On the critical endpoint in lattice QCD at nonzero temperature and density

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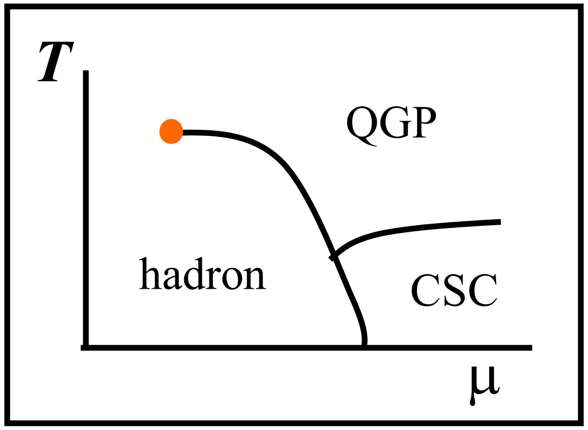
> Effective potential as a function of plquette:
arXiv:0706.3549 [hep-lat]

> Canonical approach: in preparation

xQCD @ Frascati, Roma, August 6 – 8, 2007

Study of QCD phase structure at finite density



Interesting topic:

- Endpoint of the first order phase transition

- Monte-Carlo simulations

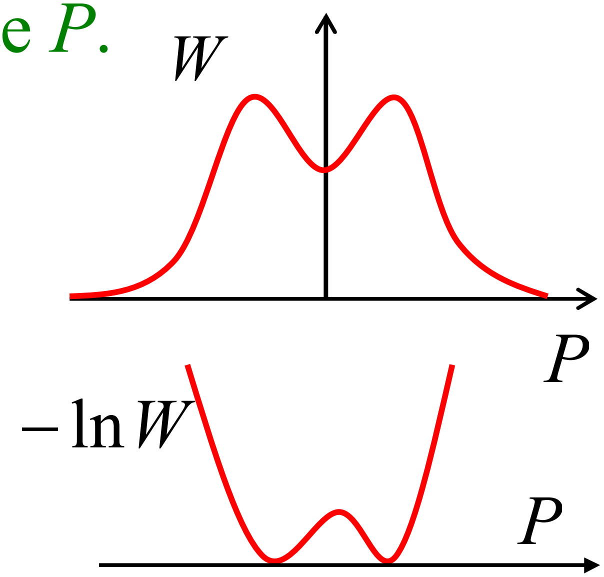
$$\langle O \rangle_{(\beta,\mu)} = \frac{1}{Z} \int \underbrace{DU \left(\det M(\mu)\right)^{N_f} e^{-S_g(\beta)}}_{\text{generate configurations}} O[U]$$

$$Z = \int DU \left(\det M(\mu)\right)^{N_f} e^{-S_g}$$

- Distribution function (histogram) of plaquette P.
  - First order phase transition:

    Two states coexist. ➡ Double peak.

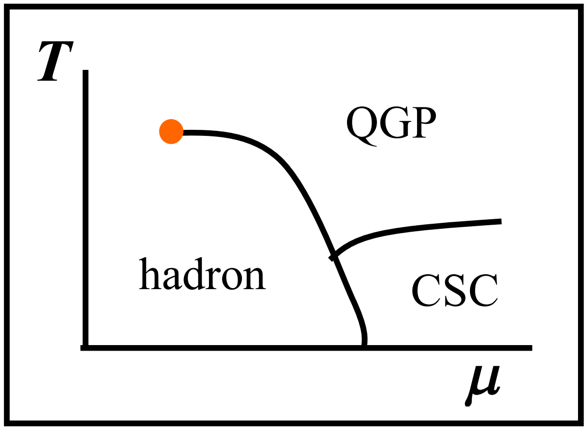
- Effective potential: $-\ln W(P)$
  - First order: Double well Curvature: negative



Study of QCD phase structure at finite density

Reweighting method for μ

- Boltzmann weight: Complex for μ>0
  - Monte-Carlo method is not applicable directly.
  - Cannot generate configurations with the probability



- Reweighting method
  - Perform Simulation at μ=0.
  - Modify the weight factor by

$$\langle O \rangle_{(\beta,\mu)} = \frac{1}{Z} \int DUO \left(\frac{\mathrm{det}M(\mu)}{\mathrm{det}M(0)} \mathrm{det}M(0) \right)^{N_{\mathrm{f}}} \mathrm{e}^{-S_g(\beta)} = \frac{\left\langle O\left(\det M(\mu)/\det M(0)\right)^{N_{\mathrm{f}}} \right\rangle_{(\beta,0)}}{\left\langle \left(\det M(\mu)/\det M(0)\right)^{N_{\mathrm{f}}} \right\rangle_{(\beta,0)}}$$

$$Z = \int DU \left(\mathrm{det}M(\mu)\right)^{N_{\mathrm{f}}} \mathrm{e}^{-S_g}$$

(expectation value at μ=0.)

Weight factor, Effective potential

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

$$Z(\mu)=\int dP\, R(P,\mu)\,W(P,\beta) \qquad\qquad S_g=-6N_{site}\beta P$$

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

(Weight factor at μ=0)

$$R(\bar{P},\mu)\equiv\frac{\int DU\ \delta(P\text{-}\bar{P})(\mathrm{det}M(\mu))^{N_\mathrm{f}}}{\int DU\ \delta(P\text{-}\bar{P})(\mathrm{det}M(0))^{N_\mathrm{f}}}=\frac{\frac{1}{Z(0)}\int DU\delta(P\text{-}\bar{P})\left(\frac{\mathrm{det}M(\mu)}{\mathrm{det}M(0)}\right)^{N_\mathrm{f}}(\mathrm{det}M(0))^{N_\mathrm{f}}\ \mathrm{e}^{-S_g}}{\frac{1}{Z(0)}\int DU\delta(P\text{-}\bar{P})(\mathrm{det}M(0))^{N_\mathrm{f}}\ \mathrm{e}^{-S_g}}$$

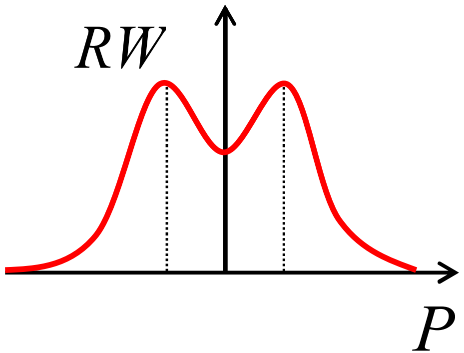
Expectation value of $O[P]$

$$\langle O[P]\rangle_{(\beta,\mu)}=\frac{1}{Z(\mu)}\int dP\, O[P]\,\underline{R(P,\mu)W(P,\beta)}$$

Weight factor at finite μ

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

Ex) 1st order phase transition



We estimate the effective potential using the data in PRD71,054508(2005).

Reweighting for μ/T, Taylor expansion

Problem 1, Direct calculation of det*M* : difficult

- Taylor expansion in μ_q (Bielefeld-Swansea Collab., PRD66, 014507 (2002))

$$\ln \det M(\mu) = N_f \sum_{n=0}^{\infty} \left[\frac{1}{n!} \left(\frac{\mu}{T} \right)^n \frac{d^n \ln \det M}{d(\mu/T)^n} \right]$$

  - Random noise method → Reduce CPU time.

