Study of QCD critical point at high temperature and density by lattice simulations

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Canonical partition function and finite density phase transition in lattice QCD

arXiv:0804.3227

xQCD, July 21-23, 2008

QCD thermodynamics at $\mu \neq 0$

- Heavy-ion collision experiment

Important roles of lattice QCD study

- Interesting properties of QCD

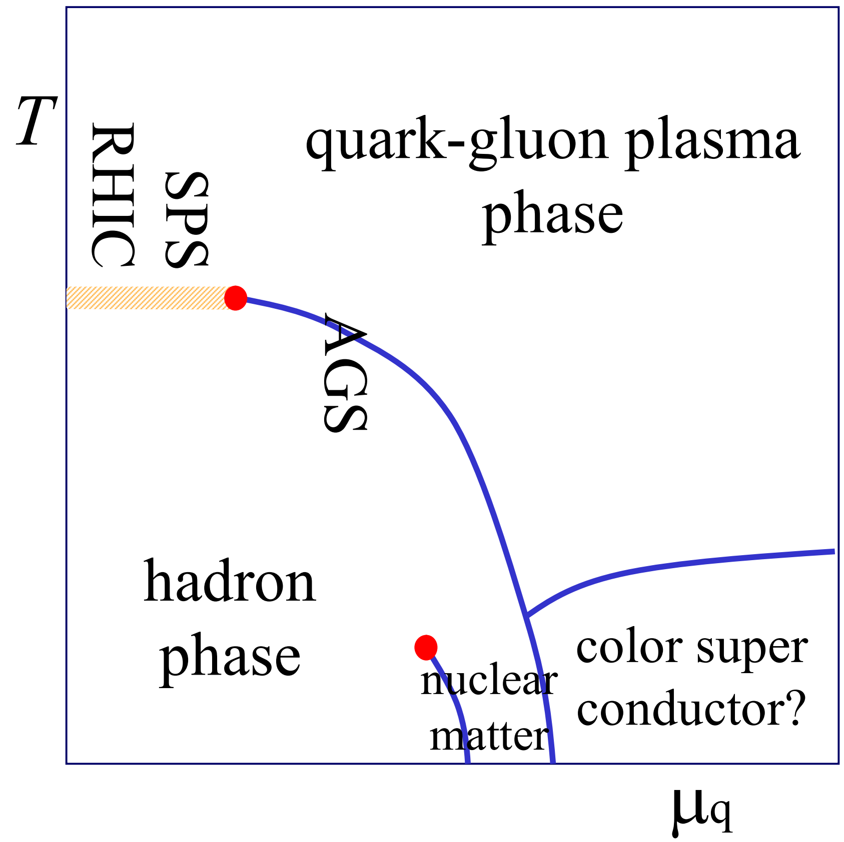
  Measurable in heavy-ion collisions

  Critical point at finite density

  – Location of the critical point ?

  – Properties of the critical point ?

    - Large fluctuation in quark number ?
    - Large bulk viscosity ?



Nature of phase transitions

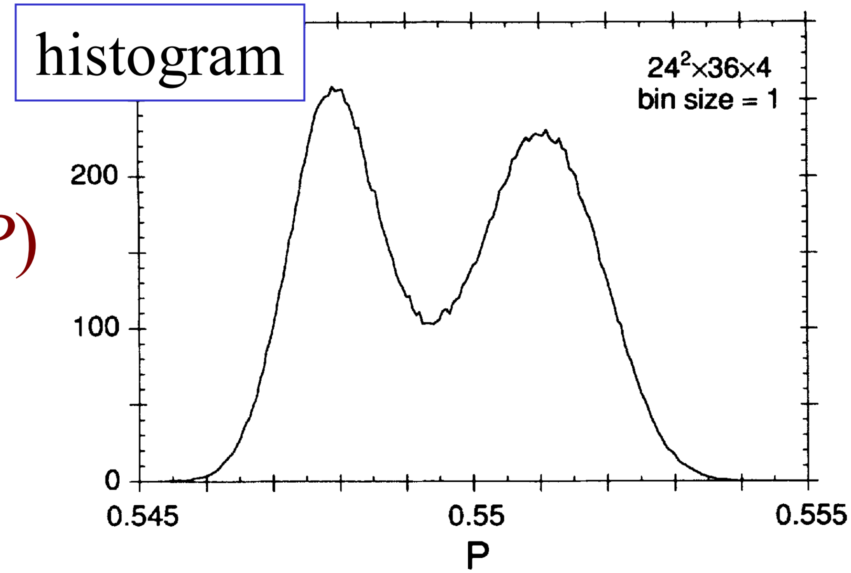
Crossover or First order

- First order phase transition

  Two phases coexists at T_c

  e.g. SU(3) Pure gauge theory

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



- Distribution function of plaquette $W(P)$

  (Plaquette histogram)

  – Gauge action $$S_g = -6 N_{site} \beta P$$

- Partition function

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

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

Existence of the critical point at $\mu \neq 0$: Suggested. S.E., Phys.Rev.D77, 014508(2008)

