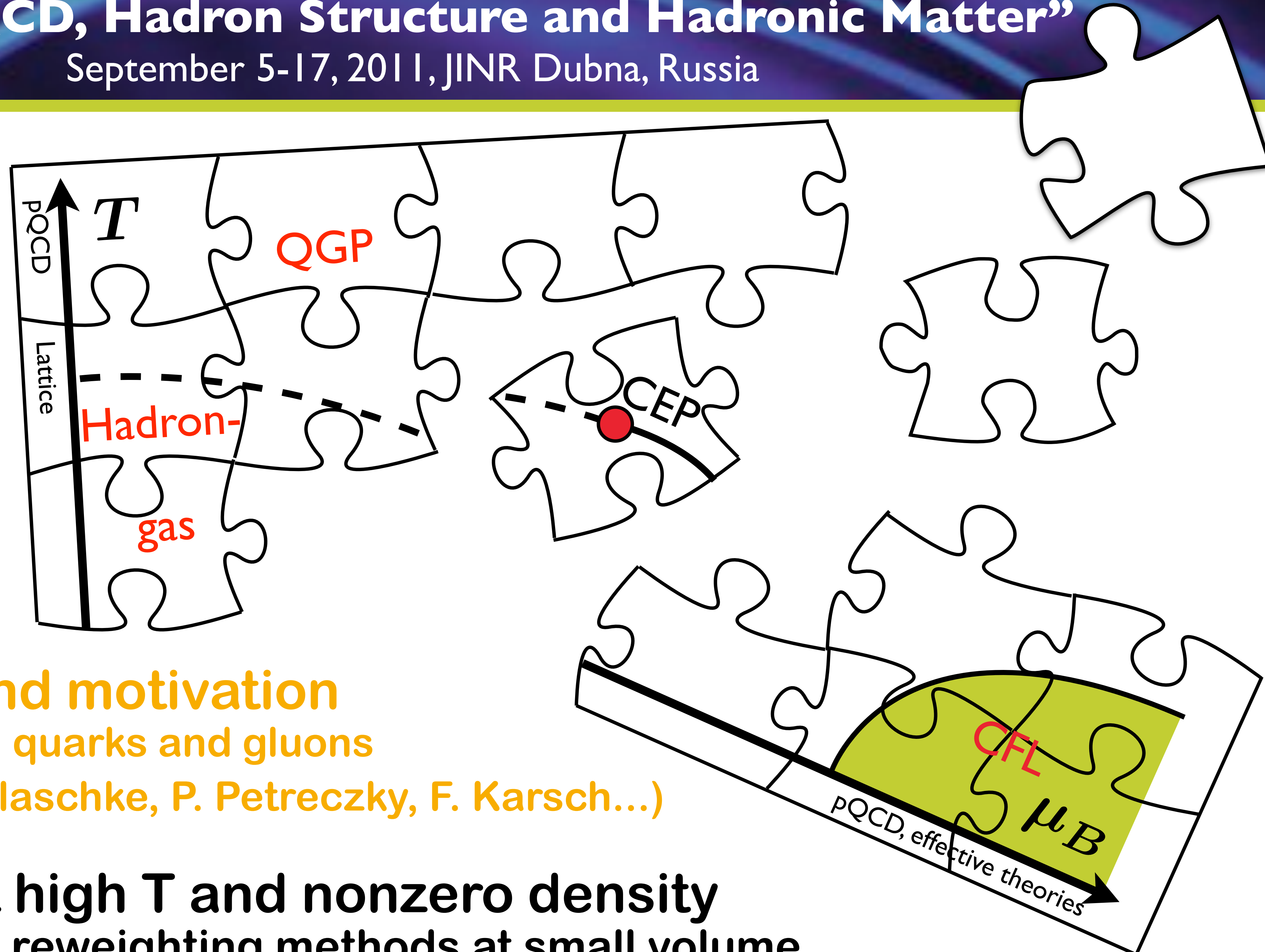
Lattice methods for QCD at nonzero baryon number density

Christian Schmidt

FIAS Frankfurt Institute for Advanced Studies

and

GSI Helmholtzzentrum für Schwerionenforschung



Overview:

★ **Introduction and motivation**
thermodynamics of quarks and gluons
(also covert by D. Blaschke, P. Petreczky, F. Karsch...)

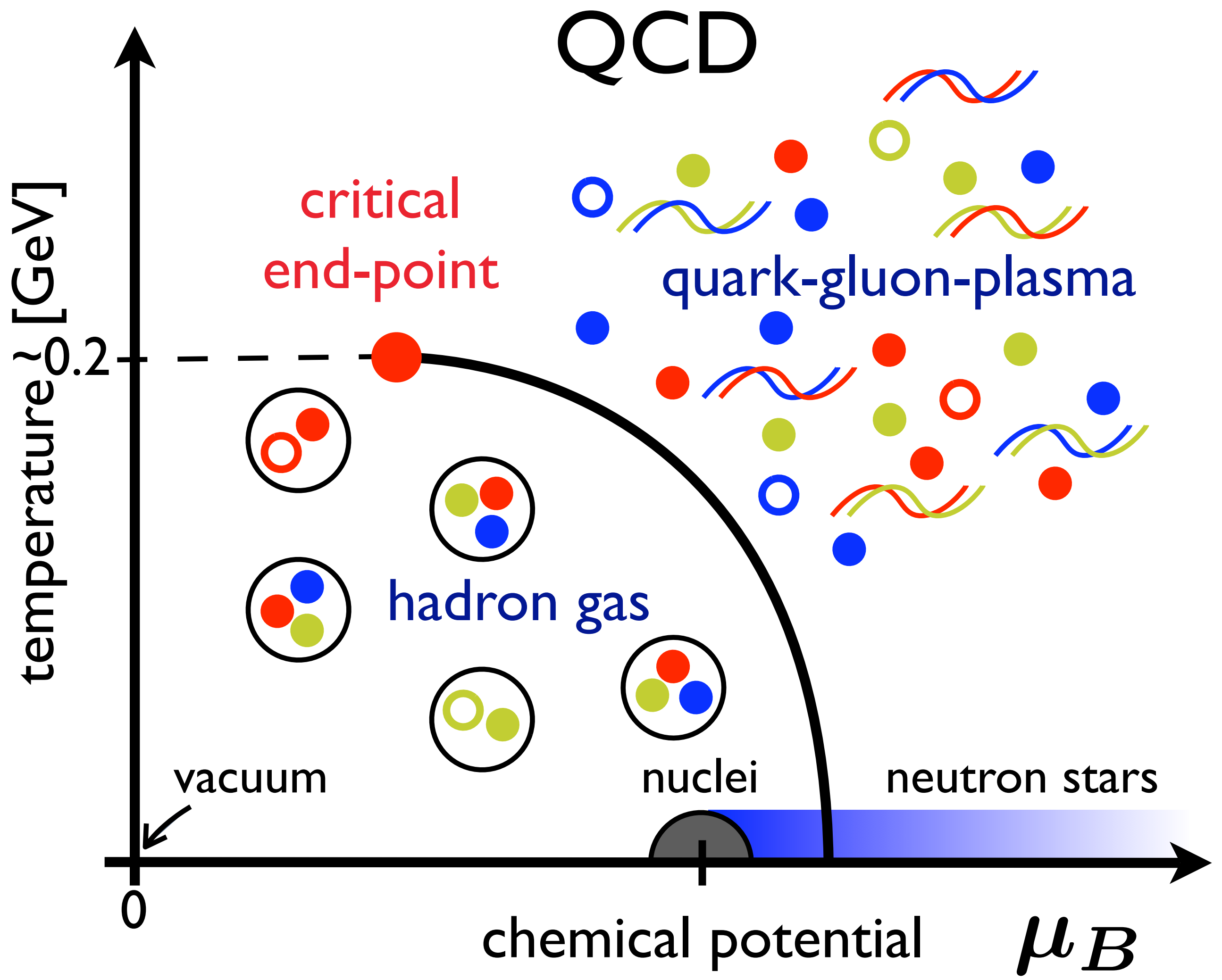
★ **Lattice QCD at high T and nonzero density**
The sign problem, reweighting methods at small volume,
extrapolation methods at large volumes

★ **Recent Results from the Taylor expansion method:**
Hadronic fluctuations and heavy ion collisions, the critical point

The phase diagram

Key questions

- What are the phases of strongly interacting matter and what role do they play in the cosmos ?
- What does QCD predict for the properties of strongly interacting matter ?
- What governs the transition from Quark and Gluons into Hadrons ?



The QCD phase diagram

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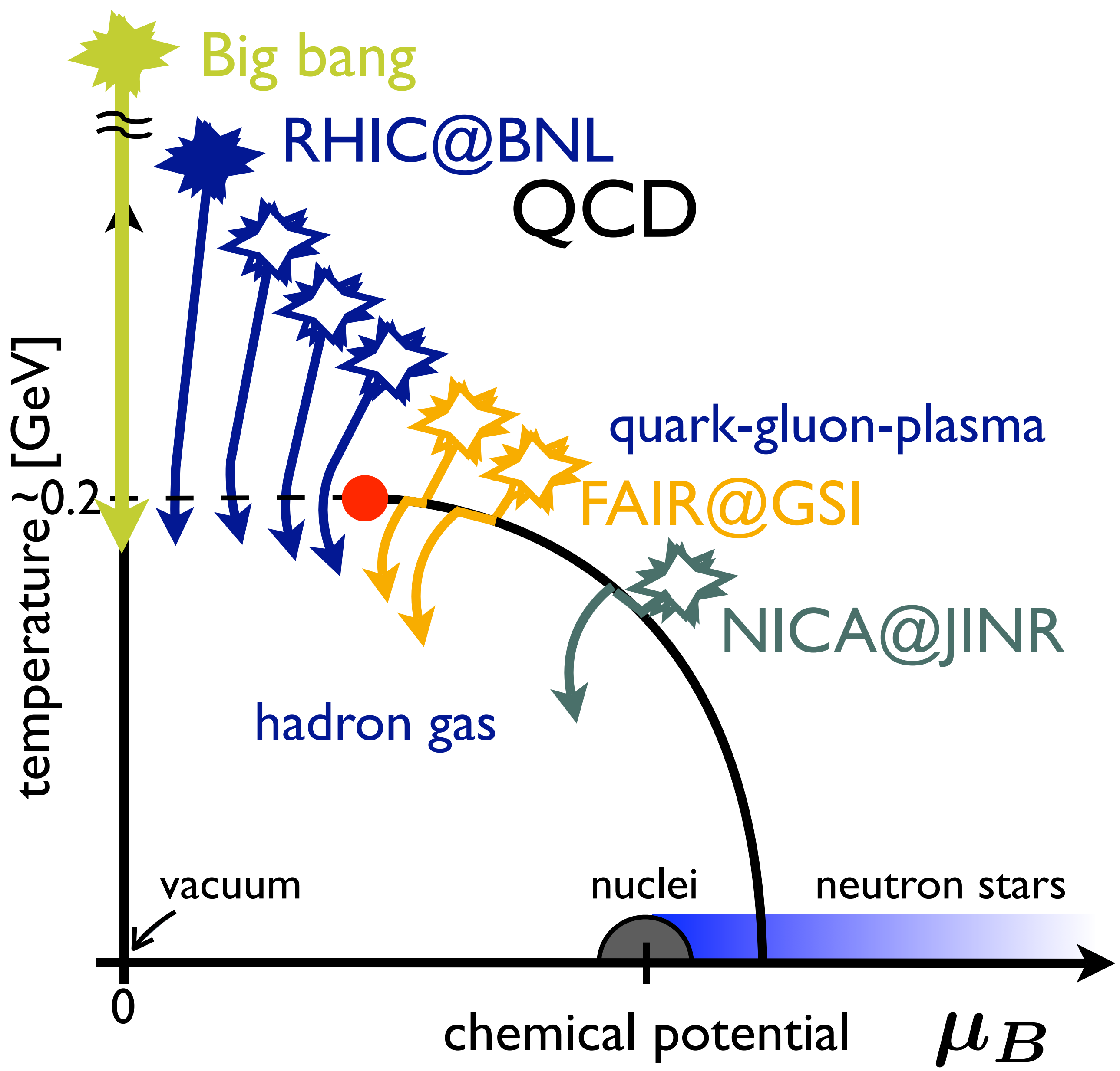
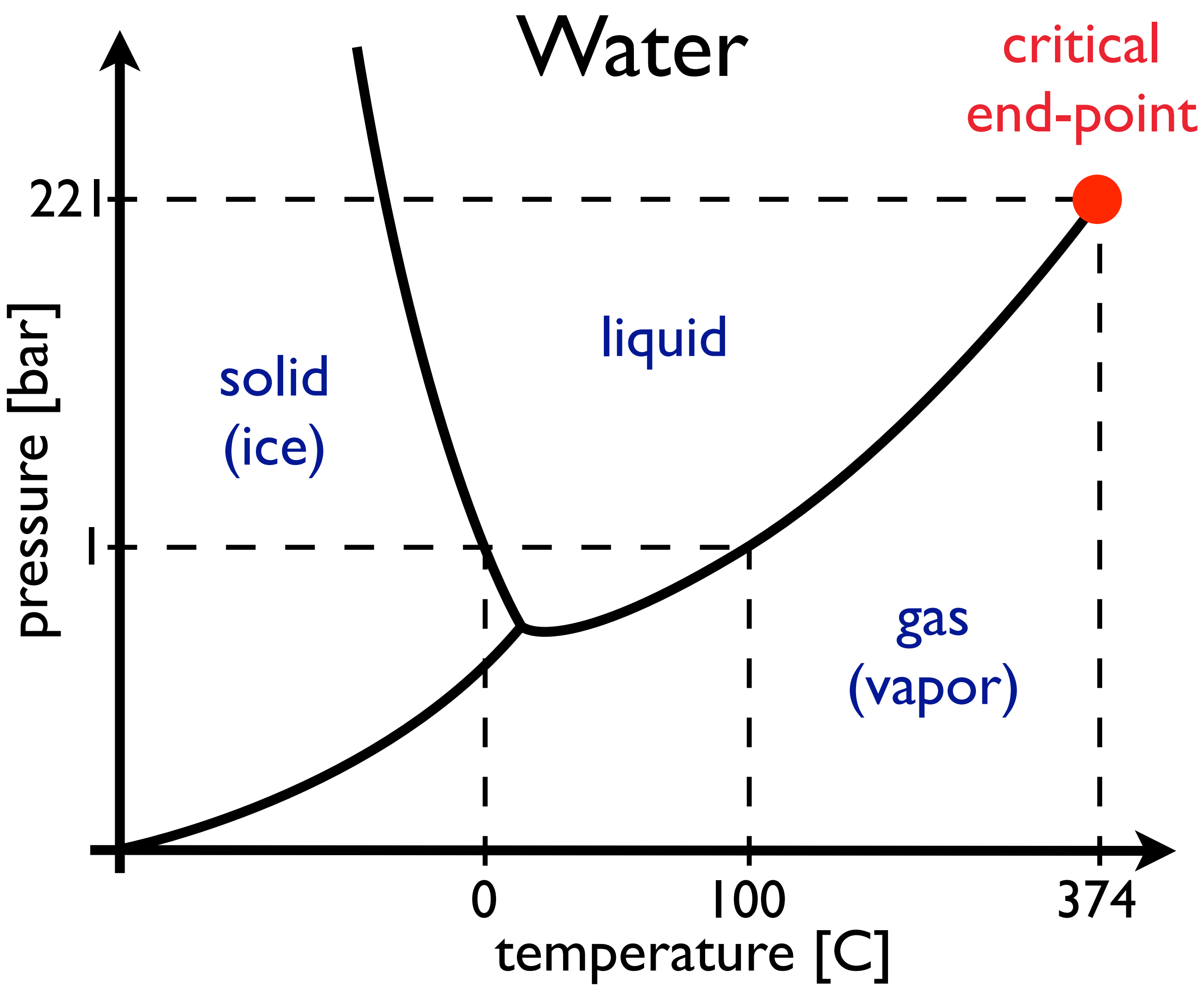
Places to find QGP ?

- In the early universe
- In the laboratory: RHIC, LHC, FAIR
- In the cores of neutron stars ?



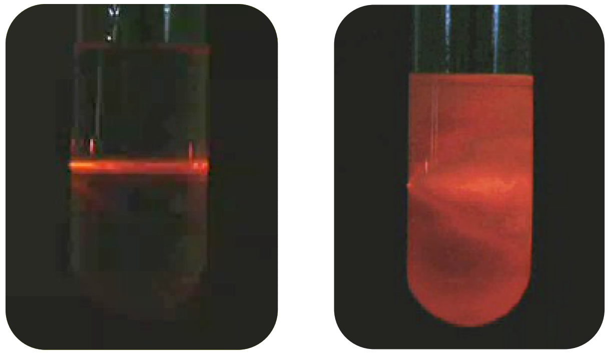
The phase diagram



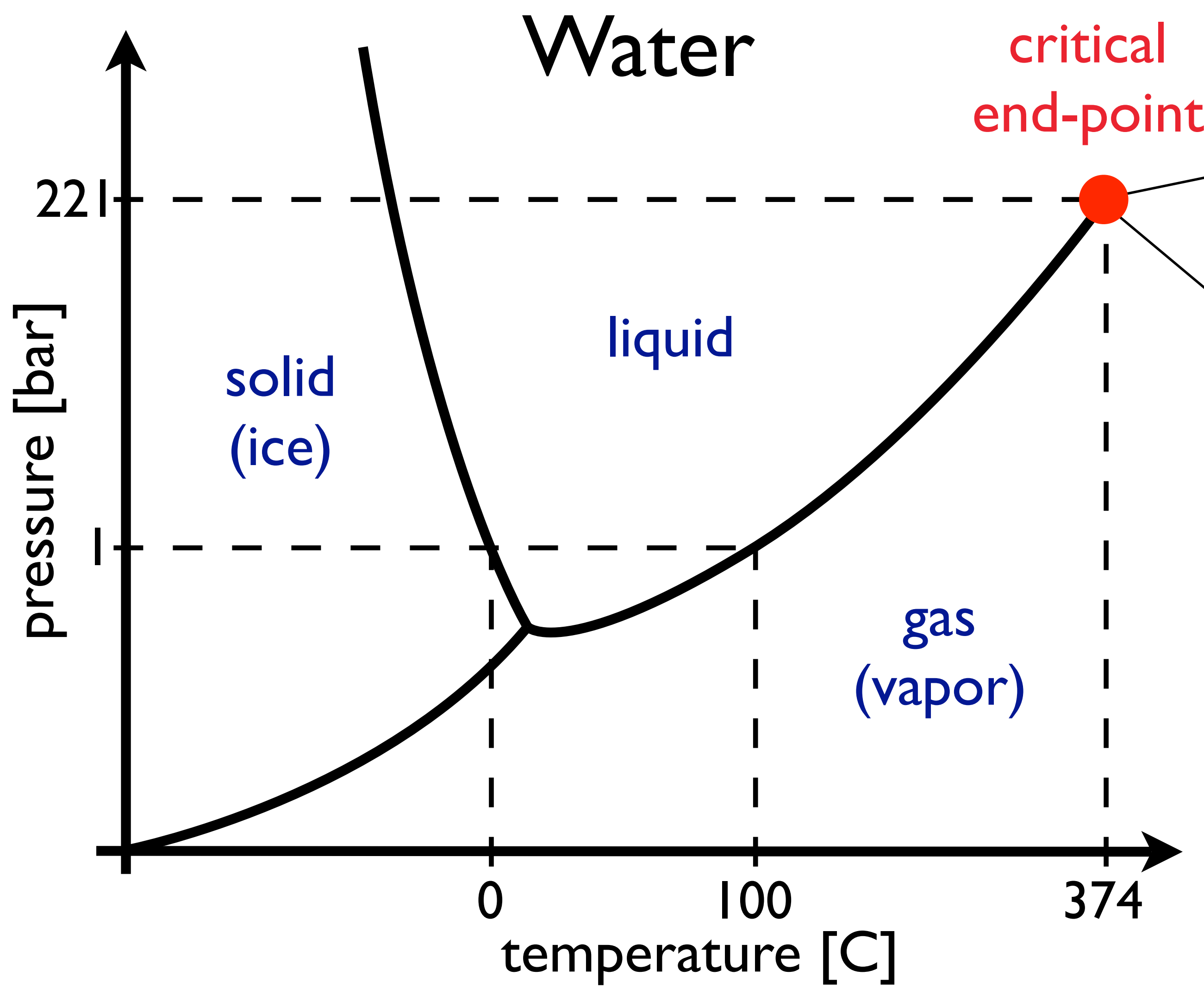
⟶ determined by the **Equation of State**

