Numerical simulations to understand QCD phase transition at high temperature and density

Shinji Ejiri (Niigata University)

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## Phase structure of QCD at high temperature and density

- Phase transition lines
- Critical point
- Equation of state
- Thermodynamic quantities

Lattice QCD Simulations

 Direct simulation: Impossible at µ≠0.



# Heavy-ion collisions at RHIC and LHC

- Beam energy scan at RHIC
  - Fluctuations
  - Higher order cumulant
  - Bryon number distribution
  - Canonical partition function

- M. Kitazawa
  - A. Nakamura

# **RHIC Beam Energy Scan**

• Investigate the density dependence changing the beam energy



# Cumulants of conserved charges

BNL-Bielefeld, Phys. Rev. Lett. 109, 192302 (2012)





# Heavy-ion collisions at RHIC and LHC

- Hydrodynamics in HIC
  - Equation of State: Energy density, Pressure

T. Umeda

- Energy-Momentum tensor from Wilson flow: useful?
   T. Hatsuda, H. Suzuki
- Transport coefficients: Viscosity etc. ???

# Viscosity in QGP



Kovtun, Son, Starinets, PRL 94, 111601 (2005)

Viscose Hydrodynamics calculation

e.g. 
$$\eta/s \approx 0.12$$

Lattice calculation: in the stage of quenched approximation





# Nature of the phase transitions in terms of quark masses

- 2-flavor QCD: the chiral limit
  - O(4) universality crass or First order transition  $- U_{A}(1)$  symmetry? S. Aoki, Y. Taniguchi
- 3-flavor QCD: critical quark mass
  - Improved staggered: very small, m<sub>PS</sub><60MeV?</p>
  - Improved Wilson? Large? Y. Nakamura
  - At the physical quark mass?
- Finite chemical potential?

S. Takeda, SE

#### O(4) scaling test by N<sub>f</sub>=2 Wilson-type quark Iwasaki gauge + Clover Wilson (CP-PACS, PRD63.034502(2000))



Consistent with O(4) scaling function.

#### Scaling test by 2+1 flavor staggered quarks BNL-Bielefeld, PRD80,094505(2009)



- Fixing the strange quark mass (ms) at the physical point, they investigated the light quark mass (ml) dependence.
- The scaling behavior agrees for ml/ms<1/20 (~ phisical point)
- (Tricritical point) < ms (physical)  $\implies$  the first order region is very small. 10

# First order transition in 2-flavor QCD by staggered quarks

- The critical line separating first order and crossover is determined in QCD with an imaginary chemical potential  $\mu_I$ .
- Extrapolate to light mass direction, the critical line crosses  $\mu_I = 0$ .





## Quark Mass dependence of QCD phase trantion



- The determination of the boundary of 1<sup>st</sup> order region: important.
- On the line of physical mass, the crossover at low density 

   → 1<sup>st</sup> order transition at high density.
- However, the 1<sup>st</sup> order region is very small, and simulations with very small quark mass are required. 
   Difficult to study.

# New and Old Approaches

- Complex Langevin
   I-O. Stamatescu
- Simulations on Lefschets Thimbles
   M. Cristoforetti, Y. Kikukawa
- Strong Coupling effective theory A. Ohnishi
- Reduction formula, Lee-Yang Zero K. Nagata
- Reweighting method SE
- TBA Handa??

# Histogram method (Reweighting method)

• Monte-Carlo method

(Sg: gauge action, M: qaurk matrix)

• Generate configurations with the probability of the Boltzmann weight.

$$\langle O \rangle_{(m,T,\mu)} = \frac{1}{Z} \int DU O \left( \det M(m,\mu) \right)^{N_{\mathrm{f}}} e^{-S_g} \approx \frac{1}{N_{\mathrm{conf.}}} \sum_{\{\mathrm{conf.}\}} O$$

Distribution function in Density of state method (Histogram method)
 *X*: order parameters, total quark number, average plaquette etc.