- Approximation: up to $O(\mu_q^6)$
  - Taylor expansion of $R(\mu_q)$

Valid, if $c_8^R \left(\frac{\mu_q}{T}\right)^8 + \cdots$ is small.

$$R(\mu_q) = \underbrace{c_2^R \left(\frac{\mu_q}{T}\right)^2 + c_4^R \left(\frac{\mu_q}{T}\right)^4 + c_6^R \left(\frac{\mu_q}{T}\right)^6}_{\text{no error}} + \underbrace{c_8^R \left(\frac{\mu_q}{T}\right)^8 + \cdots}_{\text{truncation error}}$$

  - The application range can be estimated, e.g.,

$$\boxed{\sqrt{\left| \frac{c_6^R}{c_8^R} \right|} >> \frac{\mu_q}{T}} \Leftrightarrow \left| c_6^R \left(\frac{\mu_q}{T}\right)^6 \right| >> \left| c_8^R \left(\frac{\mu_q}{T}\right)^8 \right|$$

Reweighting for μ/T, Sign problem

Problem 2, det$M(\mu)$: complex number.

$$\boxed{(\det M)^{N_{\mathrm{f}}} \equiv |F|\,\mathrm{e}^{i\theta}}$$

Sign problem happens when det$M$ changes its sign frequently.

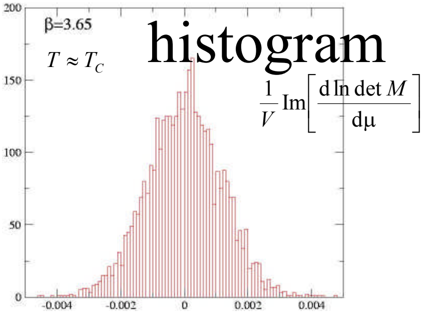
- Assumption:

Distribution function $W(P,|F|,\theta) \rightarrow$ Gaussian

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

$$\int d\theta\; e^{i\theta} W(\theta) \rightarrow \exp\left(-\frac{1}{4\alpha_{(P,|\det M|)}}\right)$$

➡ Weight: real positive (no sign problem)



When the correlation between eigenvalues of M is weak.

- Complex phase: $\theta = N_{\mathrm{f}}\,\mathrm{Im}[\ln\det M(\mu)]$

$$\ln\det M(\mu) = \ln\left(\prod_n |\lambda_n| e^{i\theta_n}\right) = \sum_n \ln|\lambda_n| + i\sum_n \theta_n \qquad \left(|\lambda_n| e^{i\theta_n} : \text{eigenvalues}\right)$$

Central limit theorem ➡ θ: Gaussian distribution

Valid for large volume (except on the critical point)

Reweighting for μ/T, sign problem

- Taylor expansion: odd terms of ln det M (Bielefeld-Swansea, PRD66, 014507 (2002))

$$\theta = N_{\mathrm{f}} \mathrm{Im}\left[\frac{\mu}{T} \frac{\mathrm{d} \ln \det M}{\mathrm{d}(\mu/T)} + \frac{1}{3!}\left(\frac{\mu}{T}\right)^3 \frac{\mathrm{d}^3 \ln \det M}{\mathrm{d}^3(\mu/T)} + \frac{1}{5!}\left(\frac{\mu}{T}\right)^5 \frac{\mathrm{d}^5 \ln \det M}{\mathrm{d}^5(\mu/T)} + \cdots \right]$$

- Estimation of $\alpha(P, |F|)$: For fixed $(P, |F|)$,

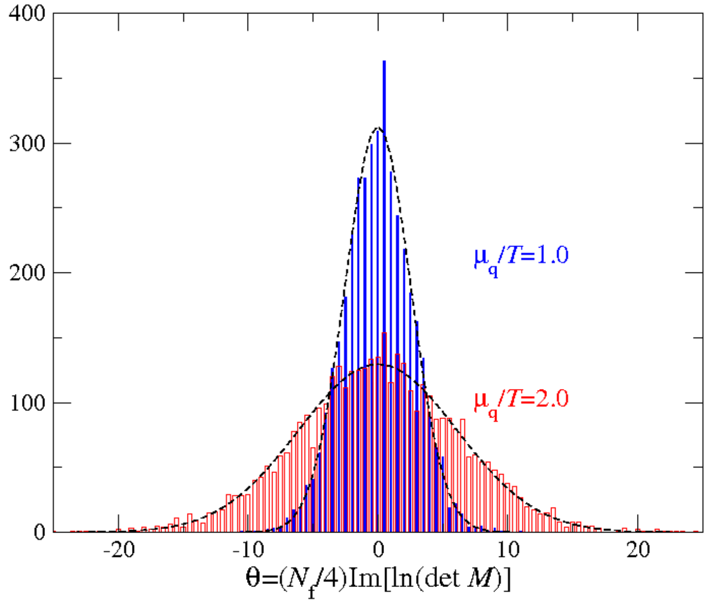
$$\frac{1}{2\alpha(P',|F|')} = \frac{\int \theta^2 W(P',|F|',\theta) d\theta}{\int W(P',|F|',\theta) d\theta} = \frac{\left\langle \theta^2 \delta(P-P')\delta(|F|-|F|') \right\rangle}{\left\langle \delta(P-P')\delta(|F|-|F|') \right\rangle}$$

$$\boxed{(\det M)^{N_{\mathrm{f}}} \equiv |F| \, \mathrm{e}^{i\theta}}$$

- Results for p4-improved staggered
  - Taylor expansion up to $O(\mu^5)$
  - Dashed line: fit by a Gaussian function