Canonical approach

- Canonical partition function

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

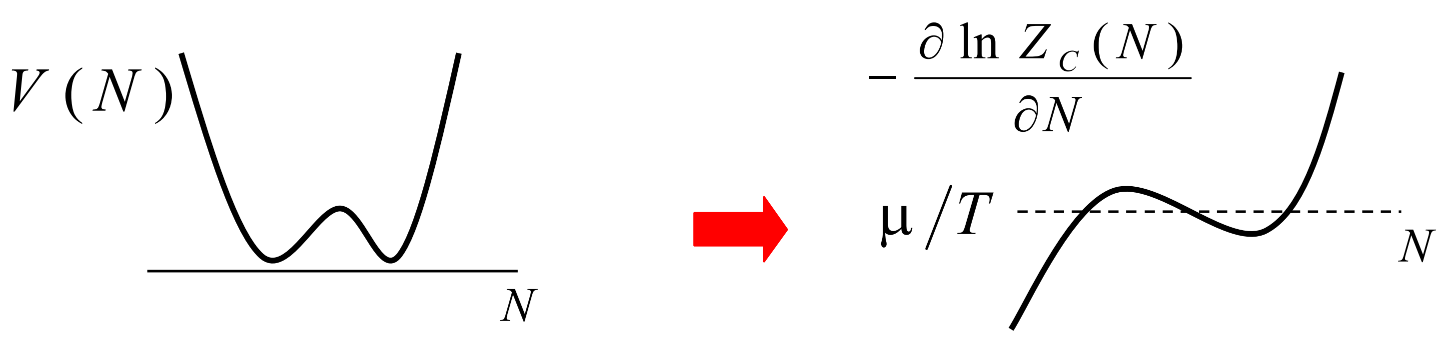
- Effective potential as a function of the quark number *N*.

$$V(N)=-\ln W(N)=-\ln Z_C(T,N)-N\mu/T$$

- At the minimum,

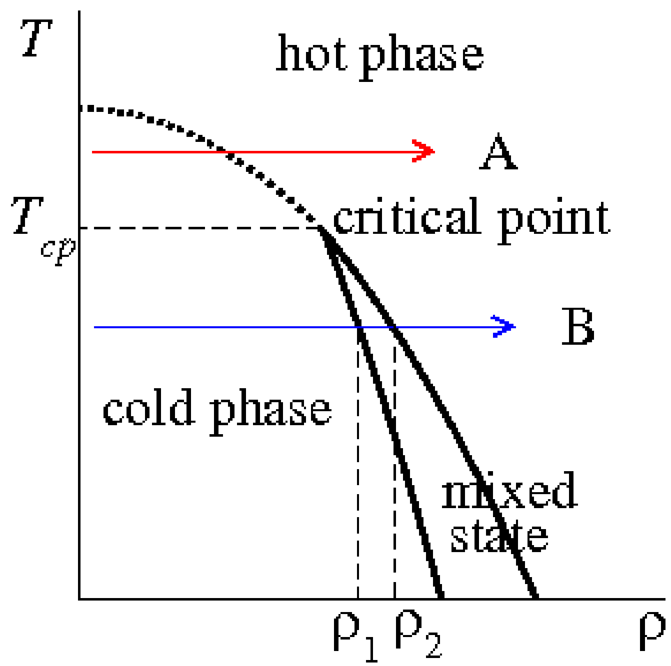
$$\frac{\partial V(N)}{\partial N}=-\frac{\partial \ln W(N)}{\partial N}=-\frac{\partial \ln Z_C(T,N)}{\partial N}-\frac{\mu}{T}=0$$

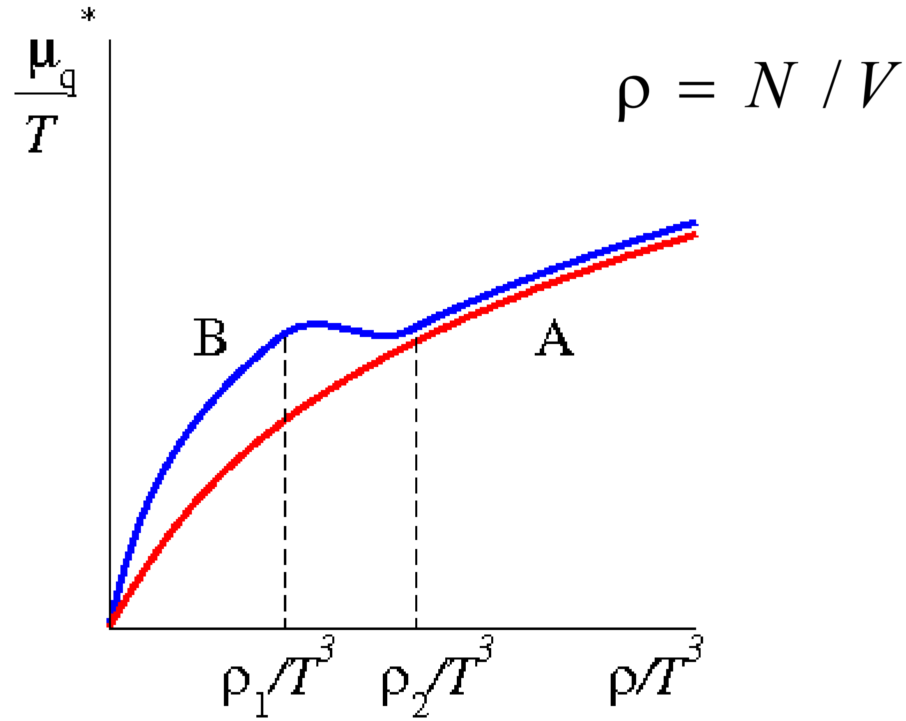
- First order phase transition: Two phases coexist.