$$W(X;m,T,\mu) \equiv \int DU \,\delta(X-\hat{X}) (\det M(m,\mu))^{N_{\rm f}} e^{-S_g}$$
$$\frac{W(X)}{Z} \approx \frac{1}{N_{\rm conf.}} \sum_{\{\text{conf.}\}} \delta(X-\hat{X}) \qquad \delta(\hat{X}) \approx \int_{\hat{X}}^{\text{Gauss}} \text{or} \qquad \hat{X}$$

• Expectation values

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



• Effective potential:  $V_{\text{eff}}(X) \equiv -\ln(W(X))$ 

# Distribution function & the effective potential $W(X;m,T,\mu) \equiv \int DU\delta(X - \hat{X}) (\det M(m,\mu))^{N_{\rm f}} e^{-S_g} \quad \text{(Histogram)}$

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



#### Reweighting method for plaquette distribution function

$$W(P,\beta,m,\mu) \equiv \int DU\delta(\hat{P}-P) \prod_{f=1}^{N_{\rm f}} \det M(m_f,\mu_f) e^{6N_{\rm site}\beta\hat{P}} \qquad S_g = -6N_{\rm site}\beta\hat{P} \qquad (\beta = 6/g^2)$$

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

 $R(P,\beta,\beta_0m,m_0,\mu) \equiv W(P,\beta,m,\mu)/W(P,\beta_0,m_0,0) \qquad \text{(Reweight factor)}$ 

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

Effective potential:

$$V_{\text{eff}}(P,\beta,m,\mu) = -\ln[W(P,\beta,m,\mu)] = V_{\text{eff}}(P,\beta_0,m_0,0) - \ln R(P,\beta,\beta_0m,m_0,\mu)$$
$$\ln R(P) = \frac{6N_{\text{site}}(\beta-\beta_0)P}{6N_{\text{site}}(\beta-\beta_0)P} + \ln\left\langle \prod_{f} \frac{\det M(m_f,\mu_f)}{\det M(m_0,0)} \right\rangle_{P:\text{fixed}}$$

# Sign problem

$$\left\langle \left( \frac{\det M(m,\mu)}{\det M(m_0,0)} \right)^{N_{\rm f}} \right\rangle_{X \text{ fixed}} = \left\langle e^{i\theta} \left| \frac{\det M(m,\mu)}{\det M(m_0,0)} \right|^{N_{\rm f}} \right\rangle_{X \text{ fixed}}$$

 $\theta$ : complex phase of  $(\det M)^{N_{\rm f}}$ 

• Sign problem: if  $e^{i\theta}$  changes the sign frequently,

$$W(X) \sim \left\langle e^{i\theta} \left| \frac{\det M(m,\mu)}{\det M(m_0,0)} \right|^{N_{\rm f}} \right\rangle_{X \text{ fixed}} << \text{(statistical error)}$$

$$\langle OR \rangle = \frac{1}{Z} \int ORW(X) dX = \frac{1}{Z} \int \exp(-V_{\text{eff}}(X) + \ln(OR)) dX$$

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

- *W* is computed from the histogram.
- Distribution function around X where  $V_{\text{eff}}(X) - \ln(OR)$  is minimized: important.<sup>0.54</sup>



• *V*<sub>eff</sub> must be computed in a wide range.



## Distribution function in quenched simulations



First order phase transition

dVeff/dP = 0 at the peak position of Veff (P). In this case, the curvature of Veff is independent of  $\beta$ .  $N_{site} = 24^3 \times 4$ 

#### Distribution function in a quenched simulation Derivative of the plaquette effective potential



#### Distribution function in the heavy quark region (WHOT-QCD Collab., Phys.Rev.D84, 054502(2011); arXiv:1309.2445)



- We study the properties of *W*(*X*) in the heavy quark region.
- Performing quenched simulations + Reweighting.
- We find the critical surface.
- Standard Wilson quark action + plaquette gauge action,  $S_g = -6N_{site}\beta P$
- $24^3x4$  lattice

Hopping parameter expansion  $\kappa \sim 1/(\text{quark mass})$  $N_{\rm f} \ln \left( \frac{\det M(\kappa,\mu)}{\det M(0,0)} \right) = N_{\rm f} \left( 288N_{\rm site} \kappa^4 P + 12 \cdot 2^{N_t} N_s^3 \kappa^{N_t} \left( \cosh(\mu/T) \Omega_R + i \sinh(\mu/T) \Omega_I \right) + \cdots \right)$ 

*P*: plaquette,  $\Omega = \Omega R + i \Omega I$ : Polyakov loop

 $\det M(0,0) = 1$ 

# Order of the phase transition Polyakov loop distribution (2-flavor)



The pseudo-critical line is determined by χ<sub>Ω</sub> peak.