➡ Well approximated

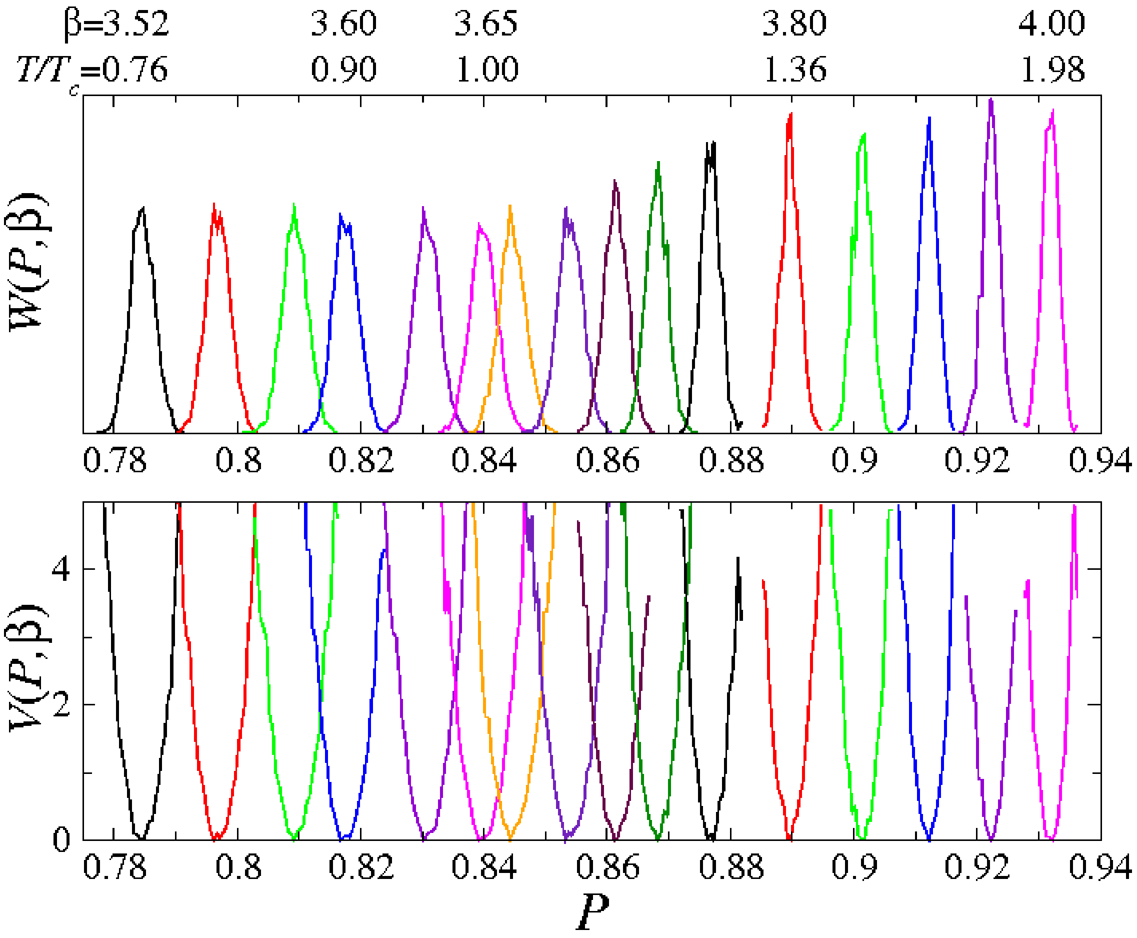
$T \approx T_C$ histogram of θ



Reweighting for $\beta(T)=6g^{-2}$

$$Z(\mu)=\int dP\, R(P,\mu)\underline{W(P,\beta)}$$

(Data: N_f=2 p4-staggared, $m_\pi/m_\rho \approx 0.7$, $\mu=0$, without reweighting)



Change: $\beta_1(T)$ ➡ $\beta_2(T)$

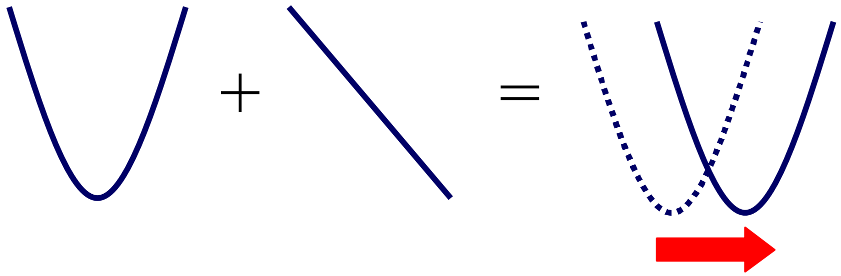
Weight:

$$W(\beta_1)\Rightarrow W(\beta_2)=e^{-S_g(\beta_2)+S_g(\beta_1)}W(\beta_1)$$

$$S_g(\beta_2)-S_g(\beta_1)=-6N_{\rm site}(\beta_2-\beta_1)P$$

Potential:

$$-\ln W(\beta_1)\underline{-6N_{\rm site}(\beta_2-\beta_1)P}=-\ln W(\beta_2)$$

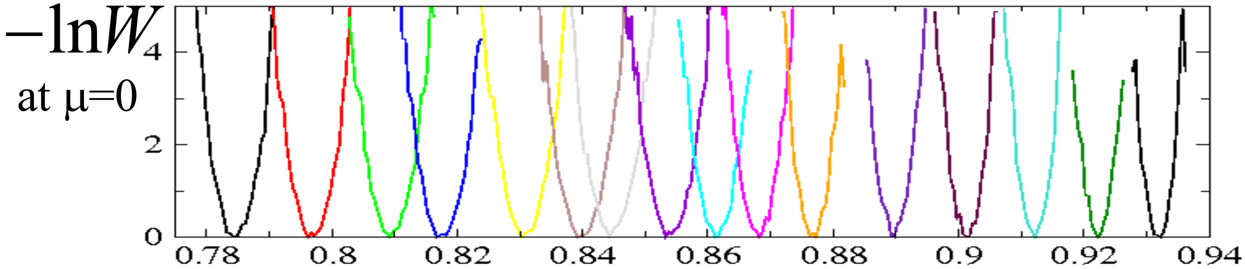


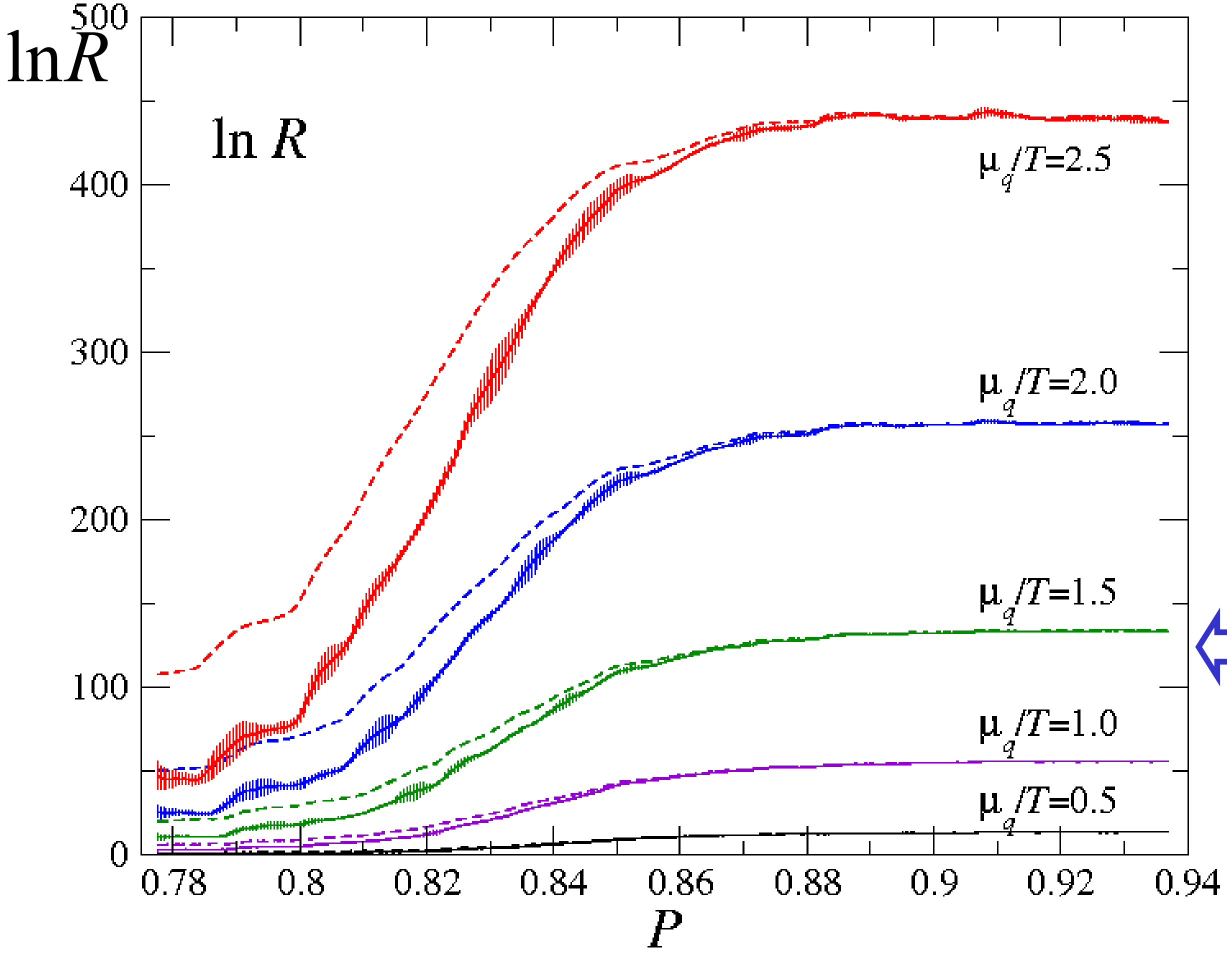
Assumption: $W(P)$ is of Gaussian.

