Density of state method for the study of finite density lattice QCD

Shinji Ejiri

(Niigata University)

WHOT-QCD collaboration

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

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

- Density of state method + Reweighting method
- Endpoint of the first order phase transition in the heavy quark mass region

Japanese German seminar 2010, (Mishima, 4-6 November, 2010)

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.

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

$$W(\bar{X},m,T,\mu) \equiv \int DU \delta(X\text{-}\bar{X}) (\det M(m,\mu))^{N_{\rm f}} \, e^{-S_g}$$

- Expectation values

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

- The density of state method is useful if we combine the reweighting method.

Order of phase transitions

Distribution function (histogram)

- First order phase transition

  Two phases coexists at T_c

  e.g. SU(3) Pure gauge theory

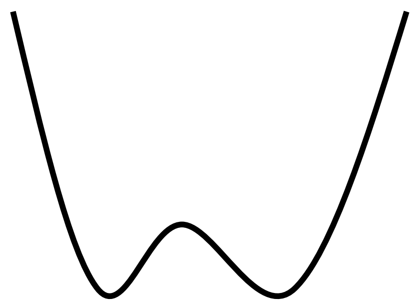
- Average plaquette (1x1 Wilson loop): P

- Partition function

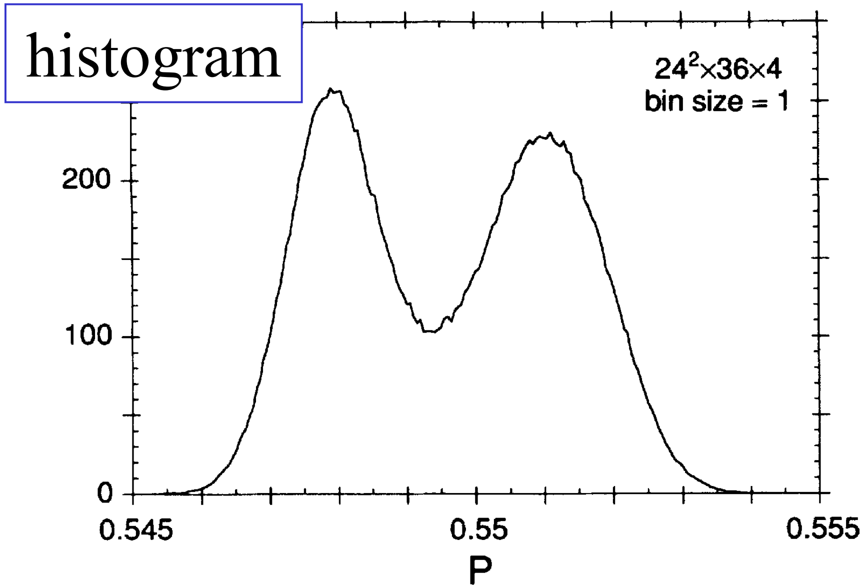
$$Z(T) = \int dP \, \underbrace{W(P,T)}_{\text{histogram}}$$

- Effective potential

$$V_{\text{eff}}(P) \equiv -\ln(W(P))$$



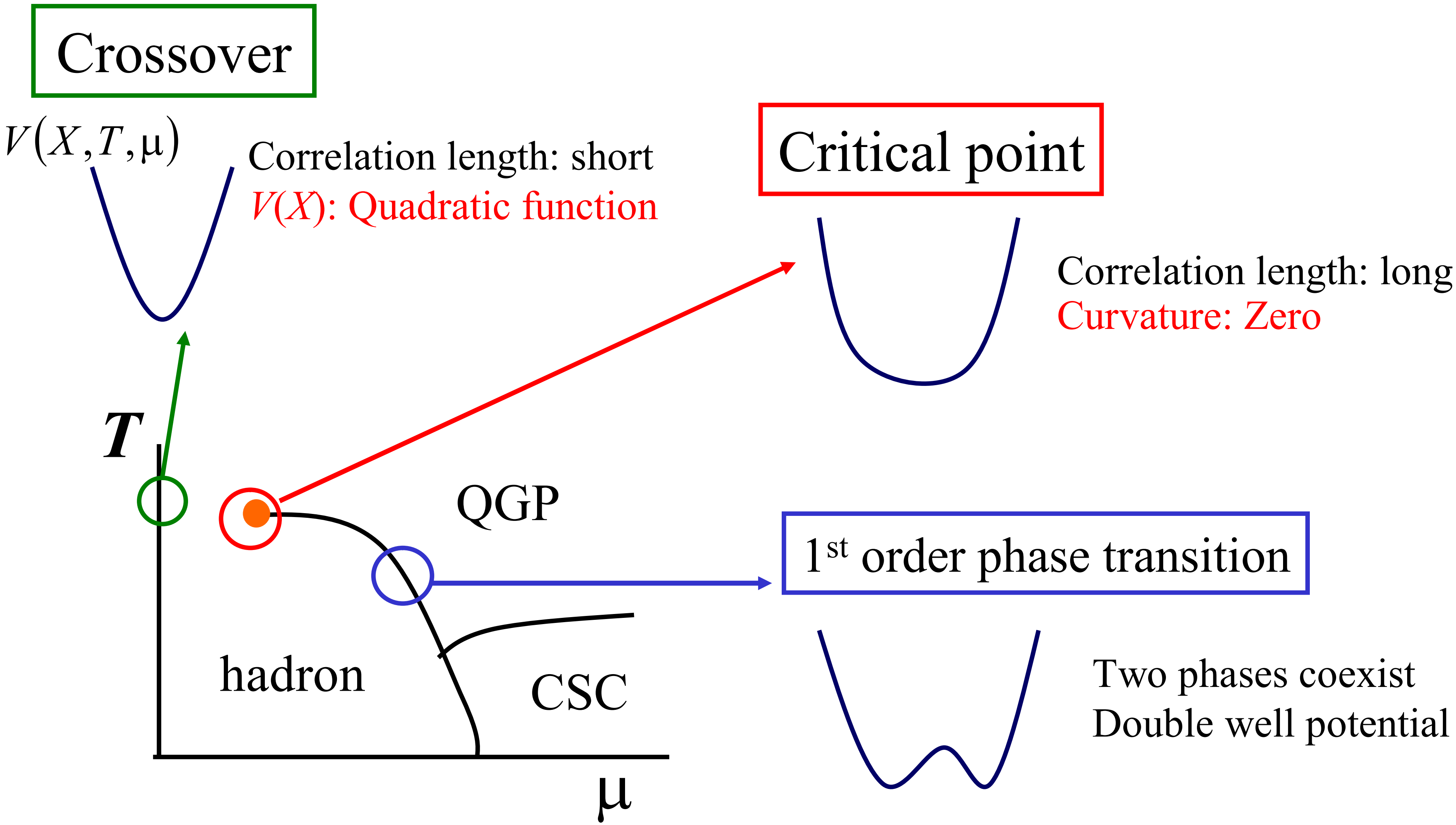
SU(3) Pure gauge theory
QCDPAX, PRD46, 4657 (1992)



μ-dependence of the effective potential

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

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

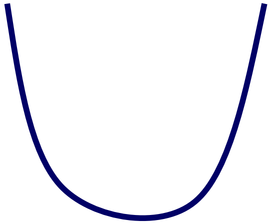


mass-dependence of the effective potential

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

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

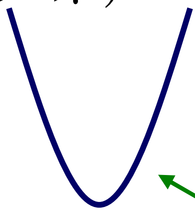
Critical point



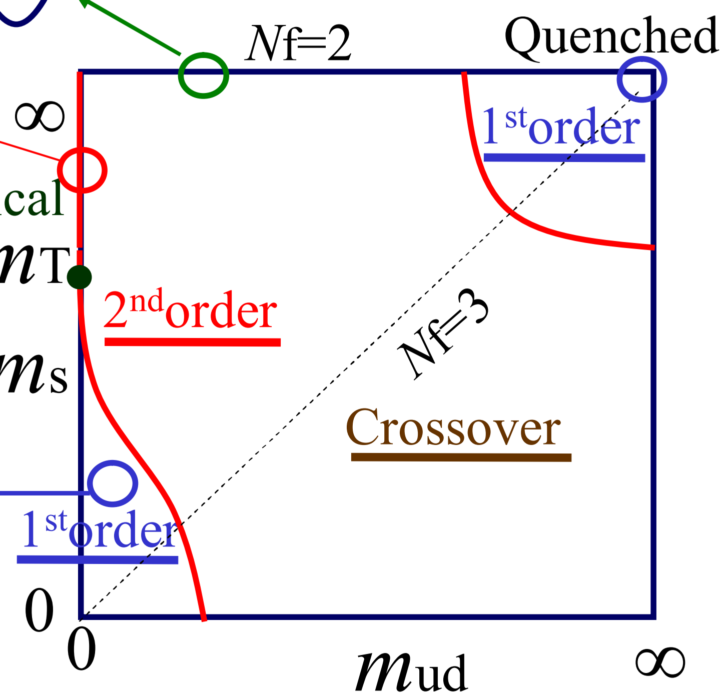
Correlation length: long
Curvature: Zero

