高温高密度での格子QCDシミュレーション
Lattice QCD Simulations at High Temperature and Density

公募研究
「状態密度法による有限密度QCDの計算方法の開発」

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WHOT-QCD collaboration

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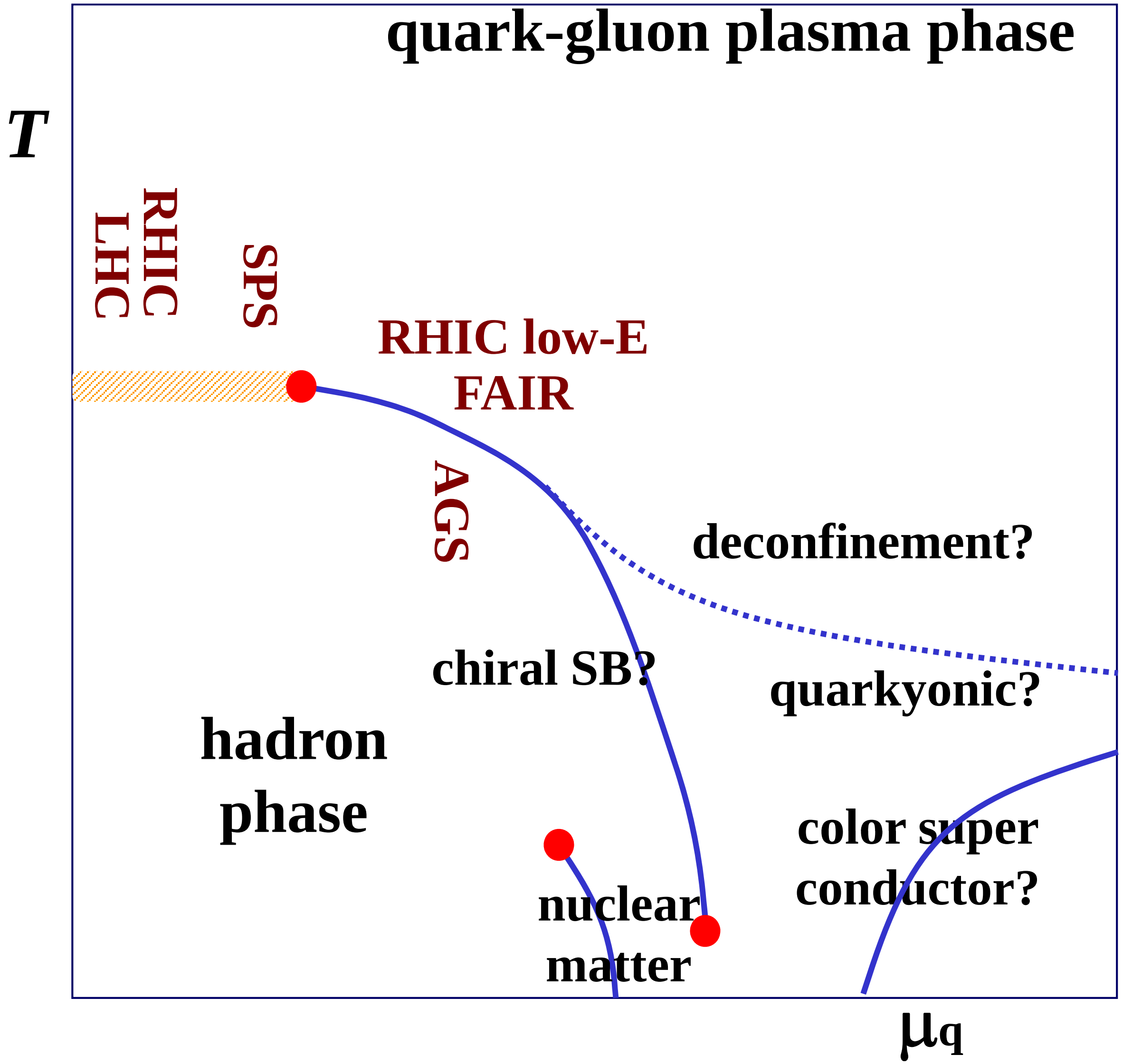
Phase structure of QCD at high temperature and density

Lattice QCD Simulations

- Phase transition lines
- Equation of state

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



Problems in simulations at μ≠0

- Problem of Complex Determinant at μ≠0
  - Boltzmann weight: complex at μ≠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.

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

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

- Expectation values

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

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 $\mu \neq 0$

$$\frac{p}{T^4}(\mu) - \frac{p}{T^4}(0) = \frac{1}{VT^3}\ln\left(\frac{Z(\mu)}{Z(0)}\right) = \left(\frac{N_t}{N_s}\right)^3 \ln\left\langle \frac{\det M(\mu)}{\det M(0)} \right\rangle_{\mu=0}$$