⟶ exciting: **critical Phenomena**

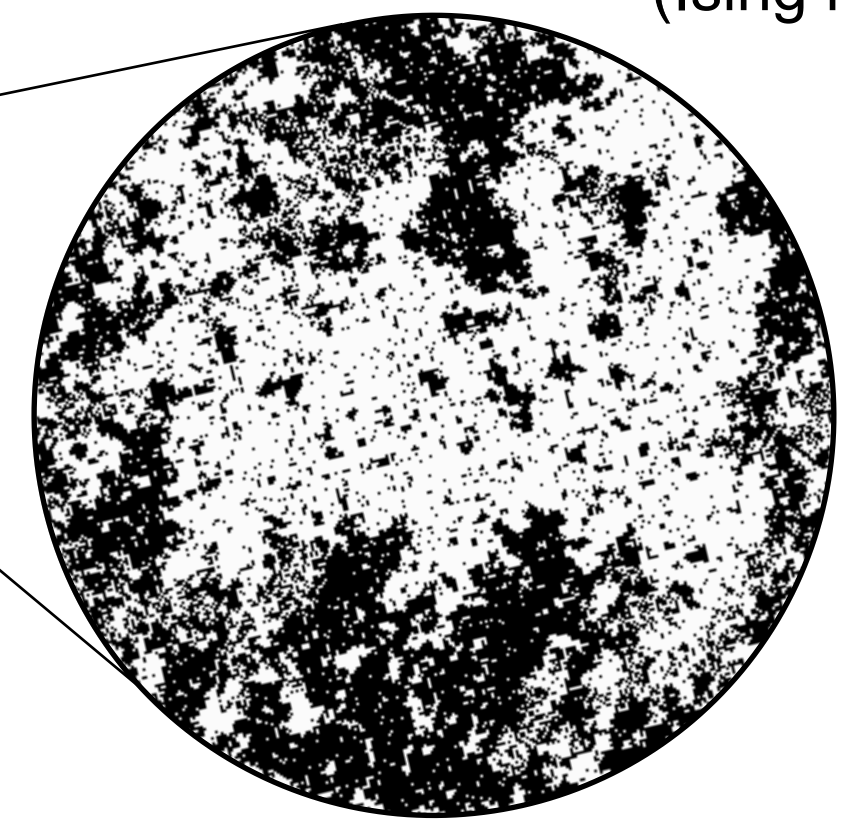
e.g. critical opalescence:



The phase diagram



(Ising model)



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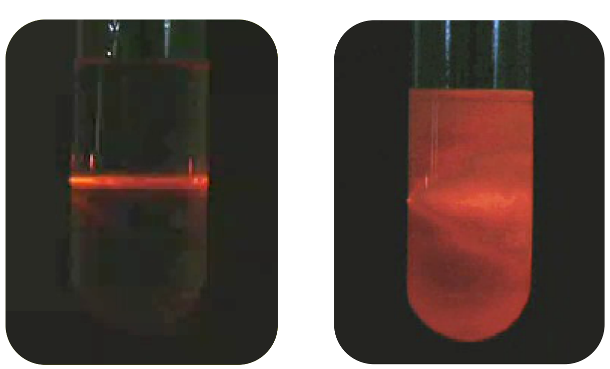


free energy density:

$$-\frac{1}{V}\ln Z = f_s(t,h) + f_r(T,V,H)$$

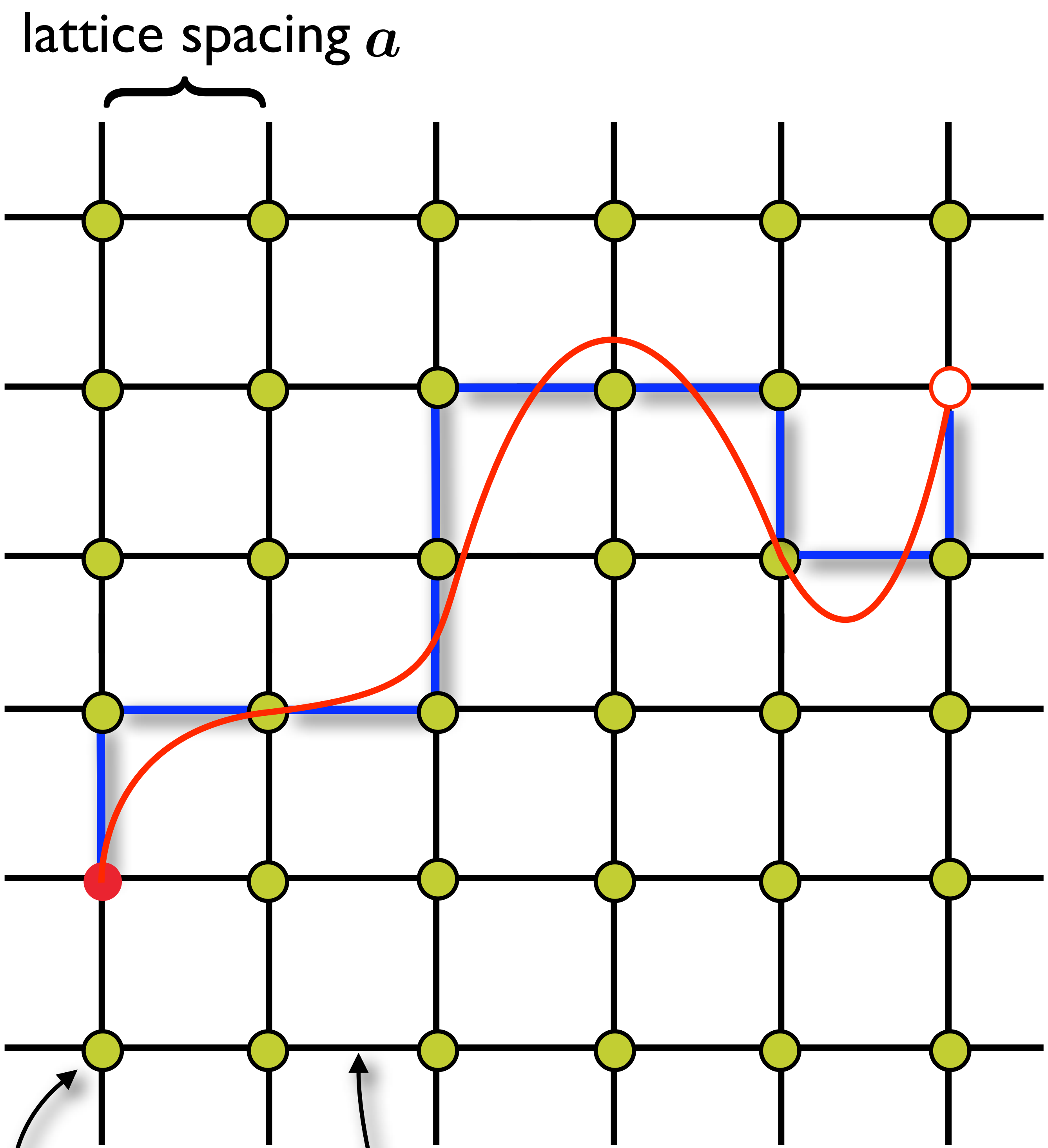
(singular part) (regular part)

scaling hypothesis:

f_s is a generalized homogenous function

$$f_s(t,h) = b^{-d} f_s(b^{y_t}t, b^{y_h}h)$$

QCD on the lattice



perform lattice QCD:
non perturbativ, ab inito

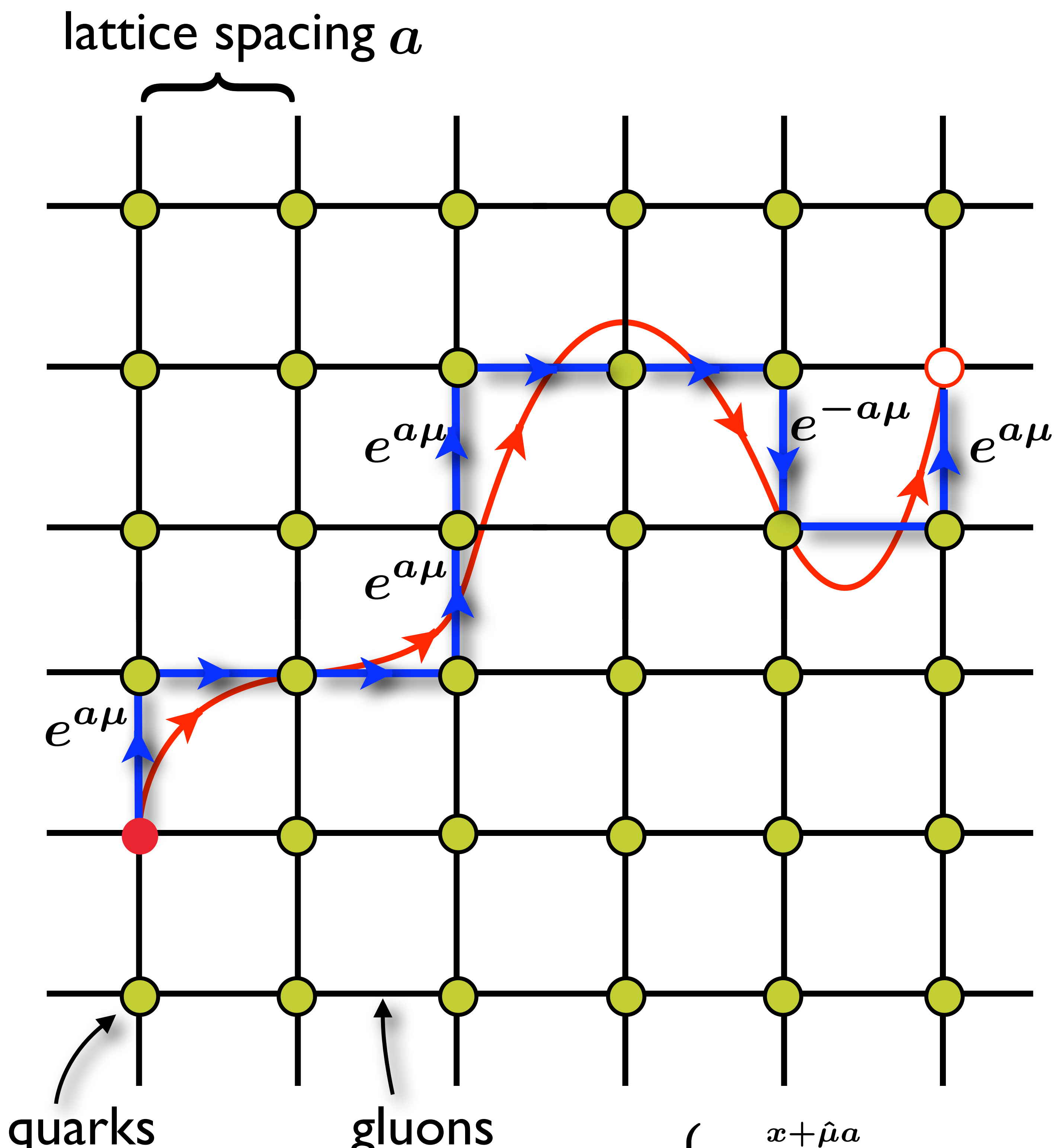
quarks

$\psi(x), \bar{\psi}(x)$

gluons

$$U_\mu(x) = P \exp\left\{ ig \int_x^{x+\hat{\mu}a} dx_\mu A_\mu(x) \right\}$$

Lattice QCD (at $T, \mu > 0$)



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$U_\mu(x) = P \exp\left\{ ig \int_x^{x+\hat{\mu}a} dx_\mu A_\mu(x) \right\}$

perform lattice QCD:
non perturbativ, ab inito

at nonzero chemical potential μ:

$$A_0 \rightarrow A_0 - i\mu$$

or equivalently:

$$U_0(x) \rightarrow e^{a\mu} U_0(x)$$
$$U_0^\dagger(x) \rightarrow e^{-a\mu} U_0^\dagger(x)$$

Hasenfratz, Karsch, PLB 125 (1983) 308.

Lattice QCD (at $T, \mu > 0$)

- the QCD partition function:

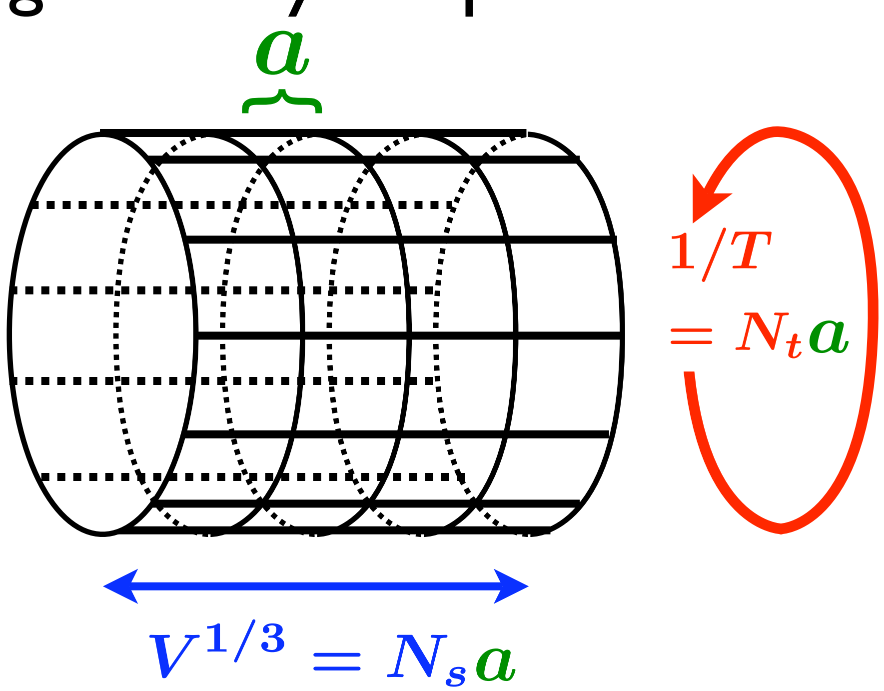
$$Z(V,T,\bar{\mu}) = \int \mathcal{D}A\, \mathcal{D}\bar{\psi}\, \mathcal{D}\psi\;\exp\{-S_E\}$$

$$S_E = \bar{\psi}_x M_{x,y} \psi_y + S_G$$

$$M_{x,y} = am\,\delta_{x,y} + \frac{1}{2}\sum_{\mu=1}^{3}\gamma_\mu \left\{U_\mu(x)\,\delta_{x+a\hat{\mu},y} - U_\mu^\dagger(y)\,\delta_{x-a\hat{\mu},y}\right\}$$

$$+\frac{1}{2}\gamma_4\left\{e^{a\bar{\mu}}U_4(x)\,\delta_{x+a\hat{4},y} - e^{-a\bar{\mu}}U_4^\dagger(y)\,\delta_{x-a\hat{4},y}\right\}$$

- geometry of space time: $N_s^3 \times N_t$ (4d - torus)



note:

- only closed loops participate to the partition function
- only loops that wind around the torus in time direction $\mathcal{W}$-times pick up a μ-dependence:

$$\exp\{\mathcal{W}\mu/T\}$$

$\longrightarrow$ alternatively (gauge-transformation):

- choose a fixed time-slice on which all temporal links get a factor $\exp\{\pm\mu/T\}$

The sign problem

- integration over fermion fields

$$Z(V,T,\mu) = \int \mathcal{D}A\mathcal{D}\psi\mathcal{D}\bar{\psi}\ \exp\{S_F(A,\psi,\bar{\psi}) - \beta S_G(A)\}$$

$$= \int \mathcal{D}A\ \det[M](A,\mu)\exp\{-\beta S_G(A)\}$$

complex for $\mu > 0$

propabilistic interpretation necessary for Monte Carlo!

we find: $[\det M(\mu)]^* = \det M(-\mu^*)$

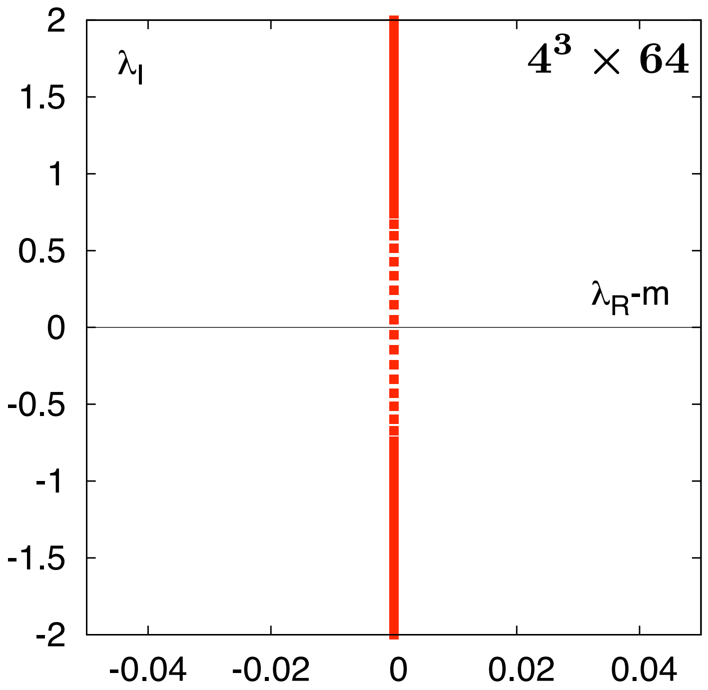
$\longrightarrow$ determinant is real only for

$\mu = 0$ or $\mu = i\mu_I$

The sign problem

- properties of the fermion matrix and eigen-spectrum

free case

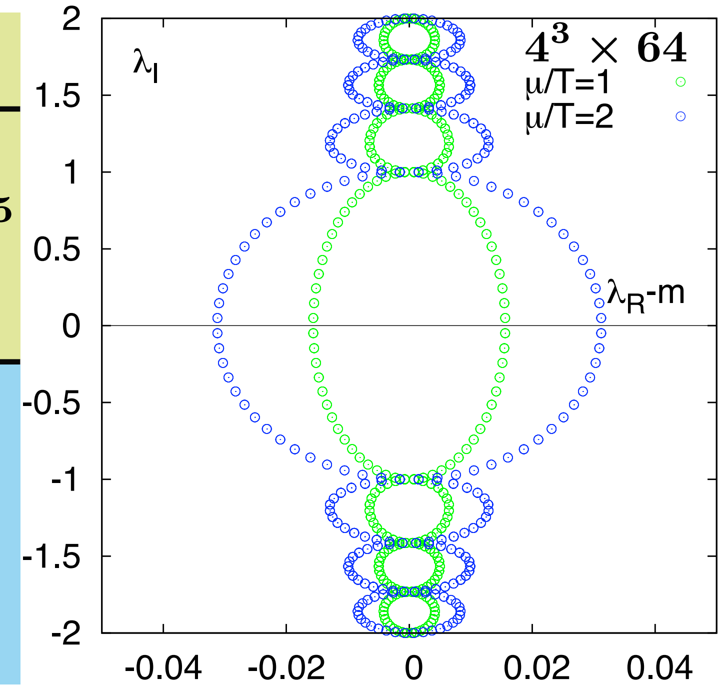


$\mu = 0$	$\mu > 0$
$M^\dagger(0) = \gamma_5 M(0)\gamma_5$ (γ_5- Hermiticity)	$M^\dagger(\mu) = \gamma_5 M(-\mu)\gamma_5$

free naive fermions

$$\lambda_p = m \pm i\sqrt{\sum_{k=1}^{3} \sin^2(p_k) + \sin^2(p_4 + i\mu)}$$

free case



$M^\dagger M$ is

- positive definite
- block diagonal in parity (even-odd) space, use even-odd preconditioning
- regulated by the mass: $\lambda_{\min} = m^2$

