A method to avoid the sign problem in finite density lattice QCD

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Existence of the critical point in finite density lattice QCD
Physical Review D77 (2008) 014508 [arXiv:0706.3549]

Canonical partition function and finite density phase transition in lattice QCD
Physical Review D 78 (2008) 074507[arXiv:0804.3227]

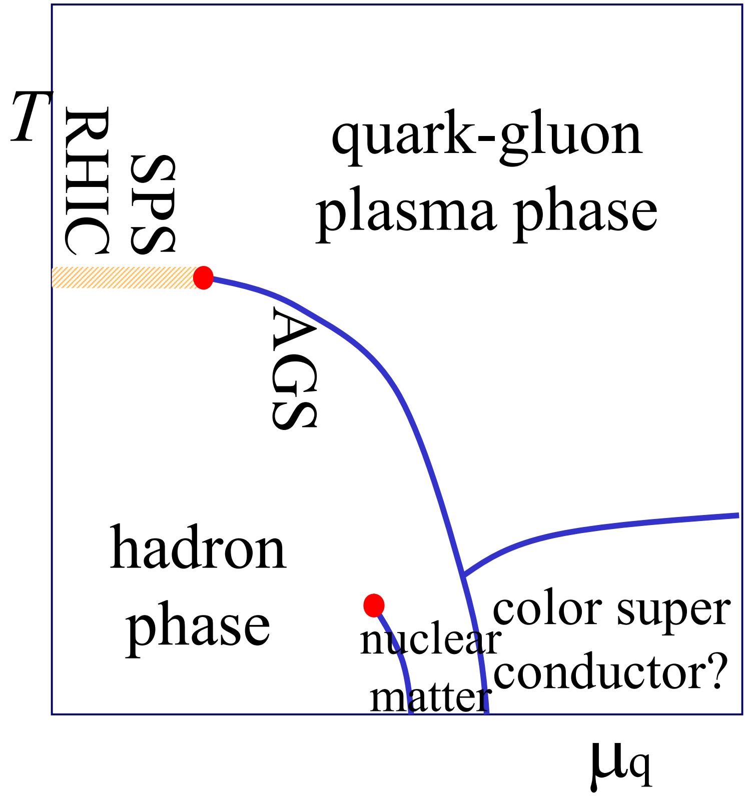
ECT* workshop ``Sign Problems and Complex Actions"
(Trento, March 2-6, 2009)

QCD thermodynamics at $\mu \neq 0$

- Interesting properties of QCD

  Measurable in heavy-ion collisions

  Critical point at finite density



- Methods for the high density region: required
- Most difficult problem: "sign problem"

In this talk

- Propose a method to avoid the sign problem.
- Discuss an effective potential as a function of the total quark number and the nature of phase transitions at finite density.

Problem of complex quark determinant at μ≠0

- Problem of Complex Determinant at μ≠0

$$\left(M(\mu)\right)^{\dagger} = \gamma_5 M(-\mu)\gamma_5 \qquad (\gamma 5\text{-conjugate})$$

$$\Rightarrow \quad \underline{\left(\det M(\mu)\right)^{*} = \det M(-\mu) \neq \det M(\mu)}$$

- Boltzmann weight: complex at μ≠0
  - Monte-Carlo method is not applicable.
  - Configurations cannot be generated.

Reweighting method for μ≠0 and Sign problem

(Ferrenberg-Swendsen → Glasgow group, Fodor-Katz)

- Reweighting method

  partition function:

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

  - Boltzmann weight: Complex for μ>0
    - Monte-Carlo method is not applicable directly.

  $$\det M \equiv \left|\det M\right| e^{i\theta}$$

  - Perform Simulation at μ=0.

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

- Sign problem
  - If $e^{i\theta}$ changes its sign frequently, $\langle O e^{i\theta} \cdots \rangle_{(\beta,0)}$ and $\langle e^{i\theta} \cdots \rangle_{(\beta,0)}$ become smaller than their statistical errors.
  - Then $\langle O \rangle_{(\beta,\mu)}$ cannot be computed.

Complex phase distribution and Gaussian approximation

Physical Review D77 (2008) 014508 [arXiv:0706.3549]

Sign problem and phase fluctuations

- Complex phase of det$M$ $\theta = N_f \, \mathrm{Im}[\ln \det M(\mu)]$
  - Taylor expansion: odd terms of ln det M (Bielefeld-Swansea, PRD66, 014507 (2002))

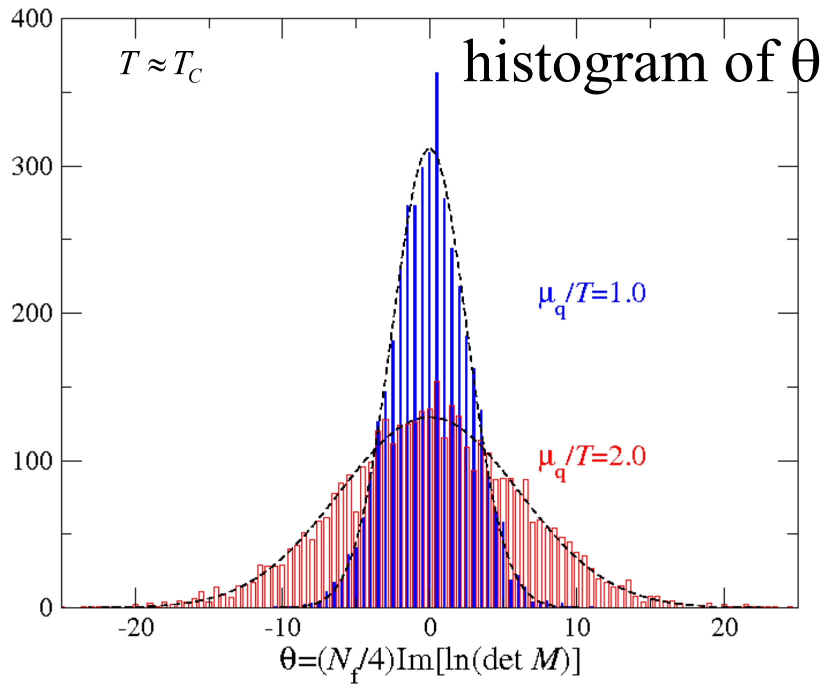
$$\theta = N_f \mathrm{Im}\left[\frac{\mu}{T} \frac{d \ln \det M}{d(\mu/T)} + \frac{1}{3!}\left(\frac{\mu}{T}\right)^3 \frac{d^3 \ln \det M}{d^3(\mu/T)} + \frac{1}{5!}\left(\frac{\mu}{T}\right)^5 \frac{d^5 \ln \det M}{d^5(\mu/T)} + \cdots \right]$$

➡ θ: NOT in the range of $[-\pi, \pi]$

- $|\theta| > \pi/2$: Sign problem happens.