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

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

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

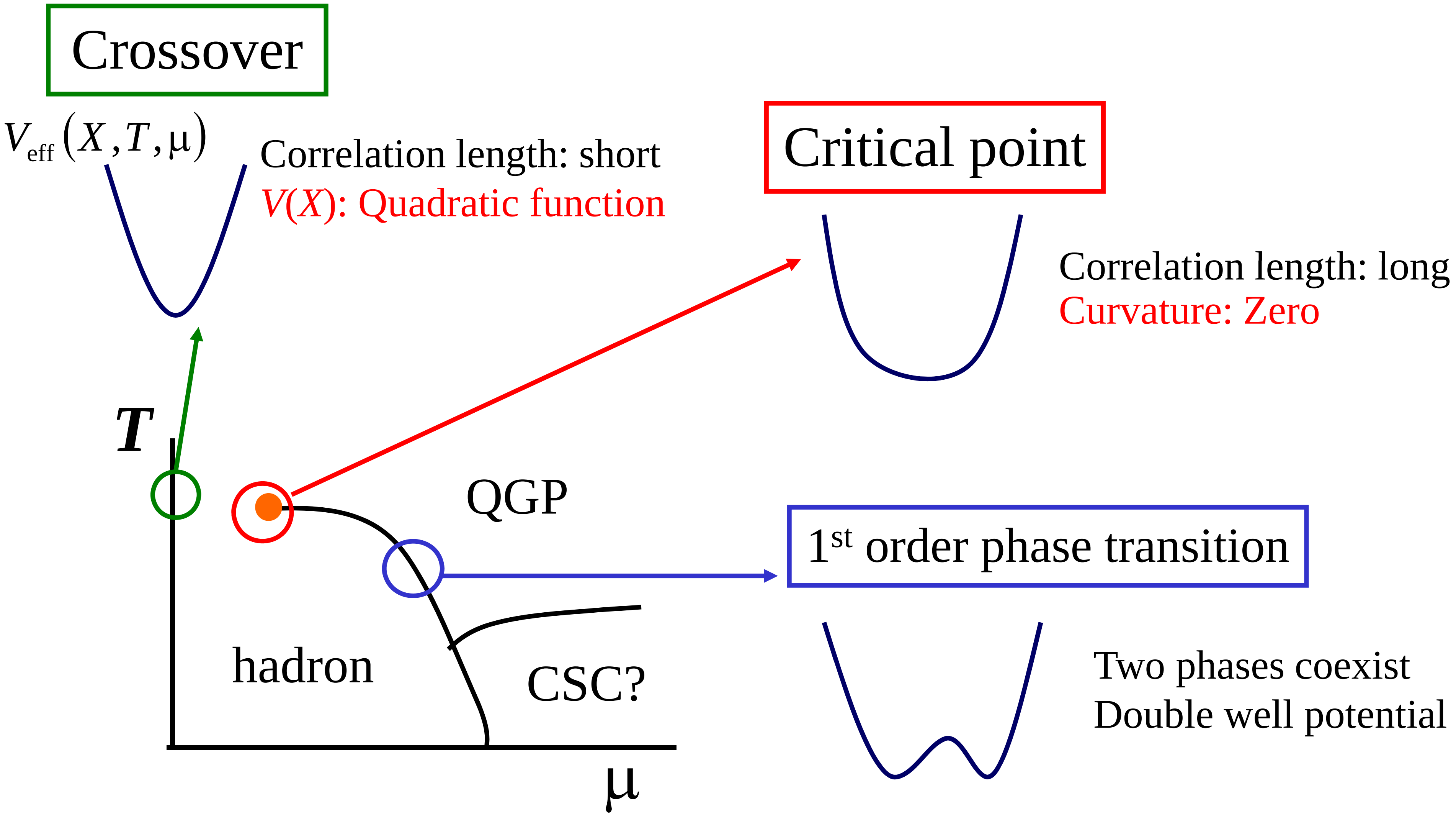
- We propose a method for the calculation of this *W*.
  - Overlap problem
  - Sign problem
- Once we get the pressure, we can calculate

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

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 and Effective potential at $\mu\neq 0$

(S.E., Phys.Rev.D77, 014508(2008))

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

$$\underline{\underline{W(\bar{P},\beta,\mu) \equiv \int DU\,\delta(P-\bar{P})\left(\det M(\mu)\right)^{N_f} e^{-S_g}}} \qquad S_g = -6N_{site}\beta P$$

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

(Reweight factor)

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

Effective potential:

$\mu=0$ crossover non-singular

1st order phase transition?

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

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

Effective potential at $\mu \neq 0$

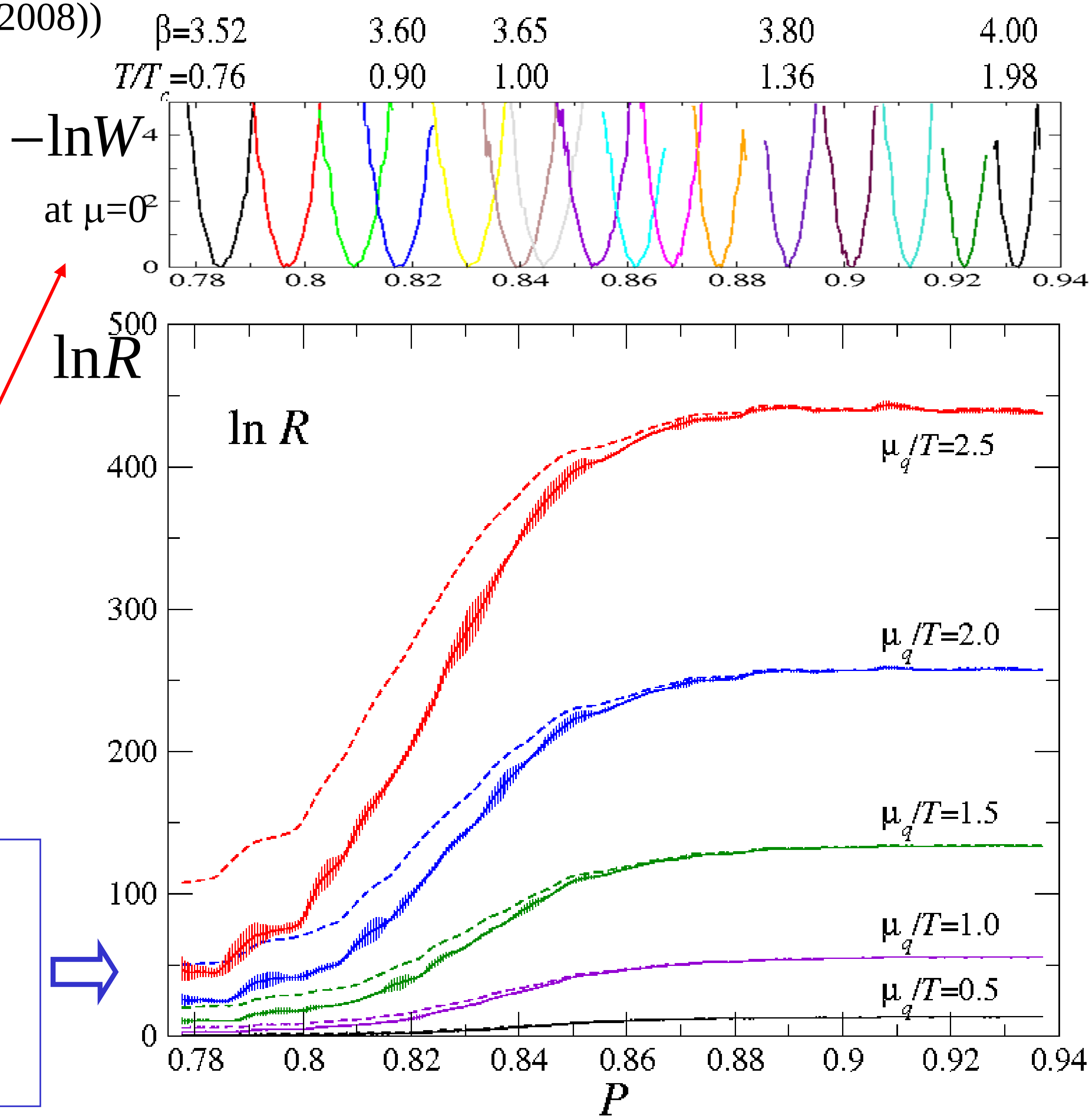
$$V_{\mathrm{eff}}(P,\beta,\mu) = -\ln W(P,\beta) - \ln R(P,\mu)$$