First order phase transition line

In the thermodynamic limit, $\frac{\partial V(N)}{\partial N} = 0, \Rightarrow \boxed{\frac{\mu^*}{T} \equiv -\frac{\partial \ln Z_C(T,N)}{\partial N}}$





- Mixed state ➡ First order transition

Canonical partition function

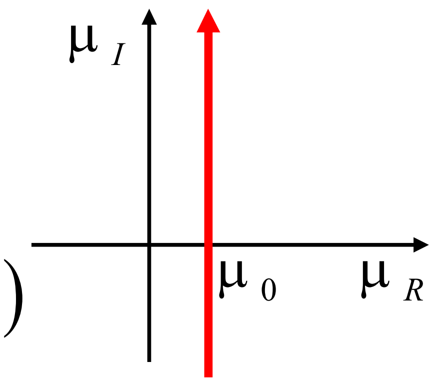
- Fugacity expansion (Laplace transformation)

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

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$Z$

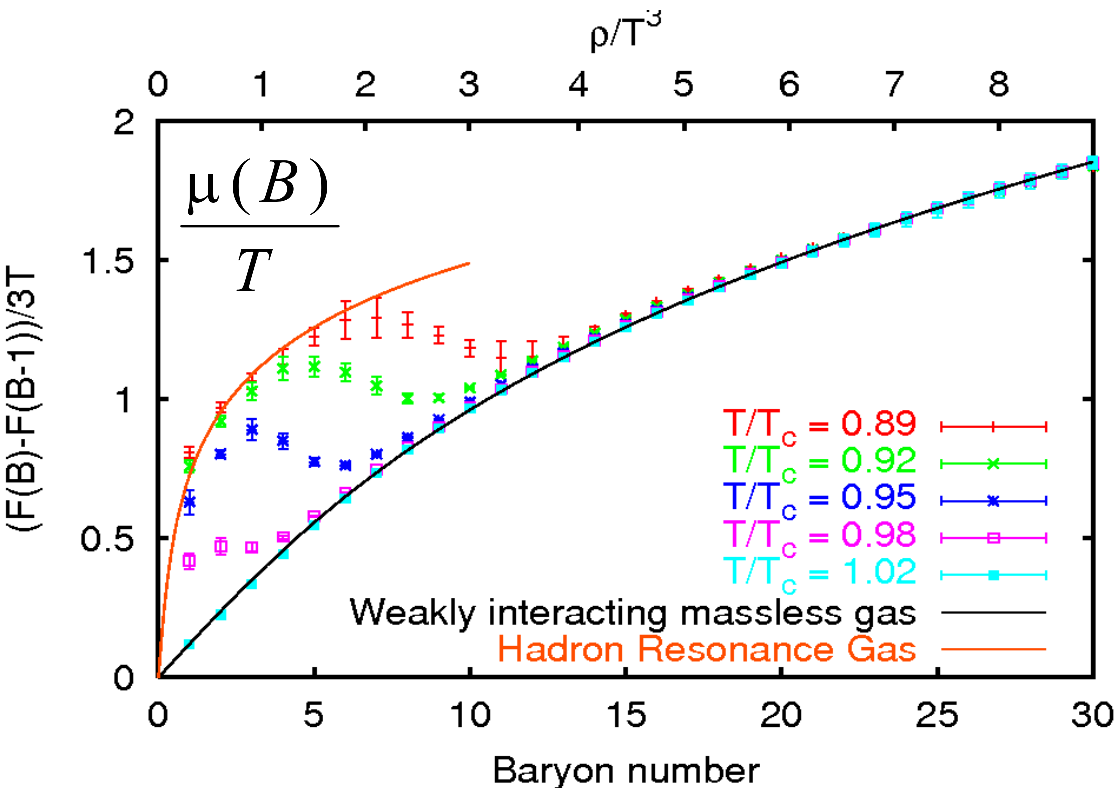
$$\boxed{\frac{\mu^*}{T} \equiv -\frac{\partial \ln Z_C(T,N)}{\partial N}}$$

Canonical partition function

Integral along the imaginary μ axis ($\mu_0=0$)

Glasgow method (calculating eigenvalues of a matrix modified from the quark matrix)

(A. Hasenfratz, D. Toussaint, Nucl. Phys. B371 (1992) 539)



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

S. Kratochvila, Ph. de Forcrand PoS (LAT2005) 167 (2005).

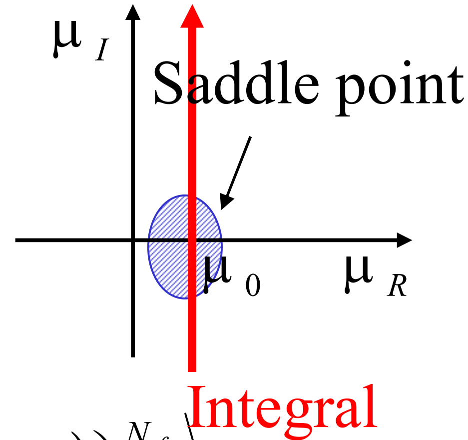
N_f=4 staggered fermions, $6^3 \times 4$ lattice

First order phase transition: Two states coexist

N_f=4: First order for all ρ.

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

- 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

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

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

Saddle point: z_0

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

- Chemical potential

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

saddle point reweighting factor

⇨ Similar to the reweighting method

(sign problem & overlap problem)

Calculation of the canonical partition function

- Simulations:
  - Bielefeld-Swansea Collab., PRD71,054508(2005).
  - 2-flavor p4-improved staggered quarks with $m_\pi \approx 770$MeV
  - 16^3x4 lattice