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

 $\kappa \sim 1/(quark mass)$ 

#### Polyakov loop distribution in the complex plane $(2-flavor, \mu=0)$







 $\kappa^4 = 1.5 \times 10^{-5}$ 





 $\kappa^4 = 2.5 \times 10^{-5}$ 



0.000025

critical point

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

# Critical surface in the heavy quark region of (2+1)-flavor QCD



# Control Parameters in W(X)

• Distribution function

$$W(X;\kappa,\beta,\mu) \equiv \int DU\delta(X-\hat{X}) \prod_{f=1}^{N_{\rm f}} \det M(\kappa_f,\mu_f) e^{-S_g}$$
$$S_g = -6N_{\rm site}\beta\hat{P}$$

Hopping parameter expansion

 $\ln\left(\frac{\det M(\kappa,\mu)}{\det M(0,0)}\right) = 288N_{\text{site}}\kappa^{4}\hat{P} + 12\cdot 2^{N_{t}}N_{s}^{3}\kappa^{N_{t}}\left(\cosh(\mu/T)\hat{\Omega}_{R} + i\sinh(\mu/T)\hat{\Omega}_{I}\right) + \cdots$ 

- Three quantities in W: P,  $\Omega_R$ ,  $\Omega_I$
- Three parameters

$$\beta^* \equiv \beta + \prod_{f=1}^{N_{\rm f}} 48\kappa_f^4, \qquad \prod_{f=1}^{N_{\rm f}} \kappa_f^{N_t} \cosh\left(\mu_f / T\right),$$

 $\left(0 \le \left| \tanh\left(\mu_{f}/T\right) \right| < 1\right)$ 

$$\prod_{f=1}^{N_{\rm f}} \kappa_f^{N_t} \sinh\left(\mu_f / T\right)$$
$$= \prod_{f=1}^{N_{\rm f}} \kappa_f^{N_t} \cosh\left(\mu_f / T\right) \tanh\left(\mu_f / T\right)$$

# Distribution function of $\Omega_{R}$ at finite density $W(\Omega_R,\beta,\kappa,\mu) = \int DU \,\delta(\Omega_R - \hat{\Omega}_R) (\det M(\kappa))^{N_{\rm f}} e^{-6N_{\rm site}\hat{P}}$

• Hopping parameter expansion

 $\frac{W(\beta,\kappa,\mu)}{W(\beta_{c},0,0)} = \left\langle \exp\left[\left(6(\beta-\beta_{0})+288N_{f}\kappa^{4}\right)N_{site}\hat{P}-12\times2^{N_{t}}N_{f}N_{s}^{3}\kappa^{N_{t}}\cosh(\mu/T)\hat{\Omega}_{R}+i\theta\right]\right\rangle_{\Omega_{R};\beta_{0},\kappa=\mu=0}$  $\left(\theta = 12 \cdot 2^{N_t} N_s^3 N_f \kappa^{N_t} \sinh(\mu/T) \hat{\Omega}_I\right)$ 

- Adopting  $\beta_0 \equiv \beta + 48N_{\rm f}\kappa^4$ ,
- Effective potential:  $V_{\text{eff}}(\Omega_{R};\beta,\kappa,\mu) = -\ln W(\Omega_{R};\beta,\kappa,\mu)$

$$V_{\rm eff}(\beta,\kappa,\mu) = V_{\rm eff}(\beta_0,0,0) - 12 \times 2^{N_t} N_f N_s^3 \underline{\kappa^{N_t} \cosh(\mu/T)} \Omega_R - \ln\langle e^{i\theta} \rangle_{\Omega_R;\beta_0,\kappa=\mu=0}$$