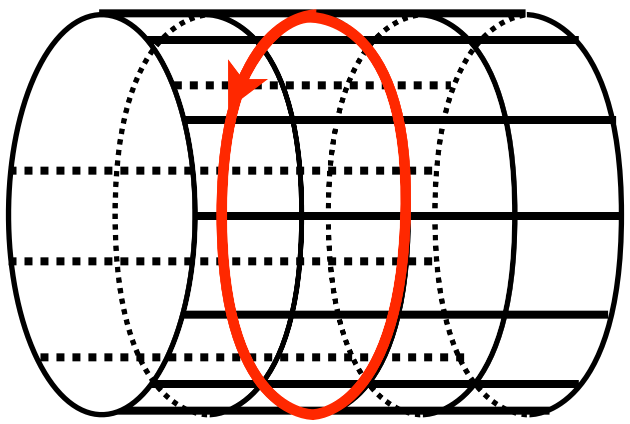
$M^\dagger M$ is

- not block diagonal in parity (even-odd) space
- not regulated, zero-modes possible for sufficiently large μ

The sign problem

- complex measure ($\mathrm{d}\omega$) needed to obtain correct physics

example Polyakov Loop (L):



$$\langle \mathrm{Tr}(L) \rangle = \exp\{-\frac{1}{T} F_q\} = \int \mathrm{Re}(\mathrm{Tr}(L))\, \mathrm{Re}(\mathrm{d}\omega) - \mathrm{Im}(\mathrm{Tr}(L))\, \mathrm{Im}(\mathrm{d}\omega)$$

$$\langle \mathrm{Tr}(L^*) \rangle = \exp\{-\frac{1}{T} F_{\bar{q}}\} = \int \mathrm{Re}(\mathrm{Tr}(L))\, \mathrm{Re}(\mathrm{d}\omega) + \mathrm{Im}(\mathrm{Tr}(L))\, \mathrm{Im}(\mathrm{d}\omega)$$

demand different free energy for quark and anti-quark:

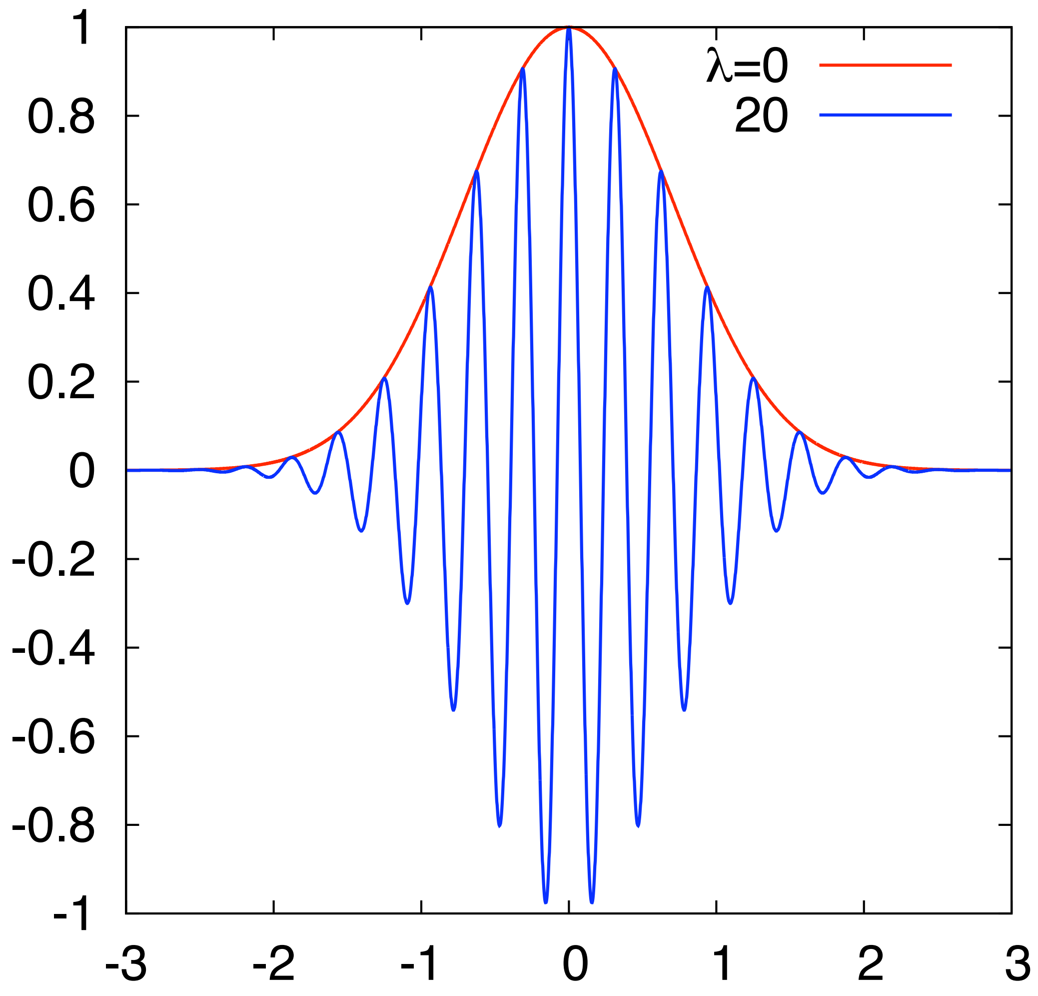
$$F_q \neq F_{\bar{q}} \Rightarrow \mathrm{Im}(\mathrm{d}\omega) \neq 0$$

The sign problem

- How to sample an oscillating partition function?

which are the dominant configurations in the path integral?

toy model: $Z(\lambda) = \int \mathrm{d}x \;\; \exp\{-\lambda x^2 + i\lambda x\}$



$\longrightarrow$ cancelations between configurations with ‘positive’ and ‘negative’ weight are exponentially large:

$$Z(\lambda)/Z(0) = \exp\{-\lambda^2/4\}$$

$\longrightarrow$ constraining the integration interval to

$$x \in [-\lambda, \lambda]$$

will give $\mathcal{O}(100\%)$ error

$\longrightarrow$ all configurations are important

Reweighing and the sign problem

- How to sample an oscillating partition function?

toy model: $Z_f \equiv \int \mathrm{d}x \; f(x)$, with $f(x) \in \mathbb{R}\,, \quad f(x) \ngeq 0$

introduce auxiliary partition function:

$$Z_g \equiv \int \mathrm{d}x \; g(x)\,, \text{ with } \; g(x) \in \mathbb{R}\,, \quad g(x) \geq 0$$

calculate observable by reweighting:

$$\langle O \rangle_f \equiv \frac{1}{Z_f} \int \mathrm{d}x \; O(x) f(x) = \frac{\int \mathrm{d}x \; O(x) \frac{f(x)}{g(x)} g(x)}{\int \mathrm{d}x \; \frac{f(x)}{g(x)} g(x)} = \frac{\left\langle O \frac{f}{g} \right\rangle_g}{\left\langle \frac{f}{g} \right\rangle_g}$$

$f/g \equiv R$ is the "reweighting factor"

$$\langle R \rangle_g = Z_f / Z_g = \exp\{-\frac{V}{T} \underbrace{\Delta \tilde{f}(\mu, T)}_{\text{difference of the free energy density}}\}$$

⟶ reweighting factor is exponentially small for large V, small T, large $\Delta \tilde{f}$

⟶ **overlap problem**, i.e. the signal gets lost quickly!

Reweighing and the sign problem

- How to sample an oscillating partition function?

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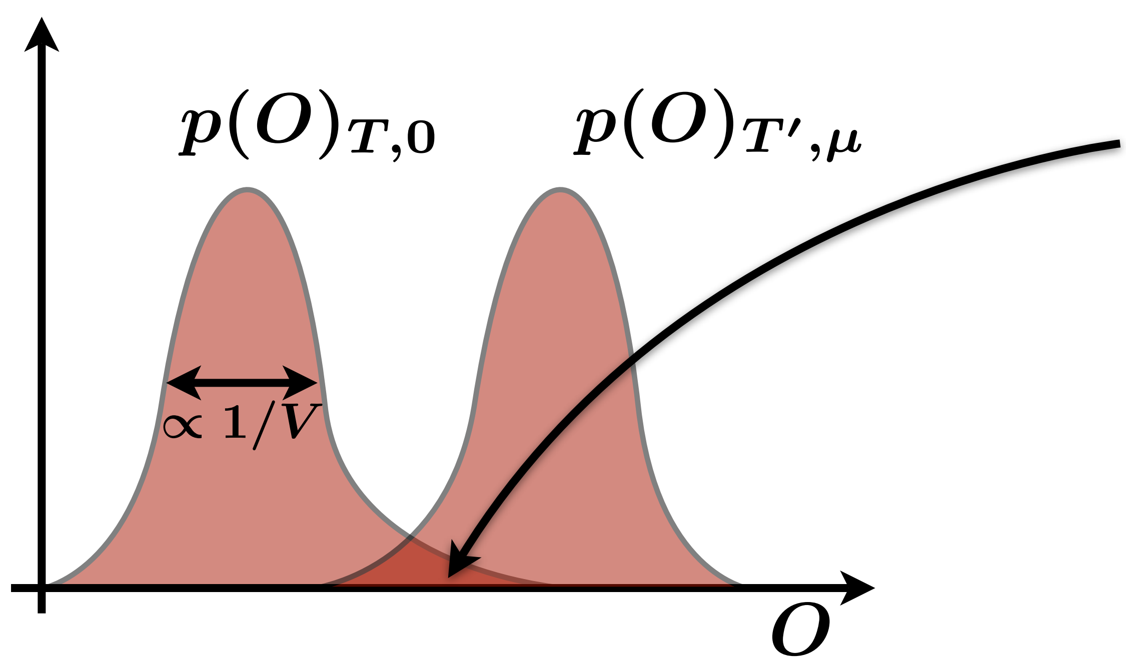

overlap problem
(schematic picture)

$\longrightarrow$ exponentially large statistics required

Reweighing and the sign problem

- How to sample an oscillating partition function?

toy model: $Z_f \equiv \int \mathrm{d}x\; f(x)$, with $f(x) \in \mathbb{R}\,,\;\; f(x) \not\geq 0$

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How to chose $g(x)$?

$\longrightarrow$ minimize $\mathrm{Var}(f/g)$

$\longrightarrow$ solution: $g(x) = |f(x)|$ and $R \equiv f/g = \mathrm{sign}(f)$

de Frocrand, Kim, Takaishi, hep-lat 0209126

Reweighting strategies in QCD

- QCD partition function (for staggered fermions):

$$Z(\mu,\beta) = \int \mathcal{D}U \;\; (\det M(U,\mu))^{N_f/4}\, e^{-\beta \tilde{S}_G}$$

factorize determinant into modulus and phase

$$Z(\mu,\beta) = \int \mathcal{D}U \;\; \underbrace{|\det M(U,\mu)|^{N_f/4}\, e^{i\theta} e^{-\beta \tilde{S}_G}}_{f}$$

$\longrightarrow$ optimal choice:

$$Z_g(\mu',\beta') = \int \mathcal{D}U \;\; |\det M(U,\mu')|^{N_f/4}\, |cos(\theta)| e^{-\beta' \tilde{S}_G}$$

prohibitively inefficient, since θ has to be evaluated in each MC step!

$\longrightarrow$ other choice:

$$Z_g(\mu',\beta') = \int \mathcal{D}U \;\; |\det M(U,\mu')|^{N_f/4}\, e^{-\beta' \tilde{S}_G}$$

"phase quenched" theory, for N_f even equivalent with non zero iso-spin chemical potential:

$$|\det M(\mu)|^{N_f} = \det M(+\mu)^{N_f/2} \times \det M(-\mu)^{N_f/2}$$

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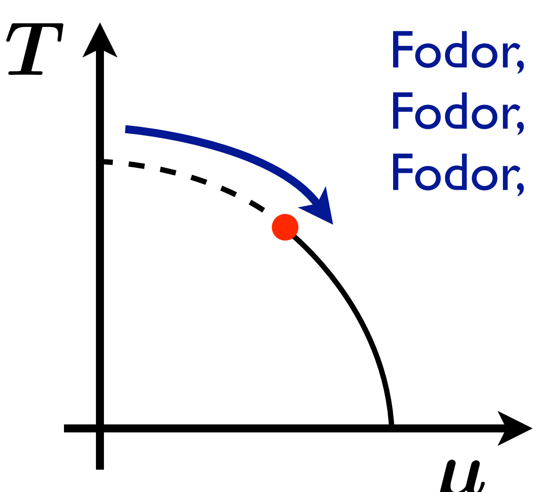
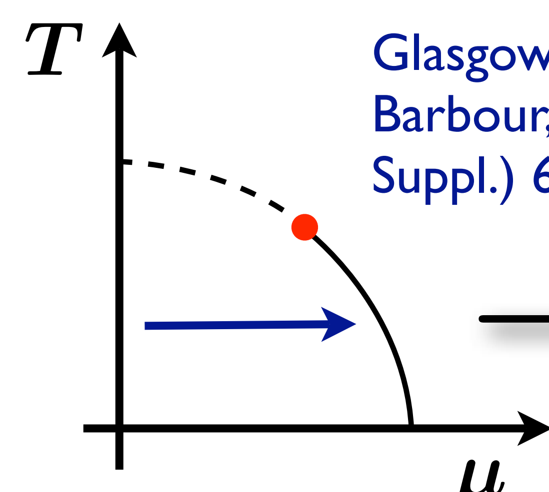
$\longrightarrow$ standard reweighting approach:

$$Z_g = Z(0,\beta') \qquad \Rightarrow \qquad f/g = \left|\frac{\det M(\mu)}{\det M(0)}\right|^{N_f/4} e^{i\theta}\; e^{-(\beta-\beta')\tilde{S}_G}$$



Fodor, Katz, JHEP 0404 (2004) 050;
Fodor, Katz, JHEP 0203 (2002) 014 ;
Fodor, Katz, PLB 534 (2002) 87.



Glasgow-method: fixed β
Barbour, et al., NPB (Proc. Suppl.) 60A (1998) 220.

$\longrightarrow$ **overlap problem**

Reweighting strategies in QCD

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exact calculation of fermion determinant, respectively all eigenvalues is required

<u>*method by Fodor and Katz:*</u>

⟶ transform μ-dependence into 2 time-slices by similarity transformations

⟶ factorize the μ -dependence of the determinant

$$\det M(\mu) = e^{-3N_\sigma^3 N_\tau \mu} \det(P - e^{N_\tau \mu})$$

$$P \in \mathbb{C}^{2N_c N_s^3 \times 2N_c N_s^3}$$

"reduced fermion matrix"

⟶ calculate all eigenvalues of the reduced fermion matrix ($\mathcal{O}(N_\sigma^9)$ operations, hard to parallelize efficiently)

$$\det M(\mu) = e^{-3N_\sigma^3 N_\tau \mu} \prod_{i=0}^{6N_\sigma^3} (e^{N_\tau \mu} - \lambda_i)$$

Fodor, Katz, PLB 534 (2002) 87.

Reweighting strategies in QCD

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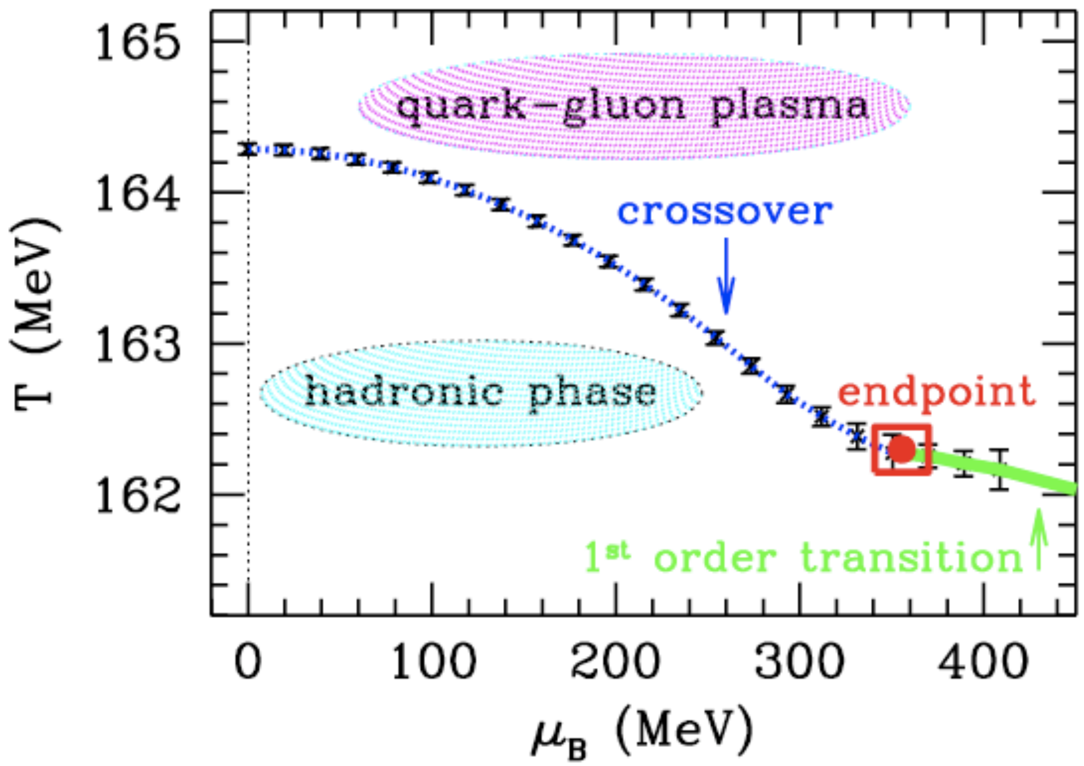
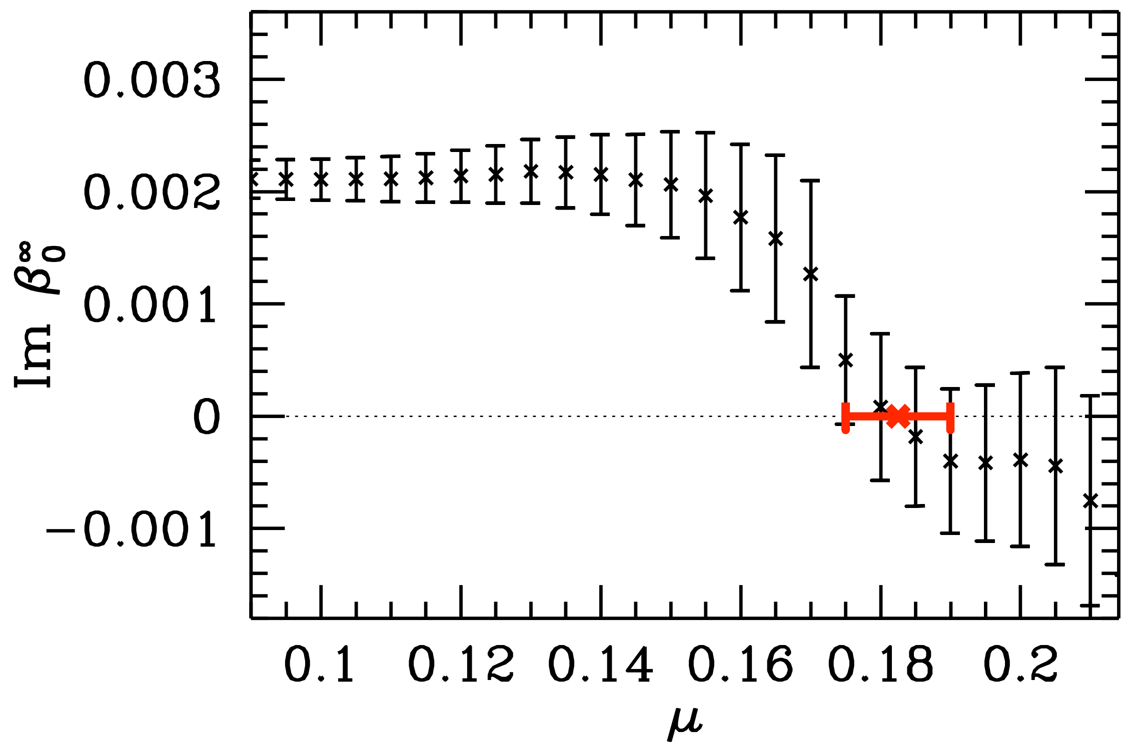
exact calculation of fermion determinant, respectively all eigenvalues is required

method by Fodor and Katz:

$\longrightarrow$ important result ($N_\tau = 4$, physical quark masses) by monitoring the first Lee-Yang zero: $(\mu_q^{\mathrm{CEP}}, T^{\mathrm{CEP}}) = (120(13), 162(2))\ \mathrm{MeV}$





Fodor, Katz, JHEP 0404 (2004) 050

Reweighting strategies in QCD

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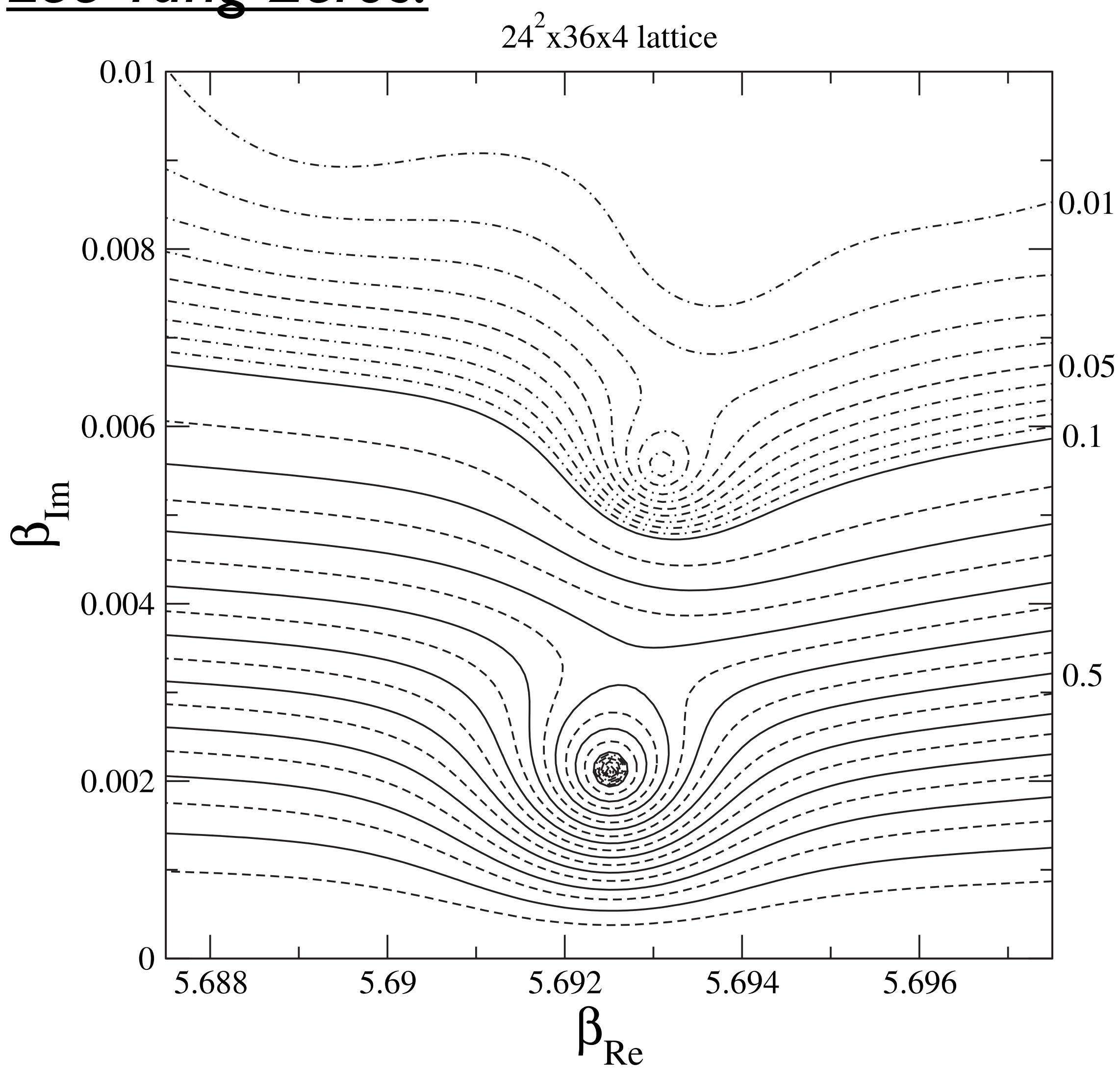
Lee-Yang zeros:



- zeros of the partition function in the complex β-plane
- move onto the real axis in the thermodynamic limit

$\longrightarrow$ detect a 1st order transition on a finite volume by studying the pattern of the Lee-Yang zeros

$$\beta_I \sim C(2n+1)$$

Ejiri, PRD 73 (2006) 054502.

Reweighting strategies in QCD

- break down of the reweighting:

standard jack-knife errors do **not** reflect the break down of the method!

⟶ study the phase factor directly

analytic results, valid in the microscopic limit of QCD:($m_\pi^2 \ll \frac{1}{\sqrt{V}}$, $\mu^2 \ll \frac{1}{\sqrt{V}}$)

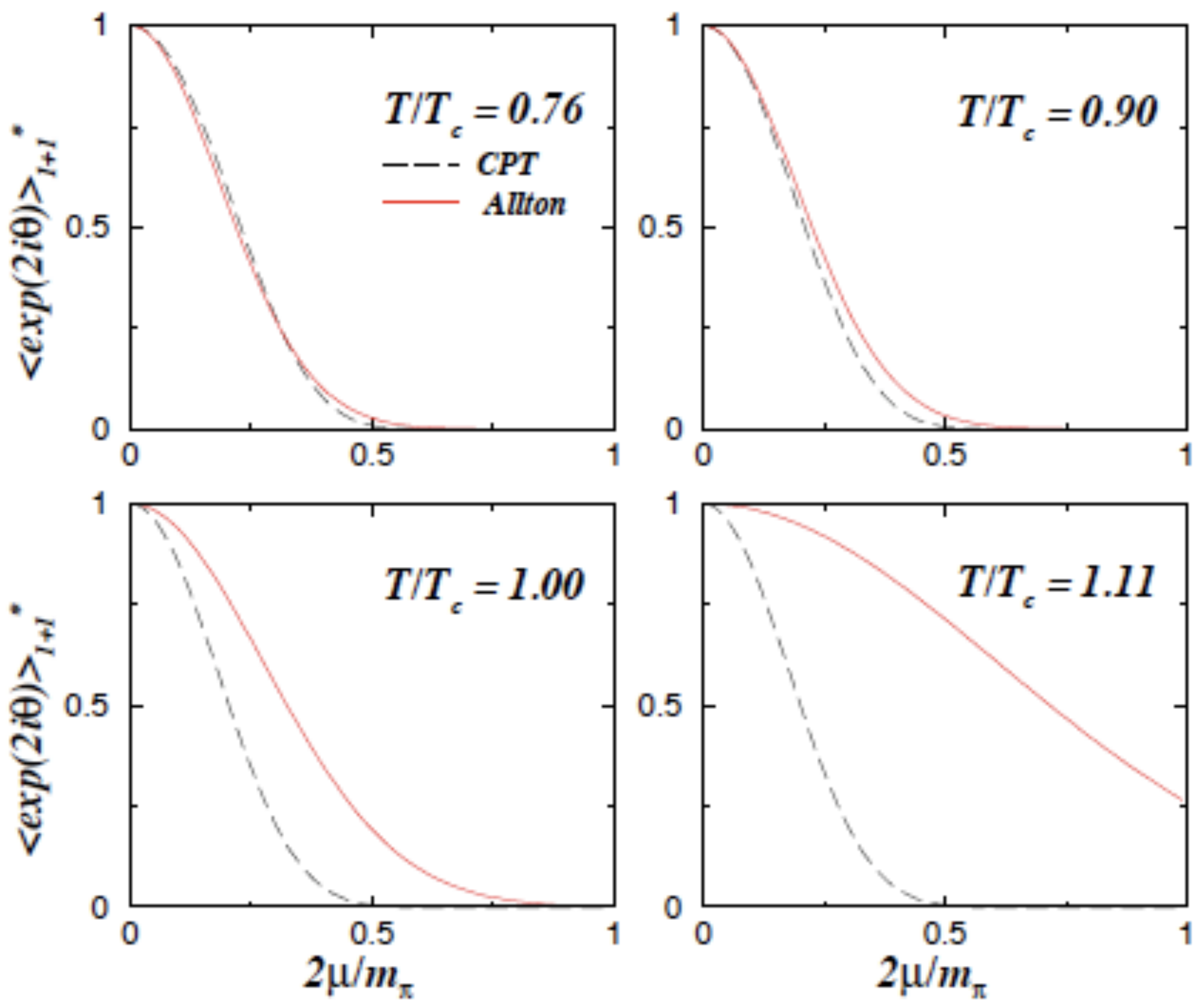
$$e^{2i\theta} = \left(1 - \frac{4\mu^2}{m_\pi^2}\right)^{N_f+1}$$

⟶ the sign problem is not severe for $\mu < m_\pi/2$

⟶ large difference in the fee energy densities of phase quenched and full theory

$$|\det M(\mu)|^{N_f} = \det M(+\mu)^{N_f/2} \times \det M(-\mu)^{N_f/2}$$

non zero iso-spin chemical potential



Splittorff, Verbaarschot, PRL98 (2007) 031601.

Lattice Data: Allton *et al.*, PRD71 (2005) 054508.

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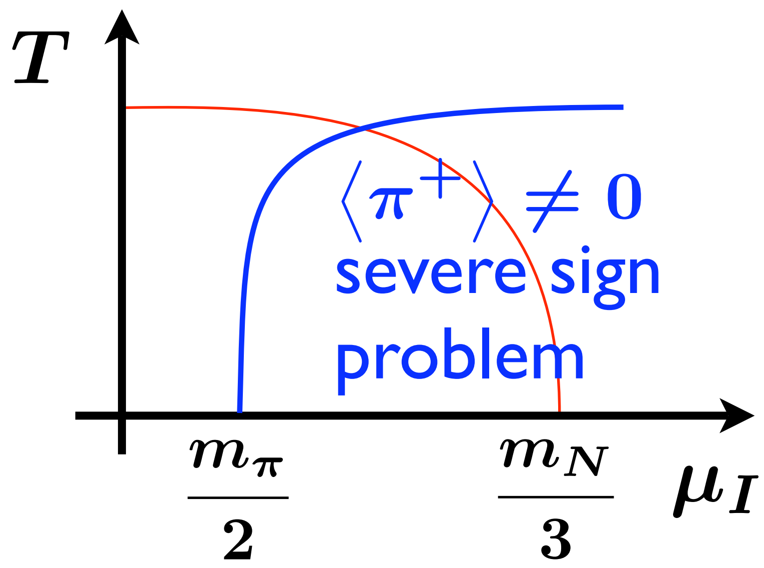


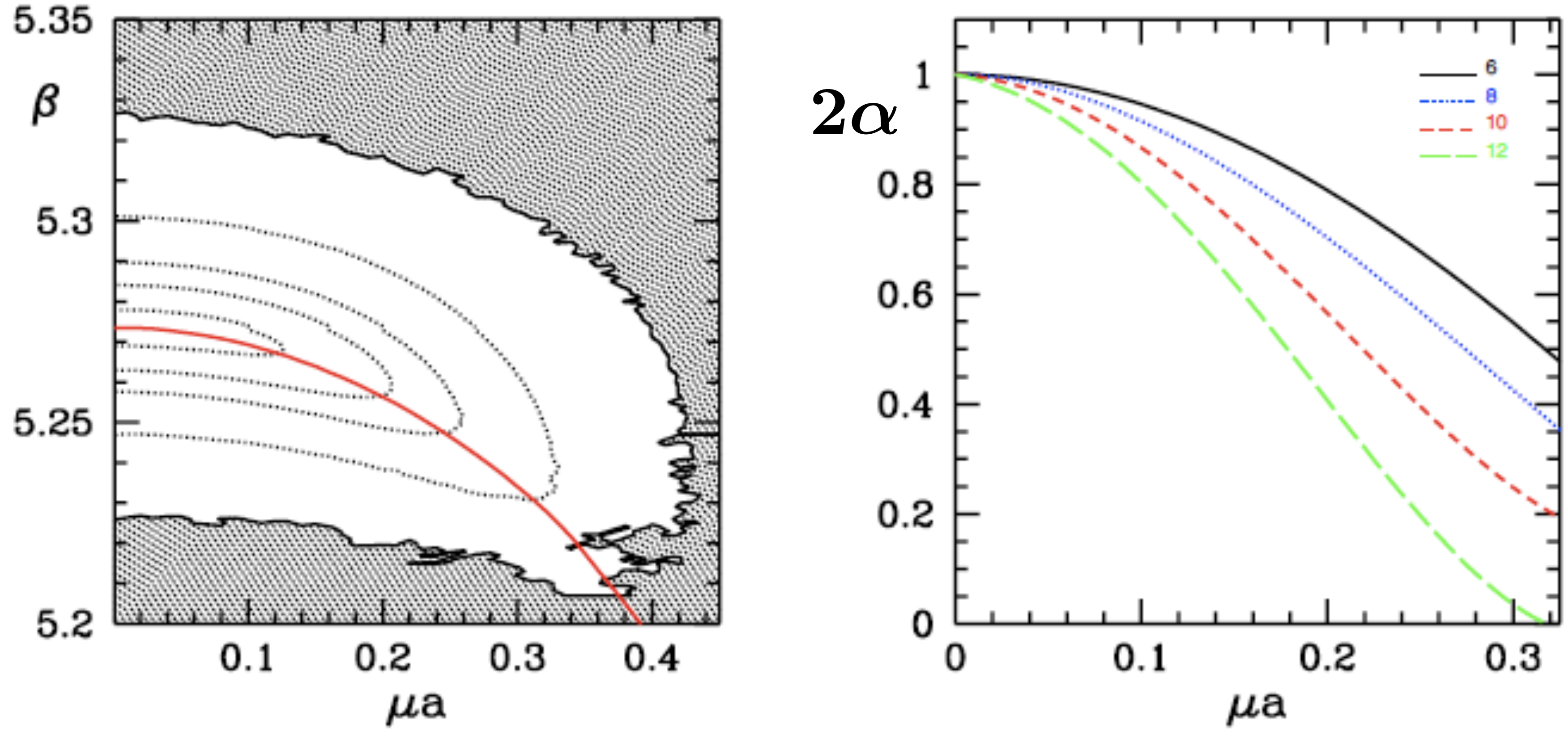
Reweighting strategies in QCD

- break down of the reweighting:

standard jack-knife errors do **not** reflect the break down of the method!

$\longrightarrow$ estimate the overlap measure 2α :
α is the fraction of the configurations that contributes the fraction $1-\alpha$ to the weight; optimal is $\alpha = 50\%$

contour lines of 2α



Csikor, et al., JEHP 0405 (2004) *046*.

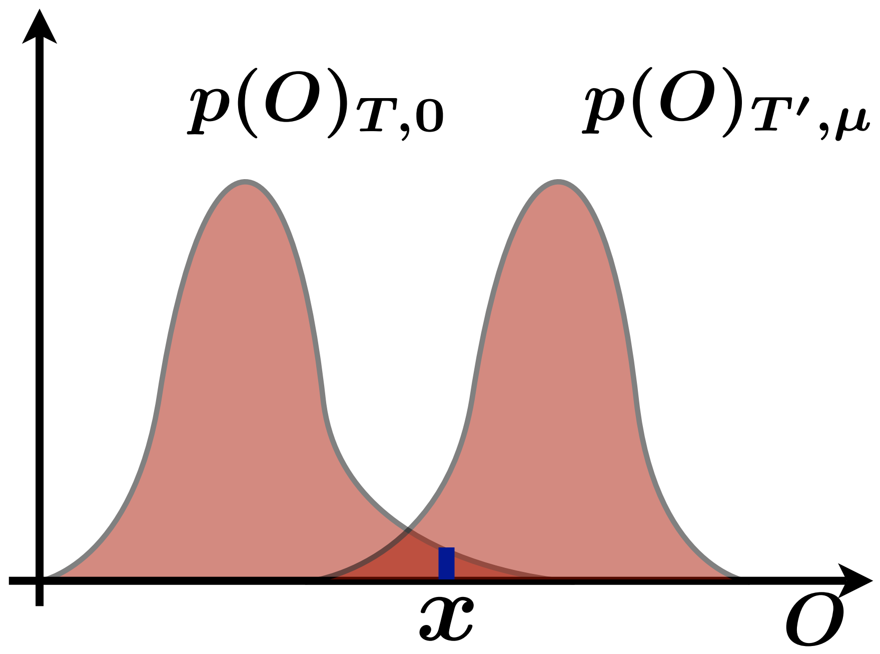
Reweighting strategies in QCD

- "density of state" modification of the reweighting

$$Z_{g,O}(\mu',\beta',x)=\int \mathcal{D}U\ \left|\det M(U,\mu')\right|^{N_f/4} e^{-\beta'\tilde{S}_G}\delta(x-O)$$

$\longrightarrow$ improve accuracy of the tail by simulating at a fixed value of O. In practice: replace delta function by a strongly peaked gaussian.

