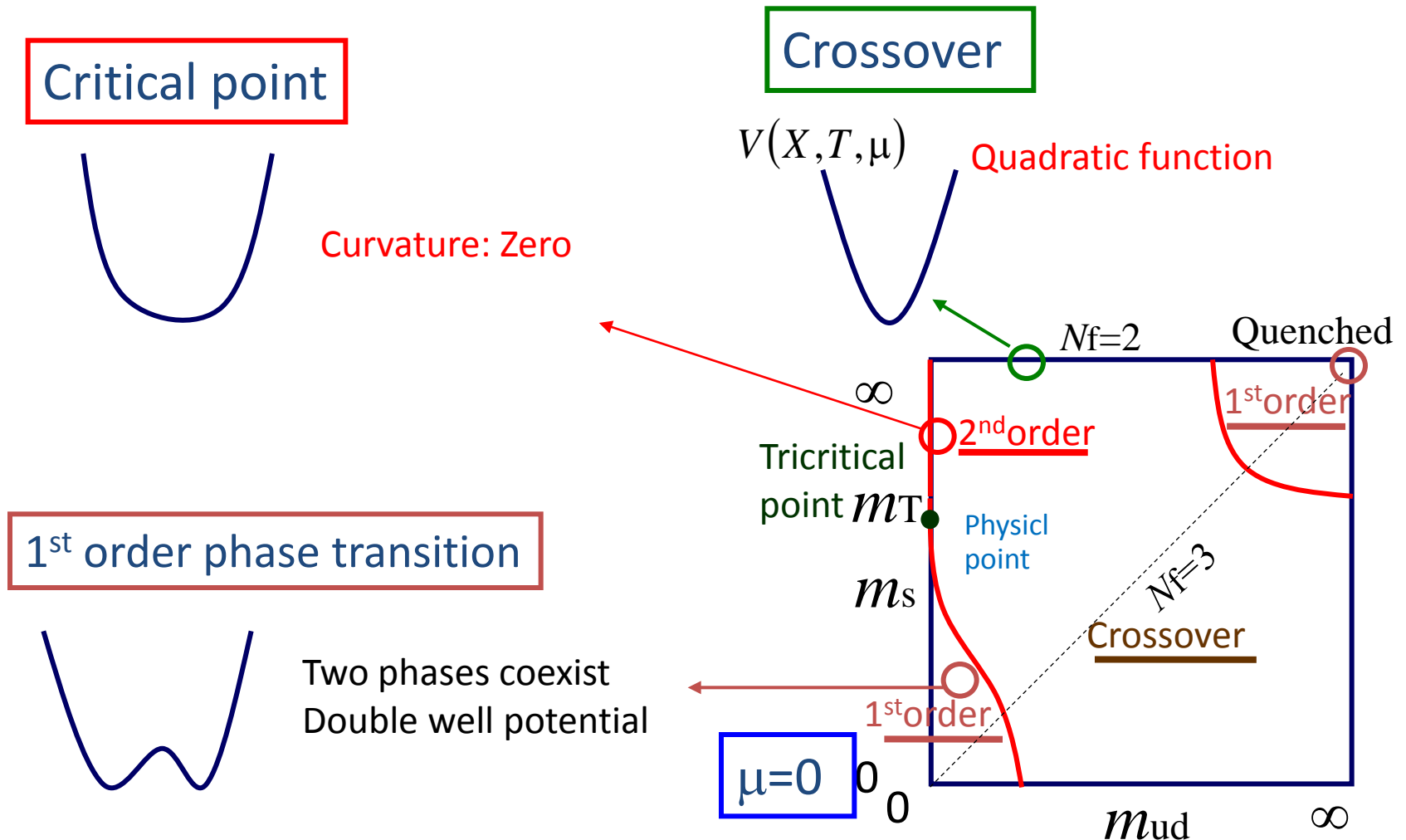
**1st order phase transition**



# Mass-dependence of the effective potential

$$W(X', m, T, \mu) \equiv \int DU \delta(X - X') \sum_{f=1}^{N_f} \det M(m_f, \mu_f) e^{-S_g}, \quad V_{\text{eff}}(X) = -\ln W(X)$$

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



# $(\beta, m, \mu)$ -dependence of the Distribution function

$$W(X, \beta, m, \mu) \equiv \int DU \delta(\hat{X} - X) (\det M(m, \mu))^{N_f} e^{6N_{\text{site}} \beta \hat{P}} \quad (\beta = 6/g^2)$$

plaquette  $P$  (1x1 Wilson loop for the standard action)

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

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

Effective potential:

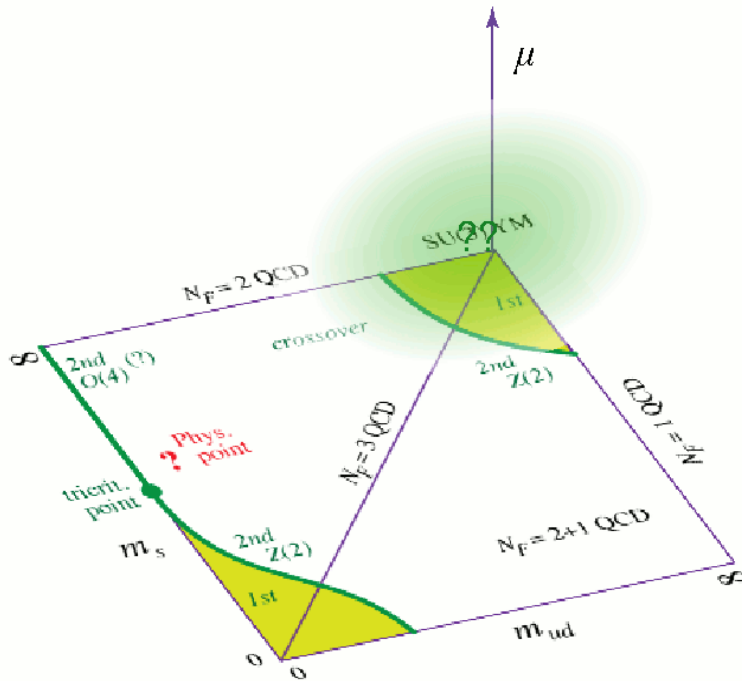
$$V_{\text{eff}}(X, \beta, m, \mu) = -\ln[W(X, \beta, m, \mu)] = V_{\text{eff}}(X, \beta_0, m_0, 0) - \ln R(X, \beta, \beta_0 m, m_0, \mu)$$

$$\ln R(X) = \ln \left\langle \exp \left[ 6N_{\text{site}} (\beta - \beta_0) \hat{P} \right] \left( \frac{\det M(m, \mu)}{\det M(m_0, 0)} \right)^{N_f} \right\rangle_{X:\text{fixed}}$$