➡ $e^{i\theta}$ changes its sign.

$$\left\langle \left(\frac{\det M(\mu)}{\det M(0)} \right)^{N_f} \right\rangle \equiv \left\langle e^{i\theta} e^{F} \right\rangle << \text{(statistical error)}$$



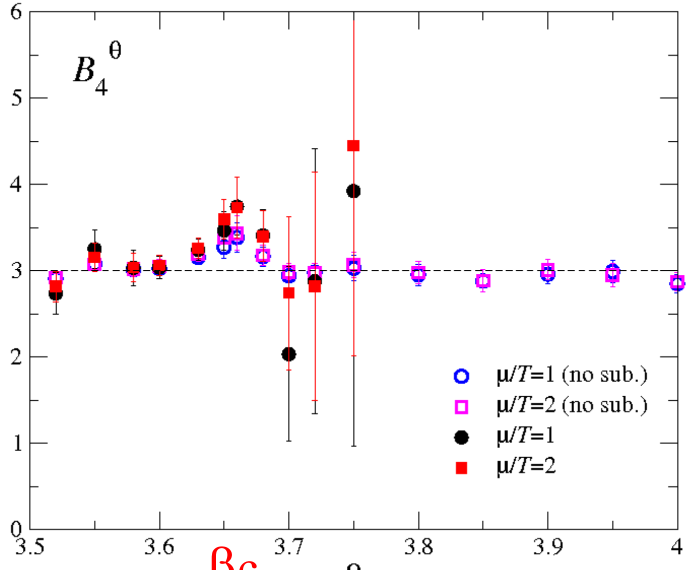
- Gaussian distribution
  - Results for p4-improved staggered
  - Taylor expansion up to $O(\mu^5)$
  - Dashed line: fit by a Gaussian function

Well approximated

Complex phase distribution (S.E., Phys.Rev.D77, 014508(2008))

Binder cumulant

$$B_4^\theta \equiv \frac{\langle \theta^4 \rangle}{\langle \theta^2 \rangle^2} = 3 \quad \text{for Gaussian}$$



Assume: Gaussian distribution

➡ Sign problem is avoided.

- Distribution function (histogram): $W(F,\theta)$
- Gaussian integral:

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

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

➡

$$\left\langle e^F e^{i\theta} \right\rangle \approx \left\langle e^F e^{-\langle \theta^2 \rangle_F / 2} \right\rangle$$

real and positive (No sign problem)

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

$$\left\langle e^F e^{i\theta} \right\rangle > \text{(statistical error)}$$

Why Gaussian distribution?

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

– e.g. 1st term: $\mathrm{Im}\left[\frac{d \ln\det M}{d(\mu/T)} \right] = \mathrm{Im}\left[Tr\left(M^{-1} \frac{\partial M}{\partial(\mu/T)} \right) \right]$

Diagonal element: local density operator

– If density correlation: not long & volume: large,

Central limit theorem ➡ θ: Gaussian distribution

- Valid for large volume (except on the critical point)
- Also see Splittorff and Verbaarschot, arXiv:0709.2218, chiral perturbation theory

For the case: $W(\theta) \approx \sqrt{\frac{\alpha}{\pi}} \left(1 - \frac{3\alpha_4}{4\alpha_2^2} + \cdots \right)^{-1} \exp\left(-\alpha_2 \theta^2 - \alpha_4 \theta^4 + \cdots \right),$

$\frac{\alpha_4}{\alpha_2} < O(1)$

$$\int d\theta\, e^{i\theta} W(\theta) \to \exp\left(-\frac{1}{2}\left\langle \theta^2 \right\rangle_{(P,|F|)} + \frac{1}{16\alpha_2^3} \frac{\alpha_4}{\alpha_2} + O\left[\left(\frac{\alpha_4}{\alpha_2} \right)^2 \right] \right)$$

$\sim O(\mu^6)$

because $1/\alpha_2 \sim 2\left\langle \theta^2 \right\rangle_{(P,|F|)} \sim O(\mu^2)$

- Valid for low density

Taylor expansion of $Z(T,\mu) \approx Z(T,0)\left\langle e^{F} e^{-\langle \theta^2 \rangle_F / 2} \right\rangle$

$$\frac{p}{T^4}(\mu) = \frac{p}{T^4}(0) + c_2\left(\frac{\mu_q}{T}\right)^2 + c_4\left(\frac{\mu_q}{T}\right)^4 + c_6\left(\frac{\mu_q}{T}\right)^6 + \cdots \quad \left(\frac{p(T,\mu)}{T^4} = \frac{N_t^3}{N_s^3}\ln Z(T,\mu)\right)$$

$$c_2 = \frac{N_t}{2!N_s^3}\frac{\partial^2 \ln Z}{\partial \mu^2} = \frac{N_t}{2!N_s^3}\mathrm{A}_2, \quad c_4 = \frac{1}{4!N_s^3 N_t}\frac{\partial^4 \ln Z}{\partial \mu^4} = \frac{1}{4!N_s^3 N_t}\left(\mathrm{A}_4 - 3\mathrm{A}_2^2\right),$$

$$D_n = N_f \frac{\partial^n \ln \det M}{\partial \mu^n}$$

$$\mathrm{A}_2 = \langle D_2 \rangle + \langle D_1^2 \rangle$$

$$\mathrm{A}_4 = \langle D_4 \rangle + 4\langle D_3 D_1 \rangle + 3\langle D_2^2 \rangle + 6\langle D_2 D_1^2 \rangle + \langle D_1^4 \rangle$$

$$\rightarrow 3\langle D_1^2 \rangle^2$$

- Distribution function of quark number at μ=0
  - D_1~ total quark number $\sim \sum_x \bar{\psi}\gamma_0\psi(x)$
  - Gaussian distribution except at a critical point

$$B_4^{D_1} = \frac{\langle D_1^4 \rangle_F}{\langle D_1^2 \rangle_F^2} \approx 3 \quad \longrightarrow \quad \langle D_1^4 \rangle_F \approx 3\langle D_1^2 \rangle_F^2$$

Canonical approach

Physical Review D 78 (2008) 074507[arXiv:0804.3227]

- An application of the Gaussian approximation
- Configurations; the complex phase fluctuation is large

  $\rightarrow$ do not contribute to the final results.