(S.E., Phys.Rev.D77, 014508(2008))

Results of N_f=2 p4-staggared, $m_\pi/m_\rho \approx 0.7$

[data in PRD71,054508(2005)]

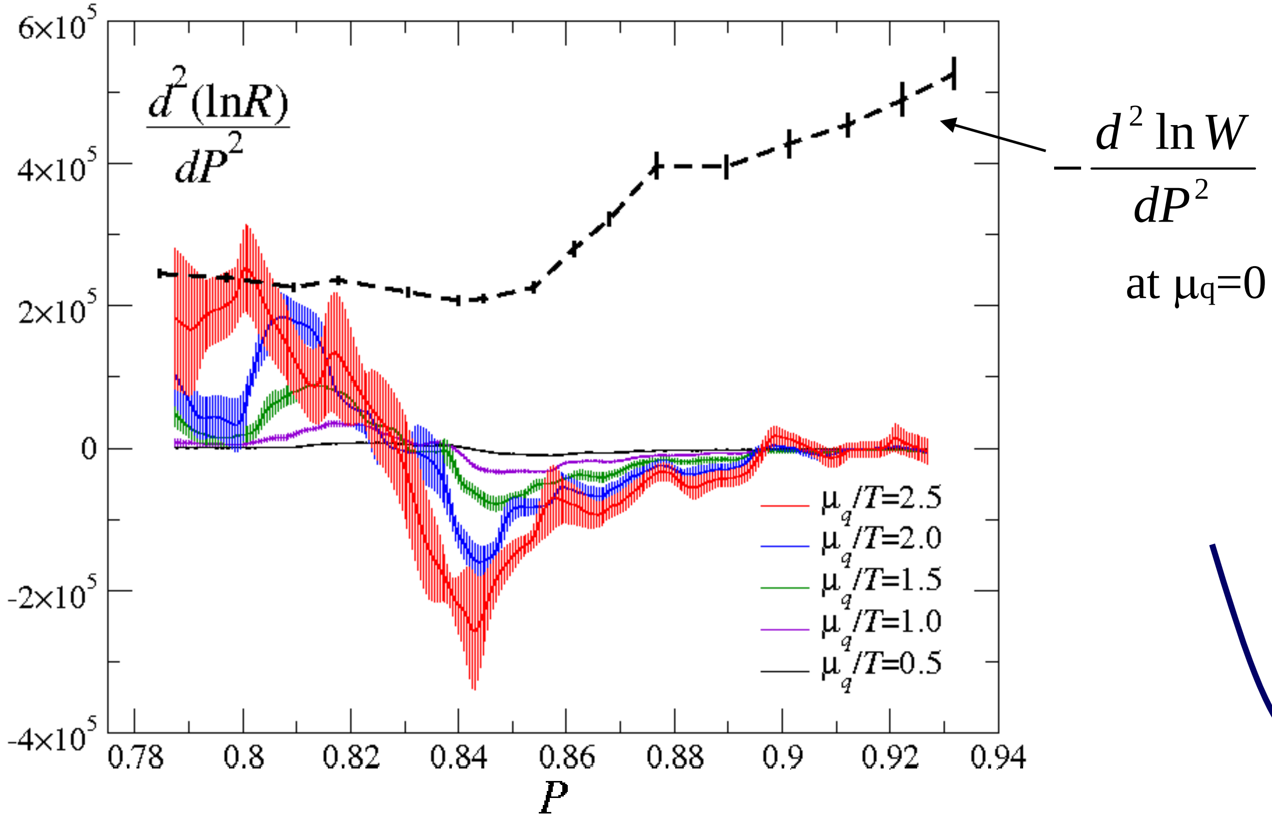
- det$M$: Taylor expansion up to $O(\mu^6)$
- The peak position of $W(P)$ moves left as β increases at μ=0.



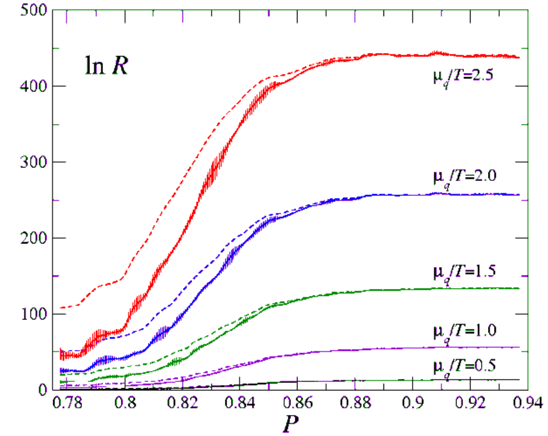
Solid lines: reweighting factor at finite μ/T, $R(P,\mu)$

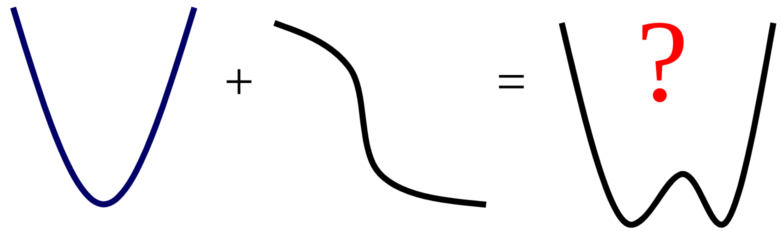
Dashed lines: reweighting factor without complex phase factor.