Performing simulations at various  $\beta$ , combine the data by multi- $\beta$  reweighting

(Ferrenberg & Swendsen, 89)

# Distribution function in the heavy quark region



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

Hopping parameter expansion ( $\kappa \sim 1/m$ )

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

phase

$P$ : plaquette,  $\Omega = \Omega_R + i\Omega_I$ : Polyakov loop (order parameter)

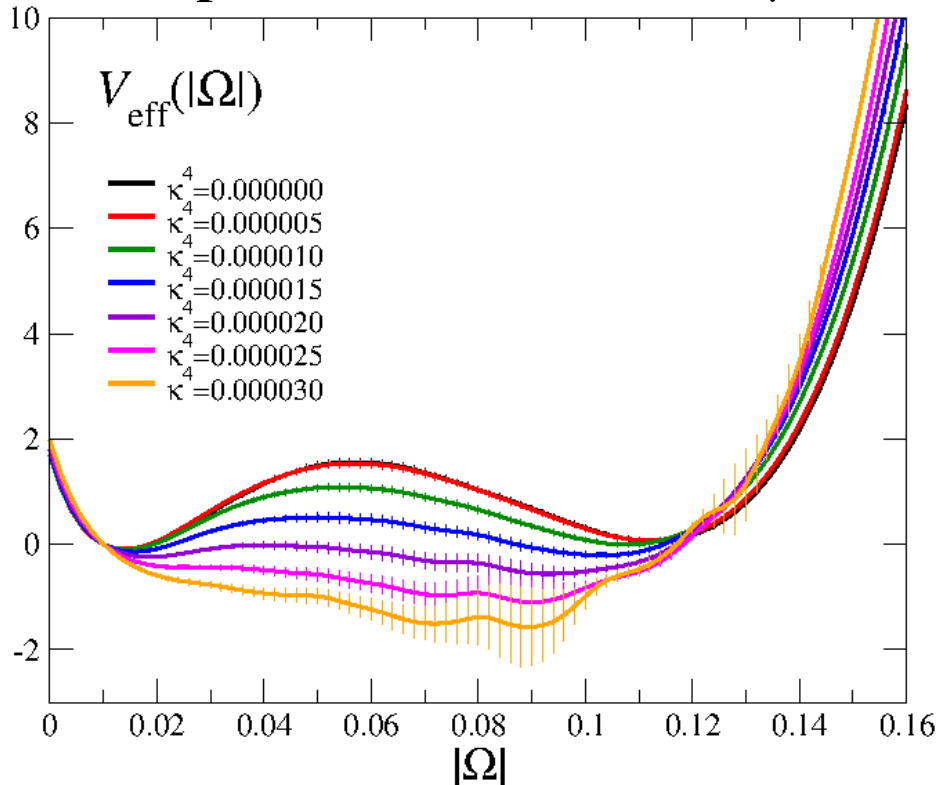
The plaquette term can be absorbed into the gauge action by redefining  $\beta$ .

# Order of the phase transition

## Polyakov loop distribution

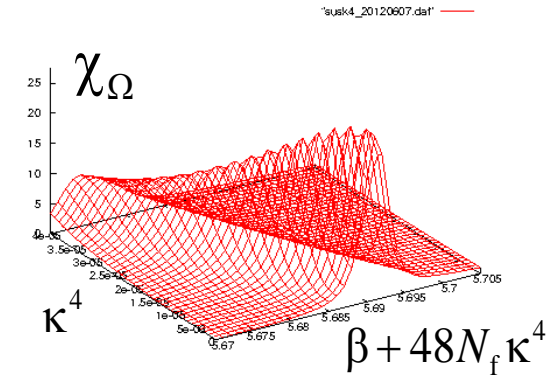
(order parameter of confinement)