➡ $$\underline{-\frac{d^2\ln W}{dP^2}=\frac{6N_{\rm site}}{\chi_P}\equiv\left\langle\left(P-\langle P\rangle\right)^2\right\rangle^{-1}}$$

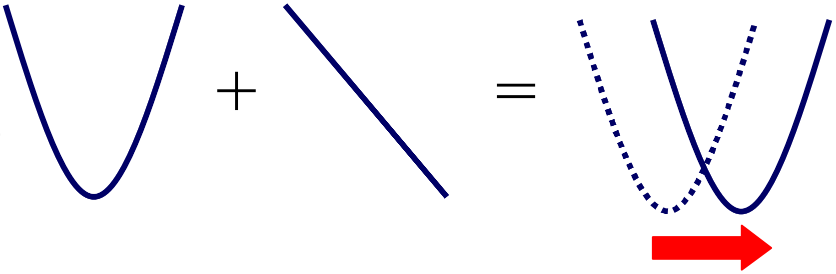
(Curvature of $V(P)$ at $\mu_q=0$)

Effective potential at finite μ/T $\boxed{-\ln W(P,\beta)-\ln R(P,\mu)}$

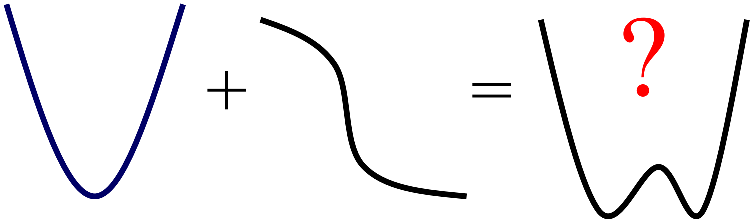




- Normal



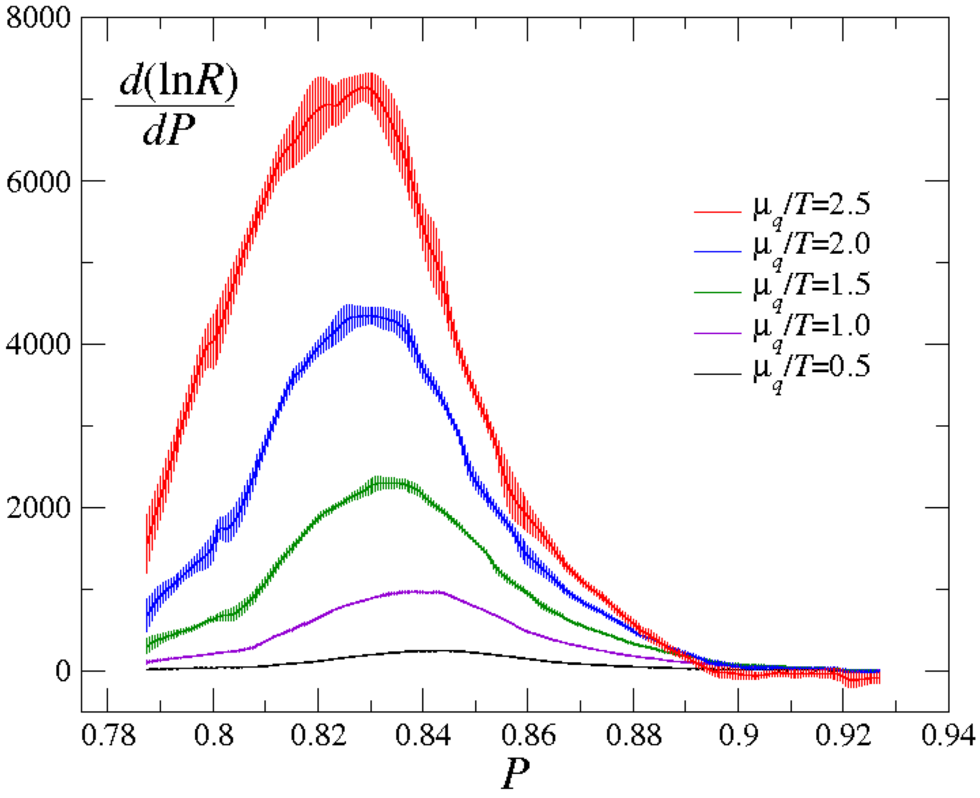
- First order

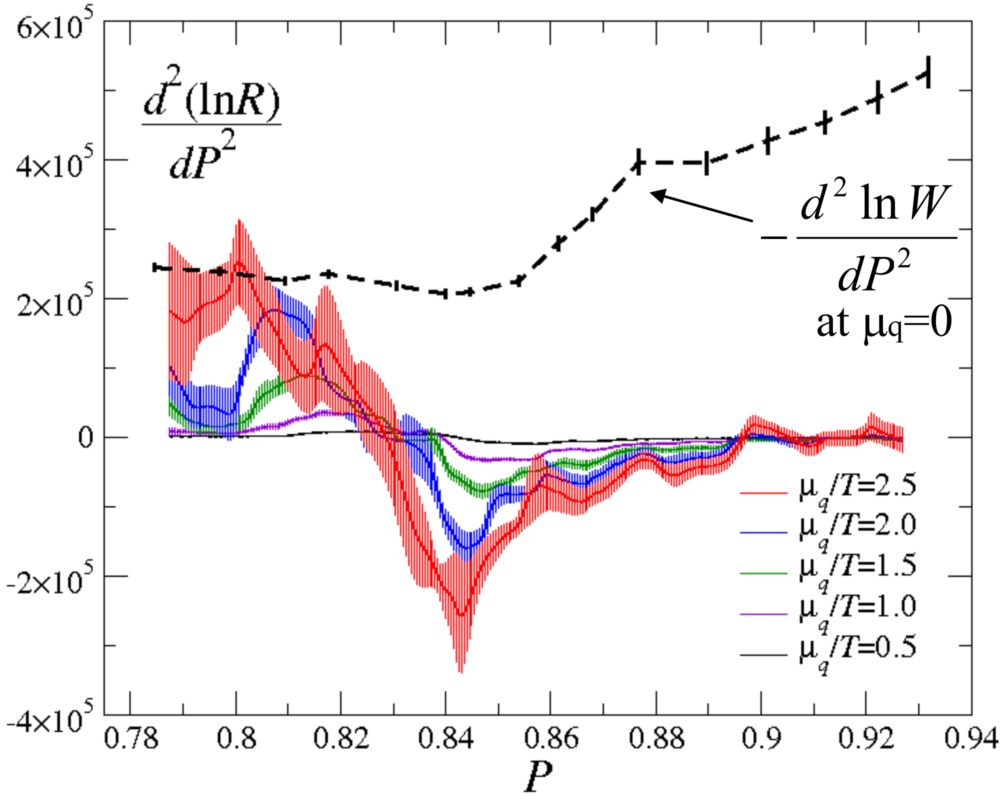


Solid lines: reweighting factor at finite μ/T, $R(P,\mu)$

Dashed lines: reweighting factor without complex phase factor.