Curvature of the effective potential



Nf=2 p4-staggared, $m\pi/m\rho \approx 0.7$





Critical point: $$\frac{d^2 V_{\text{eff}}(P,\beta,\mu)}{dP^2} = -\frac{d^2 \ln W(P,\beta)}{dP^2} - \frac{d^2 \ln R(P,\mu)}{dP^2} = 0$$

- First order transition for $\mu_q/T \geq 2.5$
- Existence of the critical point: suggested
  - although the quark mass is large.

Probability distribution function by phase quenched simulations

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:

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

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

P: plaquette $\qquad F(\mu) = N_{\mathrm{f}} \ln\left|\dfrac{\det M(\mu)}{\det M(0)}\right| \qquad \theta \equiv N_{\mathrm{f}}\ \mathrm{Im} \ln \det M$

Distribution function of the phase quenched.

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

Phase quenched simulation

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

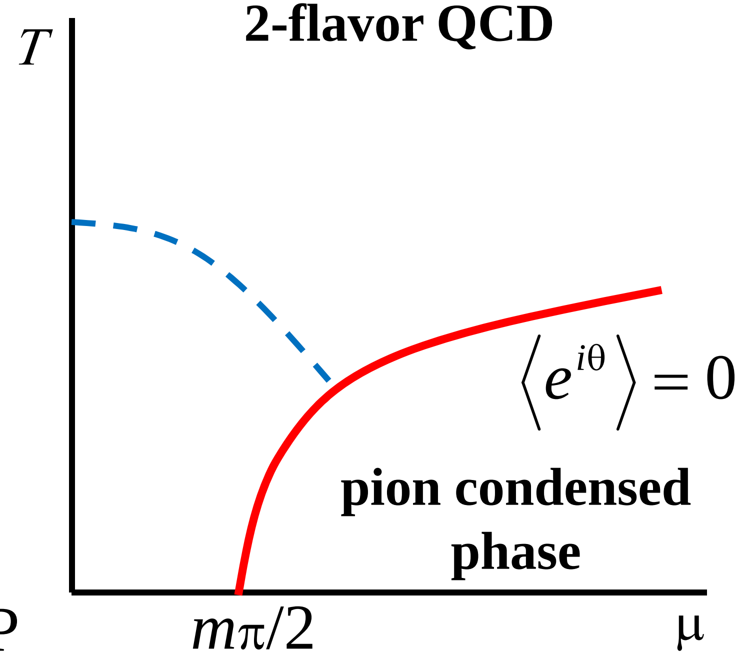
$$\det M(K,-\mu)=\left[\det M(K,\mu)\right]^*,\qquad \left|\det M(K,\mu)\right|^2=\det M(K,\mu)\det M(K,-\mu)$$

- 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 $W_0(\mu)$.

- Where is the source of the large negative curvature in V_{eff} ?
  - Phase boundary of the pion condensed phase.
  - Pseudo critical line between Hadron and QGP phases. ➡ large fluctuations in θ: expected

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.

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

$\rightarrow 0$ $\rightarrow 0$

cumulants

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

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

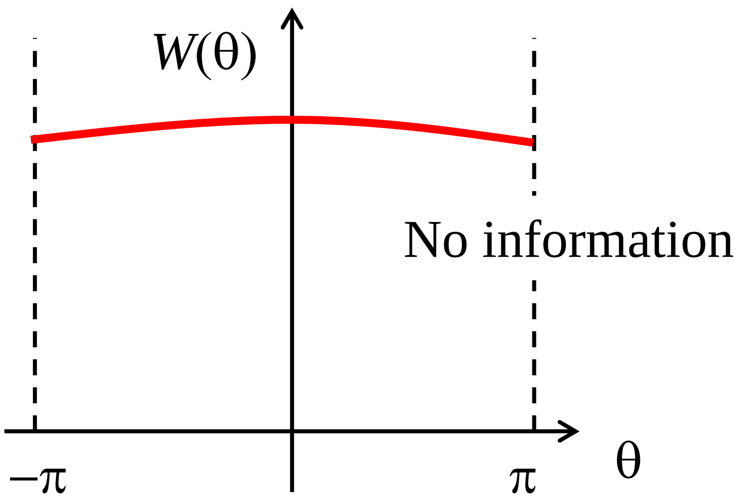
Source of the complex phase

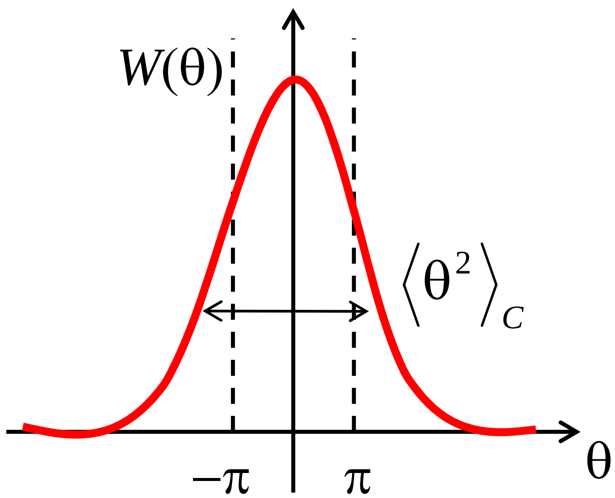
If the cumulant expansion converges, No sign problem.

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 $-\infty$ to ∞.