Effective potential of  $|\Omega|$   
on the pseudo-critical line at  $\mu=0$



Critical point :  $\kappa^4 \approx 2.0 \times 10^{-5}$

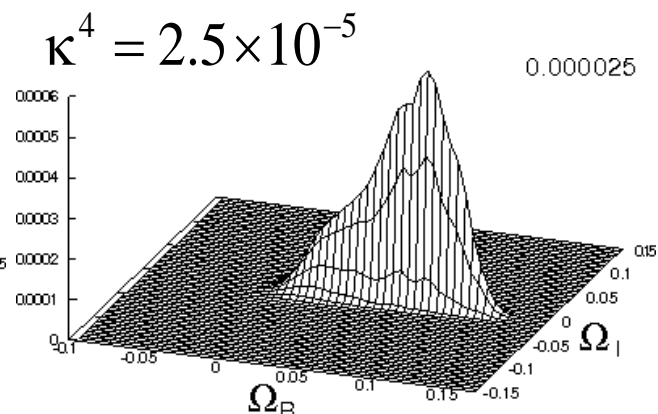
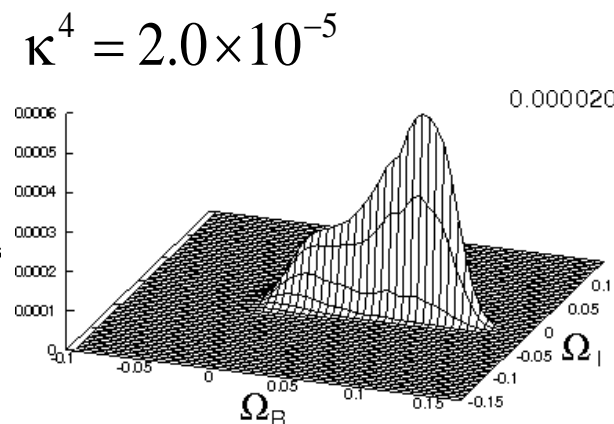
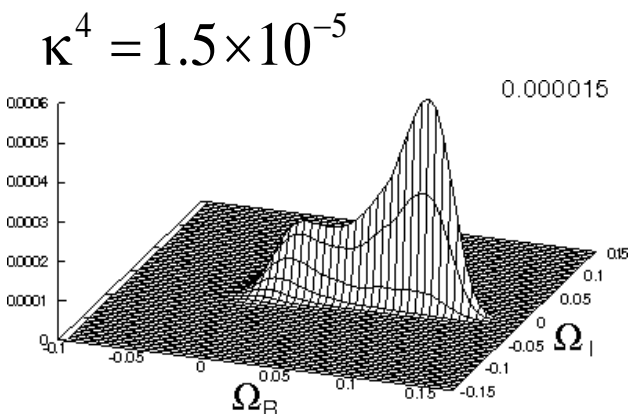
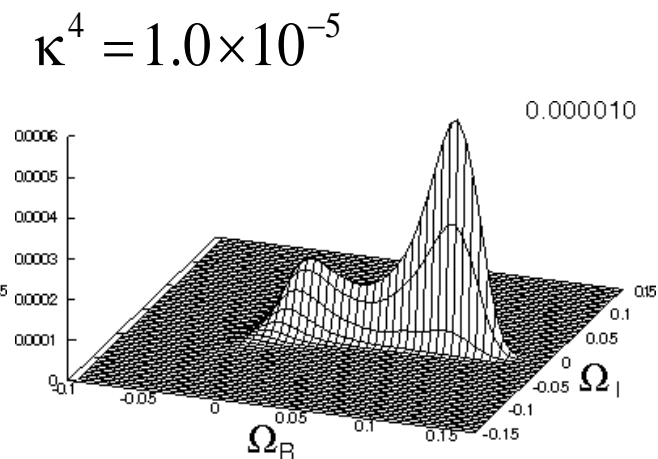
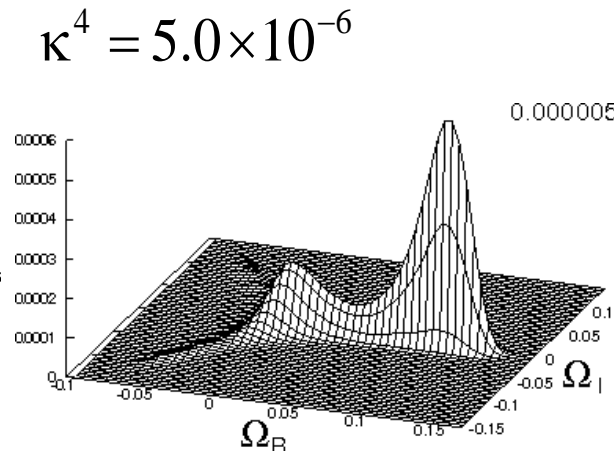
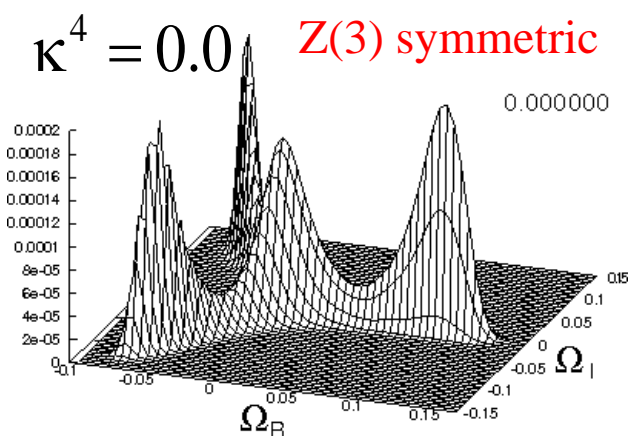
- The pseudo-critical line is determined by  $\chi_\Omega$  peak.



- Double-well at small  $\kappa$ 
  - First order transition
- Single-well at large  $\kappa$ 
  - Crossover

# Polyakov loop distribution in the complex plane

( $\mu=0$ )



**critical point**

- on  $\beta_{pc}$  measured by the Polyakov loop susceptibility.



# Distribution function of $\Omega_R$ at finite density

$$\begin{aligned}
 W(\Omega_R; \beta, \kappa, \mu) &= \int DU \delta(\Omega_R - \hat{\Omega}_R) e^{6N_{\text{site}} \hat{P}} (\det M(\kappa))^{N_f} \\
 &= \int DU \delta(\Omega_R - \hat{\Omega}_R) e^{6N_{\text{site}} \hat{P}} |\det M(\kappa)|^{N_f} e^{i\theta} \\
 &= W_0(\Omega_R; \beta, \kappa, \mu) \langle e^{i\theta} \rangle_{\Omega_R}
 \end{aligned}$$

Phase-quenched simulation:  $W_0(\Omega_R) = \int DU \delta(\Omega_R - \hat{\Omega}_R) |\det M|^{N_f} e^{6N_{\text{site}} \beta \hat{P}}$

$$(\theta = 12 \cdot 2^{N_t} N_s^3 N_f \kappa^{N_t} \sinh(\mu/T) \hat{\Omega}_I)$$

- Heavy quark region

- Effective potential:  $V_{\text{eff}}(\Omega_R) = -\ln W(\Omega_R)$ ,  $V_0(\Omega_R) = -\ln W_0(\Omega_R)$

(Phase-quenched part)

$$V_{\text{eff}}(\beta, \kappa, \mu) = V_0(\beta, \kappa, \mu) - \ln \langle e^{i\theta} \rangle_{\Omega_R}$$

Phase average

- $V_0$  is equal to  $V_{\text{eff}}(\mu=0)$  when we replace  $\kappa^{N_t} \Rightarrow \kappa^{N_t} \cosh(\mu/T)$ 
  - Critical point (phase-quenched)

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

$$N_f=2 \text{ at } \mu=0: \kappa_{\text{cp}}=0.0658(3)(8)$$

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

# Avoiding the sign problem

(SE, Phys.Rev.D77,014508(2008), WHOT-QCD, Phys.Rev.D82, 014508(2010))

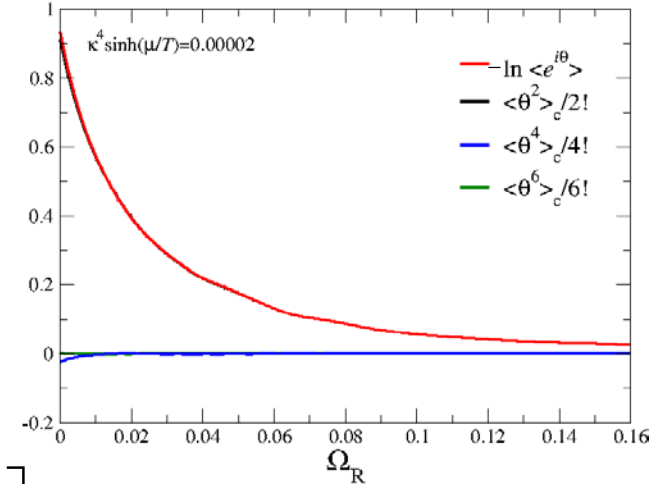
$\theta$ : complex phase  $\theta \equiv \text{Im} \ln \det M \approx 12 \cdot 2^{N_t} N_s^3 N_f \kappa^{N_t} \sinh(\mu/T) \Omega_I$