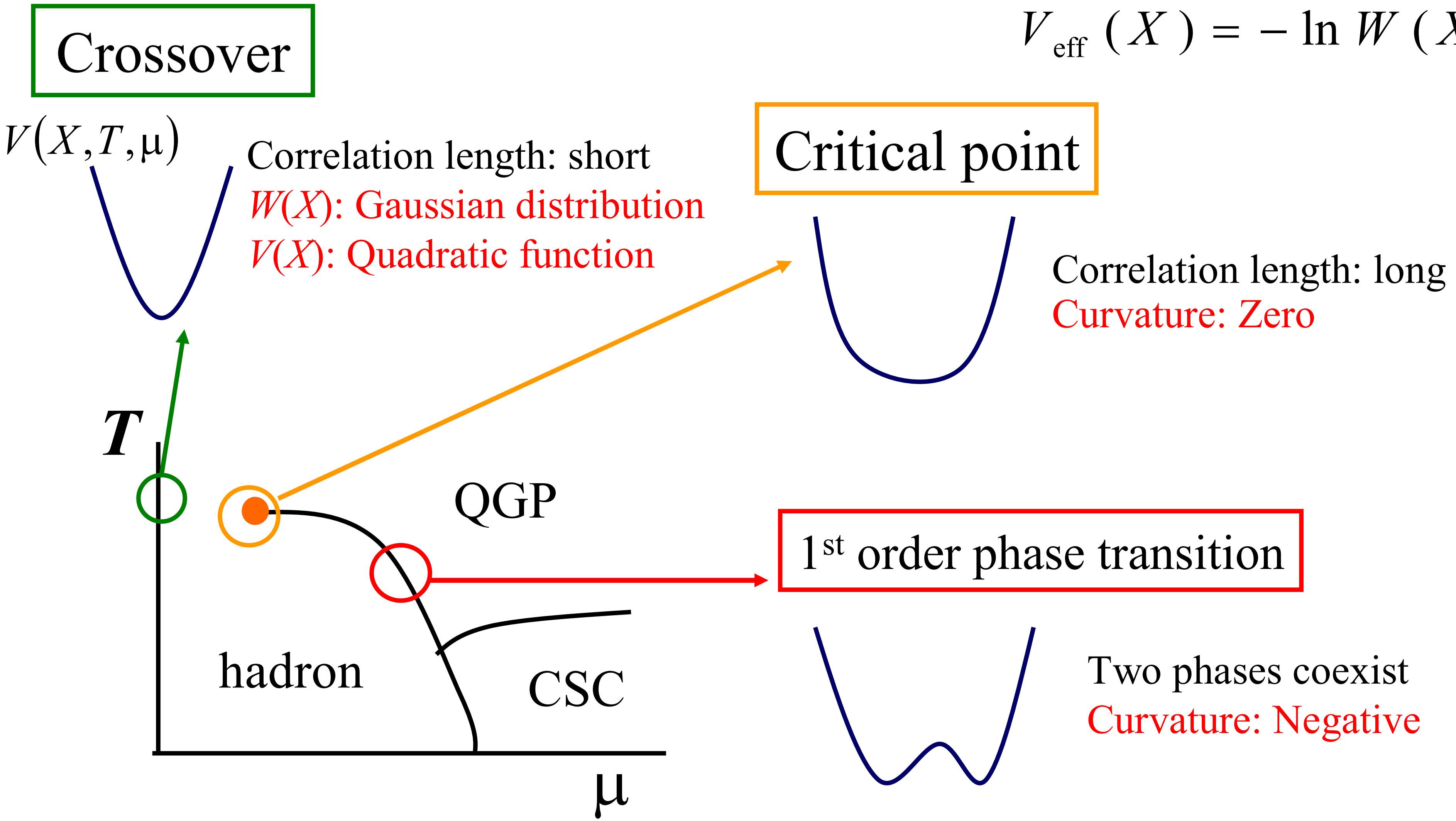
- Simulations:
  - Bielefeld-Swansea Collab., PRD71,054508(2005).
  - 2-flavor p4-improved staggered quarks with $m_\pi \approx 770$MeV
  - 16^3x4 lattice
  - ln det M: Taylor expansion up to $O(\mu^6)$

μ-dependence of the effective potential

$$Z(T,\mu) = \int dX\, W(X,T,\mu), \qquad W(X',T,\mu) = \int DU\, (\det M(0))^{N_f}\, e^{-S_g}\, \delta(X - X')$$

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

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



Canonical approach

- Canonical partition function

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

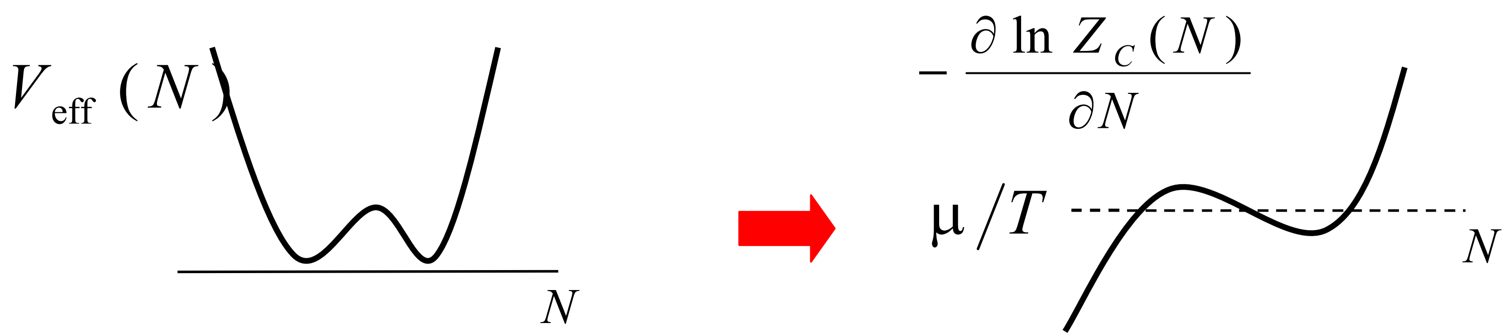
- Effective potential as a function of the quark number *N*.

$$V_{\text{eff}}(N) = -\ln W(N) = -\ln Z_C(T,N) - N\mu/T$$

- At the minimum,

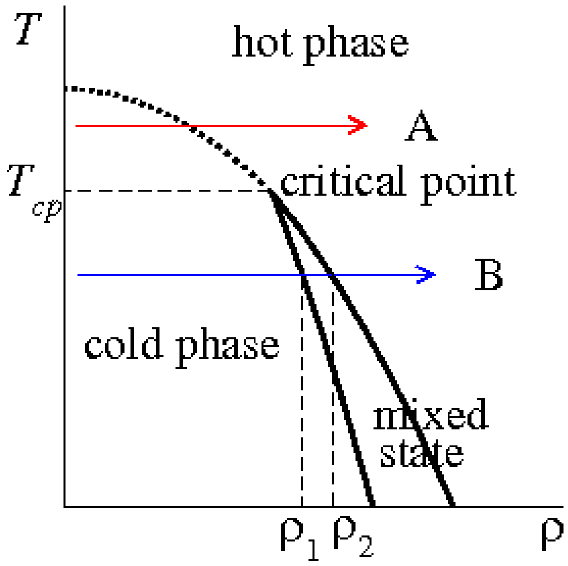
$$\frac{\partial V_{\text{eff}}(N)}{\partial N} = -\frac{\partial \ln W(N)}{\partial N} = -\frac{\partial \ln Z_C(T,N)}{\partial N} - \frac{\mu}{T} = 0$$

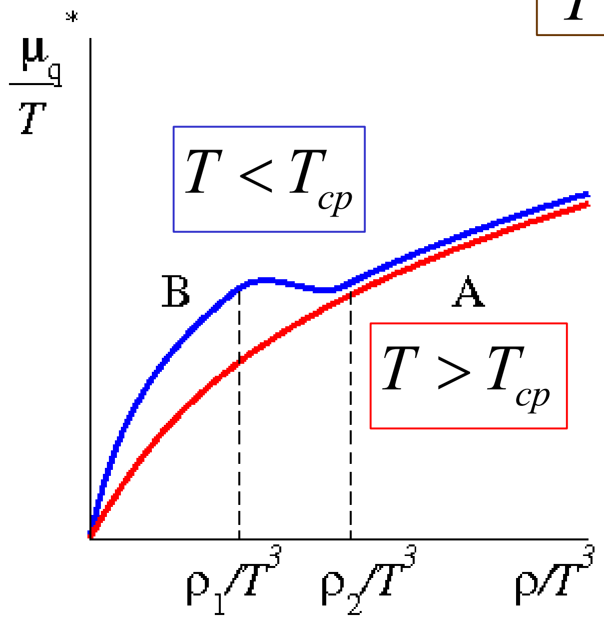
- First order phase transition: Two phases coexist.