Phase-quenched part Phase average

 $\equiv V_0(\beta,\kappa,\mu) \qquad -\ln\langle e^{\prime \circ} \rangle_{\Omega_R;\beta_0,\kappa=\mu=0}$ 

*V*<sub>0</sub> is *V*<sub>eff</sub> (µ=0) when we replace  $\underline{\kappa}^{N_t} \Rightarrow \kappa^{N_t} \cosh(\mu/T)$ (at  $\mu = 0$ ,  $V_{\text{eff}}(\beta, \kappa, 0) = V_{\text{eff}}(\beta_0, 0, 0) - 12 \times 2^{N_t} N_f N_s^3 \kappa^{N_t} \Omega_R$ )

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

- $\theta = \text{Im} \ln \det M \approx 12 \cdot 2^{N_t} N_s^3 N_f \kappa^{N_t} \sinh(\mu/T) \Omega_I$
- Sign problem: If  $e^{i\theta}$  changes its sign,

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

• Cumulant expansion

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

cumulants

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

- <u>Odd terms</u> vanish from a symmetry under  $\mu \leftrightarrow -\mu (\theta \leftrightarrow -\theta)$ Source of the complex phase
- If the cumulant expansion converges, No sign problem.



• At the critical point of phase-quenched part, the effect of higher order terms: small.  $\kappa_{cp}^{N_t}(0) = \kappa_{cp}^{N_t}(\mu) \cosh(\mu/T) > \kappa_{cp}^{N_t}(\mu) \sinh(\mu/T)$ ~0.00002 Effect from the complex phase factor (2-flavor)

• Polyakov loop effective potential at various  $\kappa^{N_t} \cosh(\mu/T)$ at the transition point. ( $\beta^*$  is adjusted at the transition point.)

- Solid lines:  $\mu=0$ , i.e.,  $\cosh(\mu/T)=1$ ,  $\tanh(\mu/T)=0$ 





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



The nature of the phase transition is controlled only by

$$\prod_{f=1}^{N_{\rm f}} \kappa_f^{N_t} \cosh\left(\mu_f / T\right)$$

# Critical surface in the heavy quark region of (2+1)-flavor QCD $(24^3 \times 4 \text{ lattice})$



# Phase transitions in many-flavor QCD

SE & Yamada, Phys. Rev. Lett. 110, 172001 (2013)

- 2 light quarks, many heavy quarks
- Technicolor model
- First order transition

Electro-weak baryogenesis

• Good test for (2+1)-flavor QCD

# Nature of phase transition of 2+N<sub>f</sub>-flavor QCD

m₅



- Assumption:  $N_{\rm f}$ -flavors are heavy.
  - Hopping parameter к expansion

• Parameter: 
$$N_{\rm f} \kappa^{N_t} \implies 1/m_{h,ct} \sim \kappa_{ct} \propto 1/N_{\rm f}^{1/N_t}$$

As increasing 
$$N_{\rm f}$$
, critical mass becomes larger.

Tricritical scaling: the same as (2+1)-flavorQCD

Tricritical point
$$m_{ud}^c \sim (m_E - m_h)^{5/2}$$
 $m_E$ : $m_{ud}^c \sim \mu^5$ 

Good test ground

#### Reweighting method for plaquette distribution function

$$W(P,\beta,m,\mu) \equiv \int DU\delta(\hat{P}-P) \prod_{f=1}^{N_{\rm f}} \det M(m_f,\mu_f) e^{6N_{\rm site}\beta\hat{P}} \qquad S_g = -6N_{\rm site}\beta\hat{P} \qquad (\beta = 6/g^2)$$

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

^

 $R(P,\beta,\beta_0m,m_0,\mu) \equiv W(P,\beta,m,\mu)/W(P,\beta_0,m_0,0) \qquad \text{(Reweight factor)}$ 