Crossover

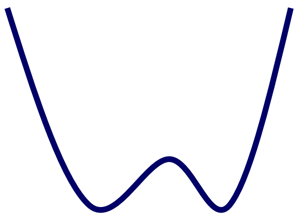
$V(X,T,\mu)$



Correlation length: short
$V(X)$: Quadratic function



1st order phase transition



Two phases coexist
Double well potential

$\mu=0$

Plaquette distribution function

$$\boxed{W(P',\beta) = \int DU\ \delta(P-P')\left(\det M(0)\right)^{N_f}\ e^{6N_{\rm site}\beta P}}$$

Change: $\beta_1(T) \Rightarrow \beta_2(T)$

P: Average plaquette (1x1 Wilson loop)

Weight: $W(\beta_1) \Rightarrow W(\beta_2) = e^{6N_{\rm site}(\beta_2-\beta_1)P}\, W(\beta_1)$

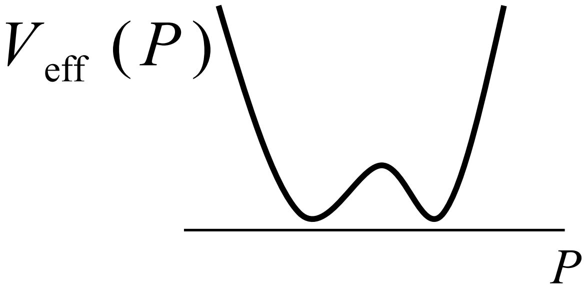
Potential: $V_{\rm eff}(P) \equiv -\ln(W(P)) \Rightarrow V_{\rm eff}(\beta_2) = V_{\rm eff}(\beta_1) - 6N_{\rm site}(\beta_2-\beta_1)P$

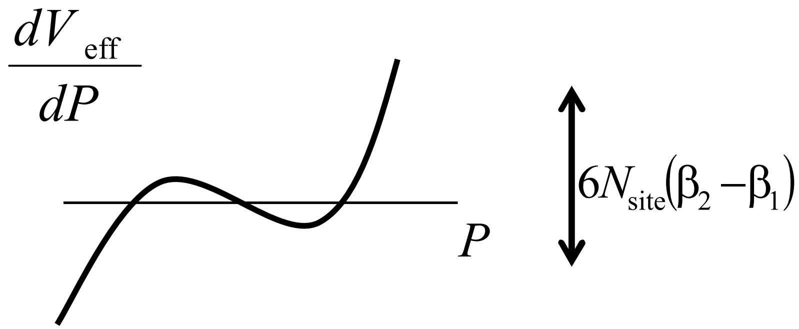
$$\Rightarrow \boxed{\frac{dV_{\rm eff}}{dP}(\beta_2) = \frac{dV_{\rm eff}}{dP}(\beta_1) - 6N_{\rm site}(\beta_2-\beta_1)}$$

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

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.

Reweighting method for quark part (S.E., Phys.Rev.D77, 014508(2008))

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

$$Z(\beta,m,\mu)=\int dP\, \underline{\underline{R(P,m,m_0,\mu)W(P,\beta,m_0,0)}} \qquad S_g=-6N_{site}\beta P \qquad (\beta=6/g^2)$$

$$W(\bar{P},\beta,0)\equiv\int DU\delta(P\text{-}\bar{P})(\det M(m_0,0))^{N_f}\ e^{-S_g}$$

(Weight factor at μ=0)

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

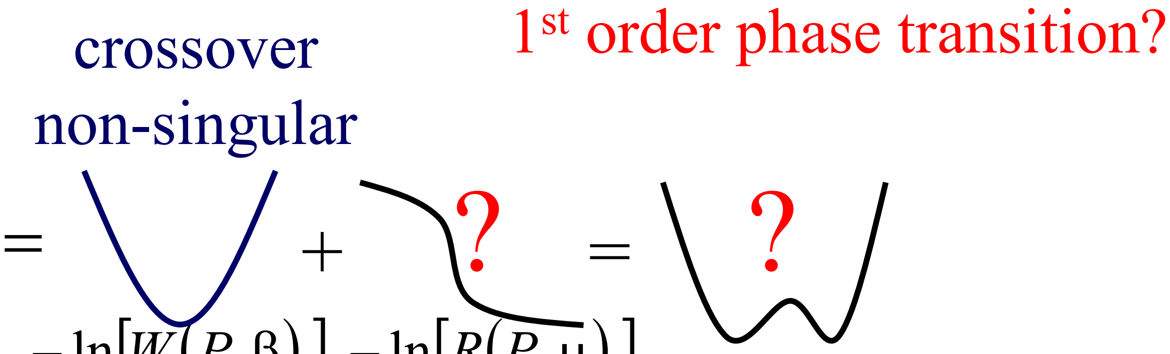
(Reweight factor)

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

R(*P*,*m*,μ): independent of β, → *R*(*P*,*m*,μ) can be measured at any β.

Effective potential:

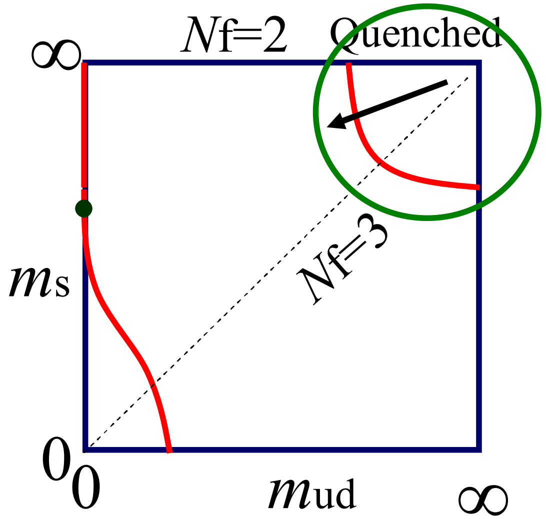
$$V_{\text{eff}}(P)=-\ln[R(P,\mu)W(P,\beta)]=$$



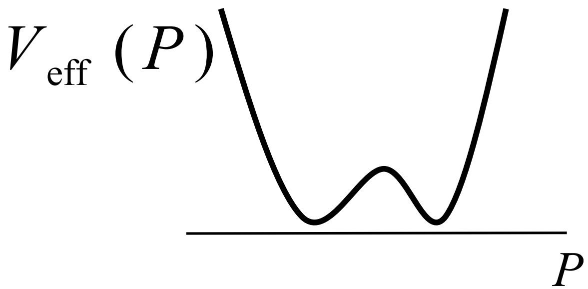
$$-\ln[W(P,\beta)]\ -\ln[R(P,\mu)]$$

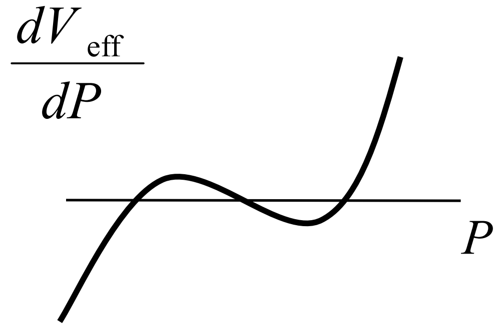
Reweighting from quenched simulations

WHOT-QCD Collaboration, H. Saito



- Order of phase transition near the quenched limit
  - First order ($m_q \to \infty$) → crossover (small m_q)
- Quenched simulations + Reweighting method
  - det$M$ is estimated by a hopping parameter expansion.
- Action: plaquette gauge action + Wilson quark action
- Lattice size: $N_{site} = 24^3 \times 4$, Simulation points: 5 β points
- Derivative of the effective potential