First order phase transition line

In the thermodynamic limit, $\dfrac{\partial V_{\text{eff}}(N)}{\partial N} = 0,$ $\Rightarrow$ $\dfrac{\mu^*}{T} = -\dfrac{\partial \ln Z_C(T,N)}{\partial N}$





$$\frac{\mu^*}{T} \to \frac{\mu}{T} \quad \left(N_s^3 \to \infty\right)$$

- Mixed state ➡ First order transition
- Inverse Laplace transformation by Glasgow method

  Kratochvila, de Forcrand, PoS (LAT2005) 167 (2005)

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

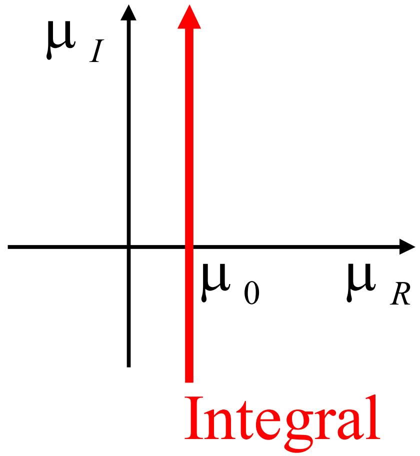
  – N_f=4: First order for all ρ.
- Simulations with canonical ensemble (Kentucky group)

Canonical partition function

- Fugacity expansion (Laplace transformation)

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

canonical partition function



- Inverse Laplace transformation

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

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

Arbitrary μ_0

  - Note: periodicity $Z_{GC}(T,\mu+2\pi i T/3)=Z_{GC}(T,\mu)$

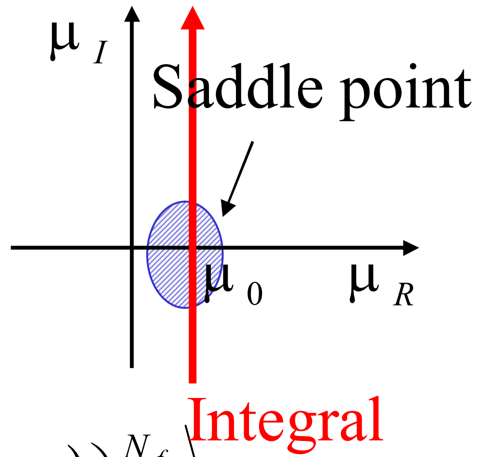
Integral path, e.g.
1, imaginary μ axis
2, Saddle point

- Derivative of ln$Z$

$$\frac{\mu^*}{T} \equiv -\frac{\partial \ln Z_C(T,N)}{\partial N}$$

Saddle point approximation

(S.E., arXiv:0804.3227)



- Inverse Laplace transformation

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

$$= \frac{3Z_{GC}(0)}{2\pi}\left\langle \int_{-\pi/3}^{\pi/3} d(\mu_I/T)\, e^{-N(\mu_0/T + i\mu_I/T)} \left(\frac{\det M(\mu_0 + i\mu_I)}{\det M(0)} \right)^{N_f} \right\rangle$$

- Saddle point approximation (valid for large *V, 1/V* expansion)
  - Taylor expansion at the saddle point.

$$\mu_0/T = z_0 \qquad \rho = N/V$$

Saddle point: z_0

$$\left[\frac{N_f}{V} \frac{\partial(\ln \det M)}{\partial(\mu/T)} - \rho \right]_{\frac{\mu}{T} = z_0} = 0 \qquad V \equiv N_s^3$$

- At low density: The saddle point and the Taylor expansion coefficients can be estimated from data of Taylor expansion around μ=0.

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

Saddle point approximation

- Canonical partition function in a saddle point approximation

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

$$\equiv \frac{3}{\sqrt{2\pi}} \left\langle \exp\left(F + i\theta\right) \right\rangle_{(T,\mu=0)}$$

Saddle point: z_0 $\qquad R''\left(\frac{\mu}{T}\right) = \frac{N_f}{V} \frac{\partial^2 (\ln \det M)}{\partial(\mu/T)^2} \equiv \left|R''\right| e^{i\alpha}$

- Chemical potential

$$\frac{\mu^*(\rho)}{T} \equiv \frac{-1}{V} \frac{\partial \ln Z_C(T,\rho)}{\partial \rho} \approx \frac{\left\langle z_0 \exp\left(F + i\theta\right) \right\rangle_{(T,\mu=0)}}{\left\langle \exp\left(F + i\theta\right) \right\rangle_{(T,\mu=0)}}$$

saddle point $\qquad$ reweighting factor

⇨ Similar to the reweighting method

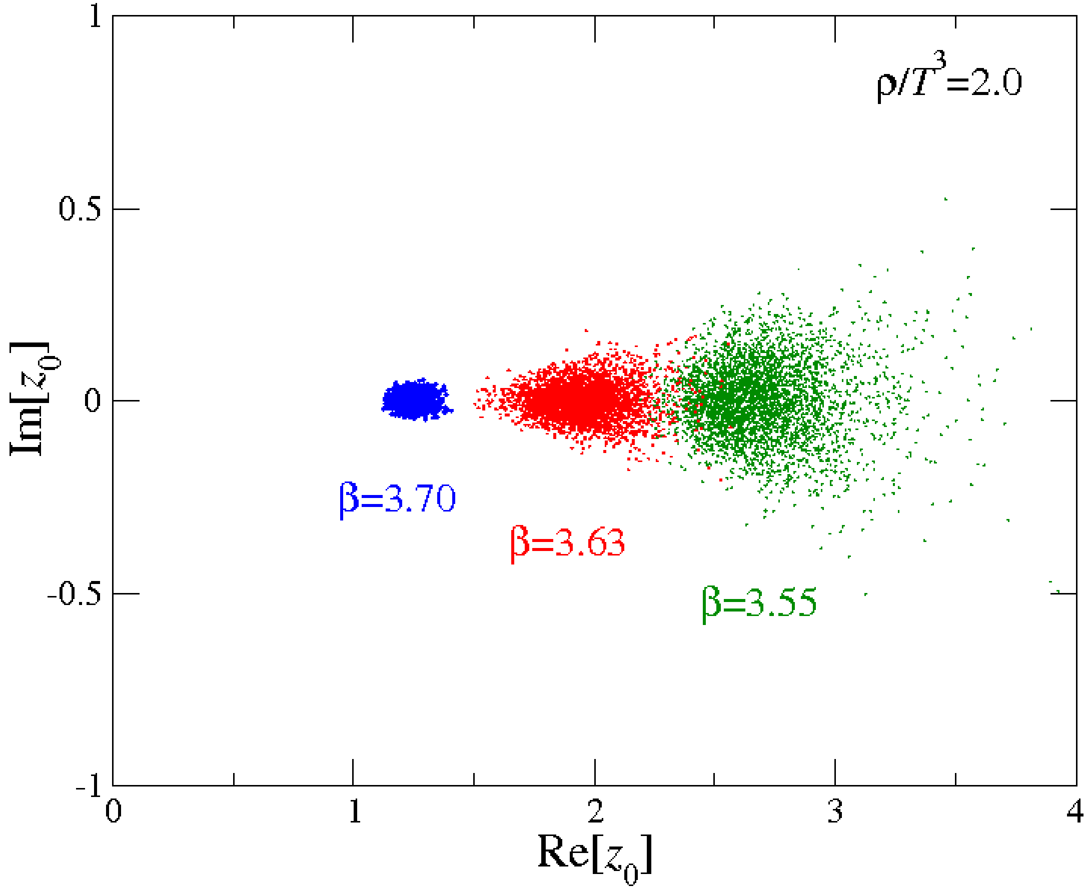
(sign problem & overlap problem)