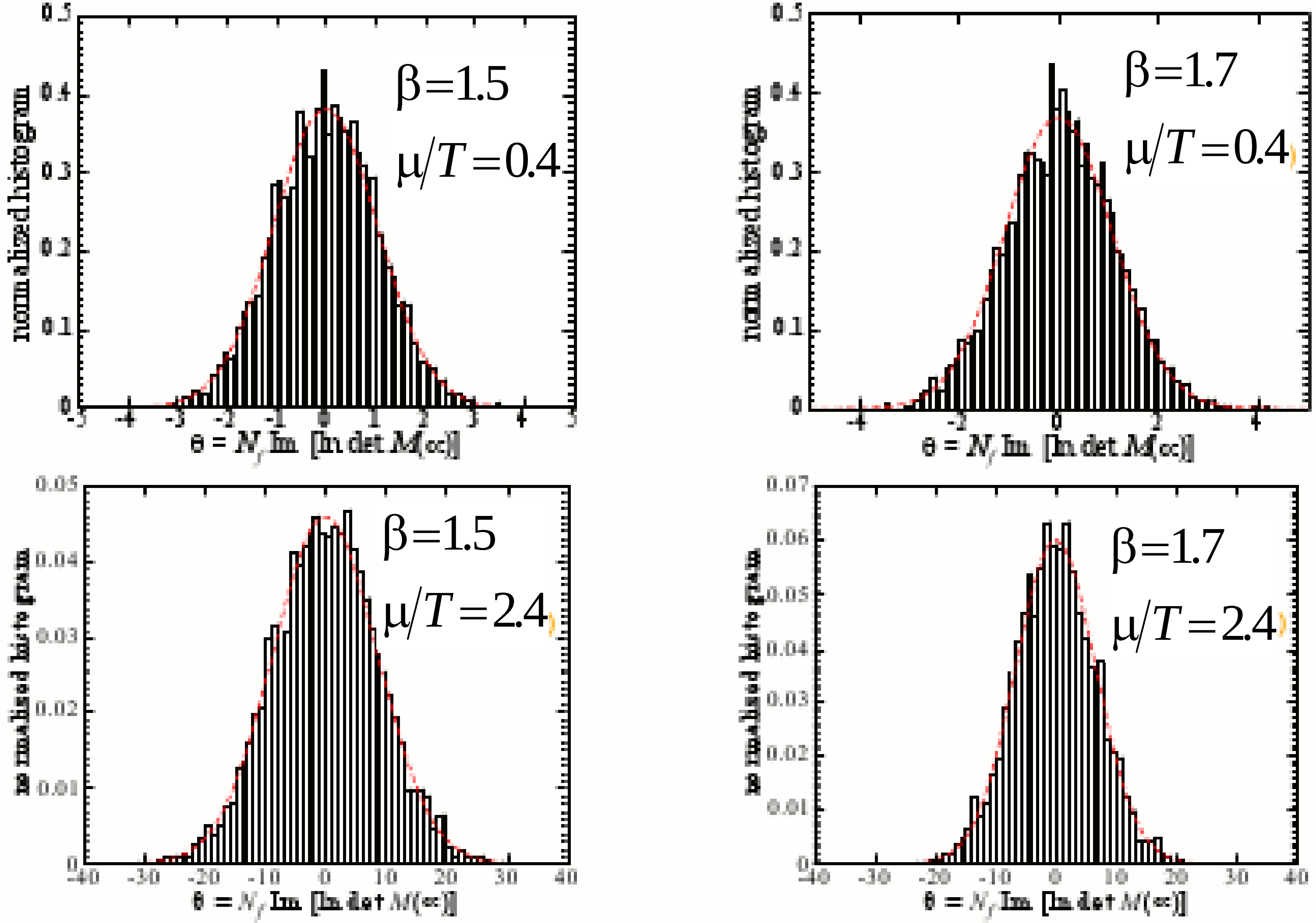
- At the same time, we calculate F as a function of μ,

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

- The reweighting factor is also computed,

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

Distribution of the complex phase

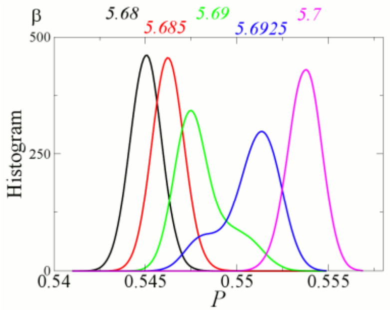


- Well approximated by a Gaussian function.
- Convergence of the cumulant expansion: good.