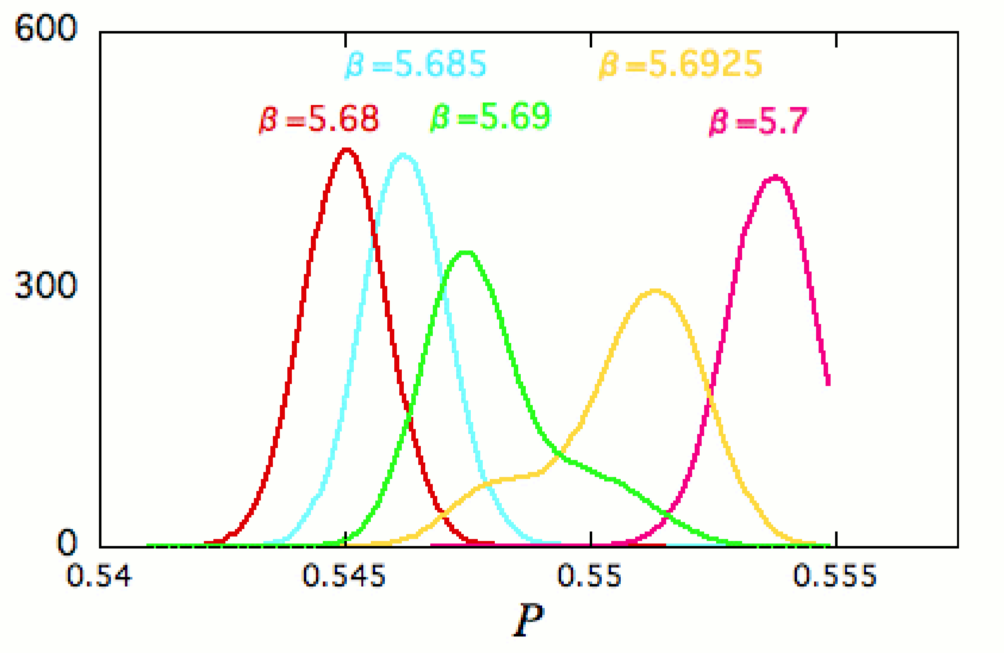


- Effective potential in a wide range of P: required.
  - We combine the data of dV_{eff}/dP obtained at different β.

Calculation of the effective potential at m=∞

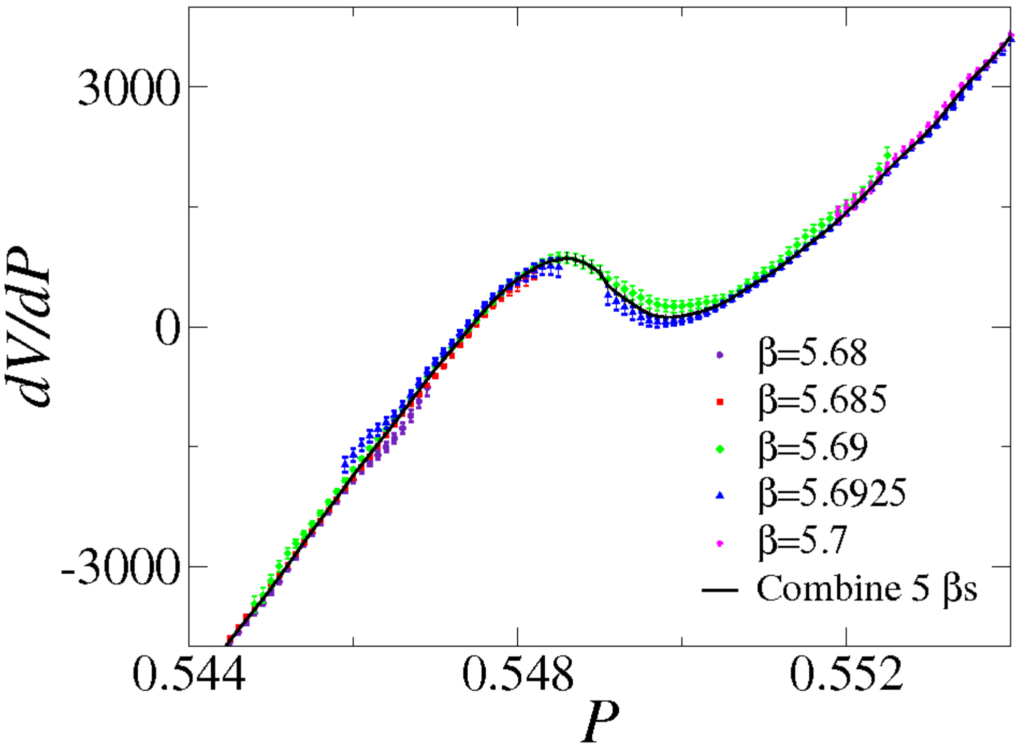
Effective potential in a wide range of P: required.

Plaquette histogram



$$N_{\rm site} = 24^3 \times 4,$$

Derivative of $V_{\rm eff}$ at β=5.69



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

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

These data are combined by taking the average.

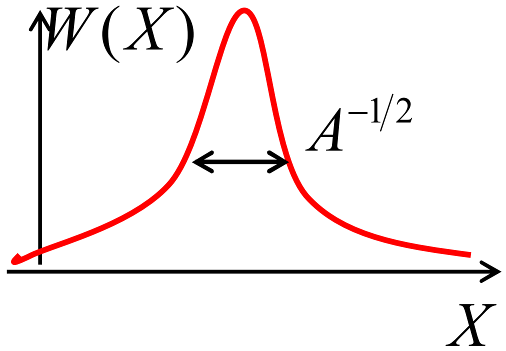
4^{th} order Binder cumulant

$$B_4 = \frac{\left\langle \left(X - \langle X \rangle\right)^4 \right\rangle}{\left\langle \left(X - \langle X \rangle\right)^2 \right\rangle^2}$$

- Normal (Gaussian distribution)

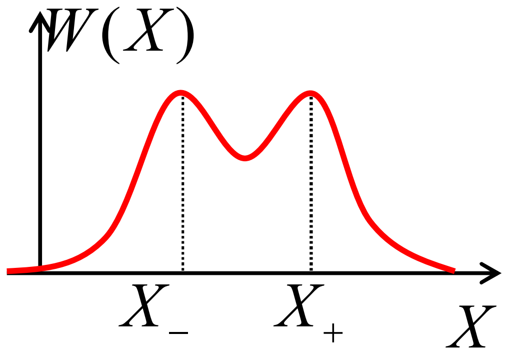
$$B_4 = \frac{\int dX \left(X - \langle X \rangle\right)^4 e^{-A\left(X - \langle X \rangle\right)^2}}{\left(\int dX \left(X - \langle X \rangle\right)^2 e^{-A\left(X - X\right)^2}\right)^2} \approx \frac{\frac{d^2}{dA^2}\left[\int dX \left(X - \langle X \rangle\right)^4 e^{-A\left(X - \langle X \rangle\right)^2}\right]}{\left(\frac{d}{dA}\left[\int dX \left(X - \langle X \rangle\right)^4 e^{-A\left(X - \langle X \rangle\right)^2}\right]\right)^2}$$

$$\approx \frac{\sqrt{A}\,\frac{d^2}{dA^2}\sqrt{1/A}}{\left(-\sqrt{A}\,\frac{d}{dA}\sqrt{1/A}\right)^2} = \frac{\frac{3}{4A^2}}{\left(\frac{1}{2A}\right)^2} = 3$$



- 1^{st} order transition

$$B_4 = \frac{\int dX \left(X - \langle X \rangle\right)^4 W(X)}{\left(\int dX \left(X - \langle X \rangle\right)^2 W(X)\right)^2} \approx \frac{\left[\left(X_+ - X_-\right)/2\right]^4}{\left(\left[\left(X_+ - X_-\right)/2\right]^4\right)^2} \sim 1$$



Measurement of $W(X)$ and $B4$ is essentially equivalent.