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

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

- Cumulant expansion

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



$$\kappa^4(\mu) \sinh(\mu/T) = 0.00002$$

$$\beta = 5.69$$

cumulants

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

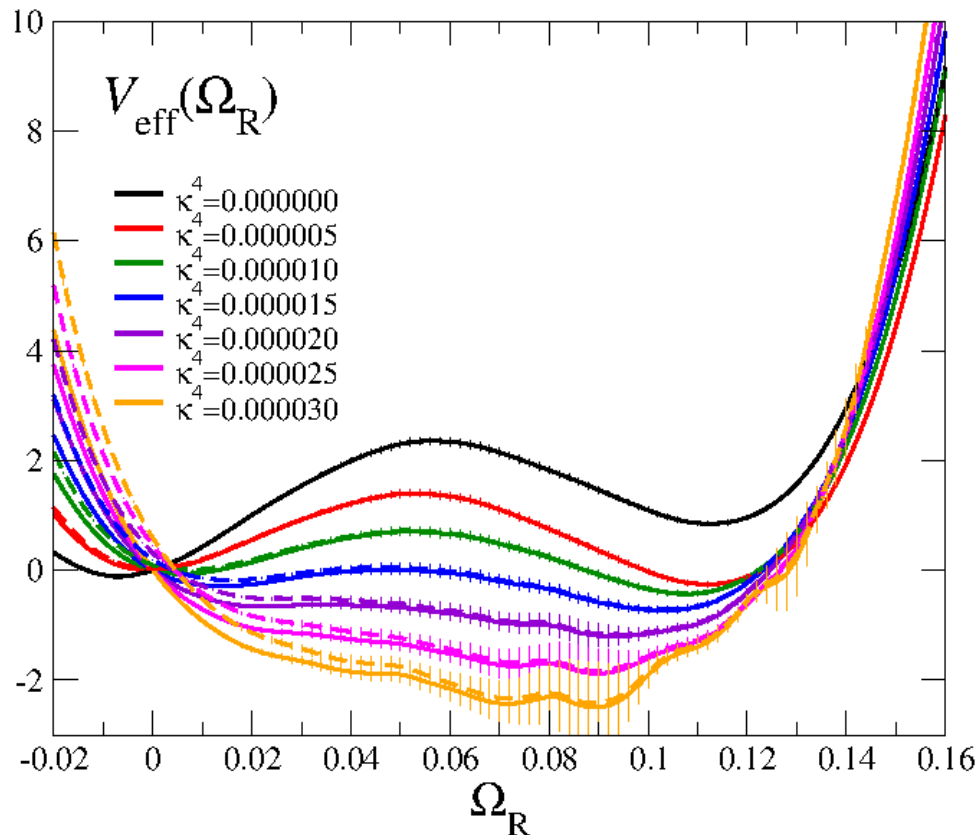
– Odd terms vanish from a symmetry under  $\mu \leftrightarrow -\mu$  ( $\theta \leftrightarrow -\theta$ )

Source of the complex phase

If the cumulant expansion converges, No sign problem.

# Effect from the complex phase factor

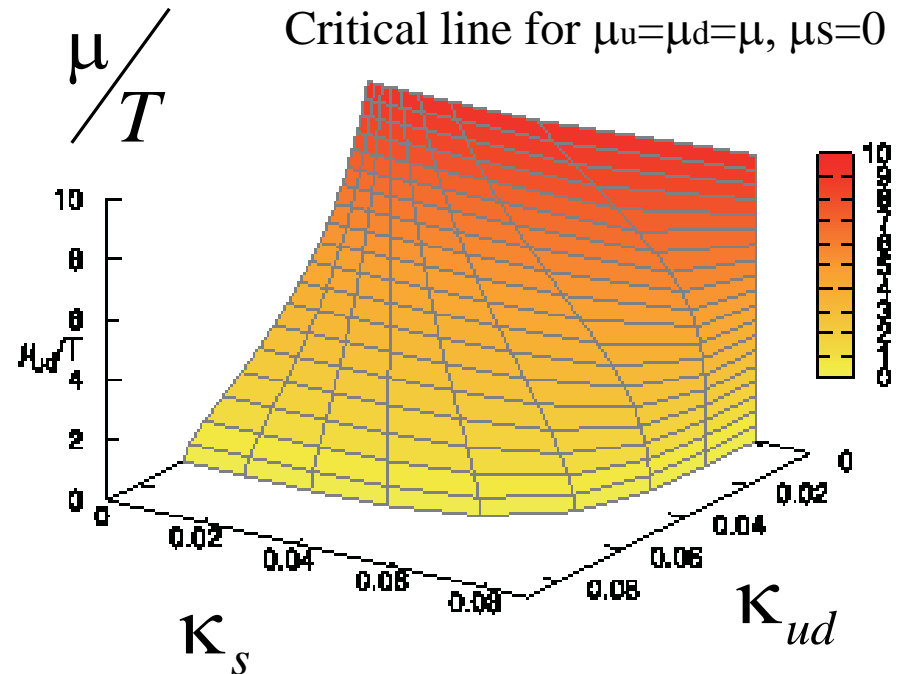
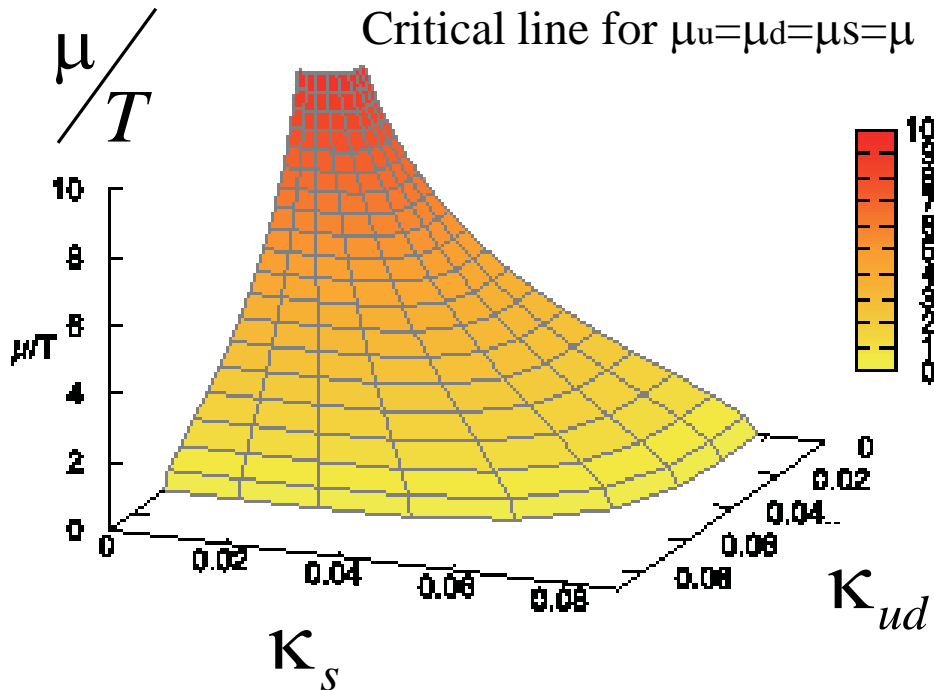
- Polyakov loop effective potential at various  $\kappa^{N_t} \cosh(\mu/T)$  at the transition point.
  - Solid lines:  $\mu=0$  , i.e.,  $\cosh(\mu/T)=1$ ,  $\sinh(\mu/T)=0$
  - Dashed lines:  $\mu = \infty$ , i.e,  $\sinh(\mu/T) = \cosh(\mu/T)$