Saddle point in complex μ/*T* plane

- Find a saddle point z_0 numerically for each conf.

$$\left[\frac{N_f}{V}\frac{\partial(\ln\det M)}{\partial(\mu/T)}-\rho\right]_{\frac{\mu}{T}=z_0}=0$$

- Two problems
  - Sign problem
  - Overlap problem



Technical problem 1: Sign problem

- Complex phase of det$M$ $\quad$ $(\text{phase}) = N_\text{f}\, \text{Im}\left[\ln \det M(\mu)\right]$
  - Taylor expansion (Bielefeld-Swansea, PRD66, 014507 (2002))

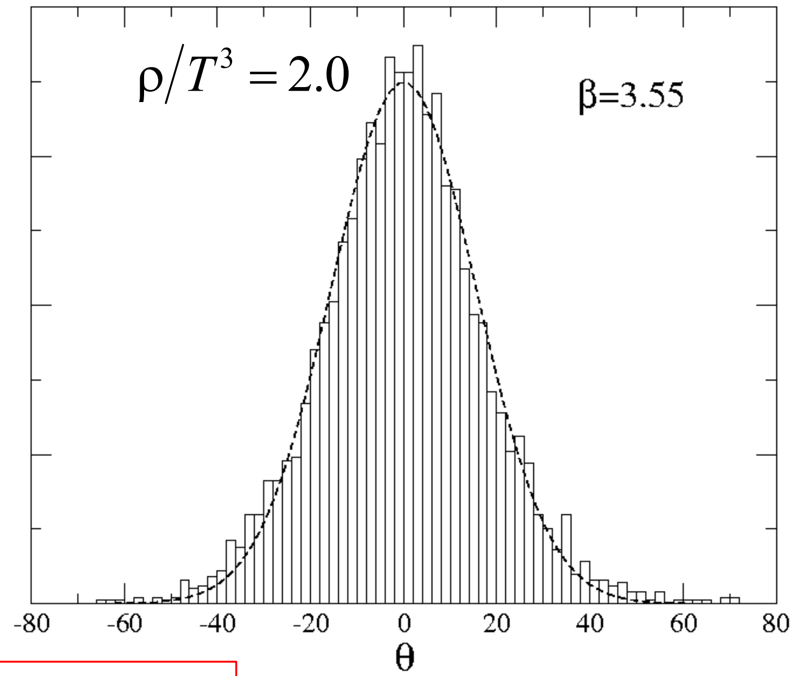
$$\theta = \text{Im}\left[V\left(N_\text{f} N_\text{t} \sum_{n=1}^{\infty} D_n z_0 - \rho z_0\right)\right] - \frac{\alpha}{2}$$

➡ θ: NOT in the range [-π, π]

- |θ| > π/2: Sign problem happens.

➡ $e^{i\theta}$ changes its sign.

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



histogram of θ

Well approximated

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

➡

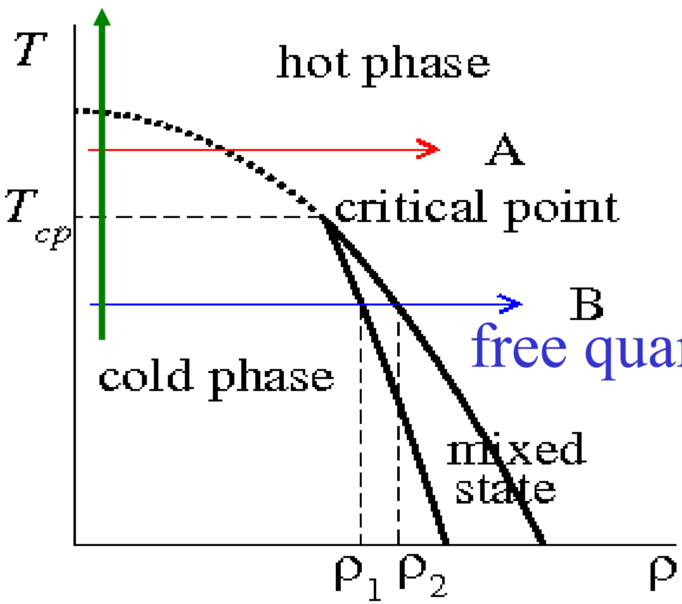
$$\left\langle e^{i\theta} e^F \right\rangle \approx \left\langle e^{-\langle\theta^2\rangle_F/2} e^F \right\rangle$$

Technical problem 2: Overlap problem
Role of the weight factor exp($F+i\theta$)

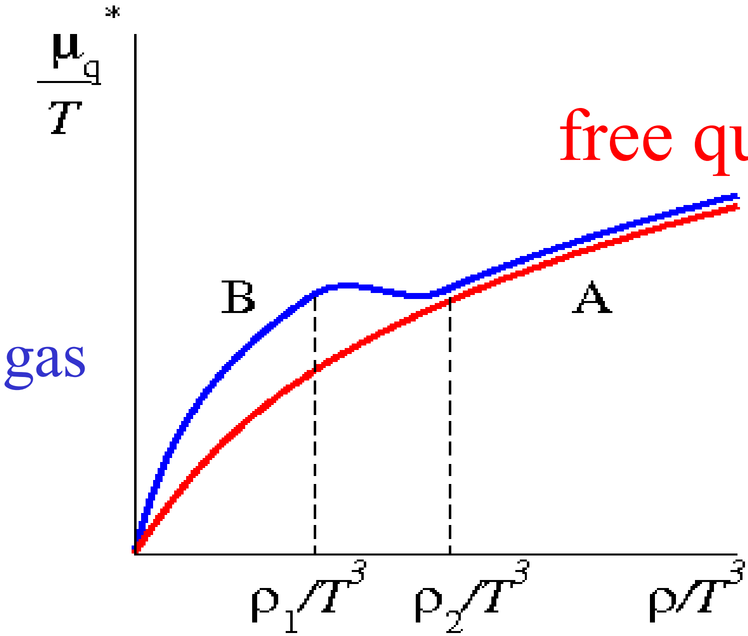
- The weight factor has the same effect as when β (T) increased.
- μ^*/T approaches the free quark gas value in the high density limit for all temperature.