Distribution function in a wide range of P: required for the calculation of $B4$.

Quark determinant in the heavy quark mass region

$$M_{x,y} = \delta_{x,y} - K\sum_{i=1}^{3}\left[(1-\gamma_i)U_i\delta_{x+\hat{i},y} + (1+\gamma_i)U_i^{+}\delta_{x-\hat{i},y}\right] - K\left[e^{\mu_q a}(1-\gamma_4)U_4\delta_{x+\hat{4},y} + e^{-\mu_q a}(1+\gamma_4)U_4^{+}\delta_{x-\hat{4},y}\right]$$

- Taylor expansion around K_0

$$\ln\left(\frac{\det M(K)}{\det M(K_0)}\right) = \sum_{n=1}^{\infty}\frac{1}{n!}\left[\frac{\partial^n(\ln\det M)}{\partial K^n}\right]_{K_0}(K-K_0)^n = \sum_{n=1}^{\infty}\frac{1}{n!}D_n(K-K_0)^n$$

$$D_n = \left[\frac{\partial^n(\ln\det M)}{\partial K^n}\right]_{K_0} = (-1)^{n+1}(n-1)!\,\mathrm{tr}\left[\left(M^{-1}\frac{\partial M}{\partial K}\right)^n\right]_{K_0}$$

- We adopt $K_0=0$ (quenched limit), then $M^{-1}_{x,y} = \delta_{x,y}$,

$\left[\dfrac{\partial M}{\partial K}\right]_{x,y}$ is the hopping term.

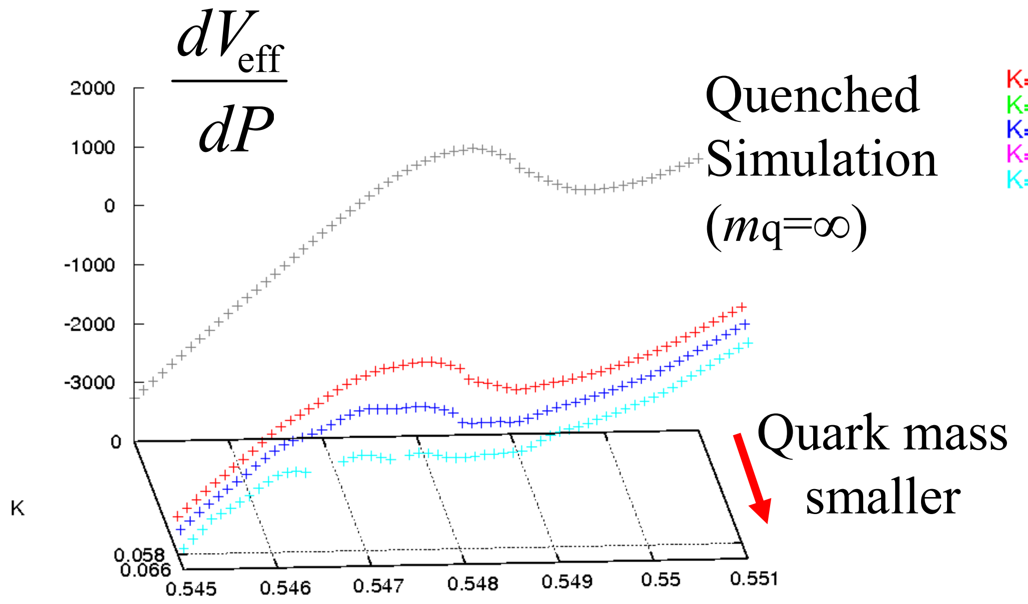
$$R(P,K,0) = \left\langle\left(\frac{\det M(K)}{\det M(0)}\right)^{N_f}\right\rangle_{P\text{ fixed}}$$

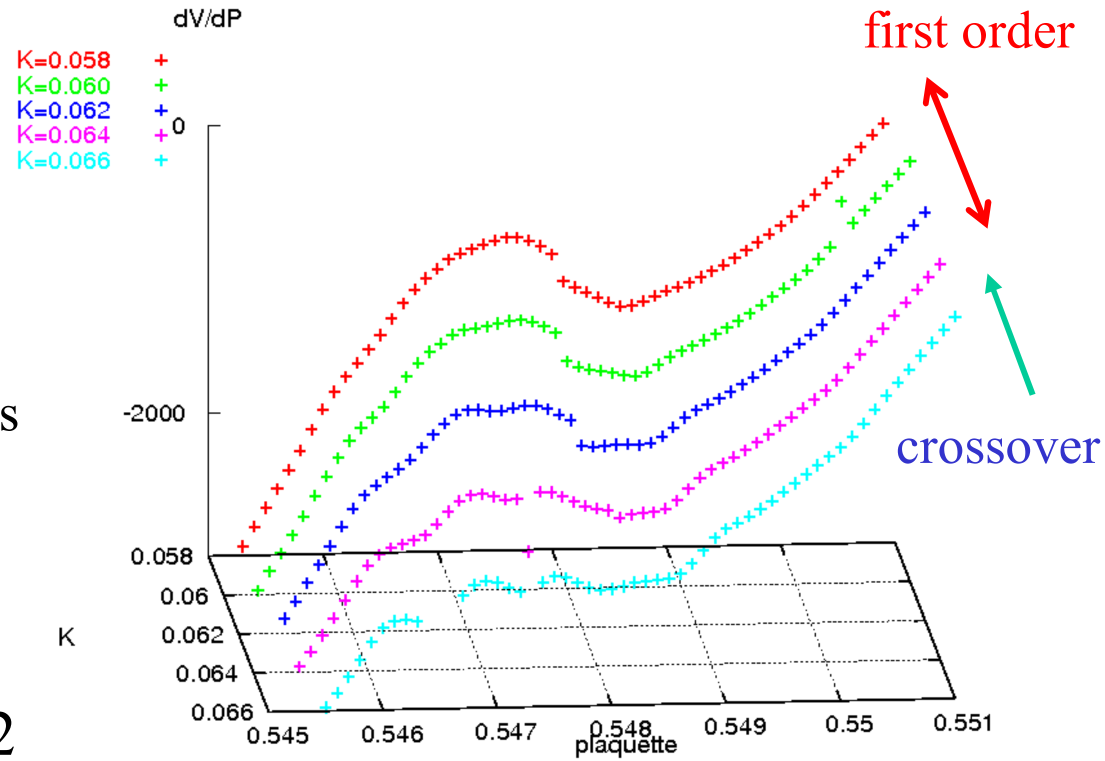
$$\ln\left(\frac{\det M(K)}{\det M(0)}\right) = N_{site}\left(\underline{288K^4P} + \underline{12\times 2^{N_t}K^{N_t}\,\mathrm{Re}\Omega} + \cdots\right)$$

Polyakov loop: $\Omega = \dfrac{1}{N_{\mathrm{site}}}\sum_{\vec{x}}\dfrac{1}{3}\mathrm{Re\,tr}\left[U_{\vec{x},4}U_{\vec{x}+\hat{4},4}U_{\vec{x}+2\hat{4},4}\cdots U_{\vec{x}+(N_t-1)\hat{4},4}\right]$

Plaquette term can be absorbed into β.