Slope and curvature of the effective potential





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

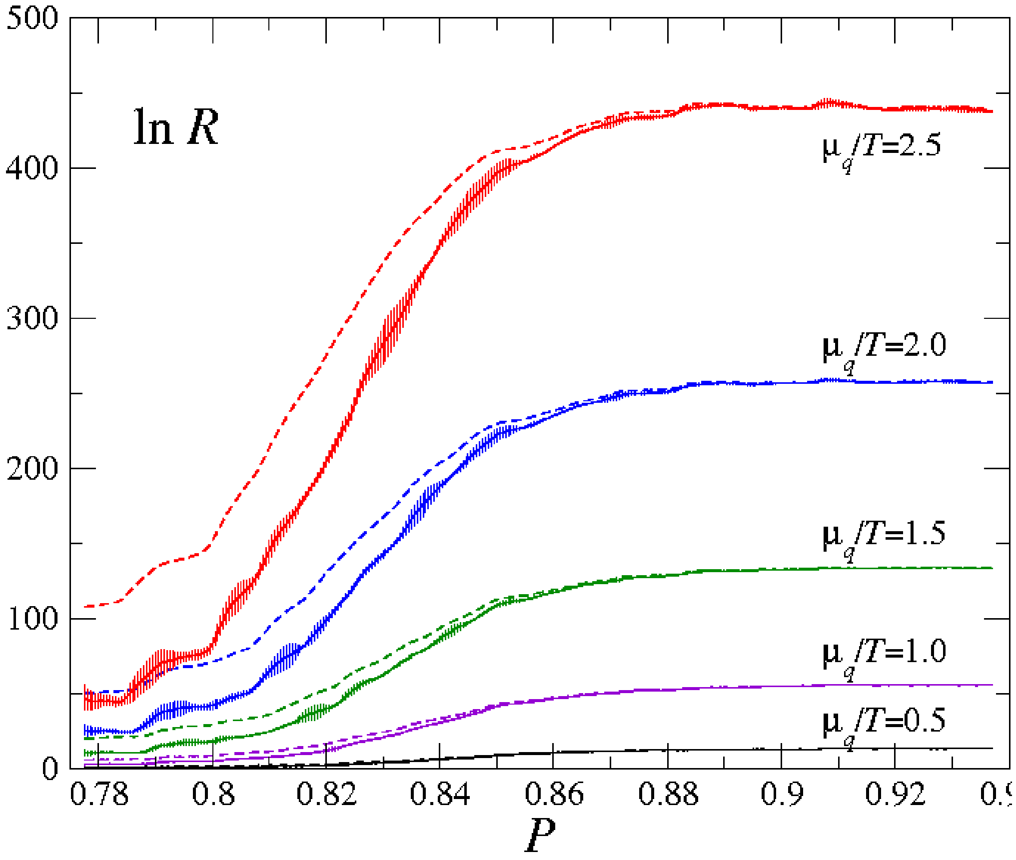
- First order at $\mu_q/T \geq 2.5$

QCD with isospin chemical potential μ_I

$$\boxed{\mu_u = -\mu_d = \mu_I, \qquad \mu_q = (\mu_u + \mu_d)/2 = 0}$$

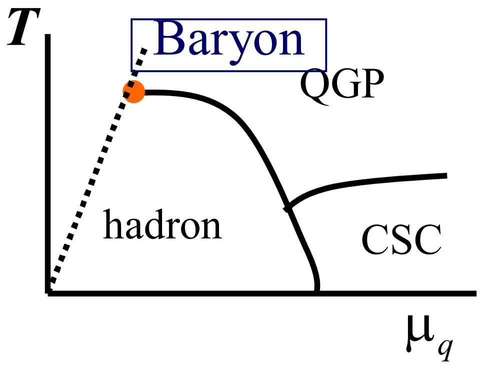
$$\det M(\mu_u)\det M(\mu_d) = \det M(\mu_I)\det M(-\mu_I) = \left|\det M(\mu_I)\right|^2$$

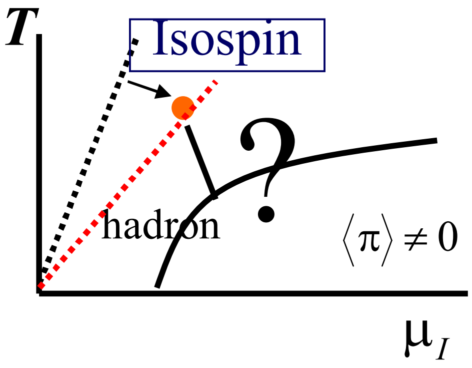
$$\left(\because \ \det M(-\mu_I) = \left[\det M(\mu_I)\right]^*\right)$$



- Dashed line: QCD with non-zero μ_I (μ_q=0)
- The slope and curvature of ln$R$ for isospin chemical potential is small.

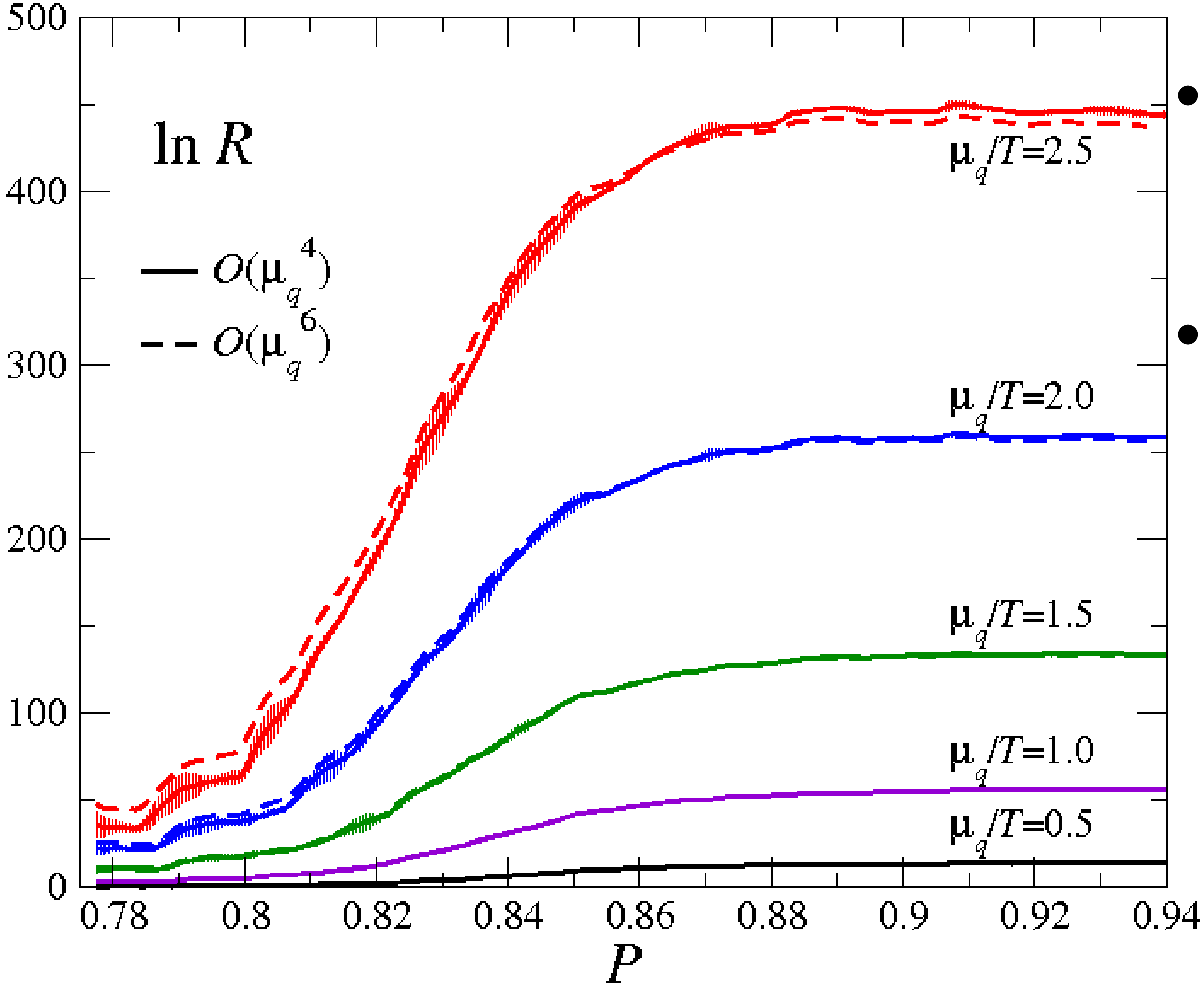
➡ The critical μ_I/T is larger than that in QCD with non-zero μ_q/T.