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

Effective potential:

$$V_{\text{eff}}(P,\beta,m,\mu) = -\ln[W(P,\beta,m,\mu)] = V_{\text{eff}}(P,\beta_0,m_0,0) - \ln R(P,\beta,\beta_0m,m_0,\mu)$$
$$\ln R(P) = \frac{6N_{\text{site}}(\beta-\beta_0)P}{6} + \ln\left\langle \prod_{f} \frac{\det M(m_f,\mu_f)}{\det M(m_0,0)} \right\rangle_{P:\text{fixed}}$$

## First order transition point: two phases coexist Plaquette distribution function

- Performing simulations of 2-flavor QCD,
- Dynamical effect of N<sub>f</sub>-flavors are included by the reweighting.
- We assume *N*<sub>f</sub>-flavors are heavy.
- Hopping parameter ( $\kappa$ ) expansion (Wilson quark)

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

• Effective potential  $2-\text{flavor} \qquad 2+\text{Nf-flavor} \qquad 1 \text{ st order transition} \\ V_{\text{eff}}(P,\beta,\kappa) = -\ln[R(P,\kappa)W(P,\beta,0)] = V_{\text{eff}}(P,\beta,0) + V_{\text{eff}}(P,\beta,0) + V_{\text{eff}}(P,\beta,0) = V_{\text{eff}}(P,\beta,0) + V_{\text{eff}}(P,\beta,0) + V_{\text{eff}}(P,\beta,0) = V_{\text{eff}}(P,\beta,0) + V$ 

# Curvature of the effective potential $V_{\text{eff}}(P,\beta,h,\mu) = V_{\text{eff}}(P,\beta_0,0,0) - \ln \overline{R}(P,h,\mu) + \text{ (linear term of }P)$ $\overline{R}(P) = \left\langle \exp(6N_s^3h\Omega_R) \right\rangle_{P:\text{fixed}} \text{ (for the case of }\mu=0)$

Wilson quark

 $h = 2N_{\rm f} \left(2\kappa_{\rm h}\right)^{N_t}$ 

Staggered quark

$$h = N_{\rm f} / (4(2m_{\rm h})^{N_t})$$

- Linear term of *P* is irrelevant to the curvature
- $\beta$ -dependence is only in the linear term.
- The curvature is independent of  $\beta$ .

$$\chi_P$$
: plaquette susceptibility  
 $\frac{d^2 V_{\text{eff}}(0)}{dP^2} \approx \frac{6N_{\text{site}}}{\chi_P}$ 

$$\frac{d^2 V_{\text{eff}}}{dP^2} (P, h, \mu) = \frac{d^2 V_{\text{eff}}}{dP^2} (P, 0, 0) - \frac{d^2 \ln \overline{R}}{dP^2} (P, h, \mu)$$
  
2-flavor

• If there exists the negative curvature region,

First order transition (double-well potential)

# **Effective potential at** $h \neq 0$ $V_{eff}(P,\beta,h) = V_{eff}(P,\beta,0) - \ln R(P,h)$

Nf=2 p4-staggared, mπ/mρ≈0.7 [data: Beilefeld-Swansea Collab.,PRD71,054508(2005)]

- det*M*: hopping parameter expansion.
- InR increases as increasing *h*.
- The curvature increases with *h*.



## Curvature of the effective potential



# $N_{\rm f}$ -dependence of the critical mass $h_c = 0.0614(69)$

• Critical mass increases as  $N_{\rm f}$  increases.

$$h = 2N_{\rm f} \left(2\kappa_{\rm h}\right)^{N_t} \quad \Longrightarrow \quad \kappa_{\rm h}^c = \frac{1}{2} \left(\frac{h_c}{2N_{\rm f}}\right)^{1/N_t}$$

- When  $N_{\rm f}$  is large,  $\kappa$  is small. Then, the hopping parameter ( $\kappa$ ) expansion is good.
- On the hand, when  $N_{\rm f}$  is small, the  $\kappa$ -expansion is bad.
- In a quenched simulation with  $N_t$ =4, the first and second terms becomes comparable around  $\kappa$ =0.18.
- For  $N_{\rm f}$ =10,  $N_{\rm t}$ =4,  $h_c = 0.0614(69)$   $\implies \kappa_h^c \approx 0.118$

– It may be applicable for  $N_{\rm f}$ ~10.