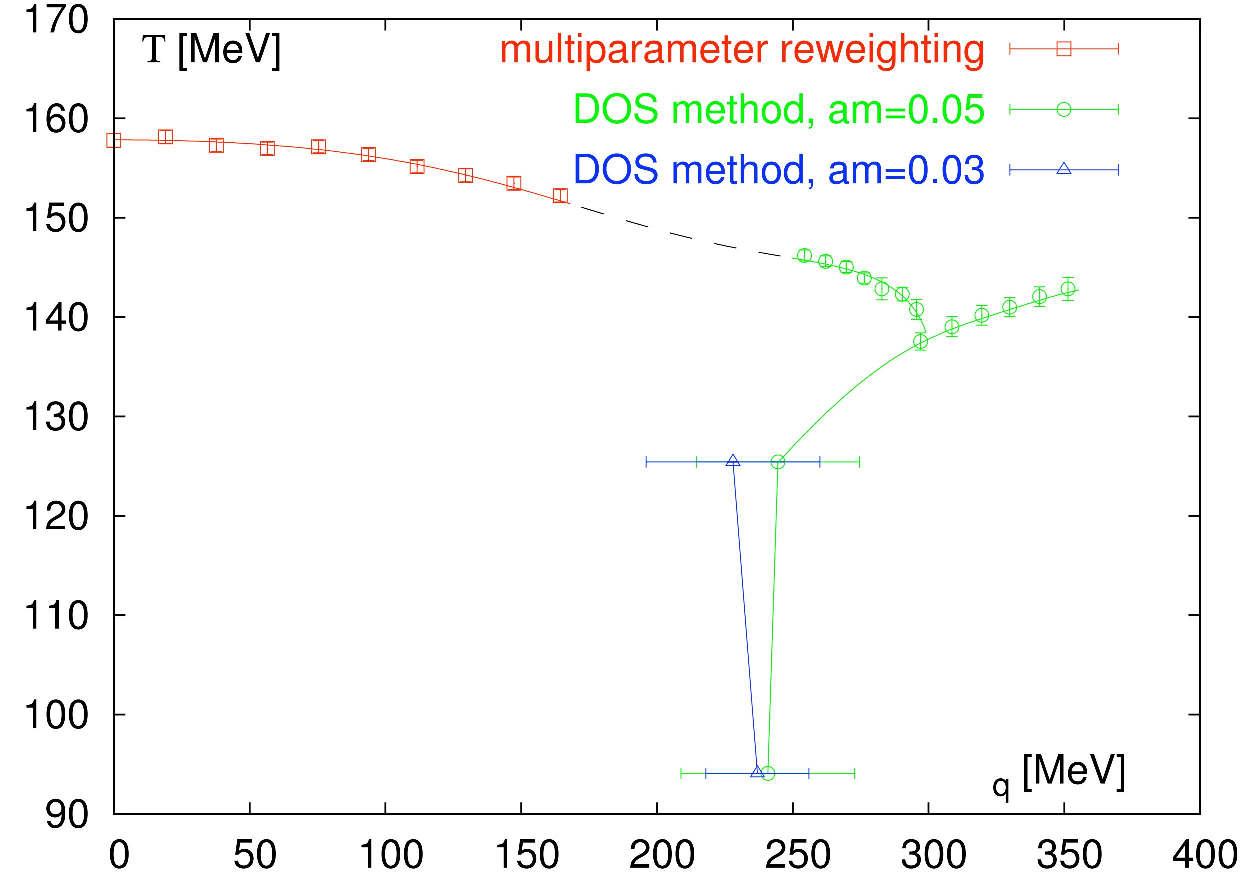
$\longrightarrow$ enlargement of the parameter space, sample many O-values



$N_f = 4$

$6^4,\ 6^3\times 8$

$am_q = 0.05,\ 0.03$



Fodor, Katz, CS, JHEP 0703:121,2007.

- canonical ensemble approach

from Z_{GC} to Z_{C}

⟶ fix quark number by introducing: $\delta(\hat{N}-Q)=\int \mathrm{d}\bar{\mu}\; e^{i\bar{\mu}(\hat{N}-Q)}$

⟶ recognize $\bar{\mu}$ as imaginary chemical potential: $i\bar{\mu}=i\mu_I/T$

⟶ exploit $2\pi/3$ symmetry of the GC partition function in $i\mu_I/T$

canonical partition function:

$$Z_{\mathrm{C}}(T,Q)=\frac{3}{2\pi}\int_{-\pi/3}^{\pi/3}\mathrm{d}\left(\frac{\mu_I}{T}\right)\; e^{-iQ\mu_I/T} Z_{\mathrm{GC}}(T,\mu_I)$$

$$\underset{Q\,=\,3B}{=}\frac{1}{2\pi}\int_{-\pi}^{\pi}\mathrm{d}\left(\frac{\mu_I}{T}\right)\; e^{-i3B\mu_I/T} Z_{\mathrm{GC}}(T,\mu_I)$$

⟶ $Z_{\mathrm{C}}(Q)$ are the coefficients in the Fourier expansion in $i\mu_I$

⟶ $Z_{\mathrm{C}}(Q)$ vanish for non integer baryon number $B=Q/3$

Reweighting strategies in QCD

- canonical ensemble approach

from Z_C to Z_GC

⟶ fugacity expansion (Laplace transformation)

$$Z_\mathrm{GC}(T,\mu) \underset{V\to\infty}{=} \int_{-\infty}^{\infty} \mathrm{d}\rho \, e^{3V\rho\mu/T} Z_\mathrm{C}(T,\rho)$$

$$= \int_{-\infty}^{\infty} \mathrm{d}\rho \, e^{-V(f(T,\rho)-3\rho\mu)/T}$$

with baryon density $\rho = B/V$

and Helmholtz fee enery $f(T,\rho) = -\frac{T}{V}\log Z_C(T,\rho)$

⟶ relation between ρ and μ :

<u>*fugacity expansion:*</u> $\langle\rho\rangle(\mu) = \frac{1}{Z_\mathrm{GC}(T,\mu)} \int_{-\infty}^{\infty} \mathrm{d}\rho \, \rho e^{3V\rho\mu/T} Z_\mathrm{C}(T,\rho)$

<u>*saddle point approxn.:*</u> $\mu(\rho) = \frac{1}{3}\frac{\partial f(T,\rho)}{\partial\rho}$

Reweighting strategies in QCD

- canonical ensemble approach

sampling strategy:

$\longrightarrow$ sample at fixed value of $i\mu_{I_0}$
(many ensembles can be combined by multi histogram reweighting)

$\longrightarrow$ calculate all eigenvalues of the reduced fermion matrix (cost $\sim N_\sigma^9$)

$\longrightarrow$ calculate ratio of partition functions as

$$\frac{Z_{\rm C}(\beta,B)}{Z_{\rm GC}(\beta,\mu)} = \left\langle \frac{\hat{Z}_{\rm C}(\beta,B)}{\det M(i\mu_{I_0})} \right\rangle_{\beta,i\mu_{I_0}}$$

$\longrightarrow$ overlap problem for large B

$\hat{Z}_{\rm C}$ Fourier coefficients of the determinant, calculated by matching term by term in

$$\det M(\mu) = e^{-3N_\sigma^3 \mu a N_\tau} \prod_{i=0}^{6N_\sigma^3} (e^{\mu a N_\tau} - \lambda_i) = \sum_{Q=-3N_\sigma^3}^{3N_\sigma^3} \hat{Z}_{\rm C} e^{-Q\mu a N_\tau}$$

de Forcrand, Kratochvila

progress:

$\longrightarrow$ Fourier transformation of $\log\det M$ — K.F. Liu *et al.*, Gattringer

$\longrightarrow$ reduced matrix also for Wilson quarks — Wenger, Gattringer, Nakamura

Reweighting strategies in QCD

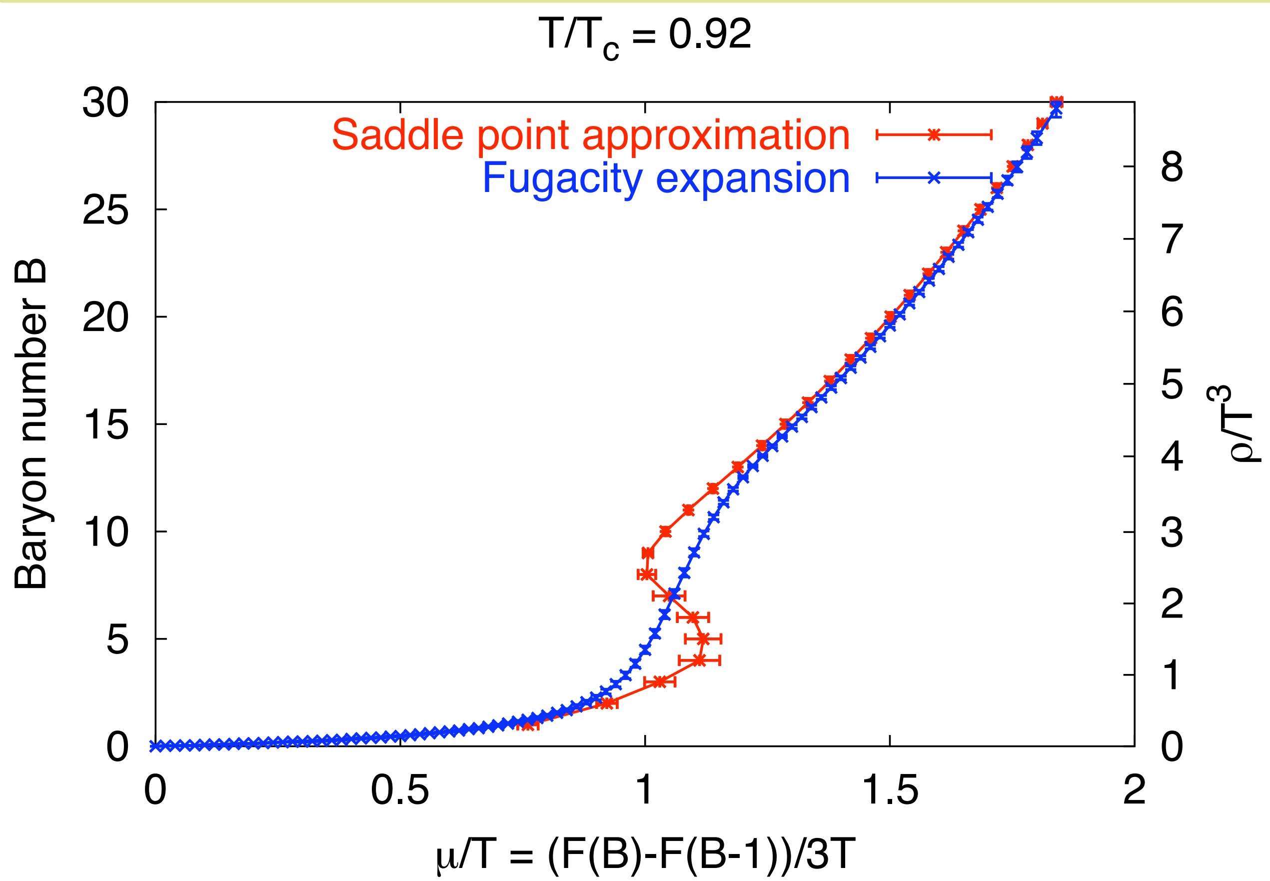
- canonical ensemble approach

results:

$\longrightarrow$ consider $F(B) \equiv -T \log \left(\frac{Z_C(B)}{Z_C(0)} \right)$

fugacity expansion: $$\rho(\mu) \equiv \frac{\langle B(\mu) \rangle}{V} = \frac{1}{V} \frac{\sum_{B=-V}^{V} B Z_C(B) e^{B3\mu/T}}{\sum_{B=-V}^{V} Z_C(B) e^{B3\mu/T}}$$

saddle point approxn.: $$\mu(B) \approx F(B) - F(B-1) = \log \left(\frac{Z_C(B)}{Z_C(B-1)} \right)$$



de Forcrand, Kratochvila

$6^3 \times 4$

$N_f = 4$

$m_\pi \approx 300$ MeV

staggered

find multi-valued density:

$\longrightarrow$ 1st order transition

Reweighting strategies in QCD

- canonical ensemble approach

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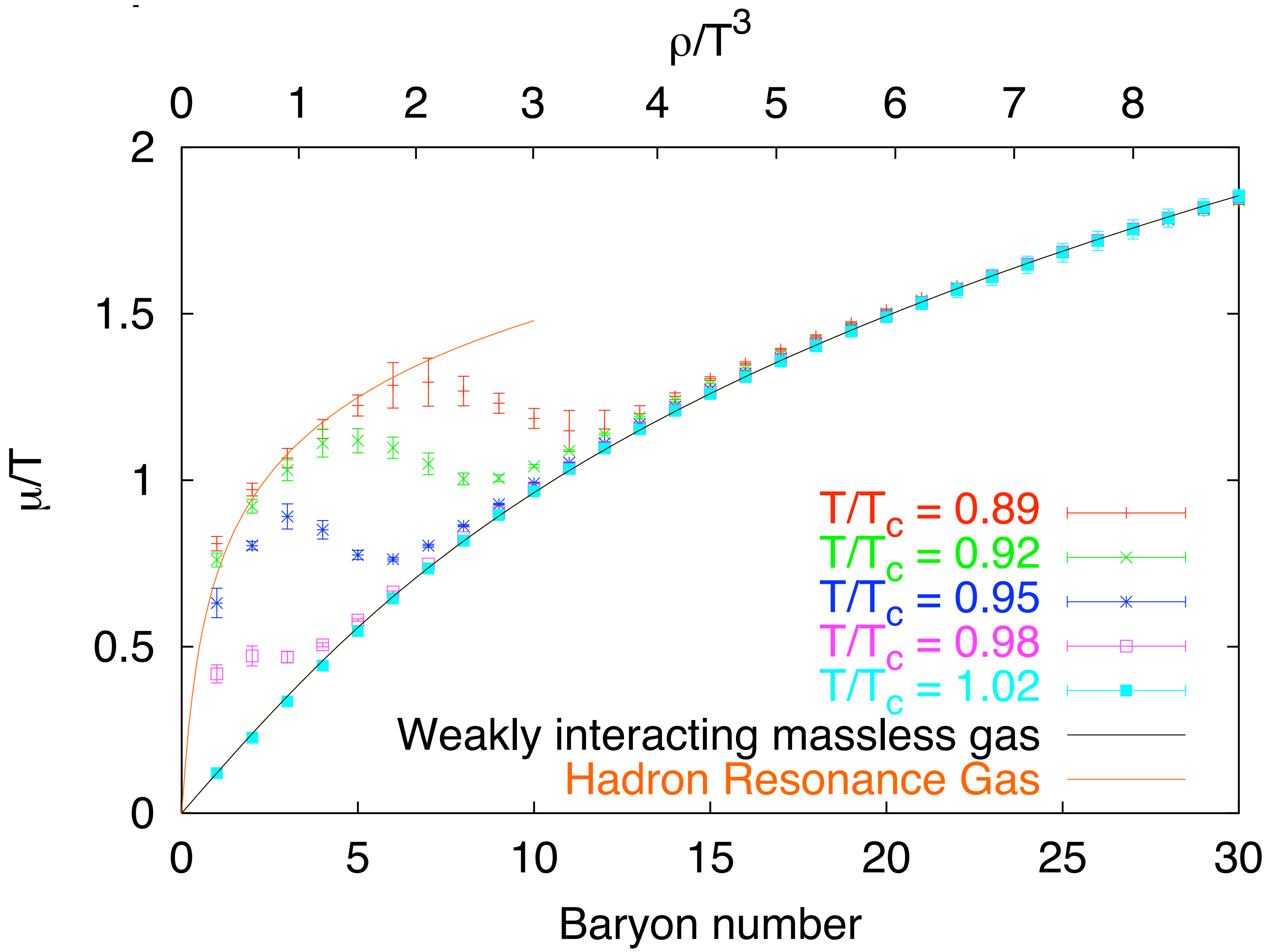


de Forcrand, Kratochvila

$6^3 \times 4$

$N_f = 4$

$m_\pi \approx 300$ MeV

staggered

⟶ good accuracy up to 30 baryons

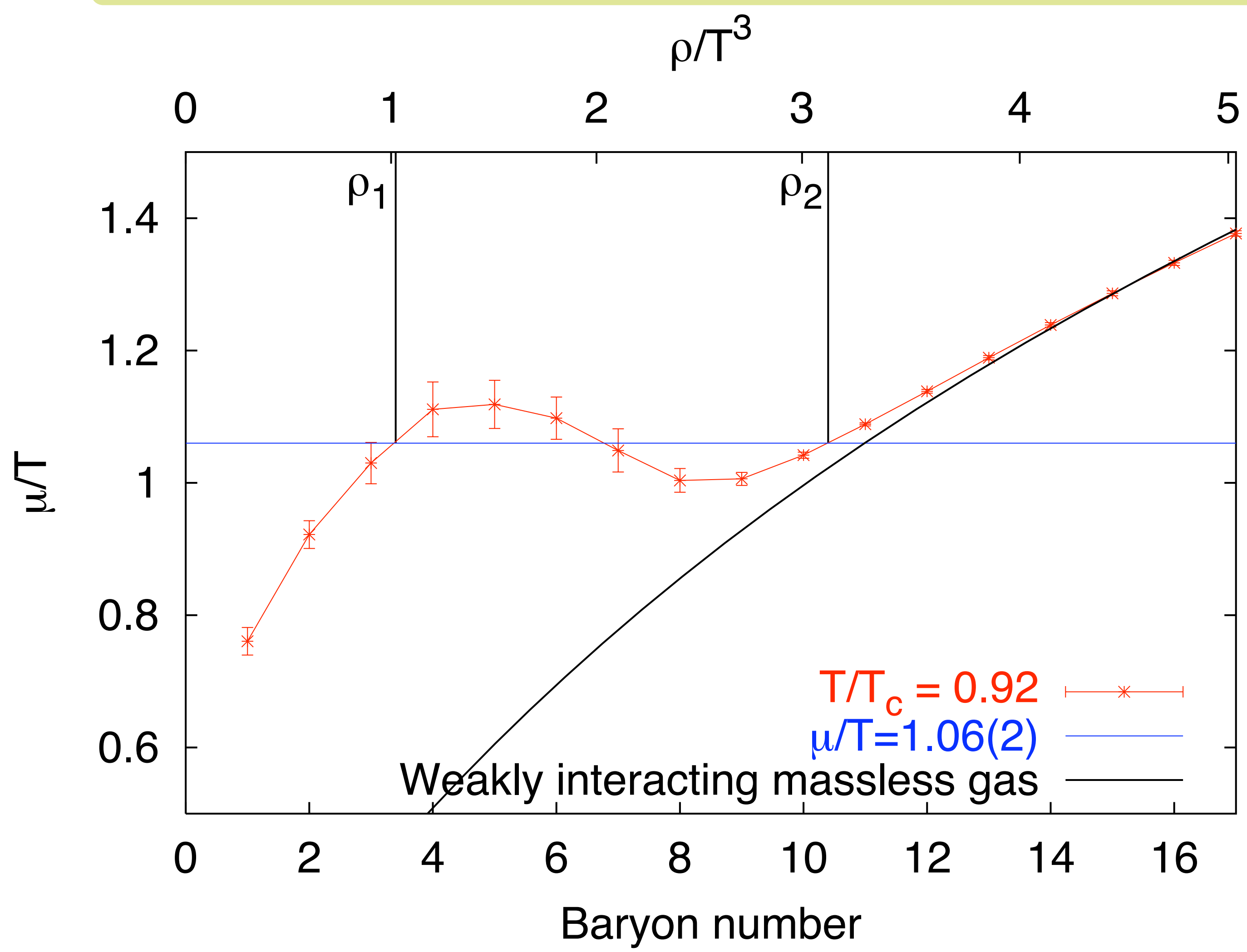
- canonical ensemble approach

results:

⟶ consider $F(B) \equiv -T \log\left(\frac{Z_C(B)}{Z_C(0)}\right)$

⟶ perform Maxwell construction:

$$\frac{1}{T}\int_{\rho_1}^{\rho_2} d\rho\,(f'(\rho)-\mu)=0 \quad \Rightarrow \quad f(\rho_1)-\rho_1\mu = f(\rho_2)-\rho_2\mu$$