Effective potential near the quenched limit

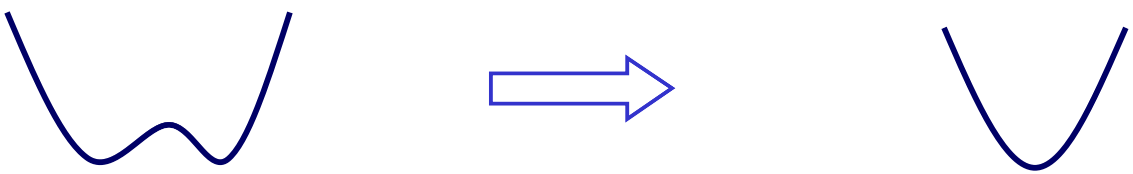




$K \sim 1/m_q$ for large m_q

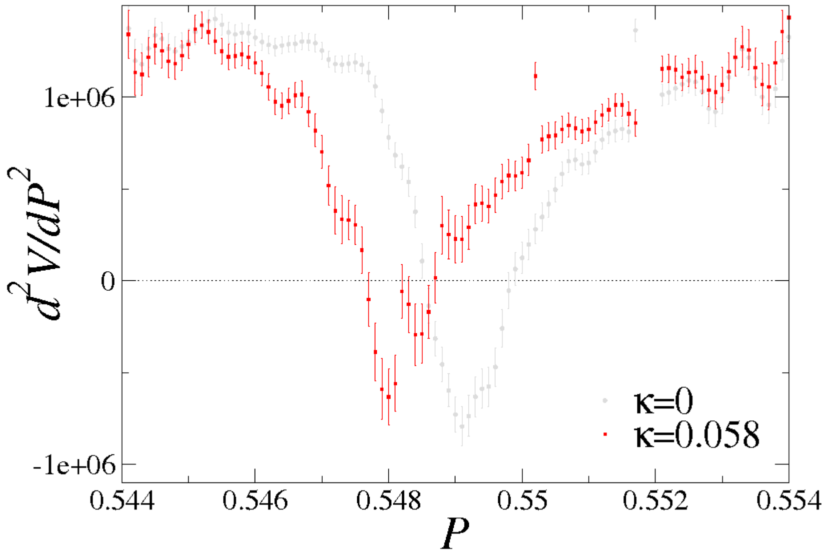
$24^3 \times 4$ lattice, 5 β points, $N_f=2$

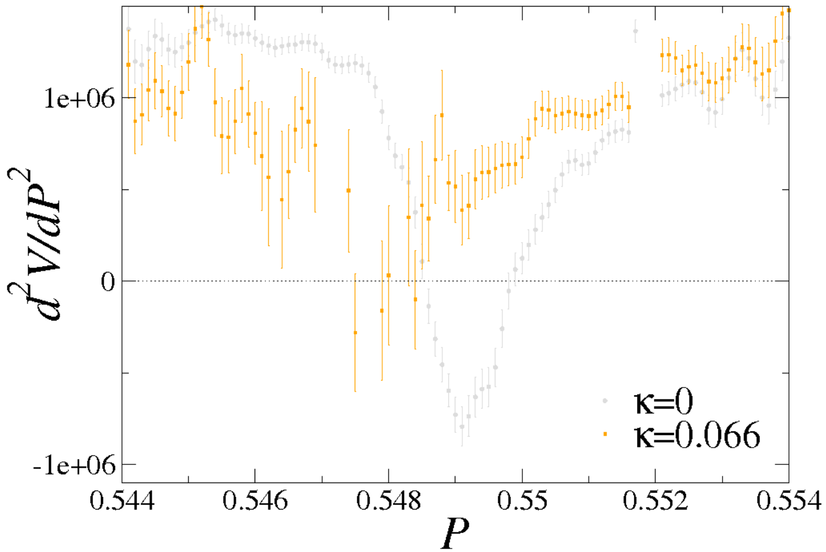
- K-dependence is calculated by the reweighting.
- First order transition at $K = 0$ changes to crossover at $K > 0$.

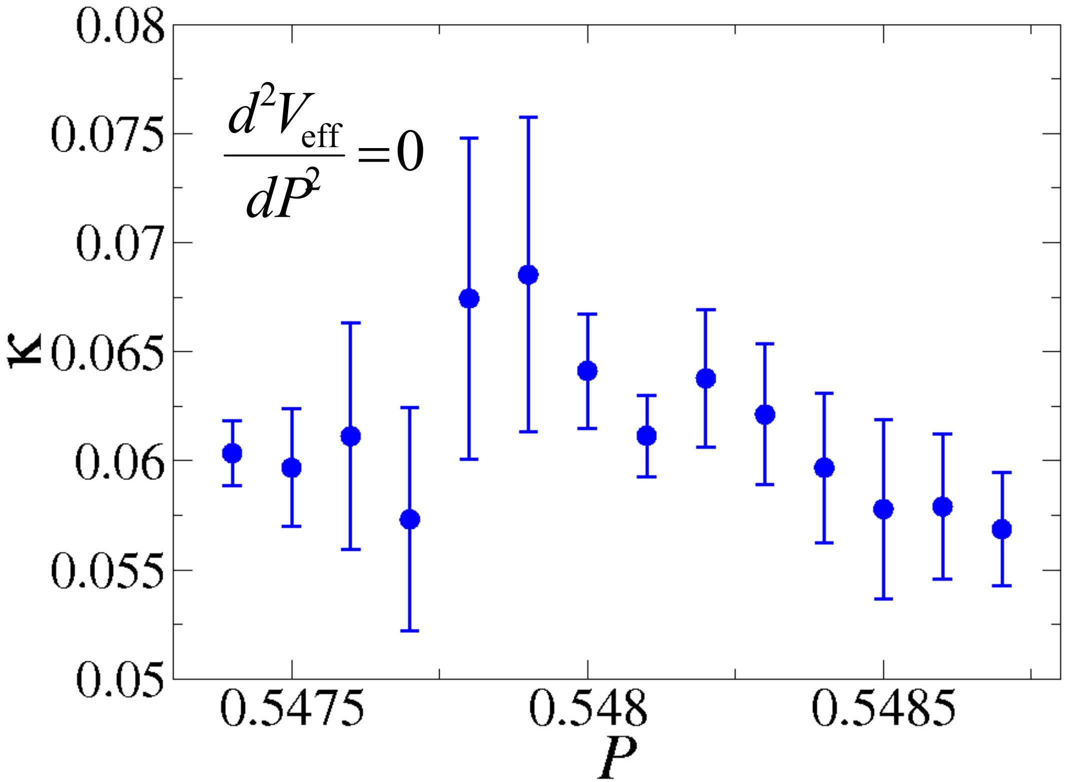


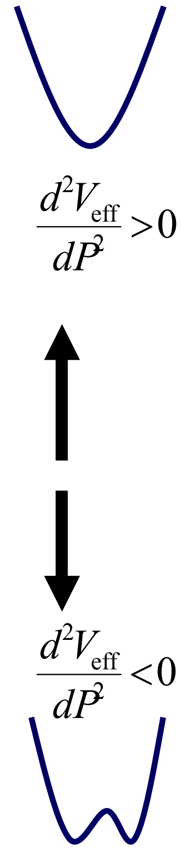
Endpoint of the first order phase transition

Curvature of Veff for Nf=2









Endpoint of the 1st order transition

Nf=1: Kep=0.081(8)

Nf=2: Kep=0.068(7)

Nf=3: Kep=0.061(6)

Cf. Nf=1 consistent with the effective Z(3) model [C. Alexandrou et al., PRD60, 034504 (1999)]

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

N_f=1: K_{ep}=0.081(8)