$$\frac{\rho}{T^3} = N_f\left[\frac{\mu}{T} + \frac{1}{\pi^2}\left(\frac{\mu}{T}\right)^3\right]$$

free quark gas



free quark gas



free quark gas

Technical problem 2: Overlap problem

- Density of state method

$$\frac{\mu^*(\rho)}{T} = \frac{\int \langle z_0 \exp(F + i\theta)\rangle_P W(P)dP}{\int \langle \exp(F + i\theta)\rangle_P W(P)dP}$$

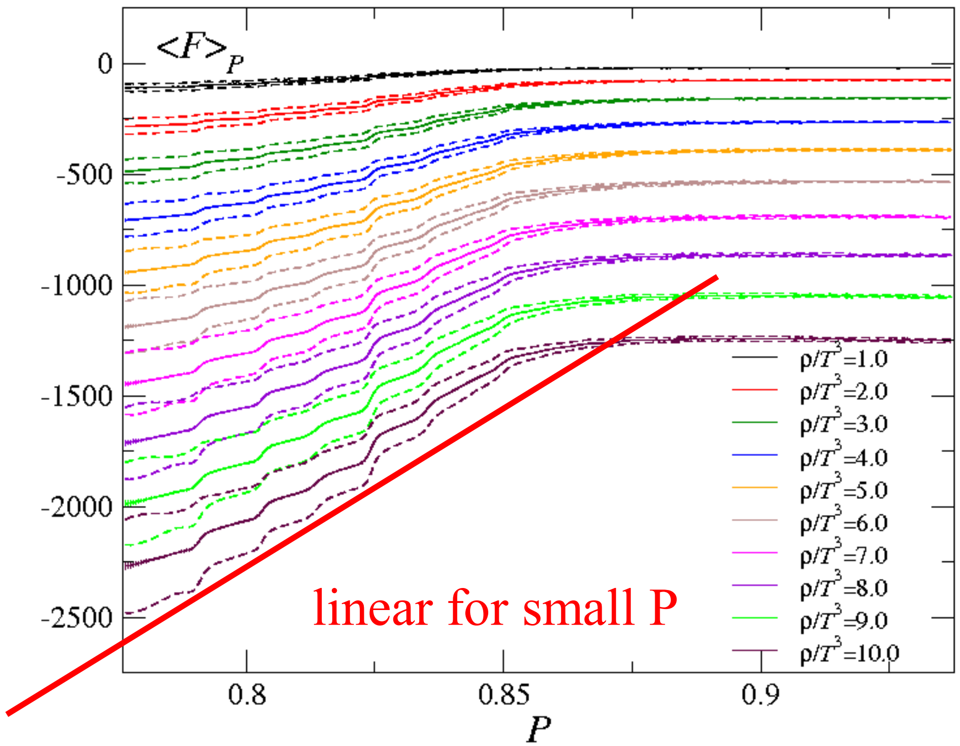
$W(P)$: plaquette distribution

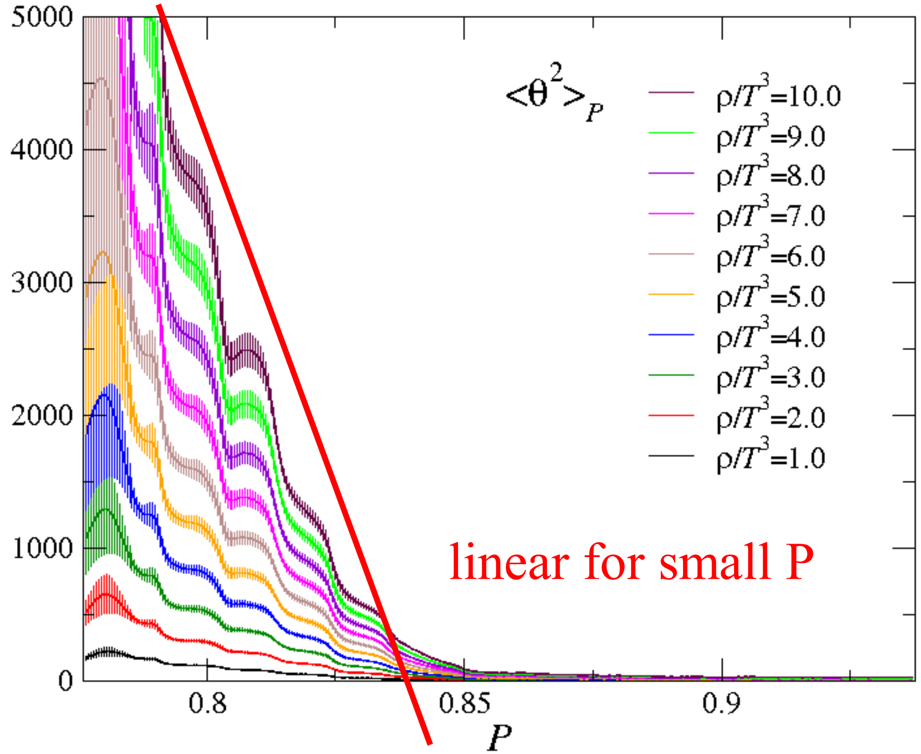
$$\langle \exp(F + i\theta)\rangle_P W(P) \approx \exp\left(\langle F\rangle_P - \langle \theta^2 \rangle_P /2 + \cdots\right) W(P)$$

Same effect when β changes.

$$\propto \exp(\Delta\beta_{\rm eff} P) W(P)$$

for small P





Reweighting for $\beta(T)$ and curvature of $-\ln W(P)$

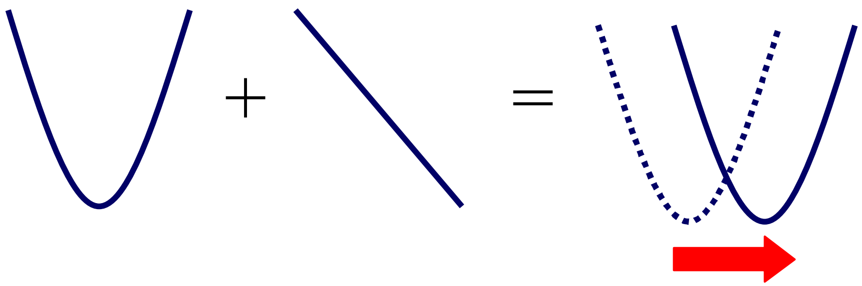
$$Z(\beta) = \int dP\, \underline{W(P,\beta)} \qquad W(P',\beta) = \int DU \left(\det M(0)\right)^{N_f} e^{-S_g} \delta(P - P')$$