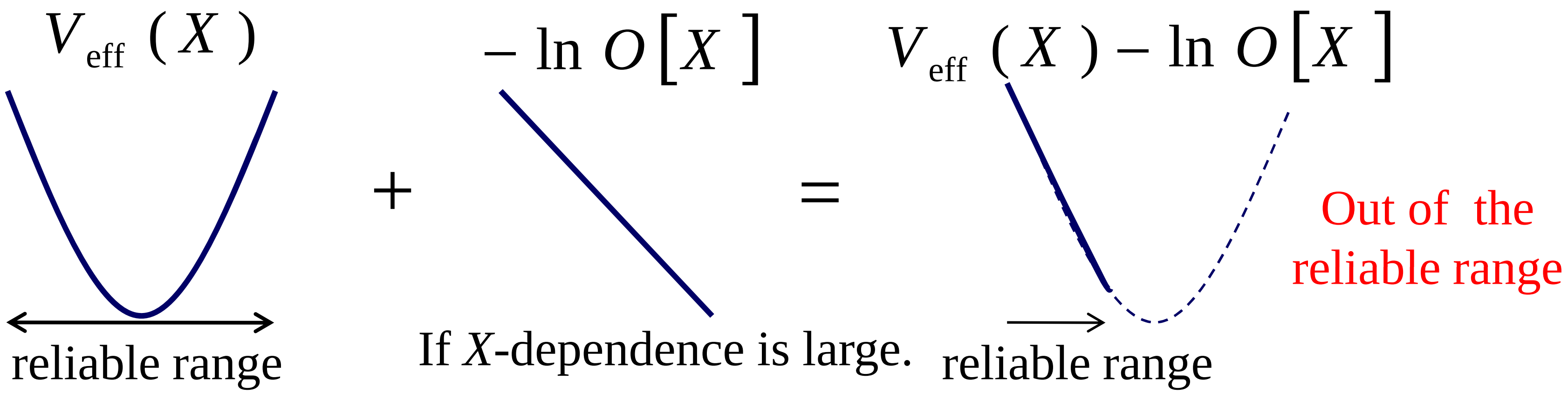
Overlap problem

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

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



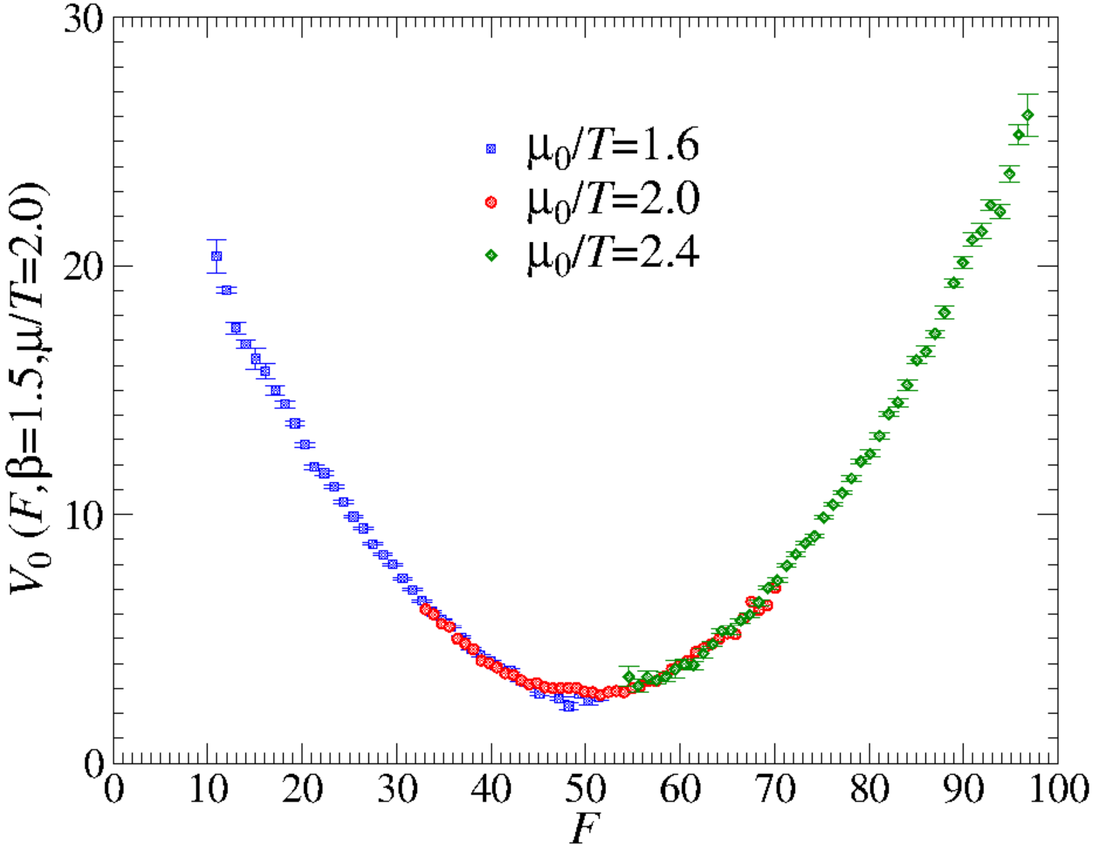
- W is computed from the histogram.
- Distribution function around X where $V_{\mathrm{eff}}(X) - \ln O[X]$ is minimized: important.
- V_{eff} must be computed in a wide range.



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.

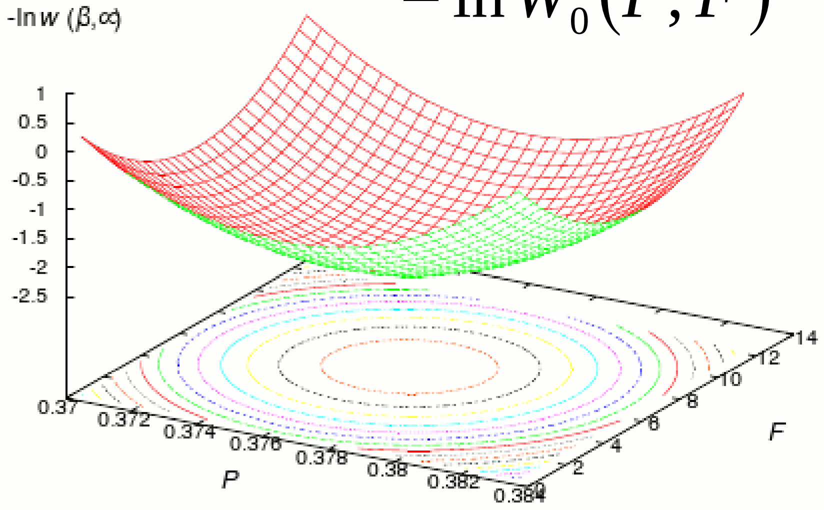
- The error of R is small because F is fixed.

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

Effective potential at finite μ

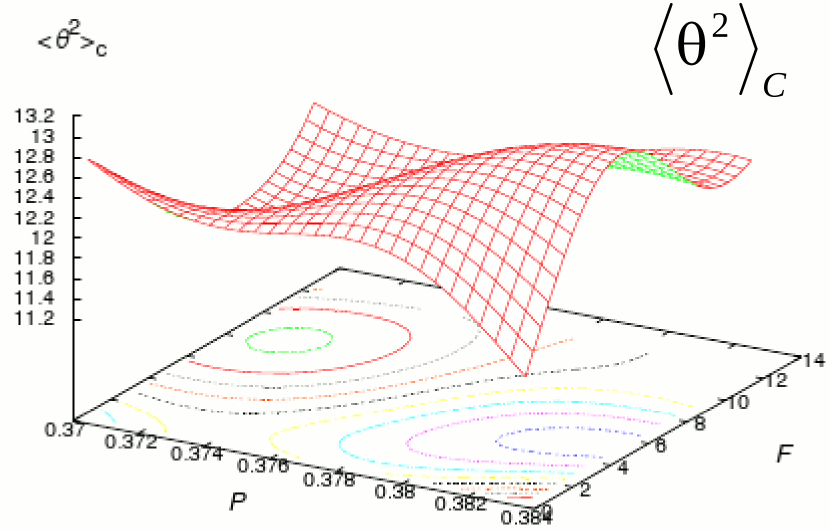
- Combine V_0 and the phase factor. Preliminary