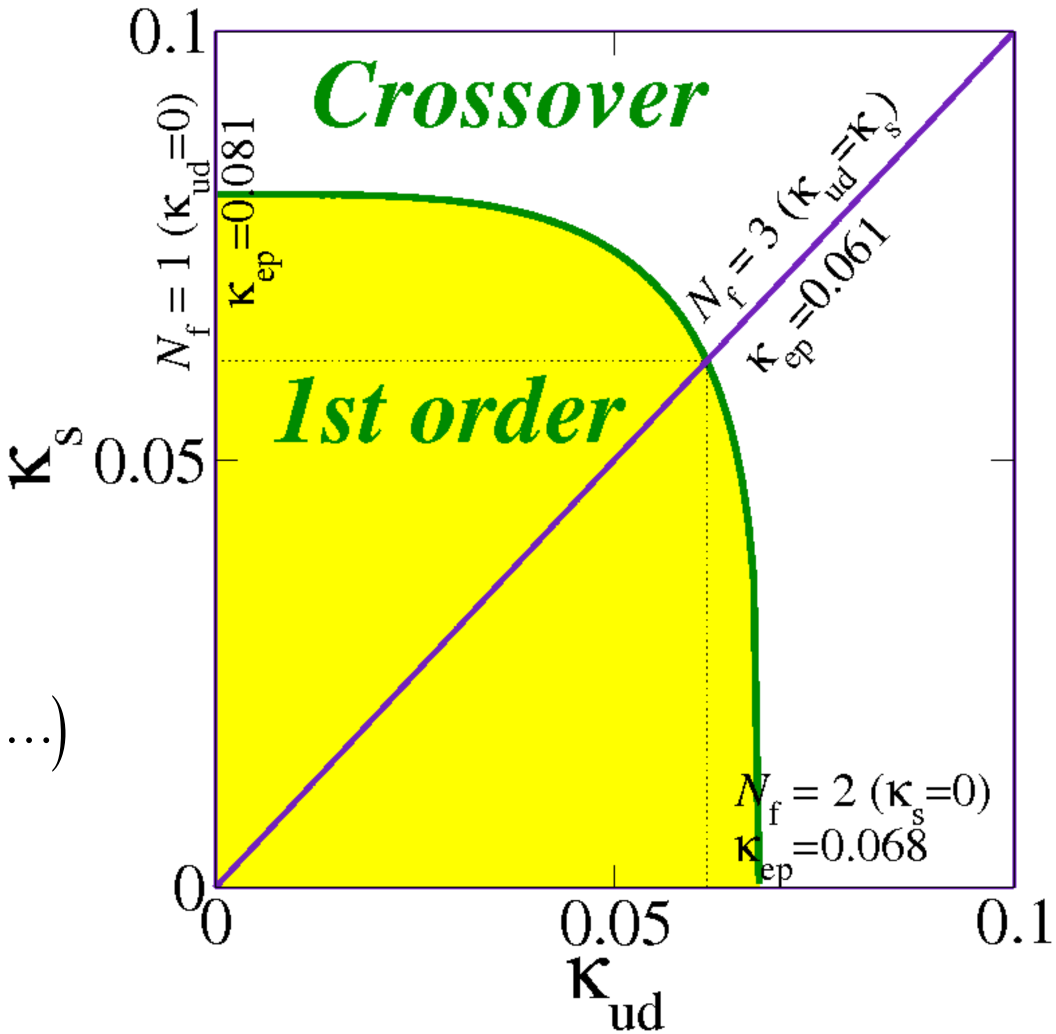
$$\ln\left(\frac{\det M(K)}{\det M(0)}\right) = N_{\rm site}\left(288K^4P + 12\times 2^{N_t}K^{N_t}\Omega + \cdots\right)$$

N_f=2+1

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

The critical line is described by

$$\boxed{2K_{ud}^{N_t} + K_s^{N_t} = \left(K_{\rm ep}^{N_f=1}\right)^{N_t}}$$



Finite density QCD

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

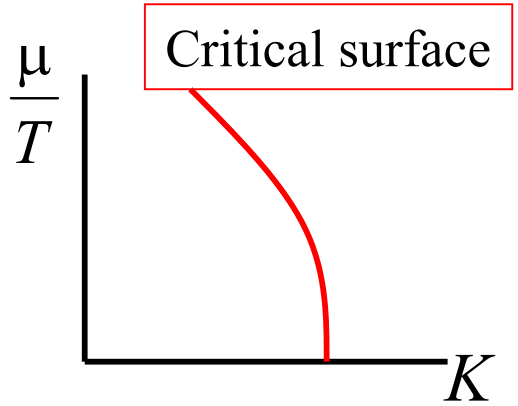
$$\Longrightarrow \quad \boxed{\Omega \Rightarrow e^{\mu_q/T}\Omega, \quad \Omega^* \Rightarrow \mathrm{e}^{-\mu_q/T}\Omega^*}$$

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

$$= N_\mathrm{f} N_\mathrm{site}\left(288K^4P + 12\cdot 2^{N_t} K^{N_t} \cosh(\mu/T)\left(\mathrm{Re}\,\Omega + \underbrace{i\tanh(\mu/T)\,\mathrm{Im}\,\Omega}_{\text{phase}}\right) + \cdots\right)$$

- Isospin chemical potential (N_f=2), $\mu_\mathrm{u} = -\mu_\mathrm{d}$. Complex phase: canceled.

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



  – Endpoint: $\underline{K_\mathrm{ep}^{N_t}(\mu)\cosh(\mu/T) = K_\mathrm{ep}^{N_t}(0)}$

- Complex phase for real chemical potential $\longrightarrow$ the sign problem

Avoiding the sign problem

(SE, Phys.Rev.D77,014508(2008))

θ: complex phase

$$F = \left| \frac{\det M(\mu)}{\det M(0)} \right|^{N_f}$$

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

$$R(P,\mu) = \left\langle \left(\frac{\det M(\mu)}{\det M(0)} \right)^{N_f} \right\rangle_{P\text{ fixed}} \equiv \left\langle e^{i\theta} F \right\rangle_P \ll \text{(statistical error)}$$

- Cumulant expansion

$\langle .. \rangle_{F,P}$: expectation values fixed F and P.

$$\left\langle e^{i\theta} F \right\rangle_P = \int F \left\langle e^{i\theta} \right\rangle_{F,P} dF$$

$$\approx \int F \exp\left[\underbrace{\cancel{i\langle\theta\rangle_C}}_{\to 0} - \frac{1}{2}\left\langle \theta^2 \right\rangle_C - \underbrace{\cancel{\frac{i}{3!}\left\langle \theta^3 \right\rangle_C}}_{\to 0} + \frac{1}{4!}\left\langle \theta^4 \right\rangle_C \cancel{+ \cdots} \right] dF$$

cumulants

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

  - 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.

Convergence of the cumulant expansion

- Because $\theta \sim O(\mu)$, $\quad \left\langle \theta^n \right\rangle_C \sim O(\mu^n)$
  - The cumulant expansion is a power expansion of μ.
    - Applicable at low density.
  - If one takes into account $\left\langle \theta^n \right\rangle_C$, the truncation error does not affect up to $O(\mu^n)$.

- Gaussian distribution function
  - The cumulants vanish except for $\left\langle \theta^2 \right\rangle_C$.

$$\left\langle Fe^{i\theta} \right\rangle = \int dF \int d\theta\, Fe^{i\theta} W\left(F,\theta\right) \approx \int dF\, Fe^{-1/(4\alpha)} W'(F)$$

$$\boxed{W\left(F,\theta\right) \approx \sqrt{\frac{\alpha(F)}{\pi}} e^{-\alpha(F)\theta^2} W'(F)}$$

$$\frac{1}{2\alpha(F')} = \frac{\int \theta^2 W(F',\theta)d\theta}{\int W(F',\theta)d\theta} \equiv \left\langle \theta^2 \right\rangle_F$$

$$\Rightarrow \quad \boxed{\left\langle Fe^{i\theta} \right\rangle \approx \left\langle Fe^{-\left\langle \theta^2 \right\rangle_F / 2} \right\rangle}$$

Chemical potential in the heavy quark mass region

$$N_{\rm f} \ln\left(\frac{\det M(K)}{\det M(0)}\right) = N_{\rm f} N_{\rm site}\left(288K^4 P + 12\times 2^{N_t} K^{N_t} \cosh(\mu/T)(\mathrm{Re}\,\Omega + \underline{i \tanh(\mu/T)\,\mathrm{Im}\,\Omega}) + \cdots\right)$$

$$\equiv N_{\rm f} N_{\rm site}\left(aP + b\,\mathrm{Re}\,\Omega + \underline{ibc\,\mathrm{Im}\,\Omega} + \cdots\right) \qquad [\Omega_R = \mathrm{Re}\,\Omega, \quad \Omega_I = \mathrm{Im}\,\Omega]$$

- Average of the complex phase:

$$\left\langle e^{i\theta}\right\rangle_{P,\Omega_R} = \left\langle e^{iN_{\rm site} bc \Omega_I}\right\rangle_{P,\Omega_R} = \exp\left[-\frac{(N_{\rm f} N_{\rm site} bc)^2}{2}\left\langle \Omega_I^2\right\rangle_c + \frac{(N_{\rm f} N_{\rm site} bc)^4}{4!}\left\langle \Omega_I^4\right\rangle_c + \cdots\right]$$

$$\left[\left\langle \Omega_I^2\right\rangle_c = \left\langle \Omega_I^2\right\rangle_{P,\Omega_R}, \quad \left\langle \Omega_I^4\right\rangle_c = \left\langle \Omega_I^4\right\rangle_{P,\Omega_R} - 3\left\langle \Omega_I^2\right\rangle_{P,\Omega_R}^2\right]$$