Truncation error of Taylor expansion

$$N_{\rm f} \ln\det M(\mu) = N_{\rm f} \sum_{n=0}^{N} \left[\frac{1}{n!} \left(\frac{\mu}{T} \right)^n \frac{{\rm d}^{\rm n} \ln\det M}{{\rm d}(\mu/T)^n} \right]$$



- Solid line: $O(\mu^4)$
- Dashed line: $O(\mu^6)$

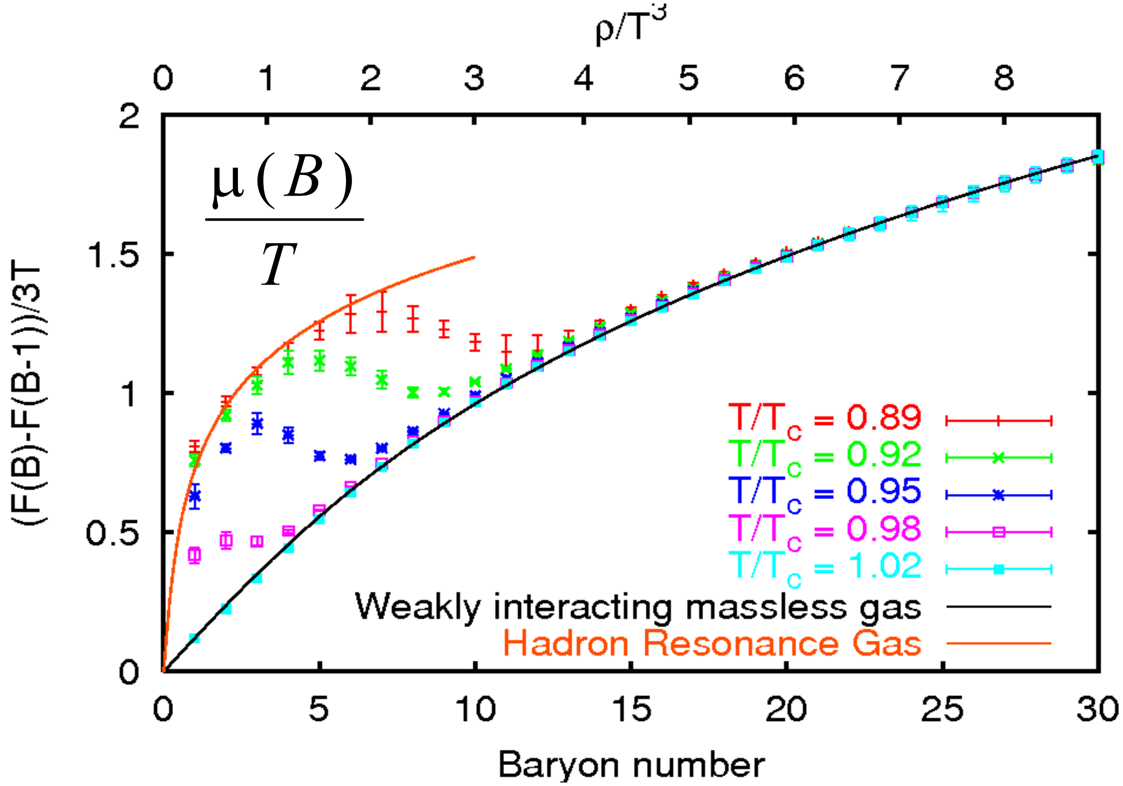
- The effect from 5th and 6th order term is small for $\mu_q/T \leq 2.5$.

Canonical approach

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

Canonical partition function $Z_{GC}(T,\mu) = \sum_N \underline{\underline{Z_C(T,N)}} \exp(N\mu/T)$

Chemical potential $\frac{\mu(N)}{T} = -\frac{\partial \ln Z_C(T,N)}{\partial N}$



S. Kratochvila, Ph. de Forcrand,
hep-lat/0509143

N_f=4 staggered fermions,
$6^3 \times 4$ lattice

First order phase transition: Two states coexist

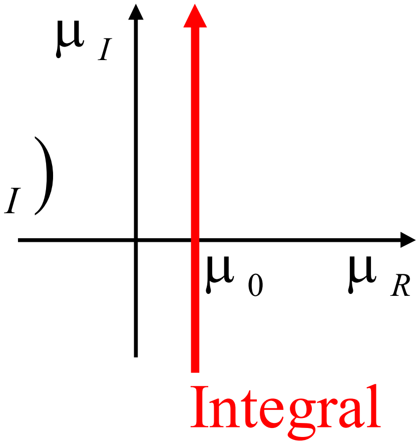
Canonical approach

- Fugacity expansion (Laplace transformation)

$$Z_{GC}(T,\mu)=\sum_N \underline{\underline{Z_C(T,N)}}\exp(N\mu/T) \qquad \rho = N / V$$

- $Z_C(T,N)$: canonical partition function

$$Z_C(T,N)=\frac{3}{2\pi}\int_{-\pi/3}^{\pi/3} d(\mu_I/T)\, e^{-N(\mu_0/T+i\mu_I/T)} Z_{GC}(T,\mu_0+i\mu_I)$$



$$\frac{Z_{GC}(\mu)}{Z_{GC}(0)}=\frac{1}{Z_{GC}(0)}\int DU\,(\det M(\mu))^{N_f}e^{-S_g}=\left\langle\left(\frac{\det M(\mu)}{\det M(0)}\right)^{N_f}\right\rangle_{\mu=0}$$

- Saddle point approximation (valid for large *V*) $V=16^3=4096$

$$\frac{Z_C(T,\rho)}{Z_{GC}(T,0)}=\frac{3}{\sqrt{2\pi}}\left\langle \exp\left[N_f\ln\left(\frac{\det M(z_0)}{\det M(0)}\right)-V\rho z_0\right]e^{-i\alpha/2}\sqrt{\frac{1}{V\left|R''(z_0)\right|}}\right\rangle_{(T,\mu=0)}$$

Saddle point: z_0

$$\left[\frac{N_f}{V}\frac{\partial(\ln\det M)}{\partial(\mu/T)}-\rho\left(\frac{\mu}{T}\right)\right]_{\frac{\mu}{T}=z_0}=0 \qquad R''\left(\frac{\mu}{T}\right)=\frac{N_f}{V}\frac{\partial^2(\ln\det M)}{\partial(\mu/T)^2}\equiv\left|R''\right|e^{i\alpha}$$

Canonical approach

- Chemical potential in saddle point approximation

$$\frac{\mu(\rho)}{T} = \frac{-1}{V}\frac{\partial \ln Z_C(T,\rho)}{\partial\rho}$$

$$\approx \frac{\left\langle \underline{z_0}\; \underline{\exp\left[\ln\left(\frac{\det M(z_0)}{\det M(0)}\right)^{N_{\rm f}} - V\rho z_0\right] e^{-i\alpha/2}\sqrt{\frac{1}{V\left|R''(z_0)\right|}}} \right\rangle_{(T,\mu=0)}}{\left\langle \underline{\exp\left[\ln\left(\frac{\det M(z_0)}{\det M(0)}\right)^{N_{\rm f}} - V\rho z_0\right] e^{-i\alpha/2}\sqrt{\frac{1}{V\left|R''(z_0)\right|}}} \right\rangle_{(T,\mu=0)}}$$

saddle point

reweighting factor

- Expectation value of plaquette

$$\langle P\rangle_{(T,\rho)} \approx \frac{\left\langle P\exp\left[\ln\left(\frac{\det M(z_0)}{\det M(0)}\right)^{N_{\rm f}} - V\rho z_0\right] e^{-i\alpha/2}\sqrt{\frac{1}{V\left|R''(z_0)\right|}} \right\rangle_{(T,\mu=0)}}{\left\langle \exp\left[\ln\left(\frac{\det M(z_0)}{\det M(0)}\right)^{N_{\rm f}} - V\rho z_0\right] e^{-i\alpha/2}\sqrt{\frac{1}{V\left|R''(z_0)\right|}} \right\rangle_{(T,\mu=0)}}$$

Calculation of the canonical partition function

- Approximation:
  - Taylor expansion of ln det M: up to $O(\mu^6)$
  - Distribution function of $\theta = N_f \,\mathrm{Im}[\,\ln \det M]$: Gaussian type.