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



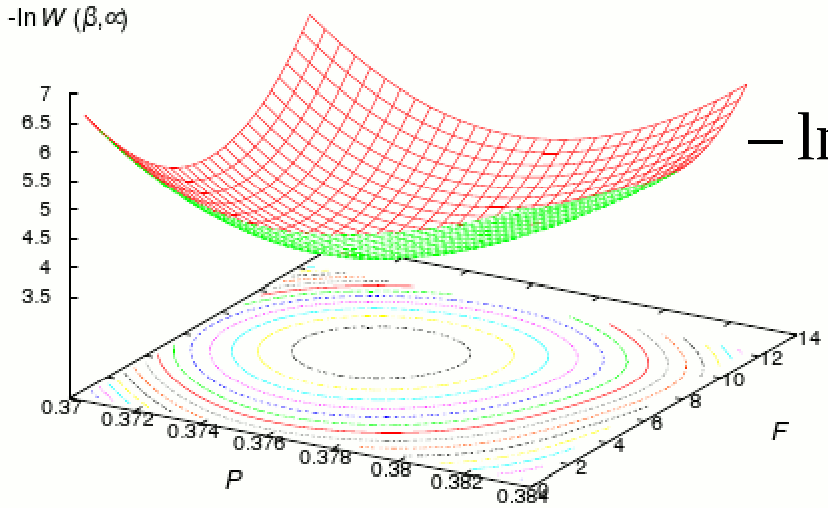
+

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



$\times 0.5$

=

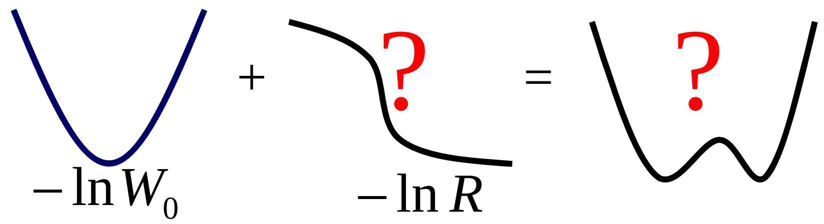


$$-\ln W(P,F)$$

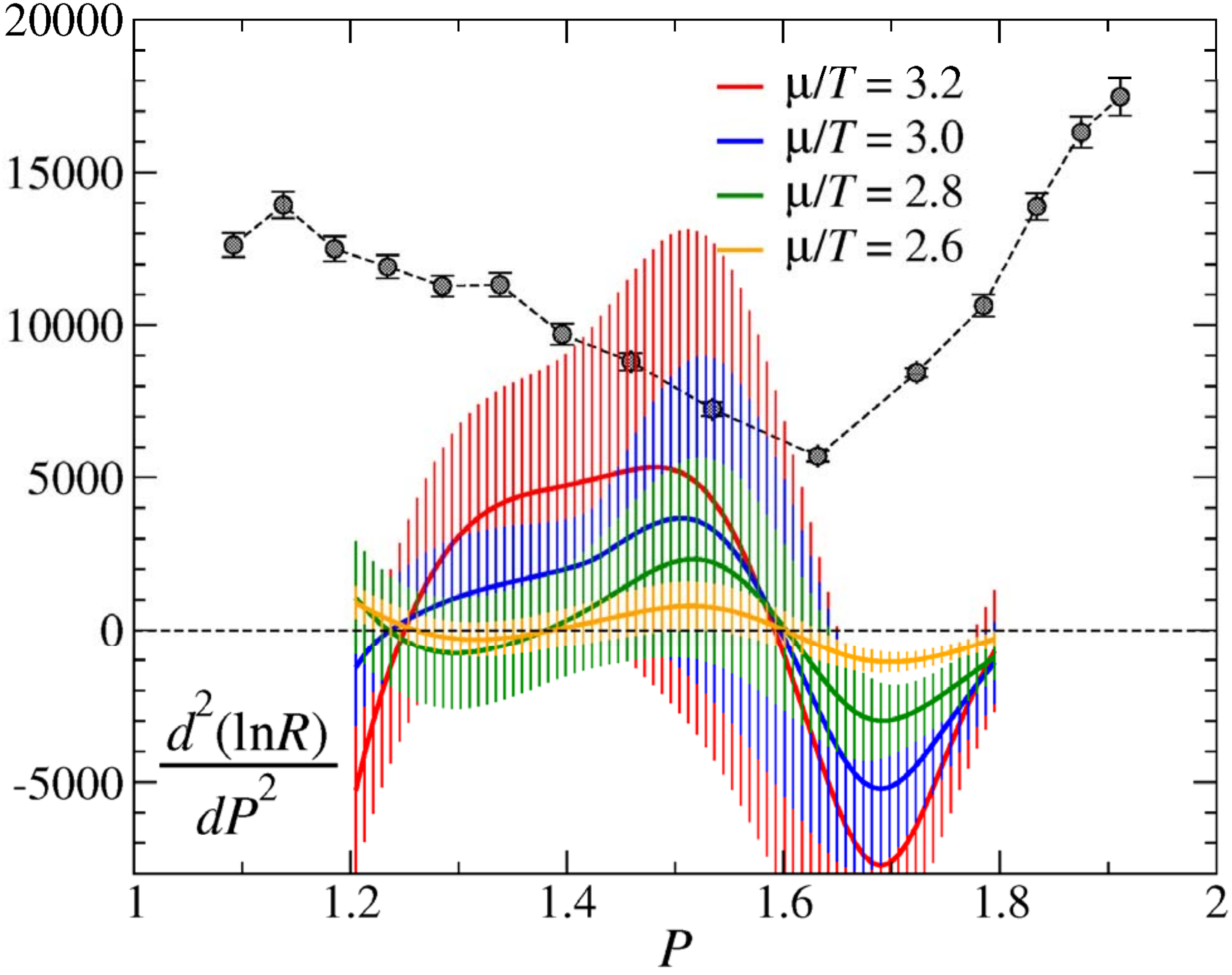
Reweighting in phase quenched simulations

very preliminary

$$\boxed{V_{\text{eff}}(P,\beta,\mu) = -\ln W_0(P,\beta,\mu_0) - \ln R(P,\mu,\mu_0)}$$



$N_f = 2,\ \ 8^3 \times 4$ lattice, $\mu_0/T = 2.4$



- Solid lines

$$R(P,\mu) \equiv \frac{W(P,\mu)}{W_0(P,\mu_0)}$$

- First order phase transition?