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

# Critical surface in 2+1-flavor finite density QCD in the heavy quark region

- The effect from the complex phase is very small for the determination of  $\kappa_{cp}$ .
- The phase effect is neglected.



# Probability distribution function in the light quark region $\rightarrow$ Nakagawa's poster

- We perform phase quenched simulations with the weight:

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

$$\begin{aligned} W(P', F', \beta, m, \mu) &= \int DU \delta(\hat{P} - P') \delta(\hat{F} - F') (\det M(m, \mu))^{N_f} e^{6N_{\text{site}}\beta\hat{P}} \\ &= \int DU \delta(\hat{P} - P') \delta(\hat{F} - F') e^{i\theta} |\det M(m, \mu)|^{N_f} e^{6N_{\text{site}}\beta\hat{P}} \\ &= \underbrace{\langle e^{i\theta} \rangle}_{P', F'} \times \underbrace{W_0(P', F', \beta, m, \mu)}_{\text{histogram}} \end{aligned}$$

expectation value with fixed  $P, F$       histogram

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

Distribution function of the phase quenched.

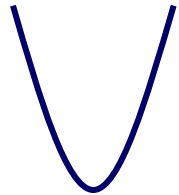
$$W_0(P', F') = \int DU \delta(\hat{P} - P') \delta(\hat{F} - F') |\det M|^{N_f} e^{6N_{\text{site}}\beta\hat{P}}$$

# $\mu$ -dependence of the effective potential

## Curvature of the effective potential

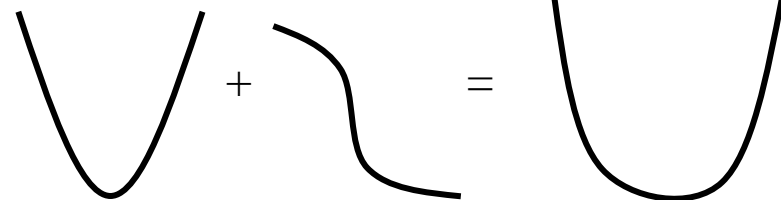
Crossover

$$-\ln[W(P, \beta)]$$

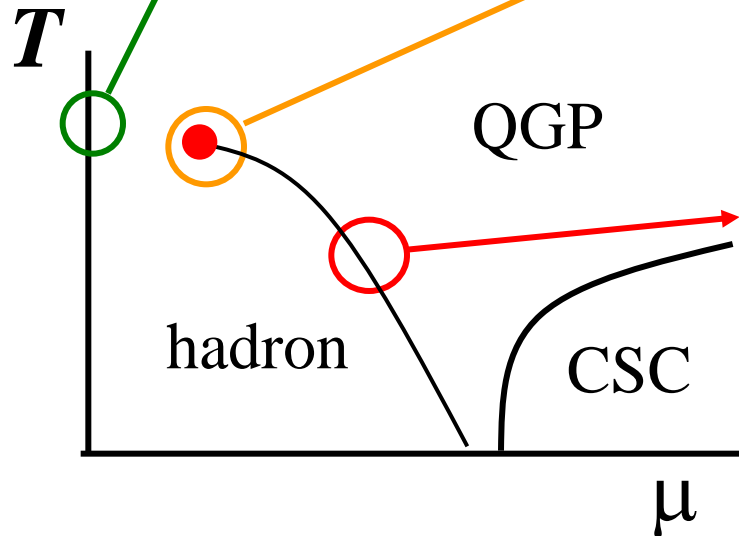


Critical point

$$-\ln[W_0(P, \beta)] \quad -\ln[\langle e^{i\theta} \rangle]$$

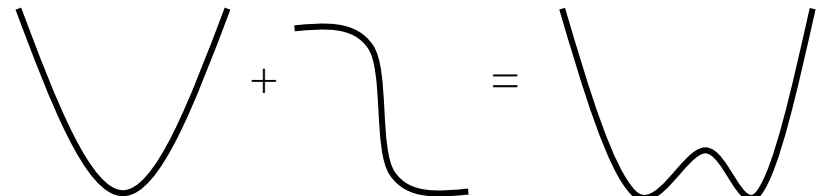


phase effect **Curvature: Zero**



1<sup>st</sup> order phase transition

$$-\ln[W_0(P, \beta)] \quad -\ln[\langle e^{i\theta} \rangle]$$



phase effect **Curvature: Negative**

# Curvature of the effective potential

- Assuming the distribution is Gaussian,

$$W_0(P, F) \approx \sqrt{\frac{6N_{\text{site}}}{2\pi\chi_P}} \exp\left[-\frac{6N_{\text{site}}}{2\chi_P} (P - \langle P \rangle)^2\right] \times \sqrt{\frac{N_{\text{site}}}{2\pi\chi_F}} \exp\left[-\frac{N_{\text{site}}}{2\chi_F} (F - \langle F \rangle)^2\right]$$

$$\chi_P = 6N_{\text{site}} \left\langle (P - \langle P \rangle)^2 \right\rangle \quad \chi_F = N_{\text{site}} \left\langle (F - \langle F \rangle)^2 \right\rangle$$