## Curvature of the effective potential at finite $\boldsymbol{\mu}$



# Critical line at finite density

$$h = 2N_{\rm f} \left(2\kappa_{\rm h}\right)^{N}$$

for Wilson quarks

$$h = N_{\rm f} \left/ \left( 4 \left( 2 m_{\rm h} \right)^{N_t} \right) \right.$$

for staggered quarks

- Calculations of detM: Taylor expansion up to O(μ<sup>6</sup>)
- Distribution function of the complex phase of detM: approximated by a Gaussian function





Phase structure of (2+many)-flavor
QCD using Wilson quark action
2-flavor QCD simulations + reweighting
Light quark mass dependence of the critical line

- Trictitical scaling behavior?
- Is there a first order transition region in 2-flavor QCD?



# Light quark mass dependence (preliminary)



1.75

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

- Perform phase quenched simulations
- Add the effect of the complex phase by the reweighting.
- 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:  $|\det M(m,\mu)|^{N_{\rm f}} e^{-S_g}$ 

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

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

Distribution function of the phase quenched.

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

#### µ-dependence of the effective potential Curvature of the effective potential



# Curvature of the effective potential

• If the distribution is Gaussian,

$$W_{0}(P,F) \approx \sqrt{\frac{6N_{\text{site}}}{2\pi\chi_{P}}} \exp\left[-\frac{6N_{\text{site}}}{2\chi_{P}} \left(P - \langle P \rangle\right)^{2}\right] \times \sqrt{\frac{N_{\text{site}}}{2\pi\chi_{F}}} \exp\left[-\frac{N_{\text{site}}}{2\chi_{F}} \left(F - \langle F \rangle\right)^{2}\right]$$
$$\chi_{P} = 6N_{\text{site}} \left\langle \left(P - \langle P \rangle\right)^{2} \right\rangle \qquad \chi_{F} = N_{\text{site}} \left\langle \left(F - \langle F \rangle\right)^{2} \right\rangle$$

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

at the peak of the distribution

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

- $\theta$ : complex phase  $\theta \equiv \operatorname{Im} \ln \det M$
- 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

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

- <u>Odd terms</u> vanish from a symmetry under  $\mu \leftrightarrow -\mu (\theta \leftrightarrow -\theta)$ Source of the complex phase
- If the cumulant expansion converges, No sign problem.

## Convergence in the large volume (V) limit

The cumulant expansion is good in the following situations.

- If the phase is given  $\mathbf{b} \mathbf{y} = \sum \theta_x$ 
  - No correlation between  $\theta_x$ .

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

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

- 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.

– The application range of  $\boldsymbol{\mu}$  can be measured on a small lattice.

# Complex phase distribution

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



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

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

- The range of  $\theta$  is from  $-\infty$  to  $\infty$ .

$$\frac{\partial \ln \det M}{\partial (\mu/T)} = Tr \left[ M^{-1} \frac{\partial \det M}{\partial (\mu/T)} \right] = \sum_{i} \left[ M^{-1} \frac{\partial \det M}{\partial (\mu/T)} \right]_{ii}$$

#### Integral method for the calculation of the quark



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# Distribution of the complex phase



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

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

$$\frac{1}{2} \left\langle \theta^2 \right\rangle_{\langle P \rangle, \langle F \rangle} \approx \frac{1}{2} \left\langle \theta^2 \right\rangle_{\beta_0, \mu_0}$$

at the peak of W<sub>0</sub> in each simulation

# Simulations

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

• Simulation point in the ( $\beta$ ,  $\mu_0/T$ )

• Peak of  $W_0(P,F)$  for each  $\mu$ 

2-flavor QCD Iwasaki gauge+ clover Wilson quark actionRandom noise method is used.





## Curvature of the effective potential $-\ln W_0$



• The curvature for F decreases as  $\mu$  increases.

## Effect from the complex phase



• Rapidly changes around the pseudo-critical point.