Canonical approach

- Canonical partition function (Laplace transformation)

$$Z_{GC}(T,\mu)=\sum_N Z_C(T,N)\exp(N\mu/T)\equiv\sum_N W(N)$$

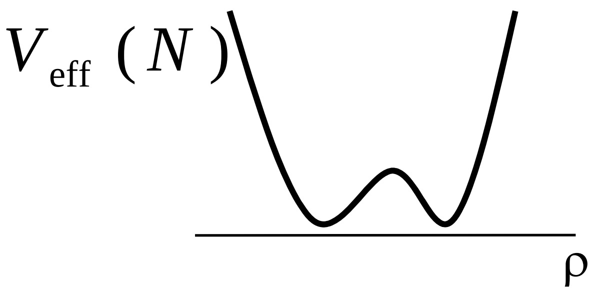
- Effective potential as a function of the quark density $\rho=N/V$

$$V_{\mathrm{eff}}(\rho)=-\ln W(\rho)=-\ln Z_C(T,\rho V)-\rho V\mu/T$$

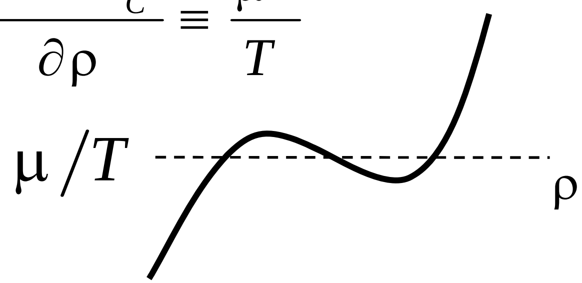
- The first derivative

$$\frac{\partial V_{\mathrm{eff}}(\rho V)}{\partial\rho}=-\frac{\partial\ln W(\rho V)}{\partial\rho}=-\frac{\partial\ln Z_C(T,\rho V)}{\partial\rho}-\frac{\mu}{T}V$$

- First order phase transition: Two phases coexist.



$$-\frac{1}{V}\frac{\partial\ln Z_C}{\partial\rho}\equiv\frac{\mu^*}{T}$$



Inverse Laplace transformation with a saddle point approximation (S.E., arXiv:0804.3227)

- Approximations:
  - Taylor expansion: $\ln \det M$ up to $O(\mu^6)$
  - Gaussian distribution: θ
  - Saddle point approximation

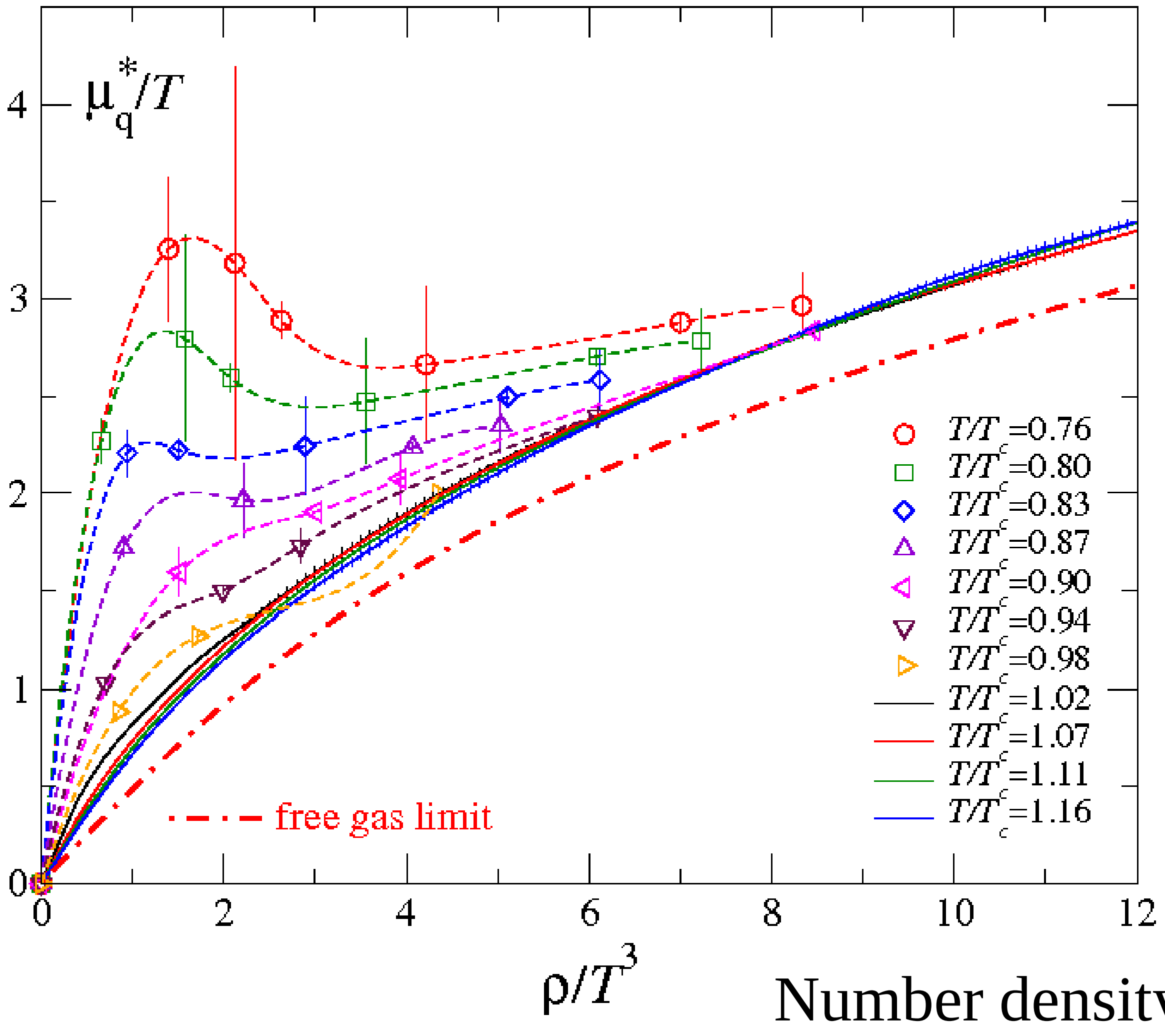
Much easier calculations

- First order transition at $T/T_c < 0.83$

- Study near the physical point important

Solid line: multi-β reweighting
Dashed line: spline interpolation
Dot-dashed line: the free gas limit

N_f=2 p4-staggered, $m_\pi/m_\rho \approx 0.7$, $16^3 \times 4$ lattice



Number density

Summary

- The histogram method is useful for the investigation of the nature of the phase transition.

- To avoid the sign problem, the method based on the cumulant expansion of θ is useful.

- Further studies are important applying this method.