- Simulations:
  - Bielefeld-Swansea collab., PRD71,054508(2005).
  - 2-flavor p4-improved staggered quarks with $m/T=0.4$
  - 16^3x4 lattice

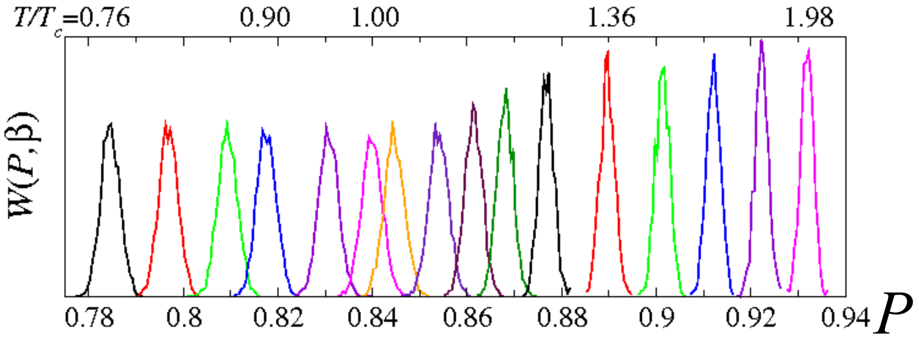
Multi-β reweighting

Ferrenberg-Swendsen, PRL63,1195(1989)

- When the density increases, the position of the importance sampling changes.
- Combine all data by multi-β reweighting

Problem:

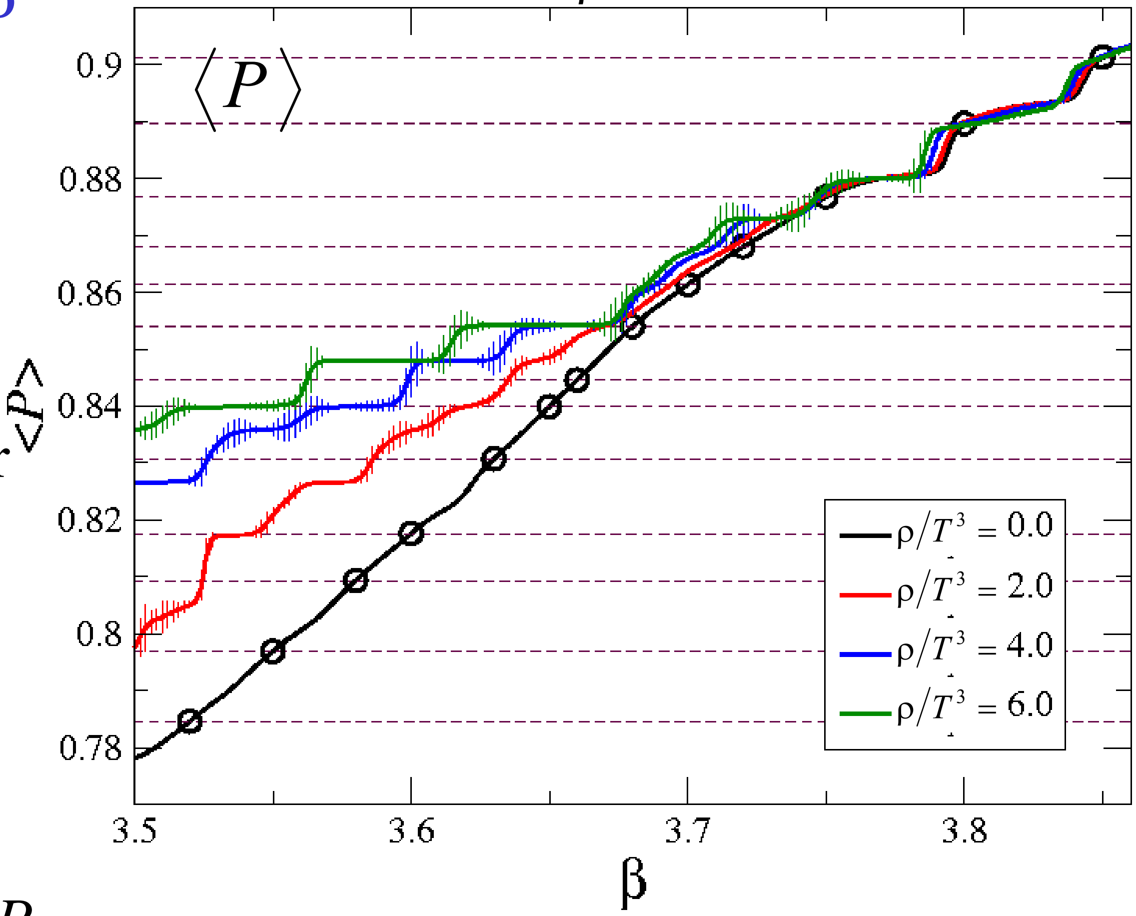
- Configurations do not cover all region of *P*.
- Calculate only when <*P*> is near the peaks of the distributions.