- Reweighting factor:

$$R(P,\mu) = \left\langle \left(\frac{\det M(\mu)}{\det M(0)}\right)^{N_{\rm f}}\right\rangle_P = \left\langle \exp\left[N_{\rm f} N_{\rm site}(aP + b\Omega_R) - \frac{(N_{\rm f} N_{\rm site} bc)^2}{2}\left\langle \Omega_I^2\right\rangle_c + \frac{(N_{\rm f} N_{\rm site} bc)^4}{4!}\left\langle \Omega_I^4\right\rangle_c + \cdots\right]\right\rangle_P$$

$$\equiv \left\langle \exp\left[N_{\rm f} N_{\rm site}(a'P + b'\Omega_R) + \text{const.} + O(P^2, \Omega_R^2)\right]\right\rangle_P \qquad (c = \tanh(\mu/T))$$

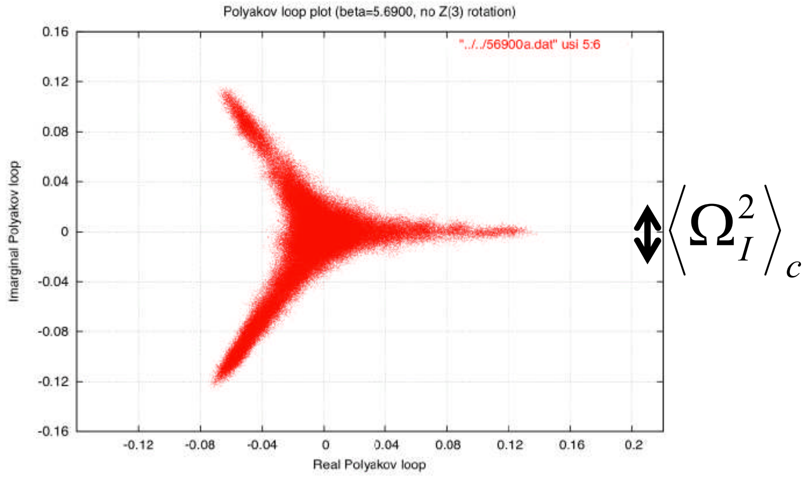
- The phase effect can be absorbed into β and K. $\quad \left(b = 12\times 2^{N_t} K^{N_t}\cosh(\mu/T)\right)$

$$b' \equiv b - \frac{N_{\rm f} N_{\rm site}(bc)^2}{2}\frac{\partial\left\langle \Omega_I^2\right\rangle_c}{\partial \Omega_R} + \frac{N_{\rm f}^3 N_{\rm site}^3 (bc)^4}{4!}\frac{\partial\left\langle \Omega_I^4\right\rangle_c}{\partial \Omega_R} - \cdots \Rightarrow \boxed{\text{Critical surface}}$$

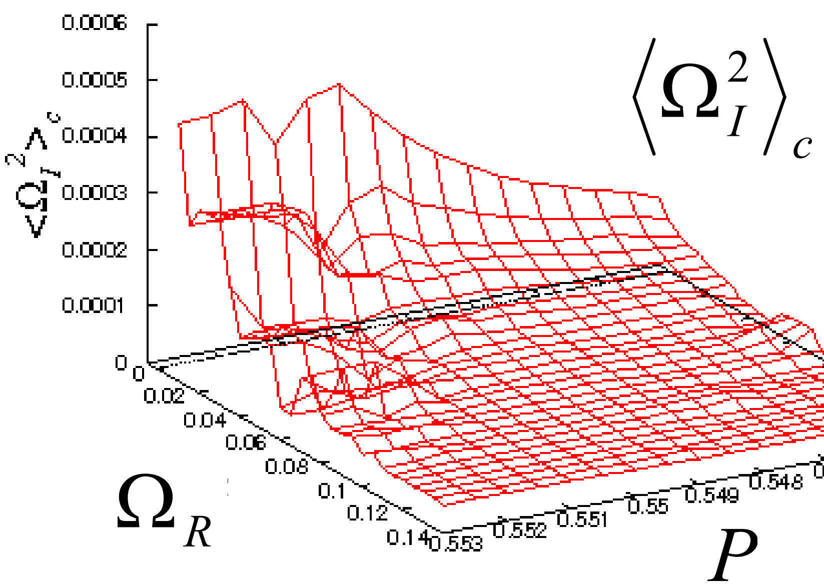
Effect from the complex phase

$$R(P,\mu)=\left\langle \exp\left[N_f N_{site}\left(aP+b\Omega_R\right)-\frac{(N_f N_{site} bc)^2}{2}\left\langle \Omega_I^2\right\rangle_c+\frac{(N_f N_{site} bc)^4}{4!}\left\langle \Omega_I^4\right\rangle_c+\cdots\right]\right\rangle_P$$

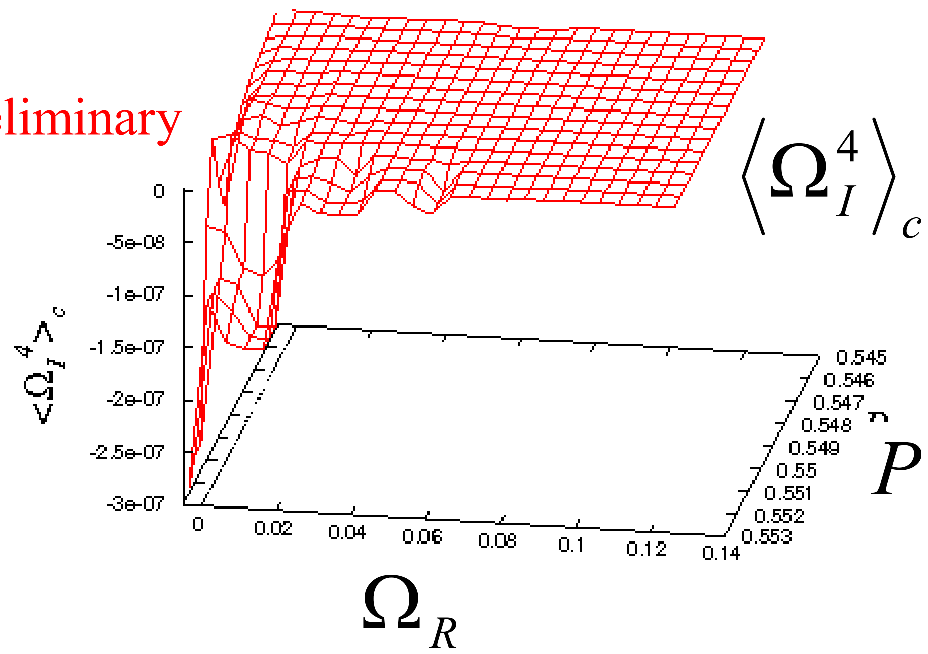
Distribution of Ω at K=0



- $\left\langle \Omega_I^2\right\rangle_c$ is large at $\Omega_R<0$.
- $W(\mu)=R(\mu)W(0)$ is suppressed by Ω_R and the large $\left\langle \Omega_I^2\right\rangle_c$ at $\Omega_R<0$.
- $\left\langle \Omega_I^4\right\rangle_c$ is small at $\Omega_R>0$.