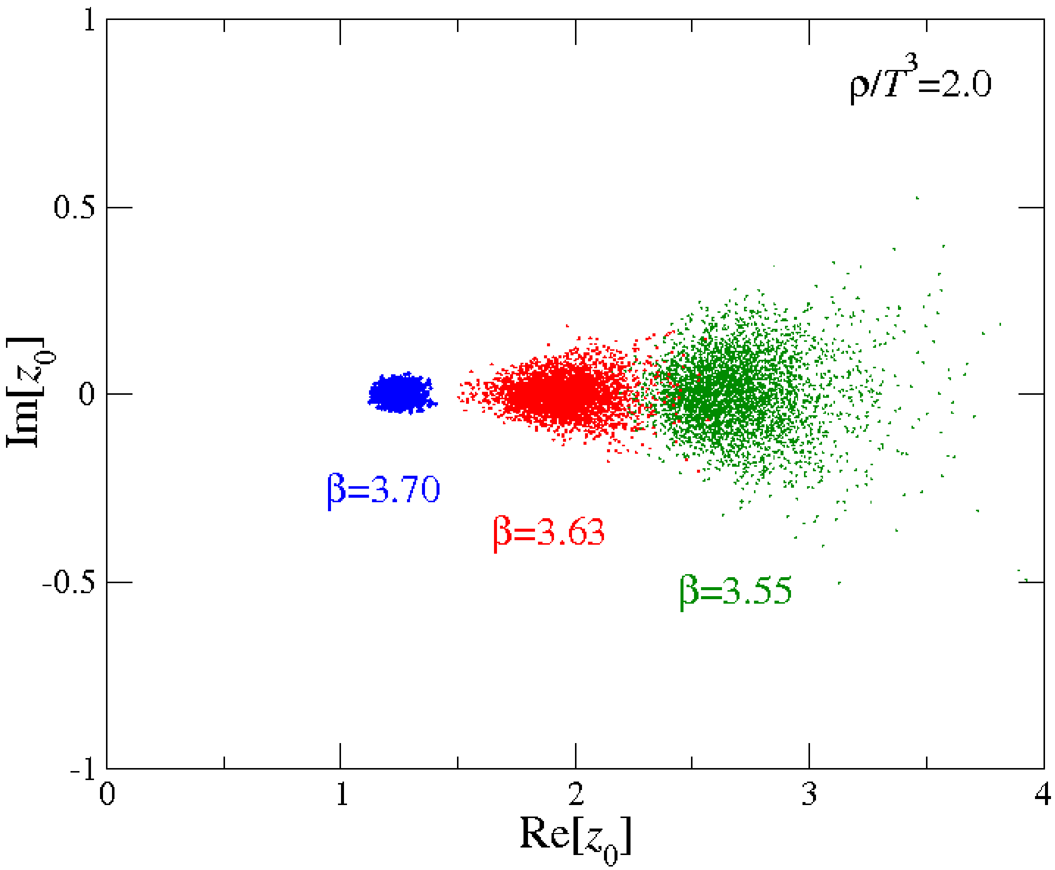
- Approximation:
  - Saddle point approximation ($1/V$ expansion)
  - ln det M: Taylor expansion up to $O(\mu^6)$
  - Distribution function of $\theta = N_f$ Im[ln det M] : Gaussian type.

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$M$ $\quad \text{(phase)} = N_f \, \mathrm{Im}\left[\ln \det M(\mu)\right]$
  - Taylor expansion (Bielefeld-Swansea, PRD66, 014507 (2002))
  - Good definition (staggered quarks: 4th root trick, θ/4?)

$$\theta = \mathrm{Im}\left[V \left(N_f N_t \sum_{n=1}^{\infty} D_n z_0 - \rho z_0 \right) \right] - \frac{\alpha}{2}$$

➡ θ: NOT in the range [-π, π]

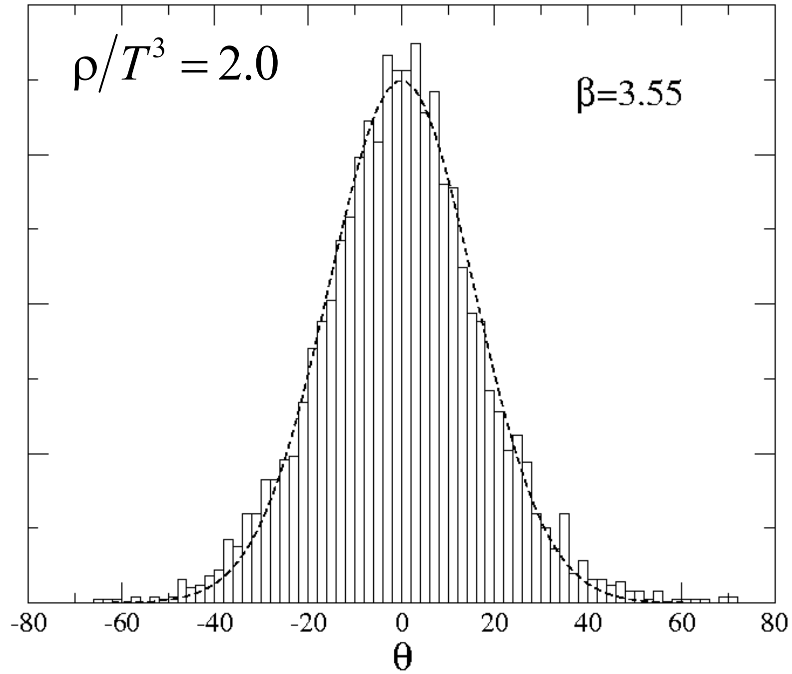
- |θ| > π/2: Sign problem happens.

  ➡ $e^{i\theta}$ changes its sign.