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

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

at the peak of the distribution

## Cumulant expansion

$$W(P, F) = W_0(P, F) \left\langle e^{i\theta} \right\rangle_{P, F: \text{fixed}} \approx W_0(P, F) \exp\left[\frac{1}{2} \left\langle \theta^2 \right\rangle_{P, F: \text{fixed}}\right]$$

$$\left\langle \theta^2 \right\rangle_{P, F: \text{fixed}} \approx \left\langle \theta^2 \right\rangle(\langle P \rangle, \langle F \rangle) \quad \rightarrow \quad \text{Curvature of } \left\langle \theta^2 \right\rangle$$

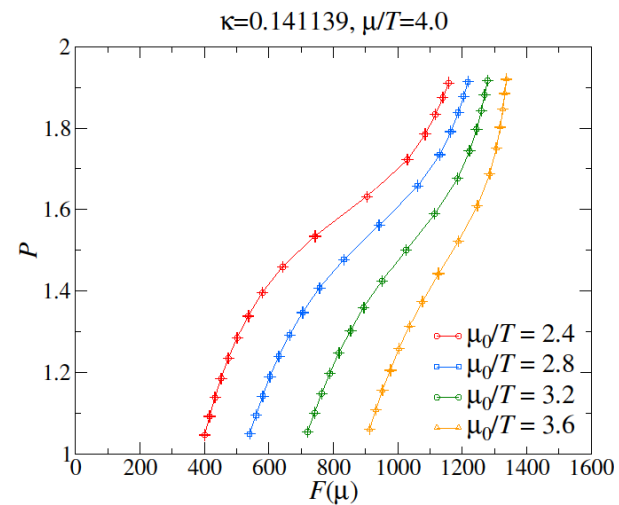
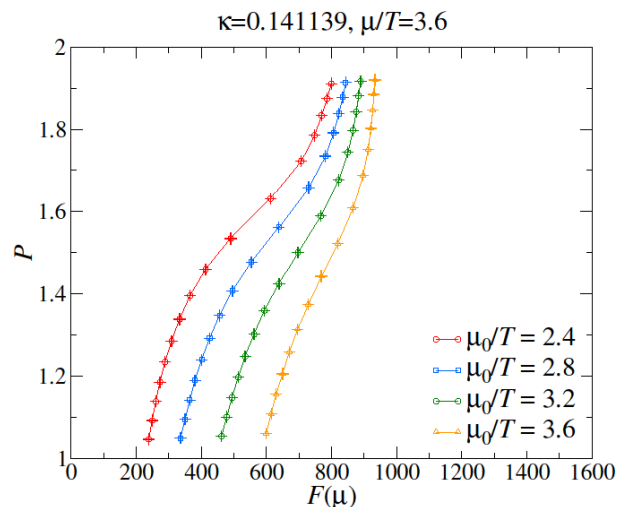
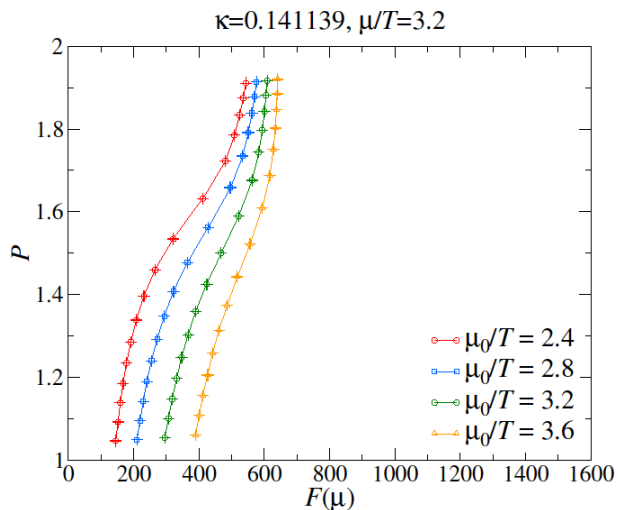
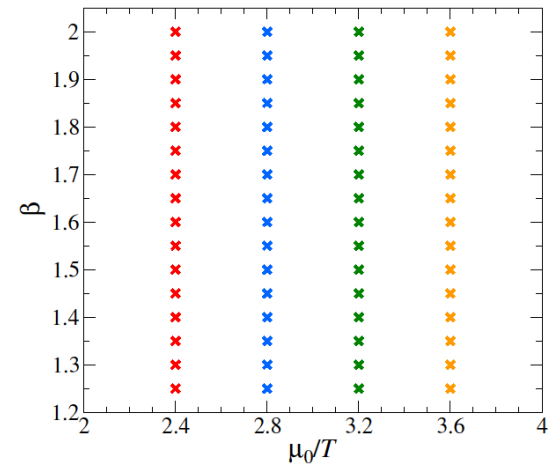
# Simulations

2-flavor QCD Iwasaki gauge  
+ clover Wilson quark action

Random noise method is used.