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

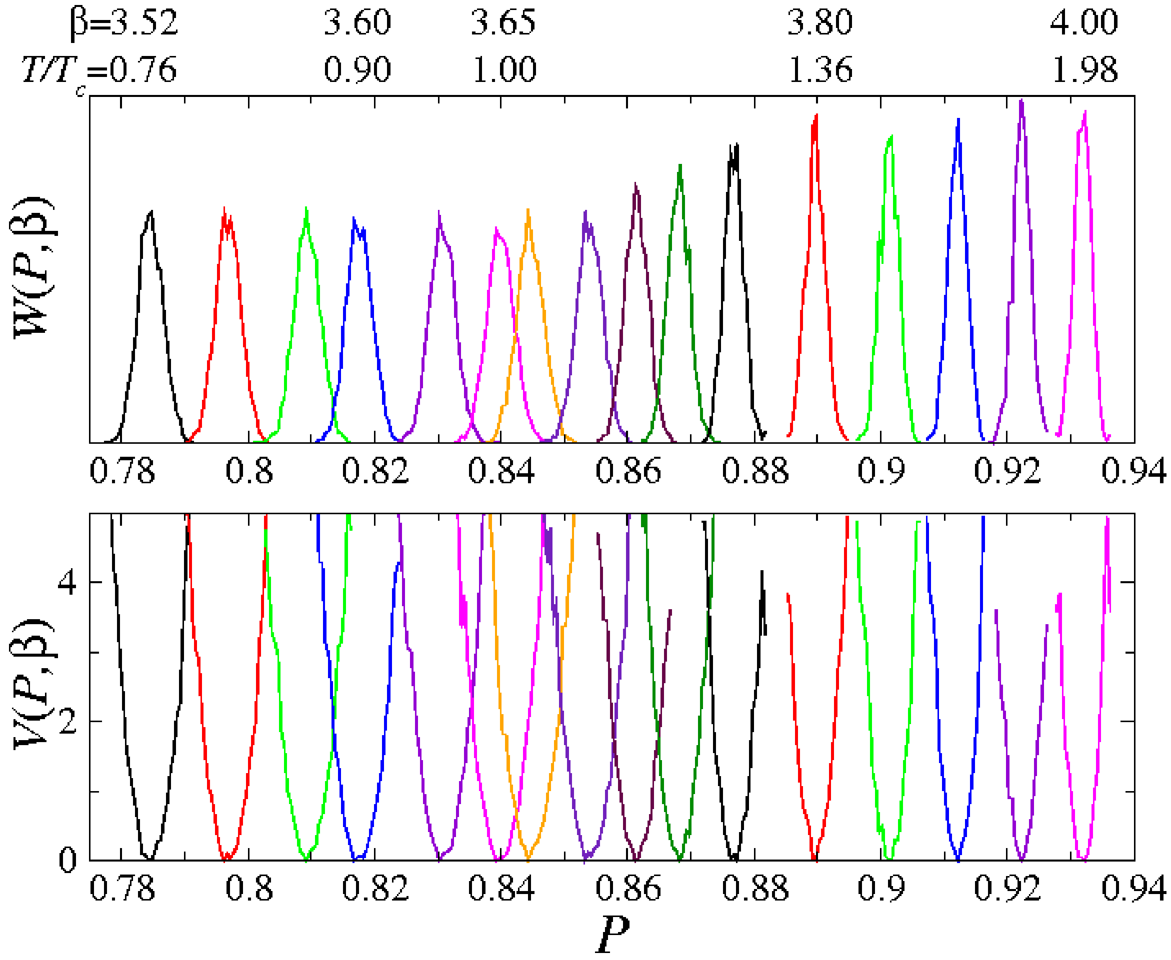


Peak position of $W(P)$ moves as b increases.

(ρ increases) ≈ (β (*T*) increases)

Plaquette histogram for each β

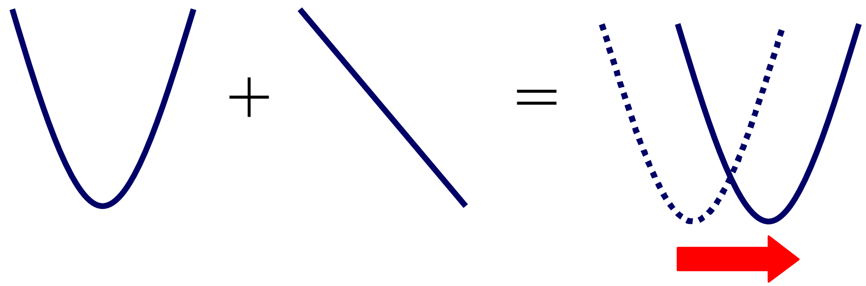
(Data: N_f=2 p4-staggared, $m_\pi/m_\rho\approx0.7$, μ=0)



$$W(P',\beta)=\int DU\,(\det M)^{N_f}\,e^{-S_g(\beta)}\delta(P-P')$$

Potential:

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



$$-\ln W(0)-\left(\langle F\rangle_P-\langle\theta^2\rangle_P/2\right)\approx-\ln W(\mu)$$

(ρ increases) ≈ (β (T) increases)

Effective β (temperature) for ρ≠0

$$\beta_{\rm eff}\equiv\beta+\left(\frac{d\langle F\rangle_P}{dP}-\frac{1}{2}\frac{d\langle\theta^2\rangle_P}{dP}\right)\frac{1}{N_{\rm site}}$$

Overlap problem, Multi-β reweighting

Ferrenberg-Swendsen, PRL63,1195(1989)

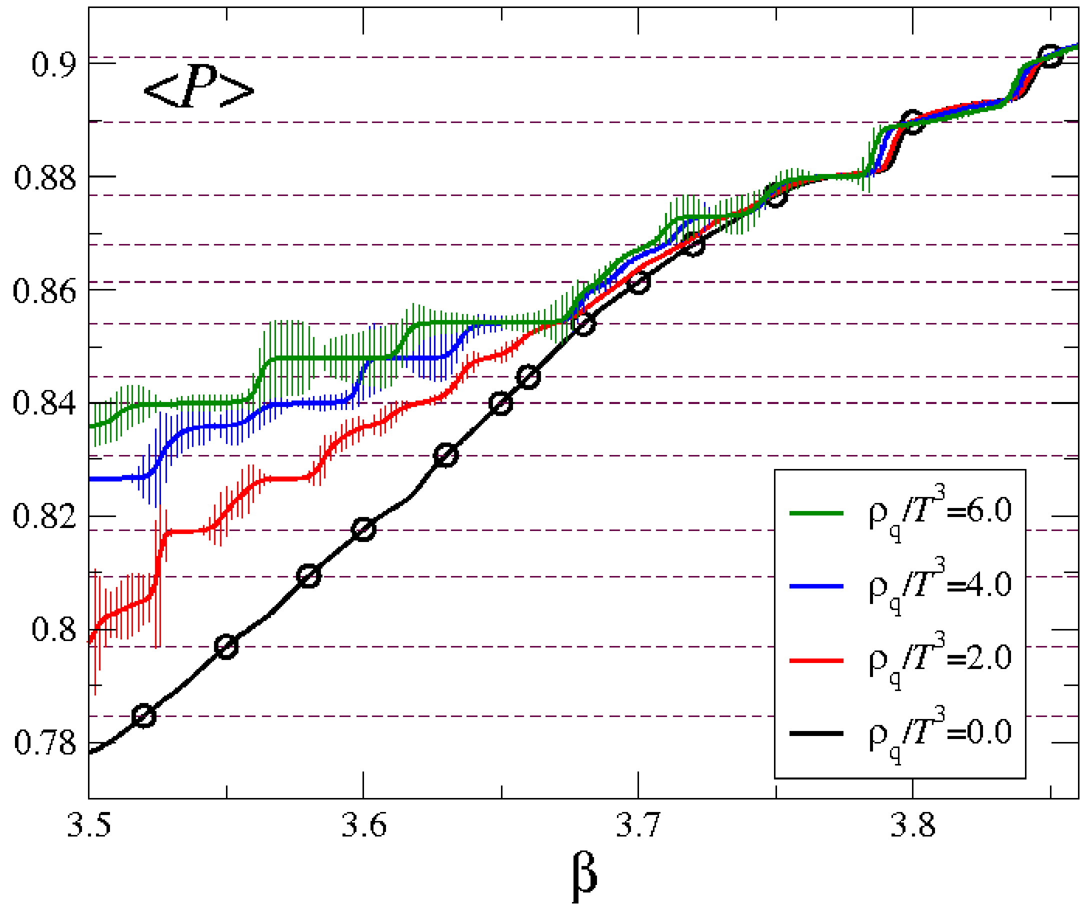
- When the density increases, the position of the importance sampling changes.
- Combine all data by multi-β reweighting

$$\langle P \rangle \approx \frac{\langle P \exp(F + i\theta) \rangle_{(T,\mu=0)}}{\langle \exp(F + i\theta) \rangle_{(T,\mu=0)}}$$