Plaquette value by multi-beta reweighting

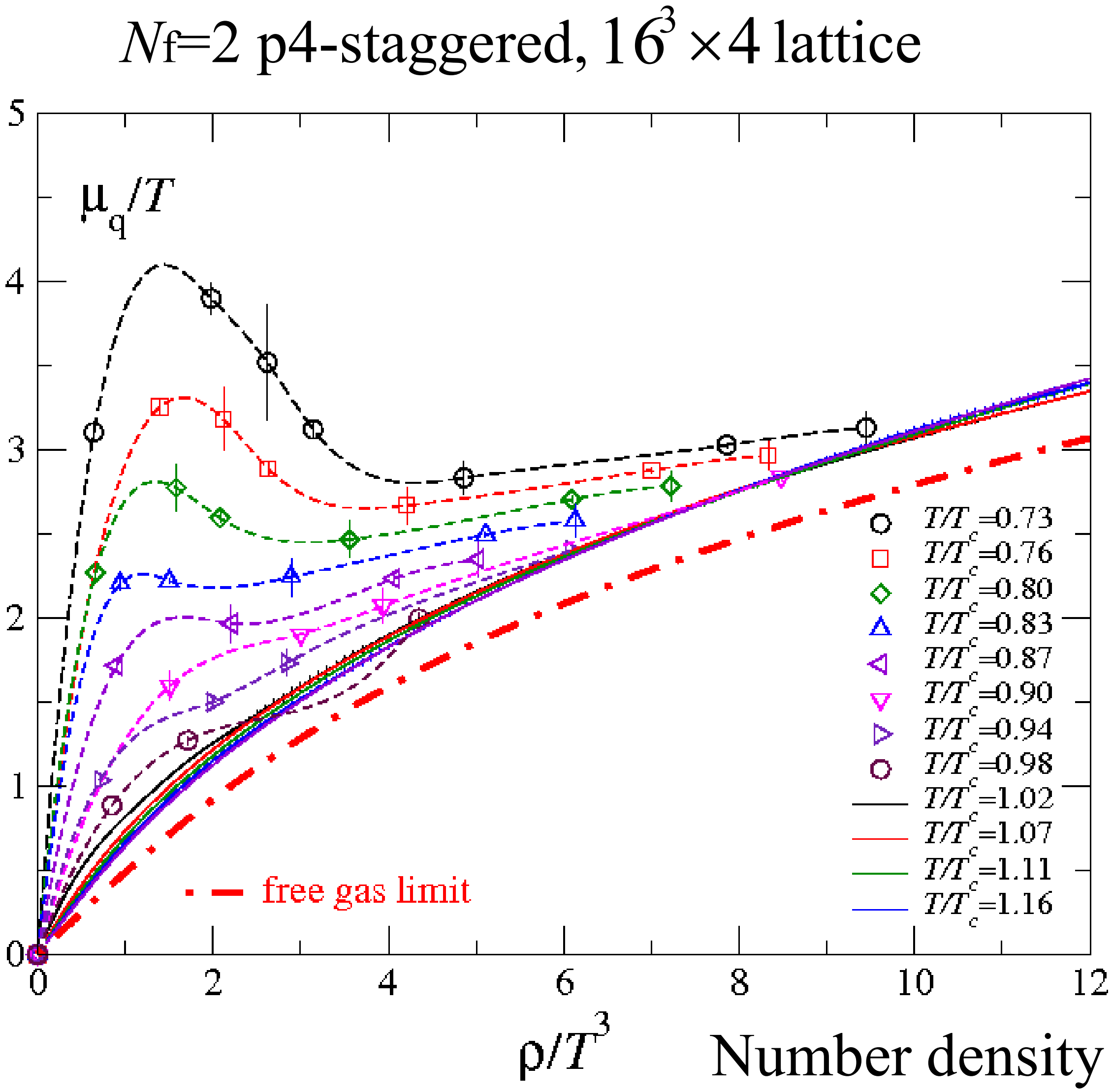
- - - peak position of the distribution

○ <*P*> at each β



Canonical approach

- Approximations:
  - Taylor expansion: ln det M
  - Gaussian distribution: θ
  - Saddle point approximation
- Two states at the same μ_q/T
  - First order transition at $\mu_q/T > 2.5$
- Similar to S. Kratochvila, Ph. deForcrand, hep-lat/0509143 (Nf=4)



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

Summary and outlook

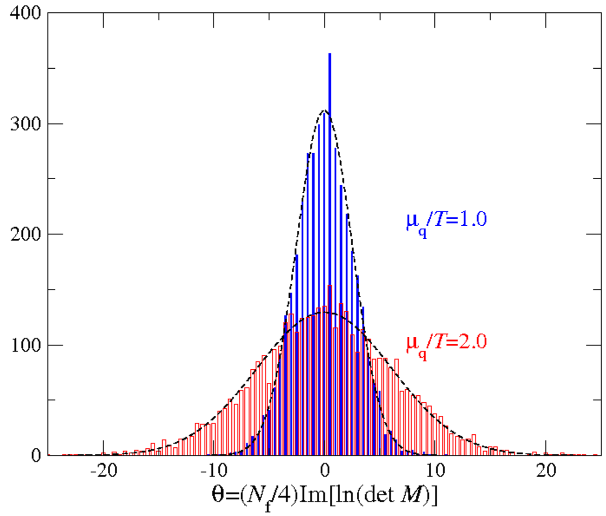
- An effective potential as a function of the plaquette is studied.

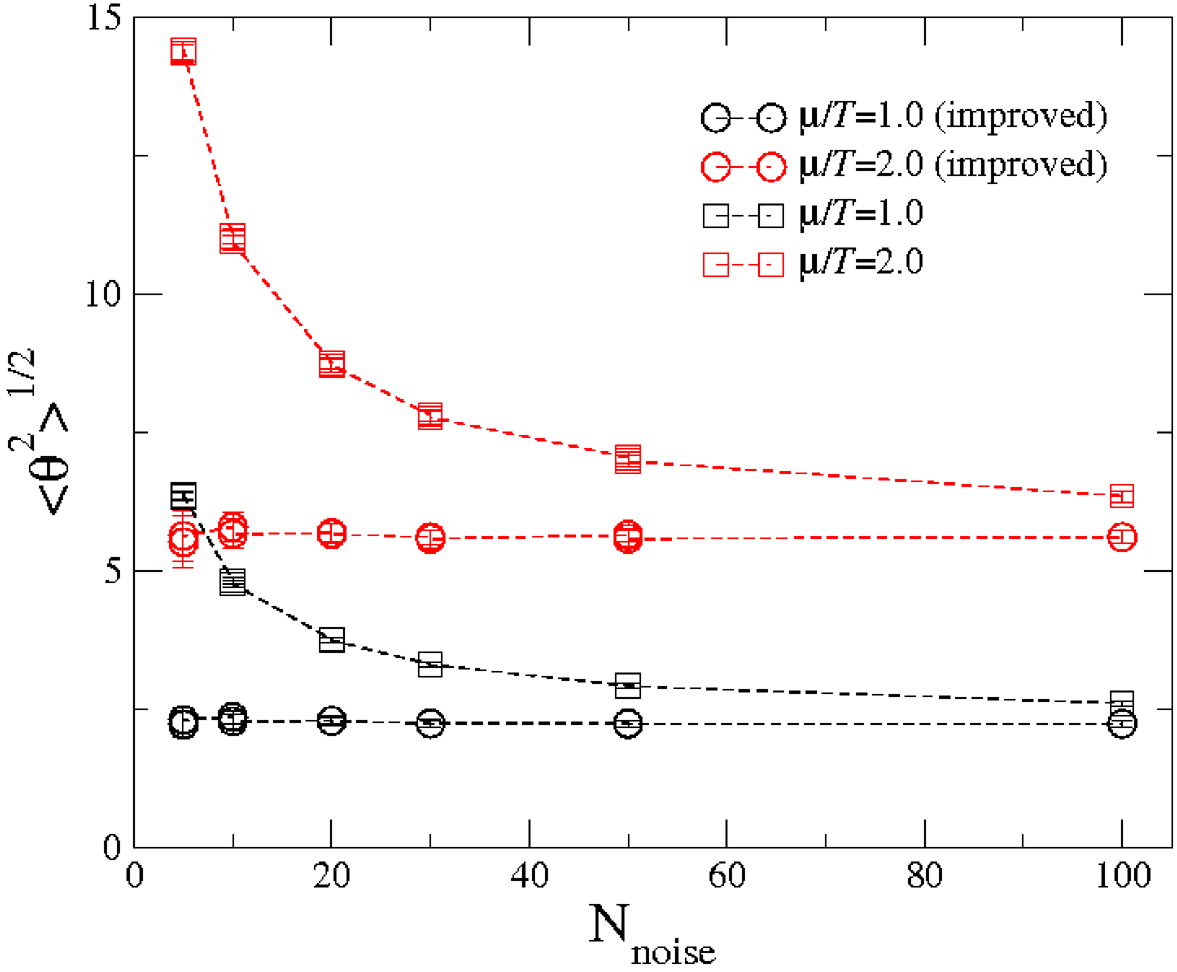
- Approximation:
  - Taylor expansion of ln det M: up to $O(\mu^6)$
  - Distribution function of $\theta = N_f$ Im[ln det M] : Gaussian type.

- Simulations: 2-flavor p4-improved staggered quarks with m/T=0.4, 16^3x4 lattice
  - First order phase transition for $\mu_q/T \geq 2.5$.
  - The critical μ is larger for QCD with finite μ_I (isospin) than with finite μ_q (baryon number).
  - The canonical partition function can be also measured.

- Studies neat physical quark mass: important.

Number of noise dependence





Relation to quark number susceptibility