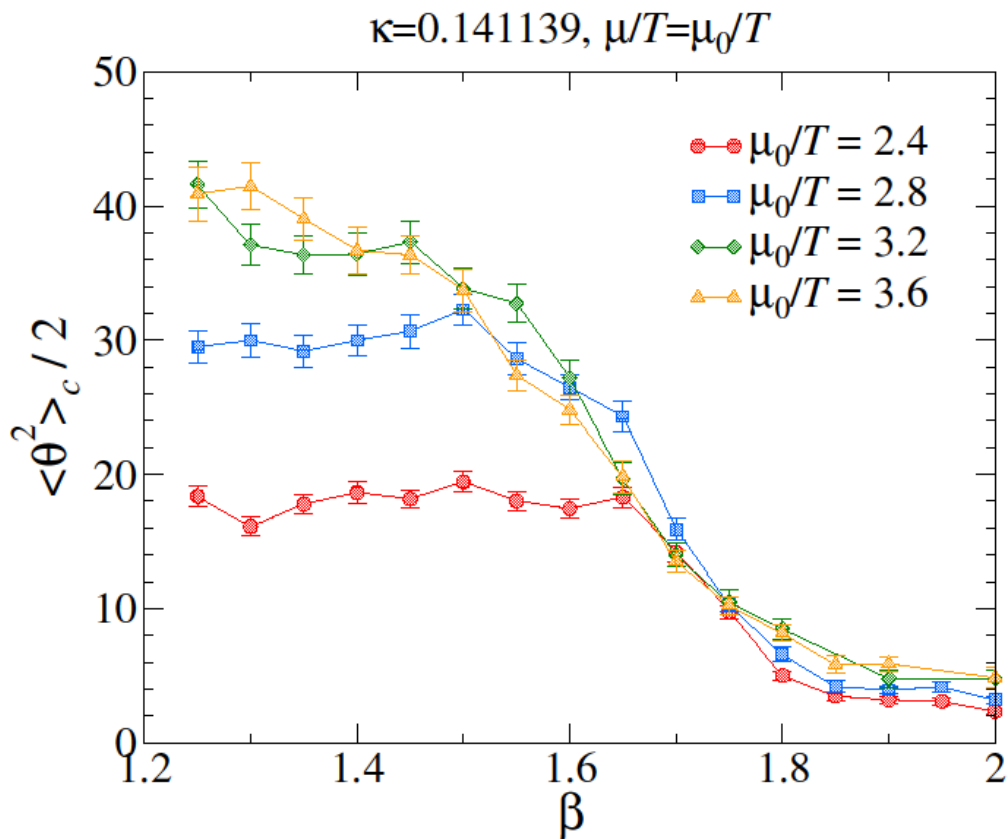
$8^3 \times 4$  lattice  $m_\pi/m_\rho \approx 0.8$

- Simulation points in the  $(\beta, \mu_0/T)$
- Peak of  $W_0(P, F)$  for each  $\mu$





# Effect from the complex phase



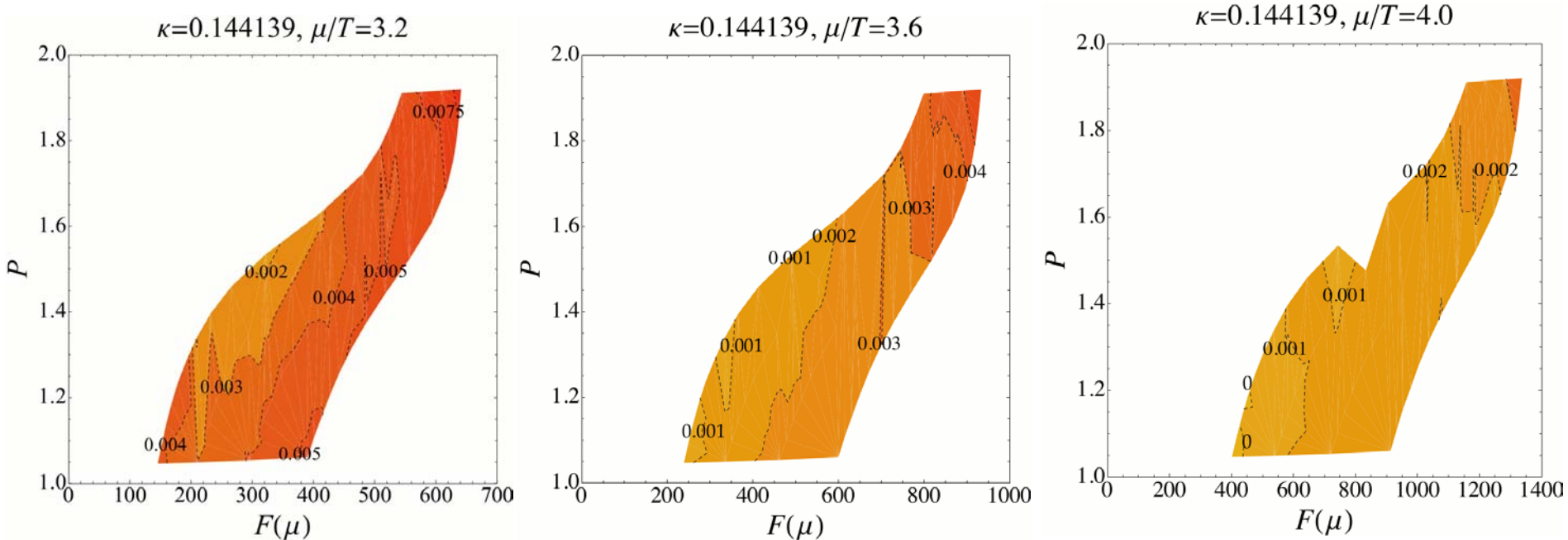
$$-\ln[W_0(P, \beta)] + \frac{1}{2} \langle \theta^2 \rangle_c$$

phase effect

Curvature: Negative

- Rapidly changes around the pseudo-critical point.
- Strong curvature in  $\langle \theta^2 \rangle_c / 2$

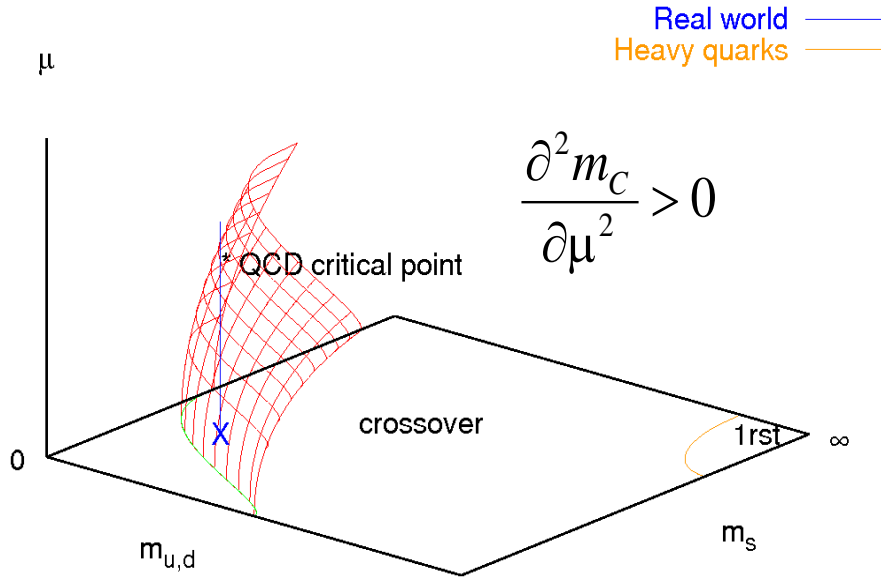
# Curvature of the effective potential for $F$ -direction