Preliminary



Effect from the complex phase

- Slope of $\left\langle e^{iN_{\rm site}bc\Omega_I} \right\rangle_{P,\Omega_R}$ changes Kep.

$$(c = \tanh(\mu/T))$$

$$R(P,\mu) = \left\langle \exp\left[N_{\rm f} N_{\rm site}\left(a'P + b'\Omega_R\right) + \cdots\right]\right\rangle_P$$

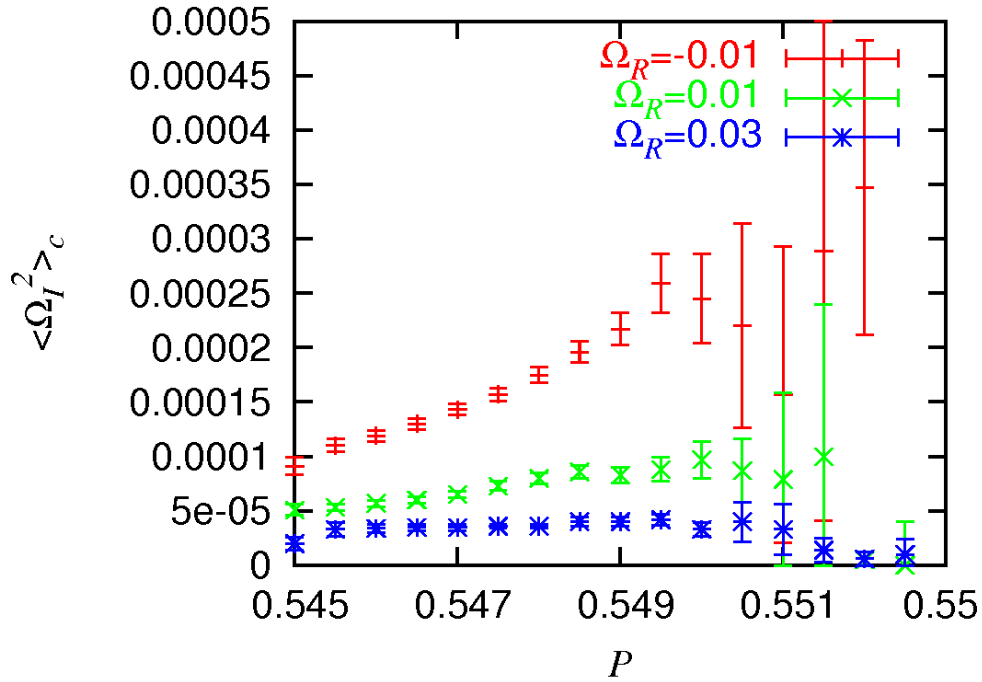
$$\left(b = 12 \times 2^{N_t} K^{N_t} \cosh(\mu/T)\right)$$

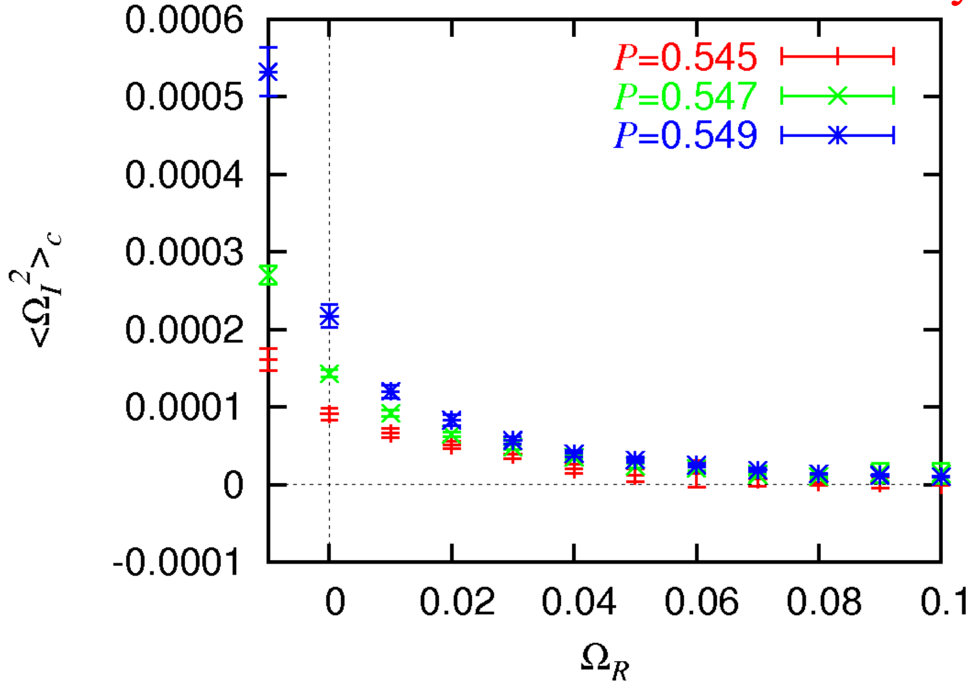
$$b' \equiv b - \frac{N_{\rm f} N_{\rm site} (bc)^2}{2} \frac{\partial \left\langle \Omega_I^2 \right\rangle_c}{\partial \Omega_R} + \frac{N_{\rm f}^3 N_{\rm site}^3 (bc)^4}{4!} \frac{\partial \left\langle \Omega_I^4 \right\rangle_c}{\partial \Omega_R} - \cdots$$

$$a' \equiv a - \frac{N_{\rm f} N_{\rm site} (bc)^2}{2} \frac{\partial \left\langle \Omega_I^2 \right\rangle_c}{\partial P} + \frac{N_{\rm f}^3 N_{\rm site}^3 (bc)^4}{4!} \frac{\partial \left\langle \Omega_I^4 \right\rangle_c}{\partial P} - \cdots$$

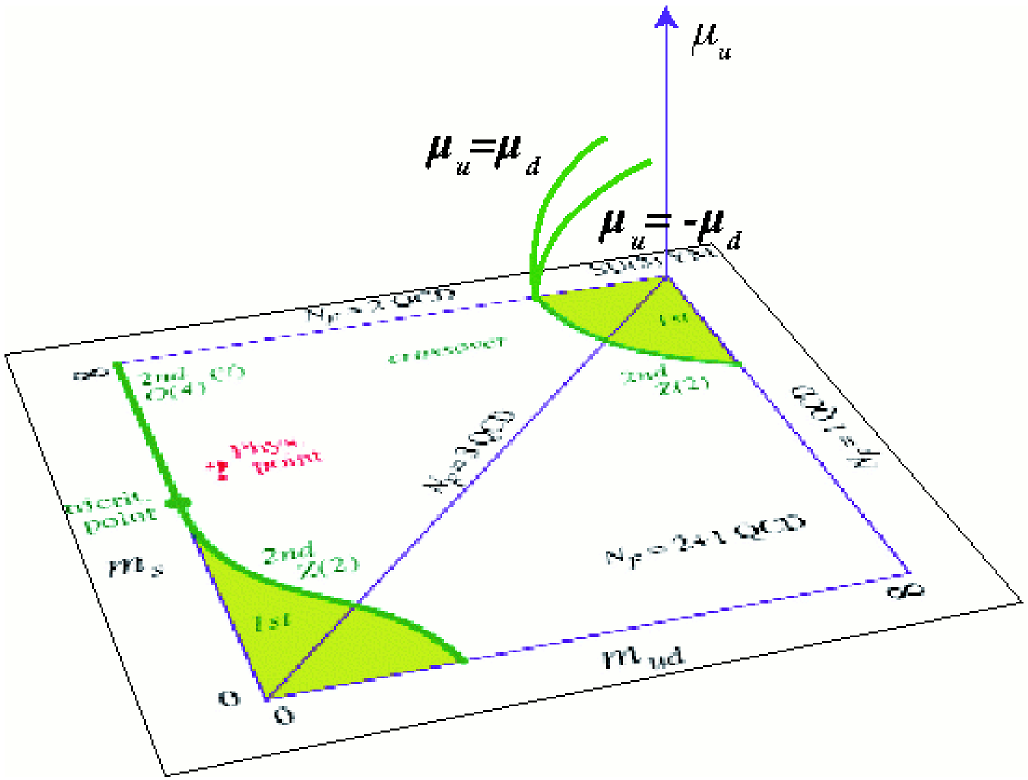
b' is constant on the critical surface

Preliminary





Critical surface in the ($m_{\rm ud}$, $m_{\rm s}$, μ) space



- The study for the light quark mass region is important.
- This method is applicable in the light quark mass region:

  Isospin chemical potential simulations + complex phase effect.

Summary

- We studied the quark mass and chemical potential dependence of the nature of QCD phase transition in the heavy quark mass region.
- Density of state method is used to identify the order of the phase transition.
- To avoid the sign problem, the method based on the cumulant expansion of θ is useful.
- The study in the light quark mass region is important applying this method.