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

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

histogram of θ



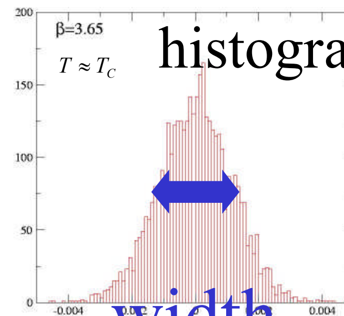
Sign problem (S.E., Phys.Rev.D77, 014508(2008))

Sign problem happens when $\exp(i\theta)$ changes its sign frequently.

$$\Rightarrow \langle e^{i\theta} e^{F} \rangle << \text{(statistical error)}$$

Assume: Gaussian distribution $\Rightarrow$ Sign problem is avoided.

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



$$\sqrt{\langle \theta^2 \rangle_F}$$

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

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

real and positive (No sign problem)

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

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

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

$$\boxed{\sim O(\mu^6)}$$

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

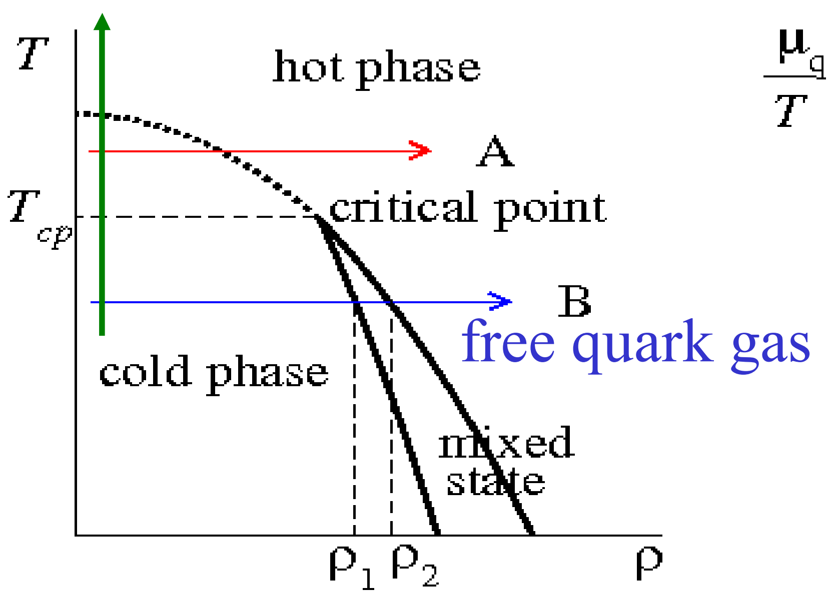
- Valid for low density

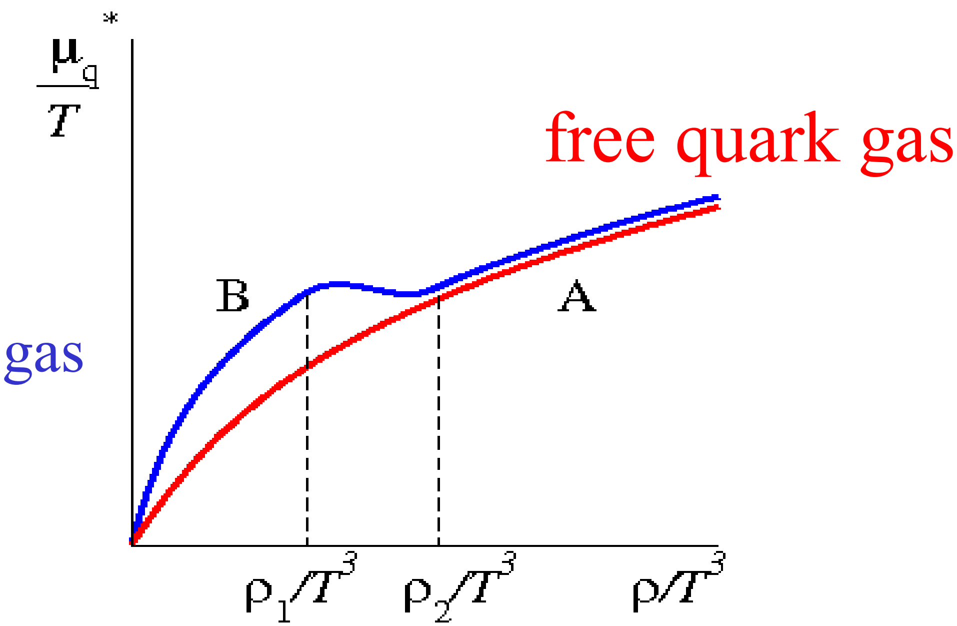
Technical problem 2: Overlap problem
Role of the weight factor exp(F+$i\theta$)

- 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.