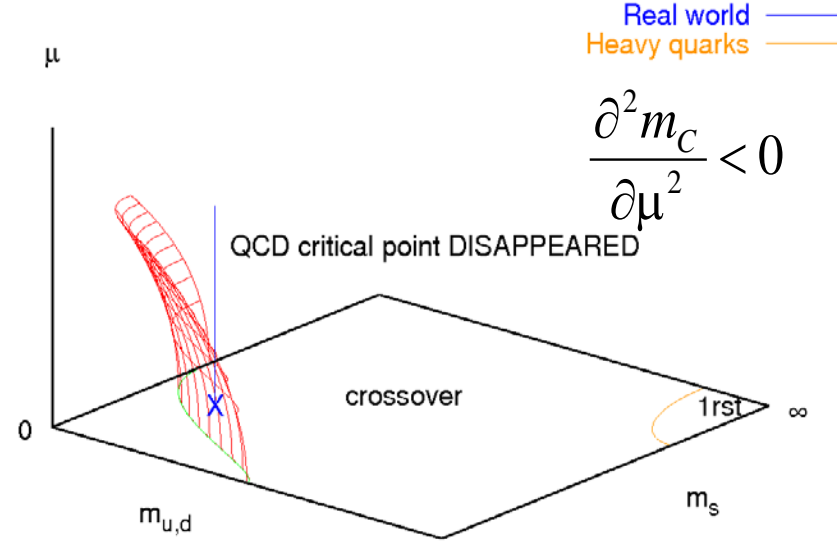
zero curvature  
Critical point

- Appearance of the critical point: suggested at  $\mu/T=4.0$   
(The quark mass is much heavier than the physical mass.)

# Curvature of the critical surface



- Usual expectation
- Critical point: exists



- de Forcrand - Philipsen, JHEP01(2007)077; PoS(LAT2007)178
  - **Curvature: slightly negative.** (3-flavor staggered,  $8^3 \times 4$  lattice)

New approach 2+ $N_f$ -flavor QCD (large  $N_f$ )  $\rightarrow$  Yamada's talk  
(2 light quarks +  $N_f$  heavy quarks)  
 $\rightarrow$  **Curvature: positive.**

# $2+N_f$ -flavor QCD ( $N_f \gtrsim 10$ )

(Ejiri, Yamada, 2012, in preparation)

$$h = 2N_f (2\kappa_h)^{N_t}$$

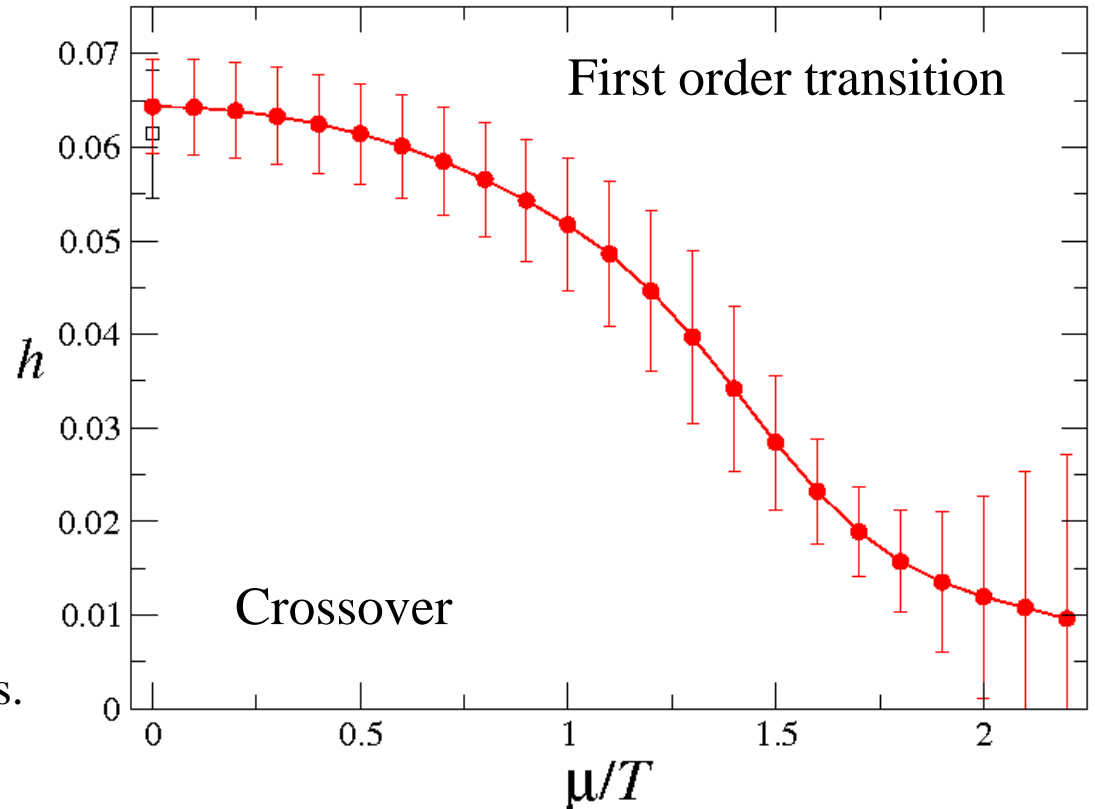
for Wilson quarks

$$h = N_f / \left( 4(2m_h)^{N_t} \right)$$

for staggered quarks

2-flavor dynamical simulation  
with p4-improved staggered quarks  
and reweighting for the heavy quarks.

$$m_\pi/m_\rho \approx 0.7$$



- The critical mass: larger with  $N_f$ .
- For large  $N_f$ , the critical mass is in the heavy quark region.
- First order transition region: wider as increasing  $\mu$ .

# Summary

- We studied the quark mass and chemical potential dependence of the nature of QCD phase transition.
- Heavy quark region: 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  $\theta$  is useful.
- Phase quenched simulations: The effective potential at large  $\mu$  suggests the the existence of the critical point.
- $2+N_f$ -flavor QCD: First order transition region: wider with  $\mu$ .
- To find the critical point at finite density, further studies in light quark region are important applying this method.