# Critical point at finite µ



• zero curvature: expected at a large  $\mu$ .

## Curvature of the effective potential

• Without the complex phase effect



$$\chi_F = N_{\rm site} \left\langle \left( F - \left\langle F \right\rangle \right)^2 \right\rangle$$



# Phase average

• 2<sup>nd</sup> order cumulant

$$\ln \left\langle e^{i\theta} \right\rangle_{P,F} \approx -\frac{1}{2} \left\langle \theta^2 \right\rangle_{P,F}$$

$$\frac{1}{2} \left\langle \theta^2 \right\rangle_{\langle P \rangle, \langle F \rangle} \approx \frac{1}{2} \left\langle \theta^2 \right\rangle_{\beta_0, \mu_0}$$



Curvature of the effective potential

• The effect of the phase incruded.



zero curvature Critical point

Peak position of W(P,F)  $\sim W$   $\partial \ln W = 0$  $-\ln W(P,F)$ at  $\frac{\partial \ln W}{\partial P} = 0, \quad \frac{\partial \ln W}{\partial F} = 0$ • The slopes are zero at the peak of W(P,F).  $\frac{\partial \ln W}{\partial P}(P,F,\beta,\mu) = \frac{\partial \ln W_0}{\partial P}(P,F,\beta,\mu) + \frac{\partial \ln \langle e^{i\theta} \rangle_{P,F}}{\partial P} \qquad \left( R(P,F,\mu,\mu_0) = \frac{W_0(P,F,\beta,\mu)}{W_0(P,F,\beta,\mu_0)} \right)$  $=\frac{\partial \ln W_0}{\partial P} (P, F, \beta_0, \mu_0) + 6N_{site} (\beta - \beta_0) + \frac{\partial \ln R}{\partial P} (P, F, \mu, \mu_0) + \frac{\partial \ln \langle e^{i\theta} \rangle_{P,F}}{\partial P}$  $\frac{\partial \ln W}{\partial F}(P,F,\beta,\mu) = \frac{\partial \ln W_0}{\partial F}(P,F,\beta,\mu) + \frac{\partial \ln \langle e^{i\theta} \rangle_{P,F}}{\partial F}$  If these terms are canceled,  $=\frac{\partial \ln W_0}{\partial F}(P,F,\beta_0,\mu_0)+\frac{\partial \ln R}{\partial F}(P,F,\mu,\mu_0)+\frac{\partial \ln \langle e^{i\theta} \rangle_{P,F}}{\partial F}$  $W(P, F, \beta, \mu) \approx W_0(P, F, \beta_0, \mu_0) \times (\text{const.})$ 

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

# 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 μ<sub>u</sub>=-μ<sub>d</sub>, pion condensation occurs.
- $\langle e^{i\theta} \rangle = 0$  is suggested in the pion condensed phase by phenomenological Tstudies. [Han-Stephanov '08, Sakai et al. '10]

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

- Near the phase boundary,
  - large fluctuations in  $\theta$ : expected.

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



# Summary

• We discussed the QCD phase transition in the heavy quark region.

WHOT-QCD(H. Saito, S. Ejiri, S. Aoki, K. Kanaya, Y. Nakagawa, H. Ohno, K. Okuno, and T. Umeda), arXiv:1309.2445 S. Ejiri, Euro. Phys. J. A 49, 86 (2013) [arXiv:1306.0295]

- The critical surface in the heavy quark region of (2+1)-flavor QCD is computed.

• We investigated the phase structure of (2+Nf)-flavor QCD.

S. Ejiri & N. Yamada, Phys. Rev. Lett. 110, 172001 (2013) [arXiv:1212.5899]

- This model is interesting for the feasibility study of the electroweak baryogenesis in the technicolor scenario.
- An appearance of a first order phase transition at finite temperature is required for the baryogenesis.
- Applying the reweighting method, we determine the critical mass of heavy flavors terminating the first order region.
  - The critical mass becomes larger with N<sub>f</sub>.
  - The first order region becomes wider as increasing μ.
- This may be a good test for the determination of boundary of the first order region in (2+1)-flavor QCD at finite density.