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

free quark gas





Technical problem 2: Overlap problem

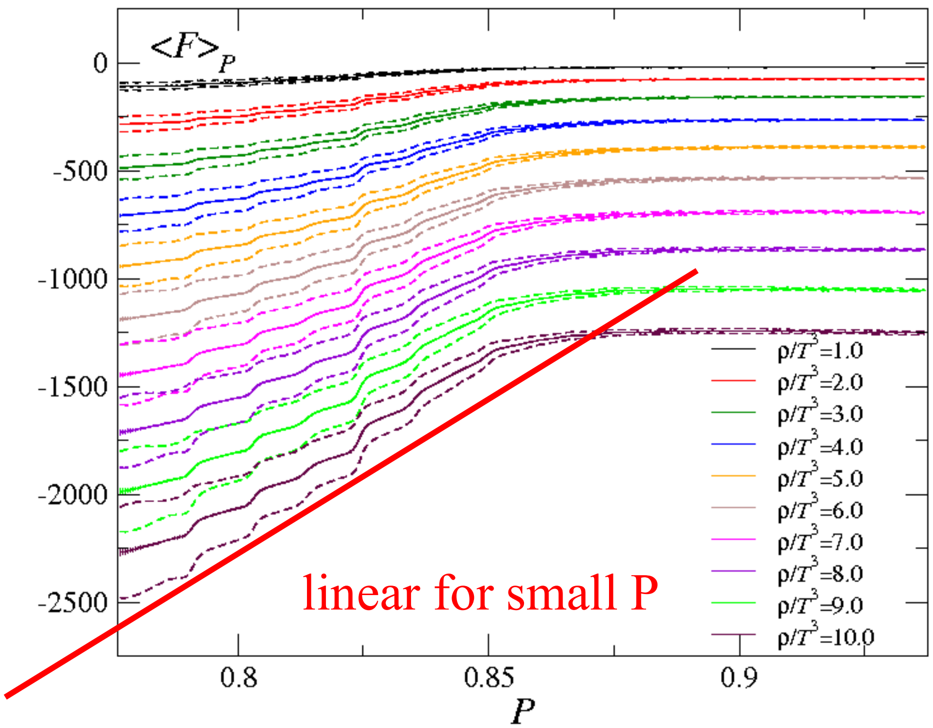
- Density of state method

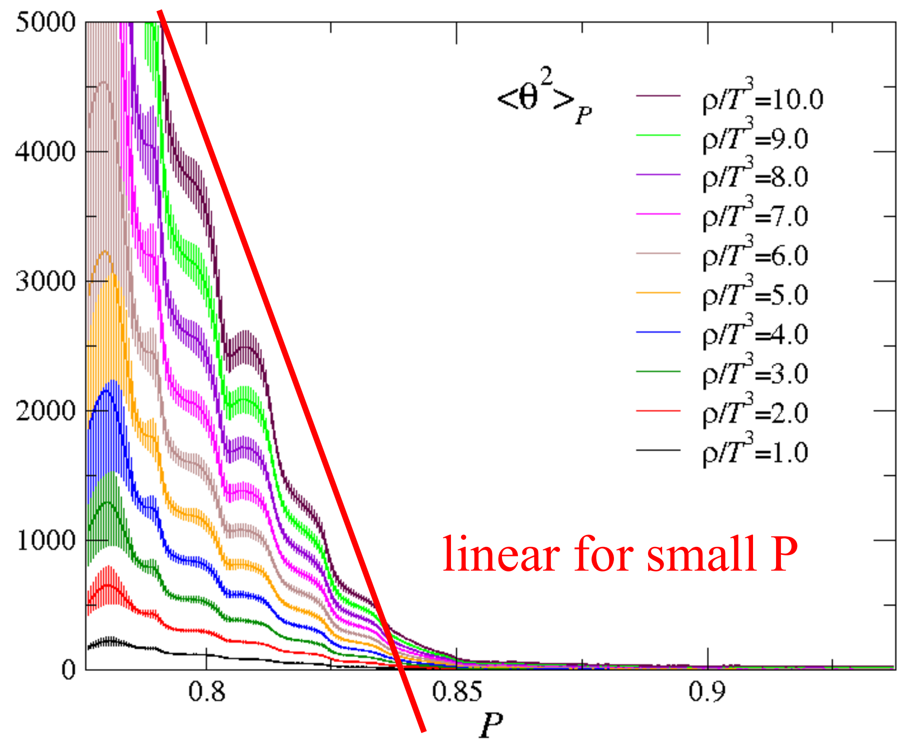
  $W(P)$: plaquette distribution

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

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

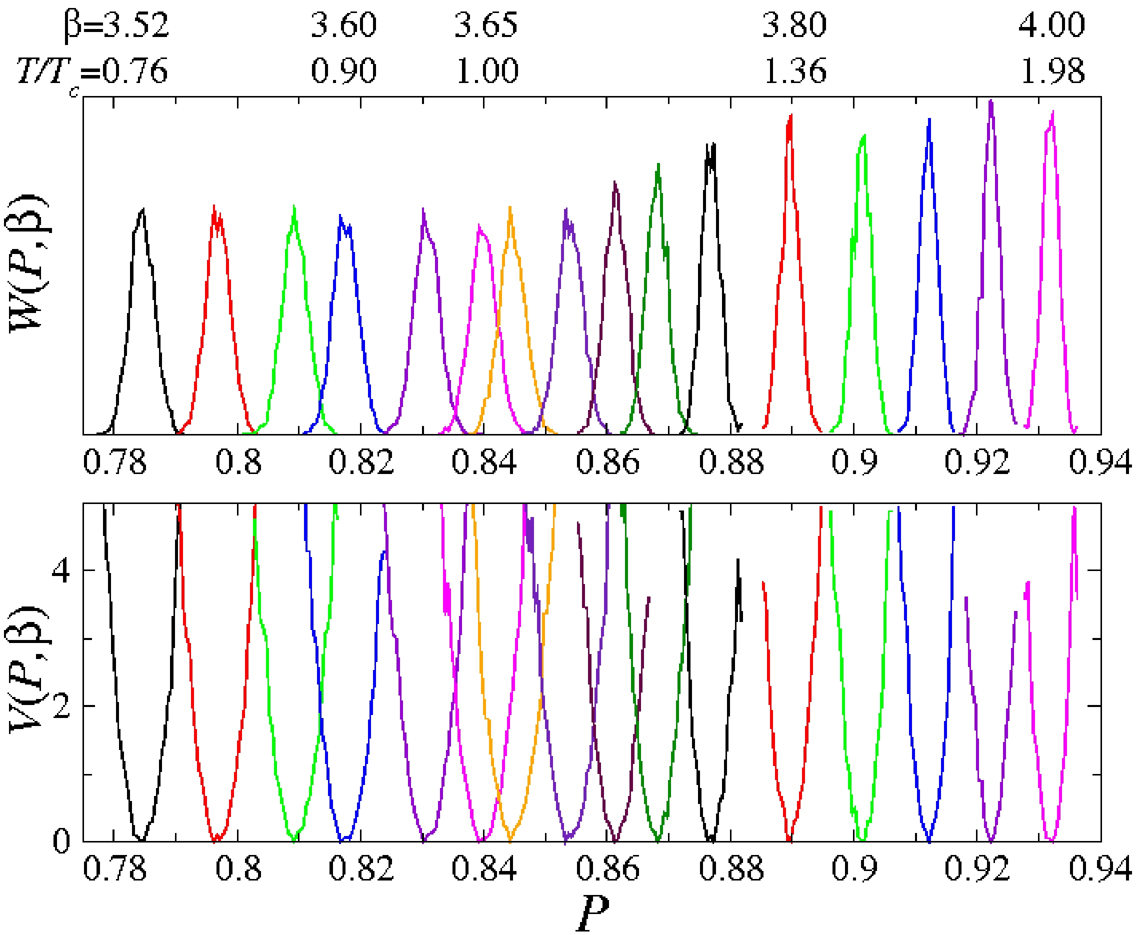
Same effect when β changes. $\propto \exp(\Delta\beta_{\mathrm{eff}} P) W(P)$ for small P