Plaquette value by multi-beta reweighting

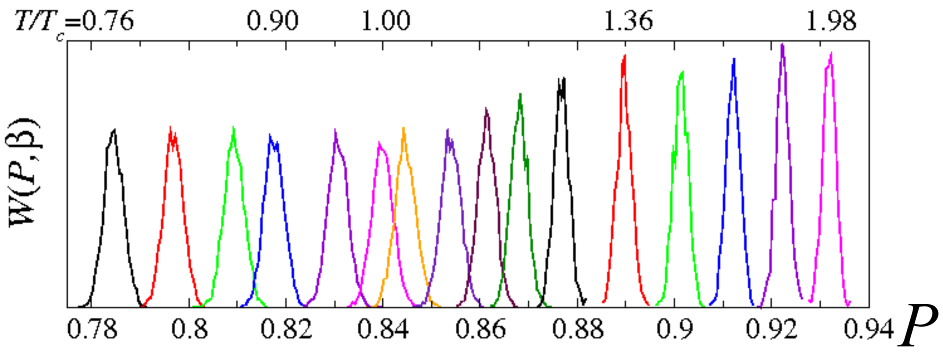
- - - peak position of the distribution

O <*P*> at each β



Problem:

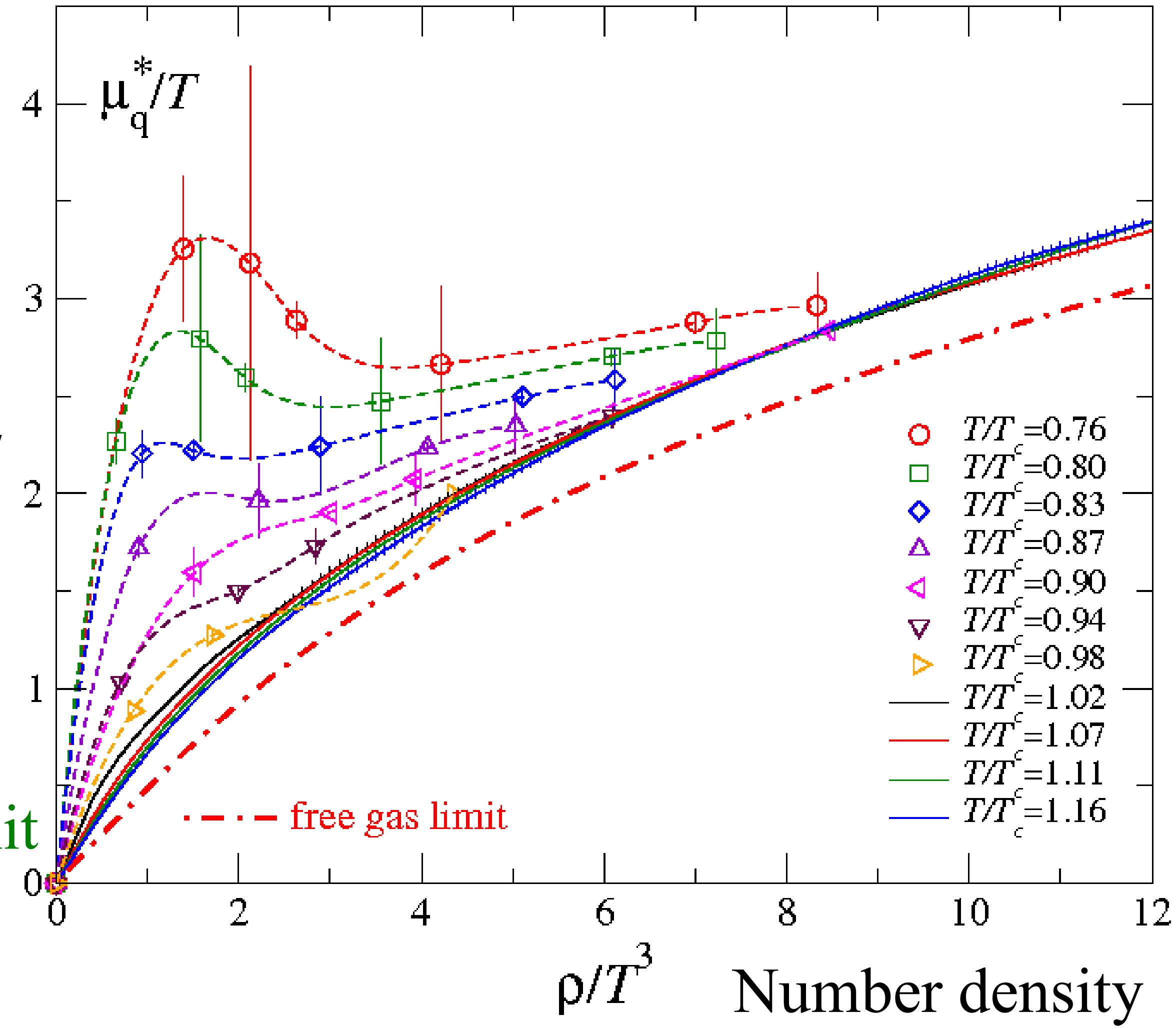
- Configurations do not cover all region of *P*.
- Calculate only when <*P*> is near the peaks of the distributions.



Chemical potential vs density

- Approximations:
  - Taylor expansion: ln det M
  - Gaussian distribution: θ
  - Saddle point approximation
- Two states at the same μ_q/T
  - First order transition at $T/T_c < 0.83$, $\mu_q/T > 2.3$
- μ^*/T approaches the free quark gas value in the high density limit for all T.

N_f=2 p4-staggered, $16^3 \times 4$ lattice



Number density

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

Summary

- Complex phase distribution:
  well approximated by a Gaussian function.
- Once we assume the Gaussian distribution,
  the sign problem is avoided.
- Applying the Gaussian method, we evaluate the canonical partition function for 2-flavor p4-improved staggered quarks with $m_\pi/m_\rho \approx 0.7$ on 16^3x4 lattice.
  - High ρ limit: μ/T approaches the free gas value for all T.
  - Configurations having large phase fluctuations do not affect to the calculation.
  - Existence of the critical point: suggested.
  - First order phase transition for $T/T_c < 0.83$, $\mu_q/T > 2.3$.
- Studies near physical quark mass: important.
  - Location of the critical point: sensitive to quark mass