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

(Data: $N_f=2$ p4-staggared, $m_\pi/m_\rho \approx 0.7$, $\mu=0$)



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

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

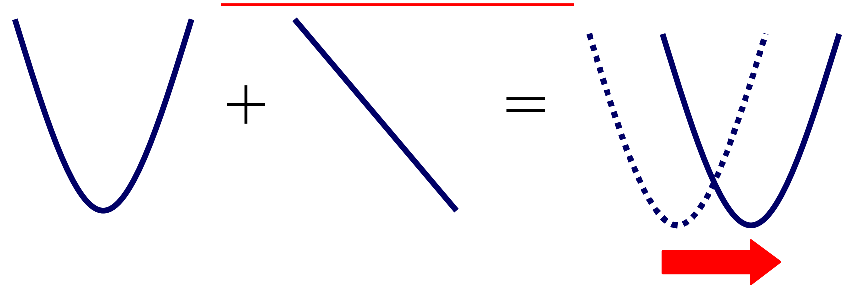
Distribution:

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

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

Potential:

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



Effective β (temperature) for ρ≠0

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

(ρ increases) ≈ (β (T) increases)

Overlap problem, Multi-β reweighting

Ferrenberg-Swendsen, PRL63,1195(1989)

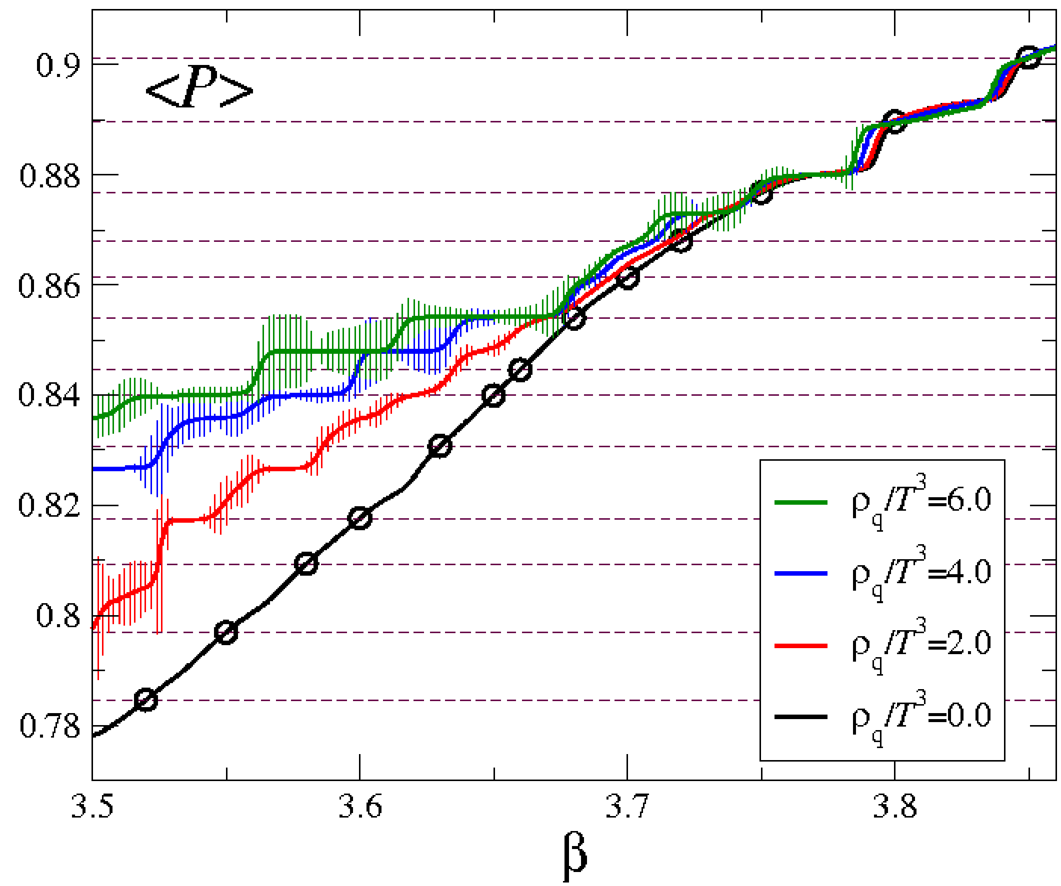
$$\langle P \rangle \approx \frac{\langle P \exp(F + i\theta) \rangle_{(T,\mu=0)}}{\langle \exp(F + i\theta) \rangle_{(T,\mu=0)}}$$

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

Plaquette value by multi-beta reweighting

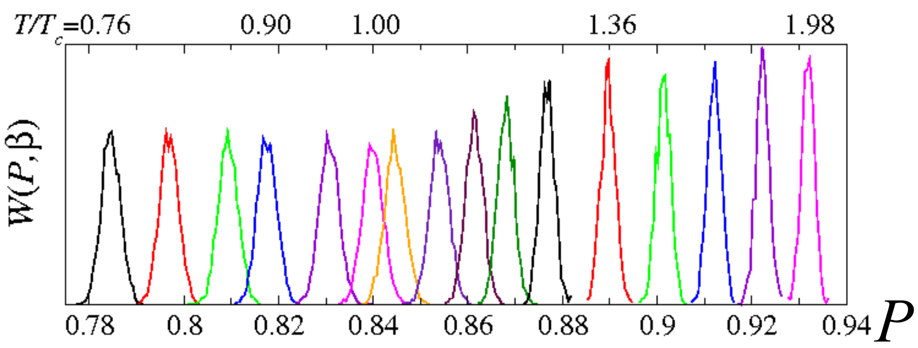
- - - peak position of the distribution

○ <*P*> at each β



Problem:

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

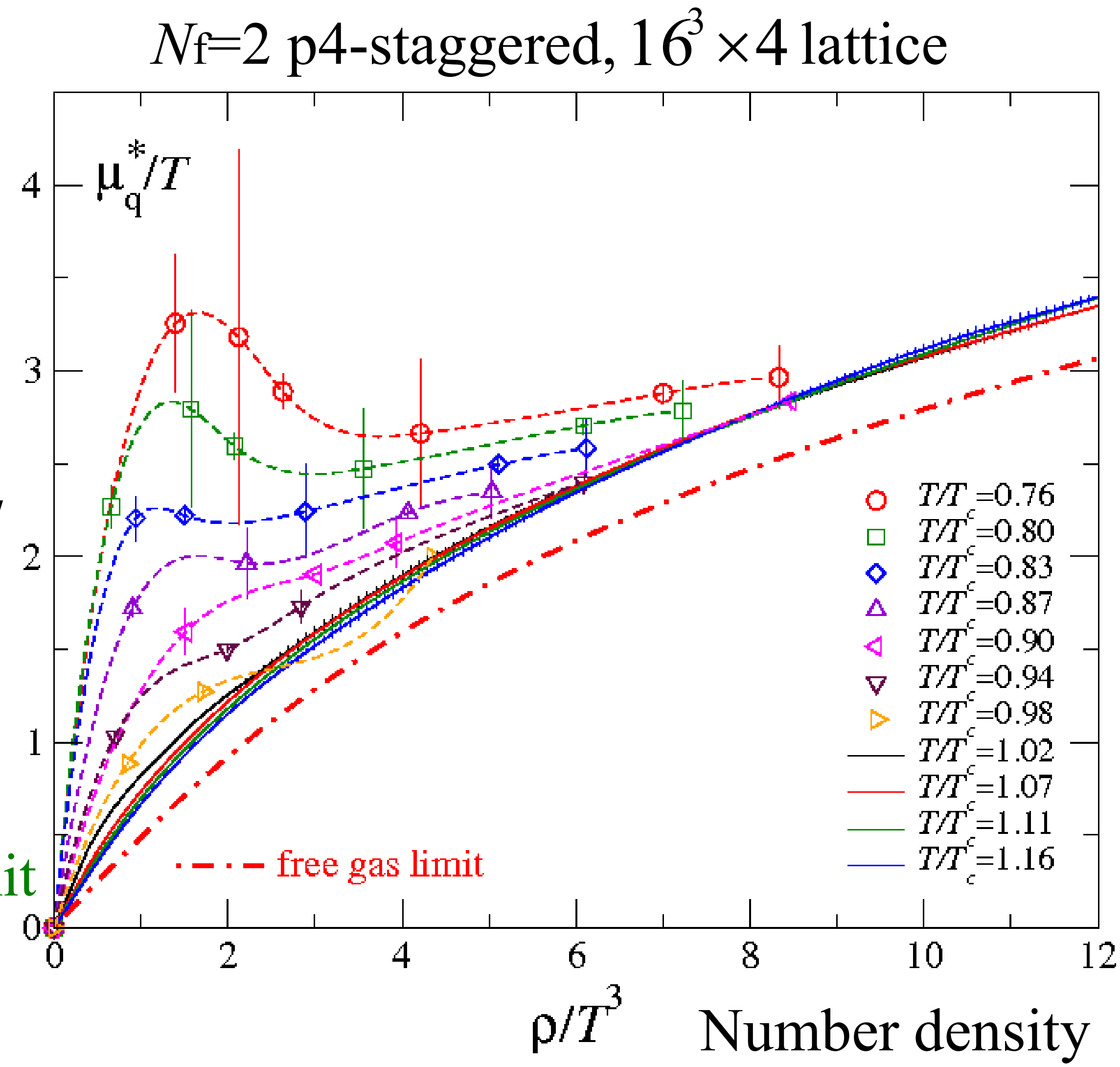


Chemical potential vs density

- 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.



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

Summary

- An effective potential as a function of the quark number density is discussed.
- 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.
  - Saddle point approximation ($1/V$ expansion)
- Simulations: 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.
  - 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