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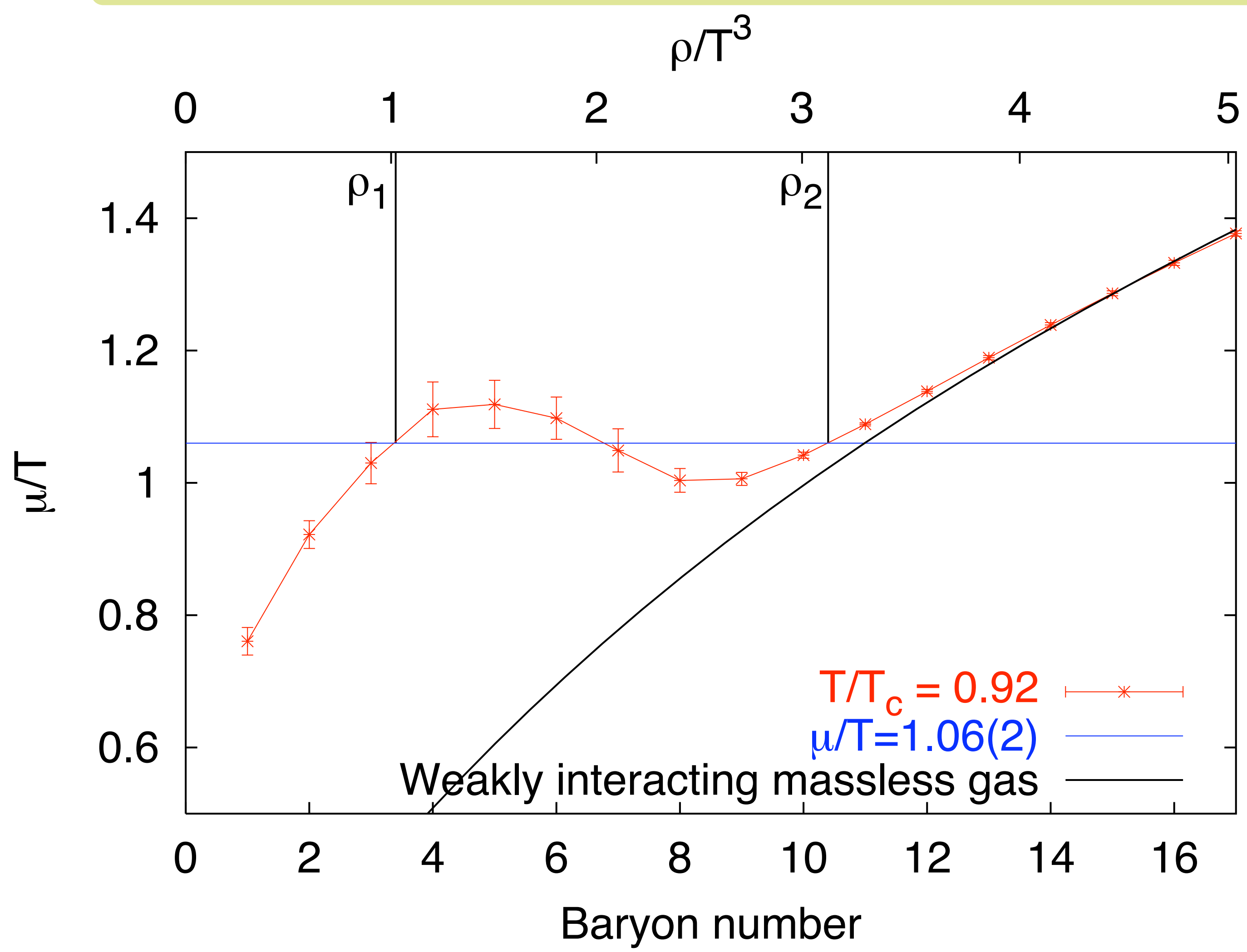

de Forcrand, Kratochvila

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$N_f = 4$
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staggered

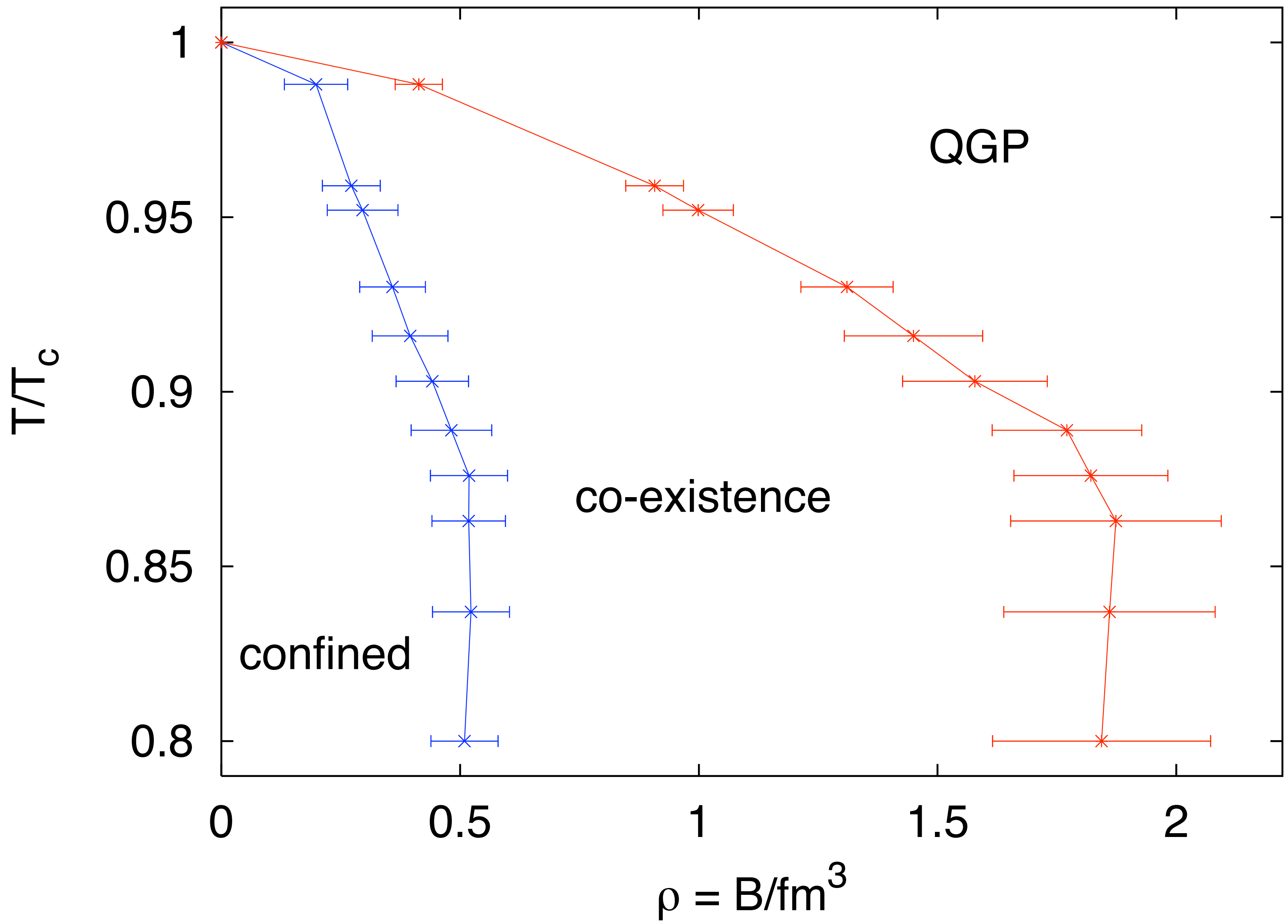
- canonical ensemble approach

results:

⟶ consider $F(B) \equiv -T \log\left(\frac{Z_C(B)}{Z_C(0)}\right)$

⟶ perform Maxwell construction

⟶ obtain the phase diagram



de Forcrand, Kratochvila

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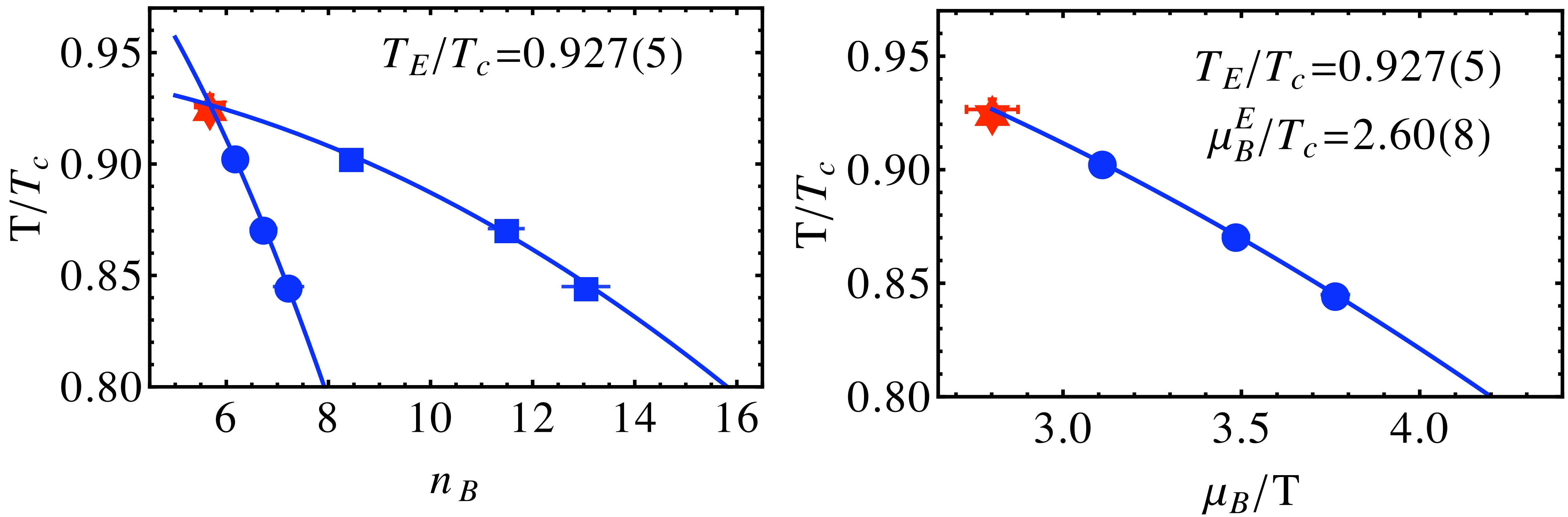


Li, Alexandru, Liu, arXiv: 1103.3045

$6^3 \times 4\,,\, N_f = 3\,,\, m_\pi \approx (700 - 800)$ MeV

Wilson-clover

Extrapolation methods

- change of strategy:

$\longrightarrow$ Reweighting is expensive and has a conceptional problem in the thermodynamic limit, but is "exact" at small volumes. Its reliabiliy is, however, hard to access.

$\longrightarrow$ confidence?

$\longrightarrow$ consider approximation methods, that have no problems in the thermodynamic limit:

$\longrightarrow$ imaginary chemical potential + fit + analytic continuations

$\longrightarrow$ systematic expansion around $\mu = 0$

Extrapolation methods

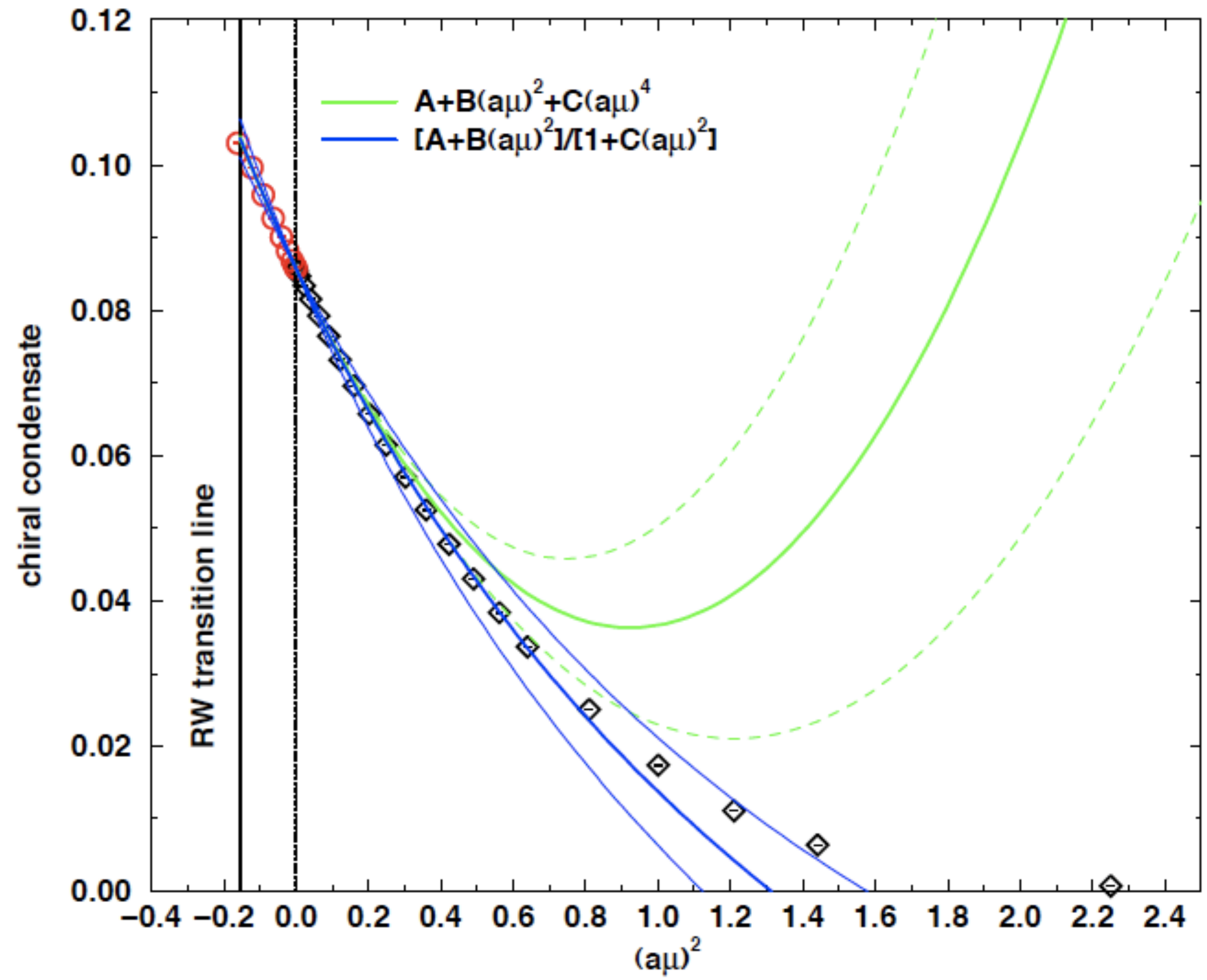
- imaginary chemical potential:

the method:

- perform HMC for $\mu^2 < 0$
- extrapolate to $\mu^2 > 0$ by fitting data to an a appropriate Ansatz and perform analytic continuation
- note: fitting range is limited by the periodicity of the partition function
$$\mu_I/T < 2\pi/3$$

- complex phase structure in the complex plane: Roberge, Weiss, NPB 275 (1986) 734
- Roberge-Weiss transition may also govern QCD thermodynamics at $\mathrm{Re}(\mu) > 0$ Philipsen, de Forcand, PRL 105 (2011) 152001.

two color QCD



Papa *et al.*, PoS Lat2006 (2006) 143

some lattice studies:

Philipsen, Forcrand, JHEP 0811 (2008) 012; D'Elia *et al.*, PRD 76 (2007) 114509;
Philipsen, Forcrand, JHEP 0701 (2007) 077; D'Elia *et al.*, PRD 70 (2004) 074509 ;
Philipsen, Forcrand, NPB 673 (2003) 170; D'Elia *et al.*, PRD 67(2003)014505 .

Extrapolation methods

- imaginary chemical potential:

results:

$\longrightarrow$ consider the Binder cumulant:

$$B_4 = \frac{\left\langle \left(\delta\bar{\psi}\psi\right)^4 \right\rangle}{\left\langle \left(\delta\bar{\psi}\psi\right)^2 \right\rangle^2}\Bigg|_{T=T_c, m=m_c} = \begin{cases} 3 & \text{crossover} \\ 1.604 & \text{2nd order} \quad Z(2) \\ 1 & \text{1st order} \end{cases}$$

$\longrightarrow$ universal, volume independent value at the critical point

Ansatz:

$$B_4(m,\mu) = 1.604 + BN_\sigma^{1/\nu}\left((m-m_c) + A\mu^2\right)$$

$\longrightarrow$ obtain the curvature of the critical surface as

$$\frac{\mathrm{d}m_c}{\mathrm{d}\mu^2} = -\frac{\partial B_4}{\partial \mu^2}\left(\frac{\partial B_4}{\partial m}\right)^{-1}$$

Extrapolation methods

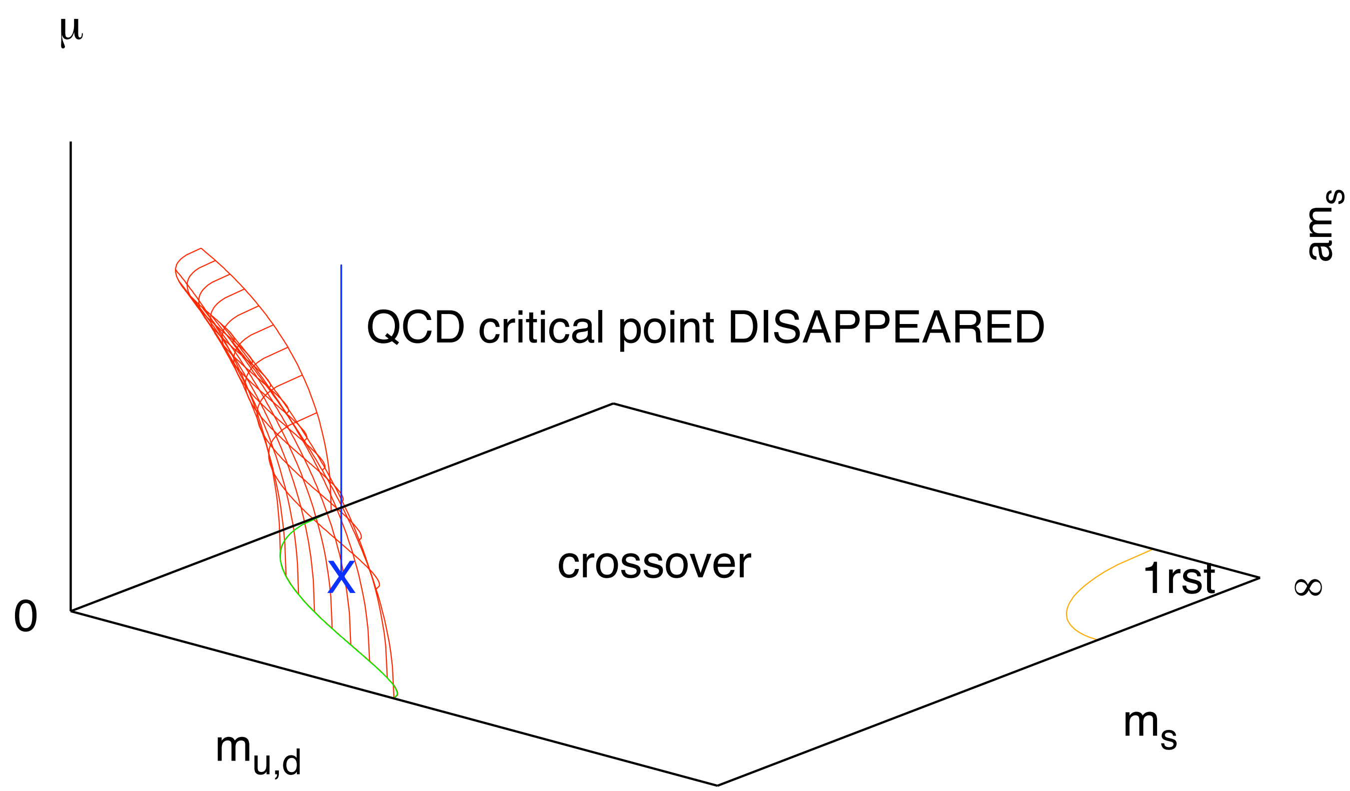
- imaginary chemical potential:

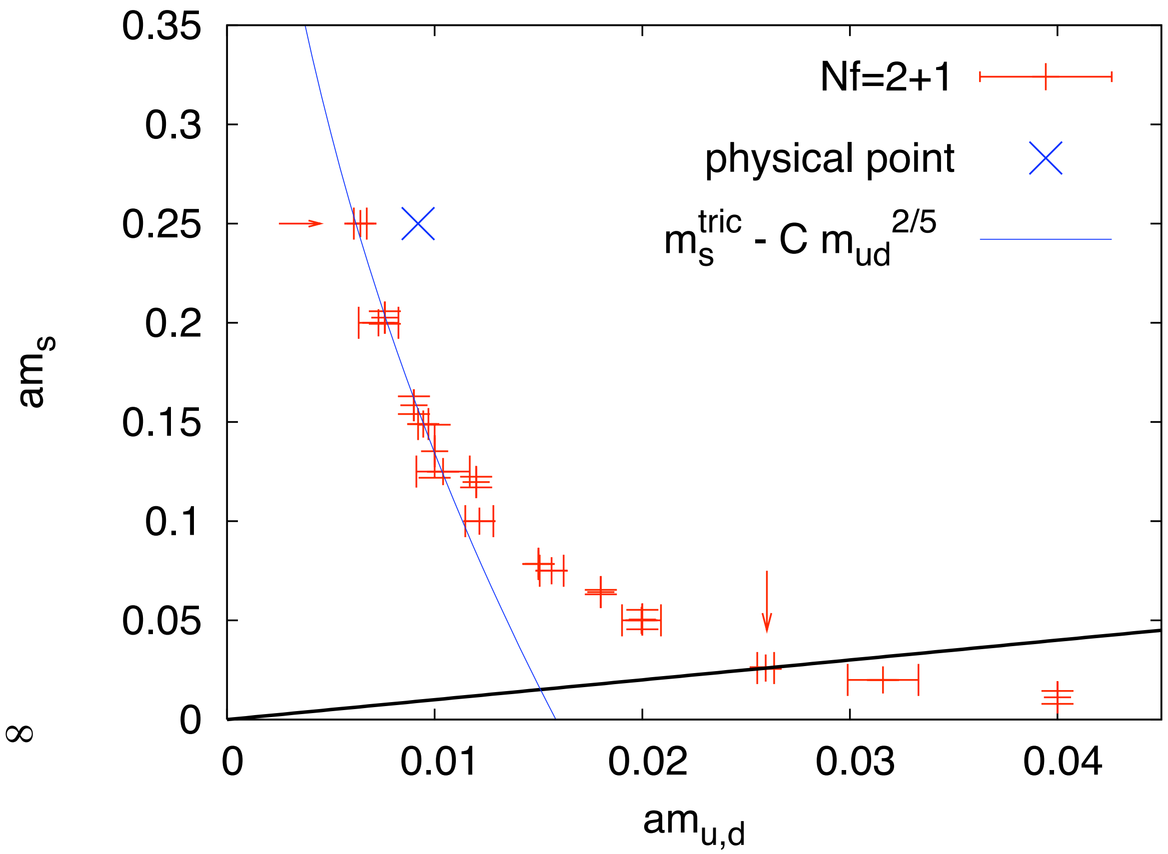
results:

$$\frac{m_c(\mu)}{m_c(0)} = 1 - 3.3(3)\left(\frac{\mu}{\pi T}\right)^2 - 47(20)\left(\frac{\mu}{\pi T}\right)^4 + \mathcal{O}(\mu^6) \quad (N_f = 3)$$

$$\frac{m_c^{u,d}(\mu)}{m_c^{u,d}(0)} = 1 - 39(8)\left(\frac{\mu}{\pi T}\right)^2 + \mathcal{O}(\mu^4) \quad (N_f = 2+1)$$

$\longrightarrow$ favored phase diagram:





de Forcrand, Philipsen, JHEP 0701 (2007) 77.

Summary

Part I:

- complex fermion determinant as origin of *sign problem*

- possible strategy is *reweighting* (includes canonical ensemble approach): shortcomings are the overlap problem, bad control over the break down of the method, problems with the thermodynamic limit and rather large costs

- simulations at pure *imaginary chemical potential* are feasible and can be analytically continued to real chemical potential

- *discussed results:* detection of a critical point for Nf=2+1 from standard reweighting and for Nf=3 for from the canonical approach, absence of critical point from imaginary chemical potential (for small values of the chemical potential)

Extrapolation methods

- Taylor expansion:
  - start from Taylor expansion of the pressure,

$$\frac{p}{T^4} = \frac{1}{VT^3} \ln Z(V,T,\mu_u,\mu_d,\mu_s) = \sum_{i,j,k} c_{i,j,k}^{u,d,s} \left(\frac{\mu_u}{T}\right)^i \left(\frac{\mu_d}{T}\right)^j \left(\frac{\mu_s}{T}\right)^k$$

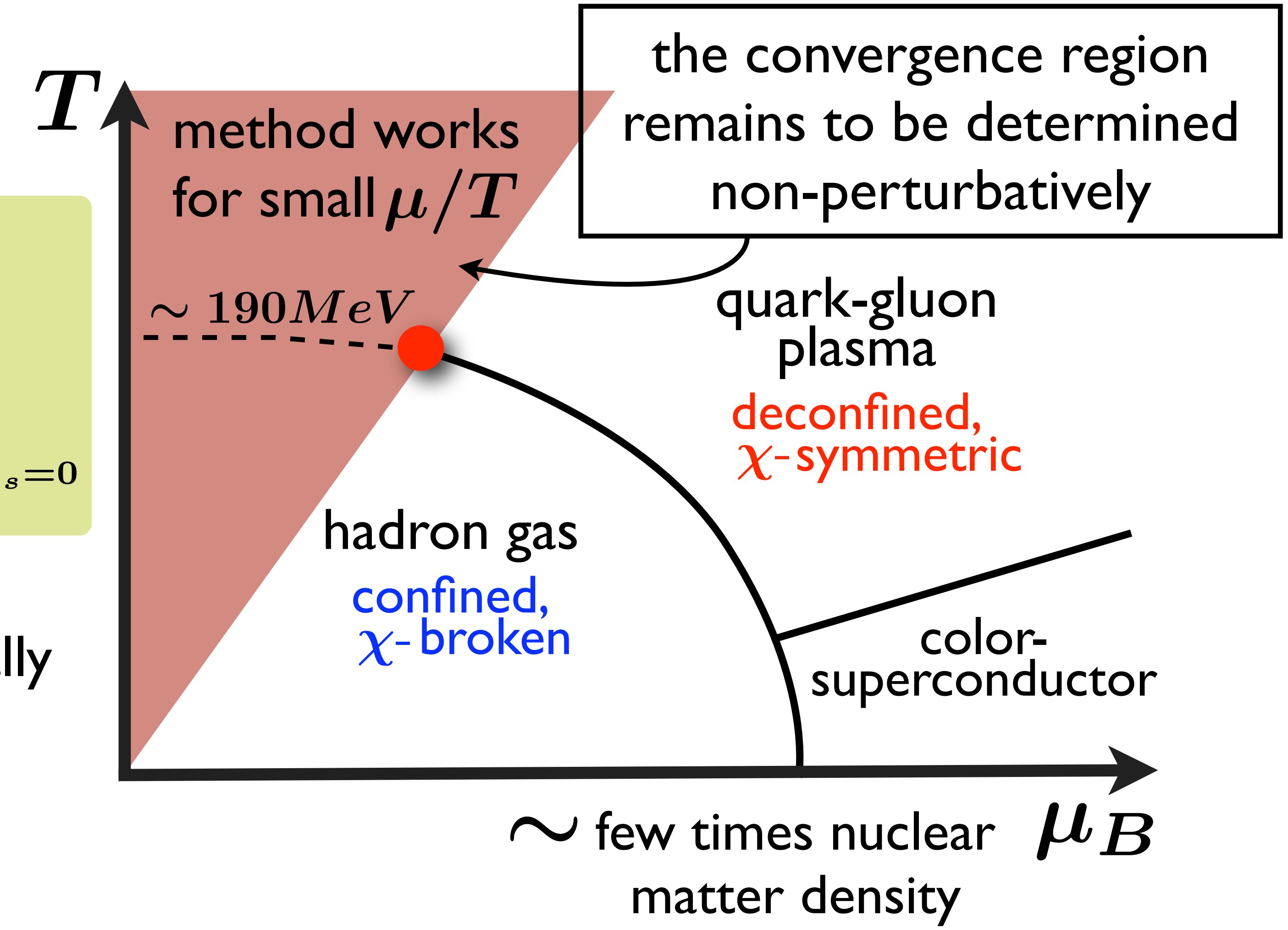
  - calculate expansion coefficients for fixed temperature

  - no sign problem: all simulations are done at $\mu = 0$

$$c_{i,j,k}^{u,d,s} \equiv \frac{1}{i!j!k!} \frac{1}{VT^3} \cdot \left. \frac{\partial^i \partial^j \partial^k \ln Z}{\partial(\frac{\mu_u}{T})^i \partial(\frac{\mu_d}{T})^j \partial(\frac{\mu_s}{T})^k} \right|_{\mu_{u,d,s}=0}$$

  - method is straight forward: all terms can be generated automatically

Allton *et al.*, PRD66:074507,2002;
Allton *et al.*, PRD68:014507,2003;
Allton *et al.*, PRD71:054508,2005.
(see also publications by MILC and Gavai, Gupta)



Extrapolation methods

- formulate all operators in term of space-time, color (and spin) traces:

$$
\begin{aligned}
\frac{\partial(\ln\det M)}{\partial\mu} &= \mathcal{D}_1 = \mathrm{Tr}\left(M^{-1}\frac{\partial M}{\partial\mu}\right)\\
\frac{\partial^2(\ln\det M)}{\partial\mu^2} &= \mathcal{D}_2 = \mathrm{Tr}\left(M^{-1}\frac{\partial^2 M}{\partial\mu^2}\right) - \mathrm{Tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}\right)\\
\frac{\partial^3(\ln\det M)}{\partial\mu^3} &= \mathcal{D}_3 = \mathrm{Tr}\left(M^{-1}\frac{\partial^3 M}{\partial\mu^3}\right) - 3\mathrm{Tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^2 M}{\partial\mu^2}\right)\\
&\quad +2\mathrm{Tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}\right)\\
\frac{\partial^4(\ln\det M)}{\partial\mu^4} &= \mathcal{D}_4 = \mathrm{Tr}\left(M^{-1}\frac{\partial^4 M}{\partial\mu^4}\right) - 4\mathrm{Tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^3 M}{\partial\mu^3}\right)\\
&\quad -3\mathrm{Tr}\left(M^{-1}\frac{\partial^2 M}{\partial\mu^2}M^{-1}\frac{\partial^2 M}{\partial\mu^2}\right) + 12\mathrm{Tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^2 M}{\partial\mu^2}\right)\\
&\quad -6\mathrm{Tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}\right)
\end{aligned}
$$

- evaluate all traces by noisy estimators:

$$\mathrm{Tr}\left(\frac{\partial^{n_1}M}{\partial\mu^{n_1}}M^{-1}\frac{\partial^{n_2}M}{\partial\mu^{n_2}}\cdots M^{-1}\right) = \lim_{N\to\infty}\frac{1}{N}\sum_{k=1}^{N}\eta_k^\dagger\frac{\partial^{n_1}M}{\partial\mu^{n_1}}M^{-1}\frac{\partial^{n_2}M}{\partial\mu^{n_2}}\cdots M^{-1}\eta_k$$

with N random vectors, satisfying $\lim_{N\to\infty}\frac{1}{N}\sum_{n=1}^{N}\eta^*_{n,i}\eta_{n,j} = \delta_{i,j}$

- construct expansion coefficients from $\mathcal{D}_n^u, \mathcal{D}_n^d, \mathcal{D}_n^s,$ with unbiased estimators

$$c_{2,0,0}^{u,d,s} = \frac{1}{2}\frac{N_\tau}{N_\sigma^3}\left(\left\langle\mathcal{D}_2^u\right\rangle + \left\langle\left(\mathcal{D}_1^u\right)^2\right\rangle\right)$$

Hadronic fluctuations

- Taylor expansion coefficients are the moments of hadronic fluctuations

$$2c_2^X = \frac{1}{VT^3}\left\langle N_X^2 \right\rangle \qquad 24c_4^X = \frac{1}{VT^3}\left(\left\langle N_X^4 \right\rangle - 3\left\langle N_X^2 \right\rangle^2\right)$$

$$X = B, Q, S, I, \ldots$$

Main ingredients:

- fast solver for the linear equation $Ax = b$, with A being a large and sparse matrix
  - iterative Krylov Subspace Methods are well suited for parallelization

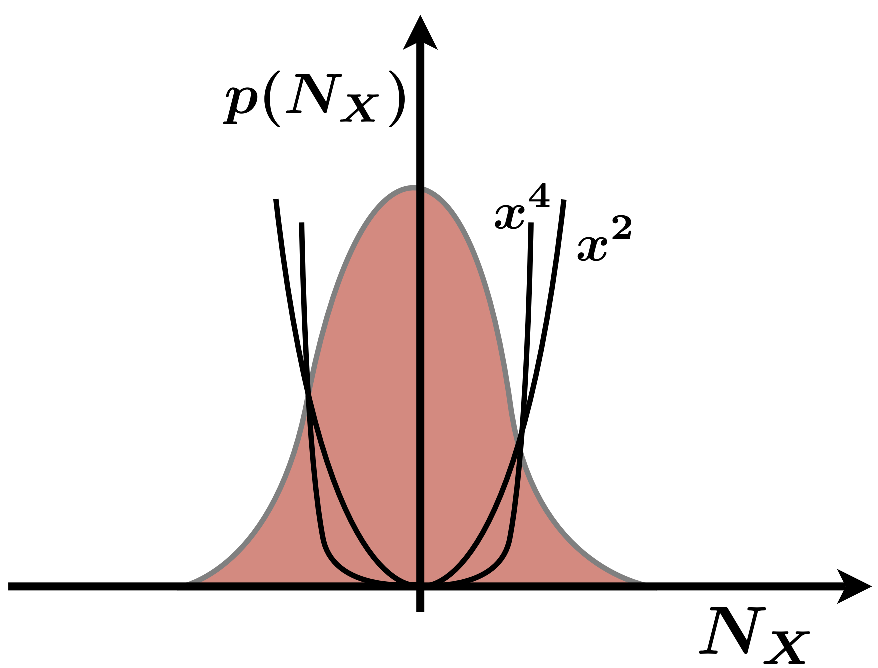
  ⟶ relatively large systems can be handled on massive parallel machines

- stochastic estimator of $\mathrm{Tr}\,A$
  - use noise reduction techniques

expansion coefficients with respect to μ_X are connected to the moments of the n_X-distribution

  - higher order moments are getting more and more sensitive to the tail of the distribution

  ⟶ high statistics required



nth-moment:

$$m_n = \int dx\, x^n p(x)$$

Hadronic fluctuations

- fluctuations in equivalent ensembles

  introduce a chemical potential for each conserved charge $\mathcal{Q}$

  $\longrightarrow$ in QCD: $SU(N_f)$ vector symmetry, introduce $\mu_f \; (f = u, d, s, \dots)$ through

$$J = \sum_f \mu_f \hat{N}_f = \mu^{\mathrm{T}} \hat{N}$$

  $\hat{N}_f$: number operator for quark with flavor f

  charges more convenient for experiment: B, Q, I_3, Y

  $\longrightarrow$ perform a coordinate change in Gibbs space

$$J = \mu^{\mathrm{T}} M^{-1} M \hat{N} = (\mu')^{\mathrm{T}} \hat{N}'$$

  example: B, Q, S-ensembles

$$B = \frac{1}{3}(N_u + N_d + N_s)$$
$$Q = \frac{1}{3}(2N_u - N_d - N_s)$$
$$S = -N_s$$

  defines transformation M

  $\longrightarrow$ invert M

$$\mu_B = \mu_u + 2\mu_d$$
$$\mu_Q = \mu_u - \mu_d$$
$$\mu_S = \mu_d - \mu_s$$

Hadronic fluctuations

- fluctuations in equivalent ensembles

introduce a chemical potential for each conserved charge Q

$\longrightarrow$ in QCD: $SU(N_f)$ vector symmetry, introduce $\mu_f \; (f = u, d, s, \dots)$ through

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example: B, Q, S-ensembles

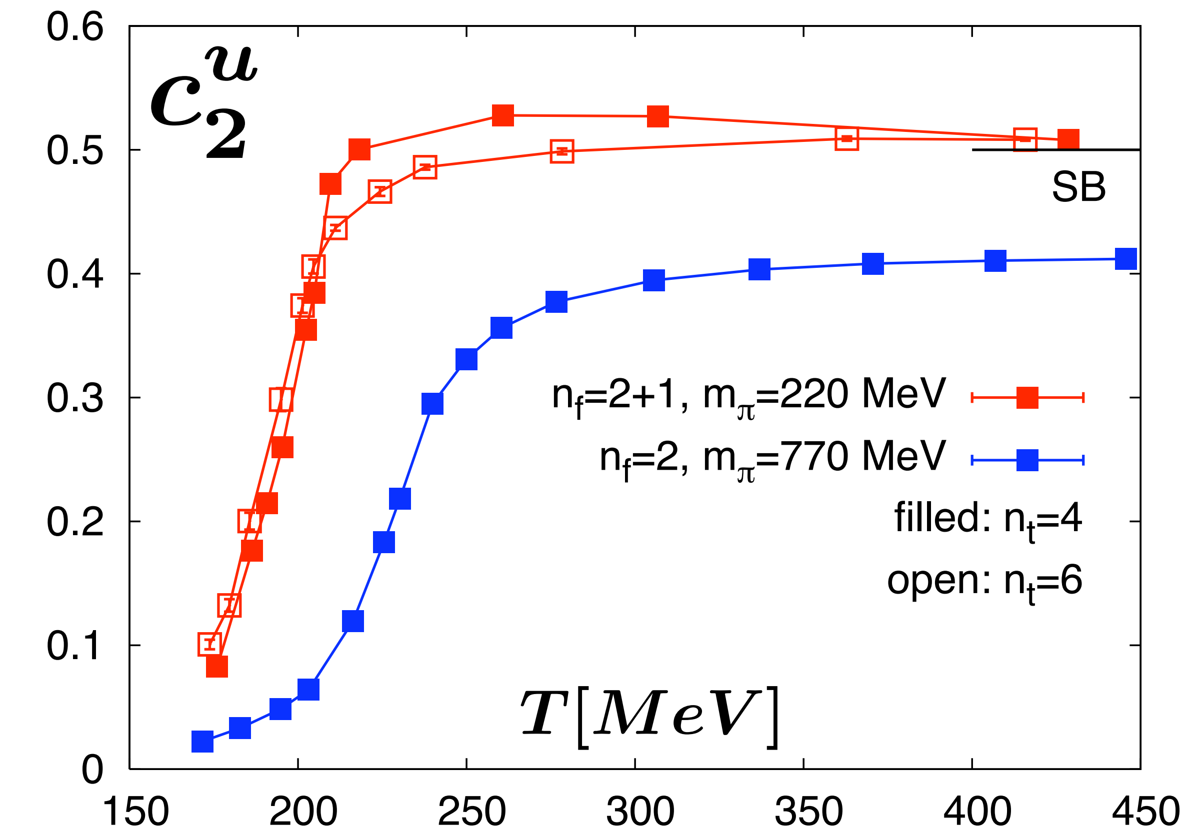
baryon number fluctuations:

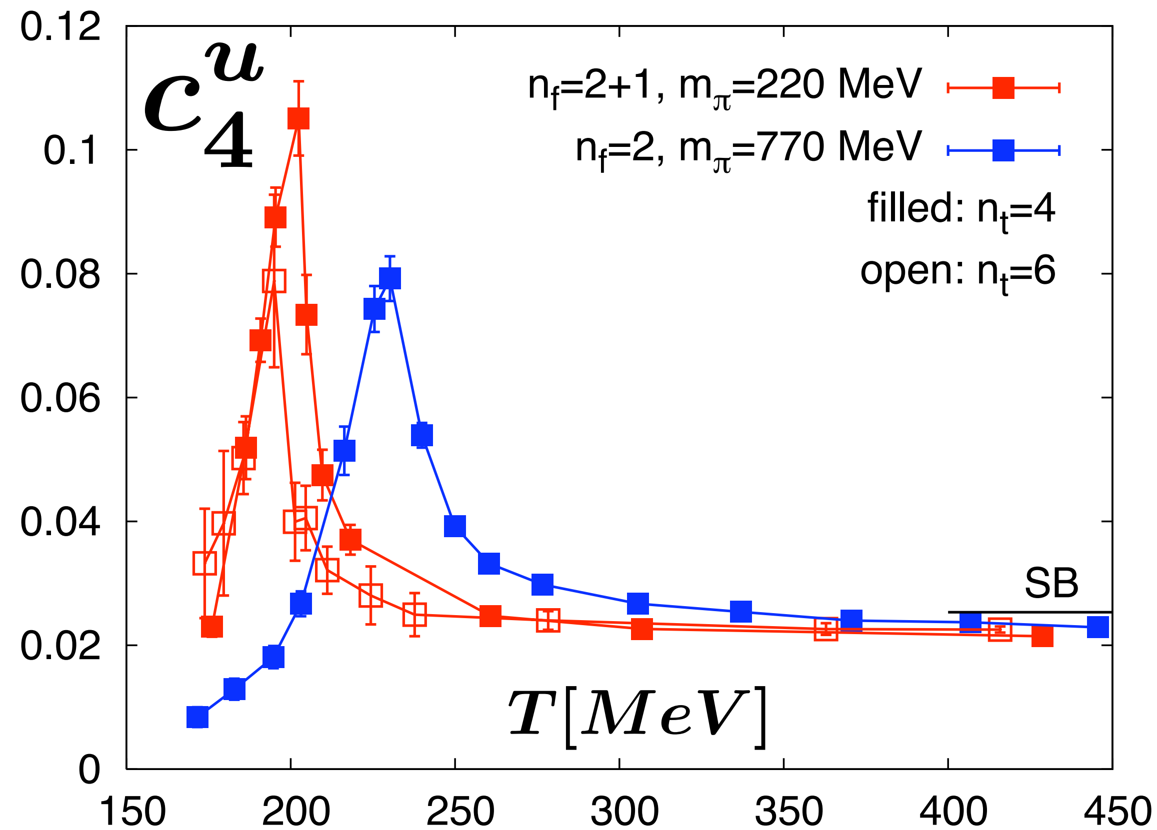
$$\chi_2^B = \frac{1}{9}(\chi_2^u + \chi_2^d + \chi_2^s + 2\chi_{1,1}^{u,d} + 2\chi_{1,1}^{u,s} + 2\chi_{1,1}^{d,s}) = \frac{1}{9}(2\chi_2^u + \chi_2^s + 2\chi_{1,1}^{u,d} + 4\chi_{1,1}^{u,s})$$

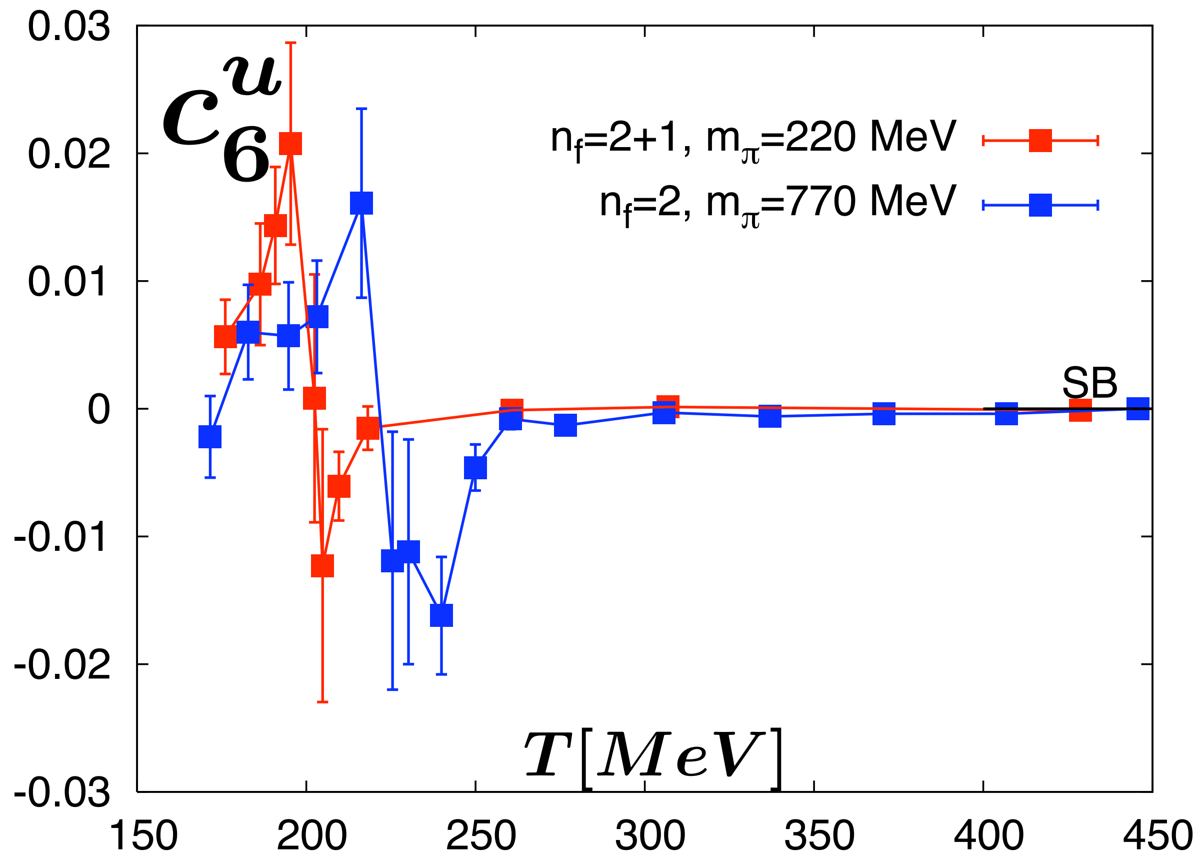
choose u, d-quarks degenerate

Hadronic fluctuations

- the building blocks:







p4-action, $N_\tau = 4, 6$:

⟶ Tc decreases with decreasing mass

⟶ fluctuations increase with decreasing mass

⟶ expect cutoff dependence, goto HISQ, $N_\tau = 6, 8, 12$

red: Cheng *et al.*, PRD79 (2009) 074505.
blue: Allton *et al.*, PRD71 (2005) 054508.

Hadronic fluctuations

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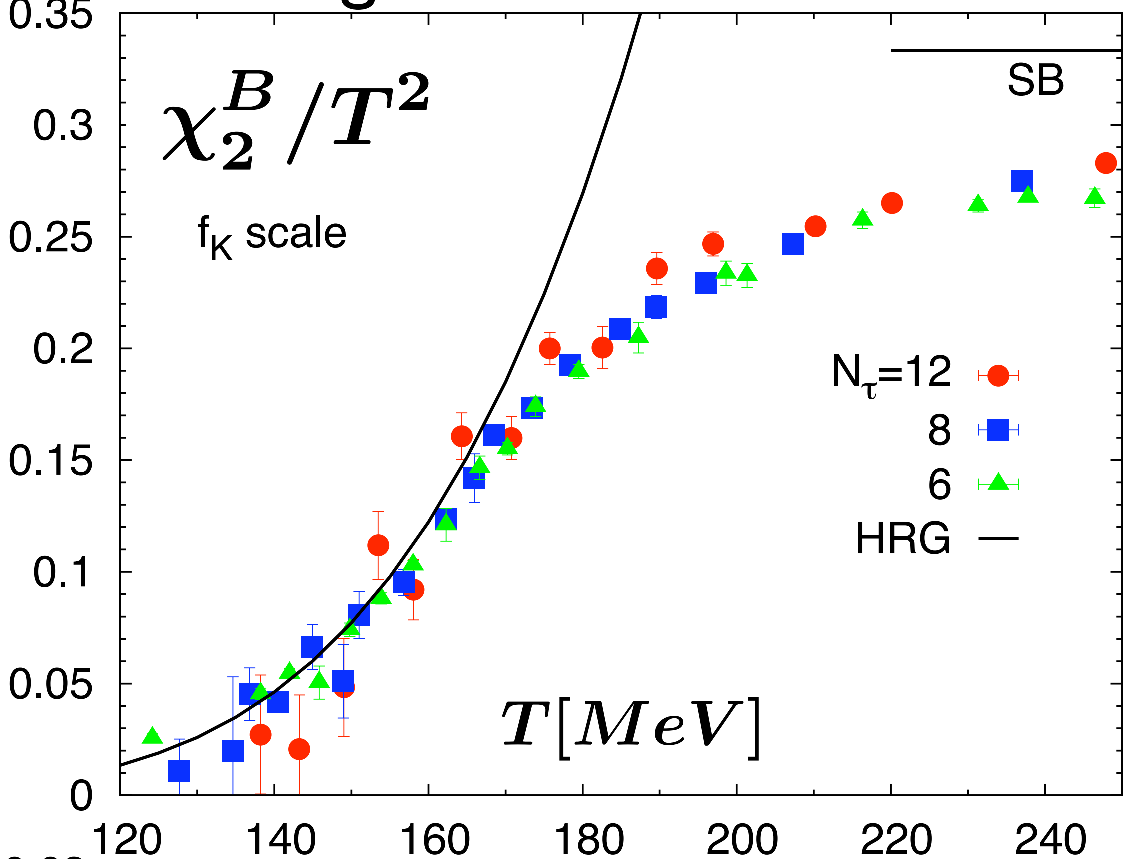

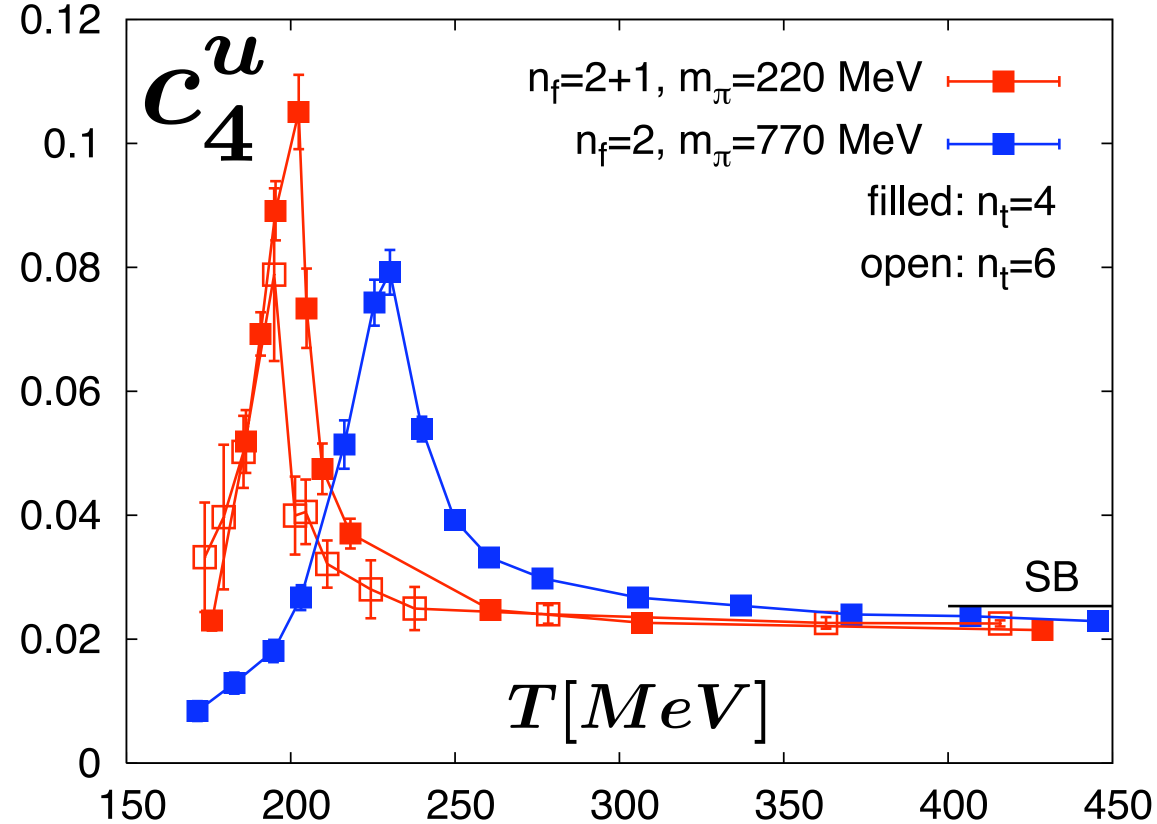

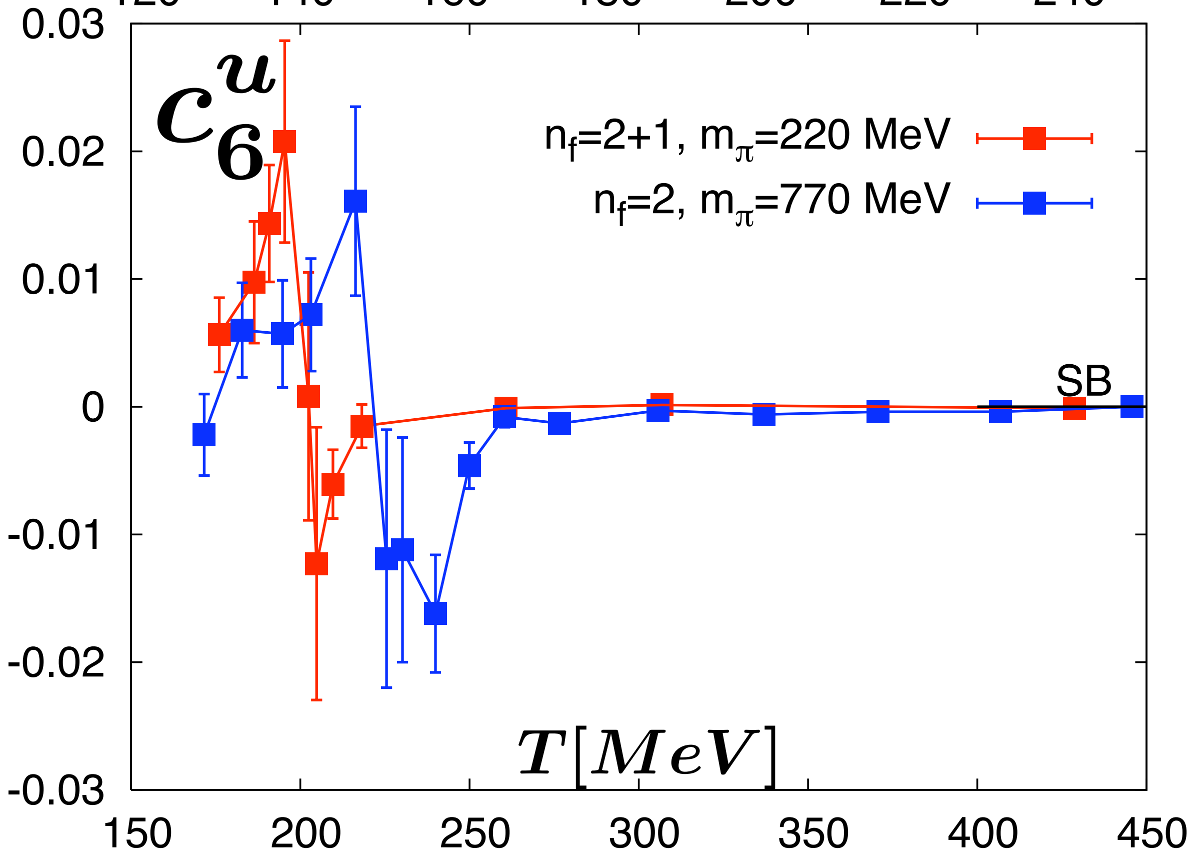

p4-action, $N_\tau = 4, 6$:

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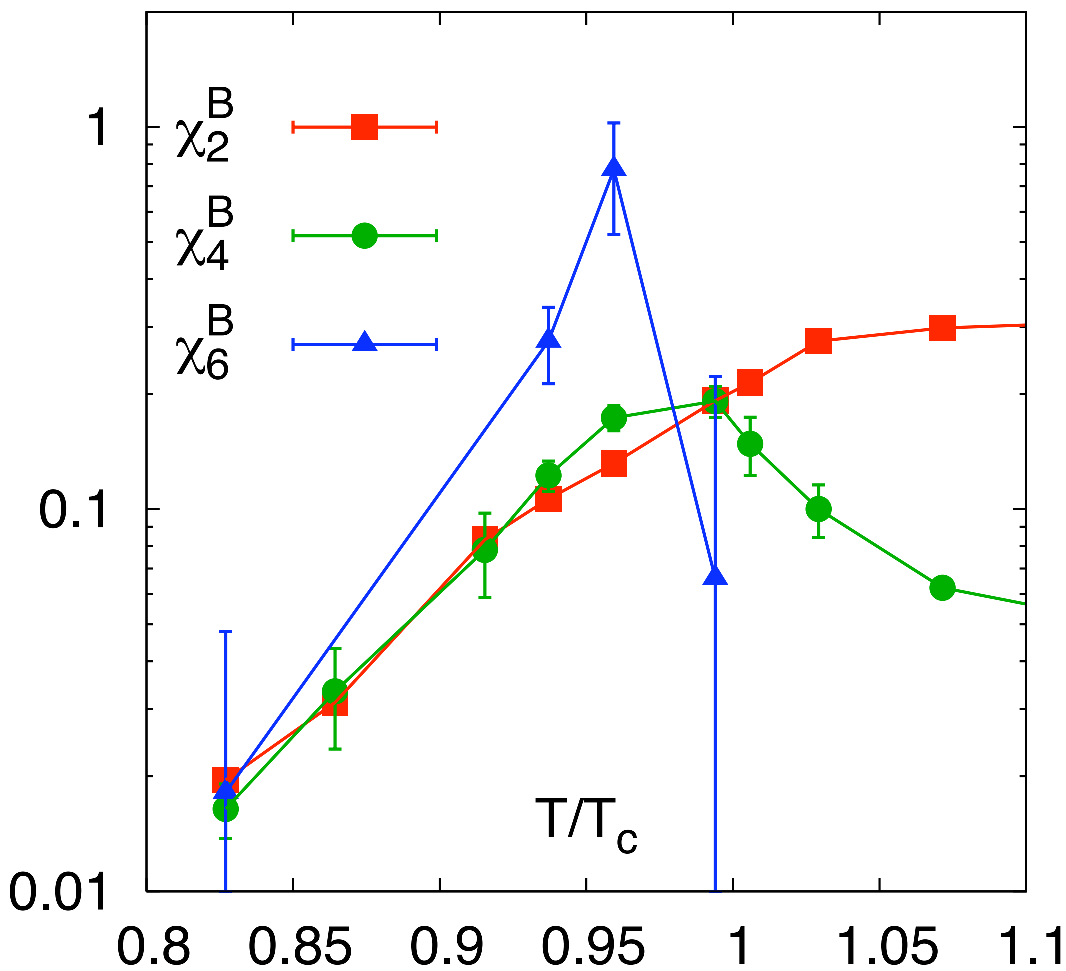
Baryonic fluctuations

- understanding the structure:

$$16^3 \times 4,\ m_q = m_s/10$$



Analyzing the critical behavior:

scaling field (chiral limit):

$$t = \frac{1}{t_0}\left(\frac{T-T_c}{T_c} + \kappa\left(\frac{\mu_B}{T}\right)^2\right)$$

free energy:

$$f = A_\pm |t|^{2-\alpha} + \text{regular}$$

critical exponent:

$$-0.15 < \alpha < -0.11$$

$$\chi_2^B \sim \mp 2A_\pm(2-\alpha)\kappa\,|t|^{1-\alpha} + \text{regular}$$

$$\chi_4^B \sim -12A_\pm(2-\alpha)(1-\alpha)\kappa^2\,|t|^{-\alpha} + \text{regular}$$ → kink (chiral limit)

$$\chi_6^B \sim \mp 120A_\pm(2-\alpha)(1-\alpha)(-\alpha)\kappa^3\,|t|^{-1-\alpha} + \text{regular}$$ → divergent (chiral limit)

Baryonic fluctuations

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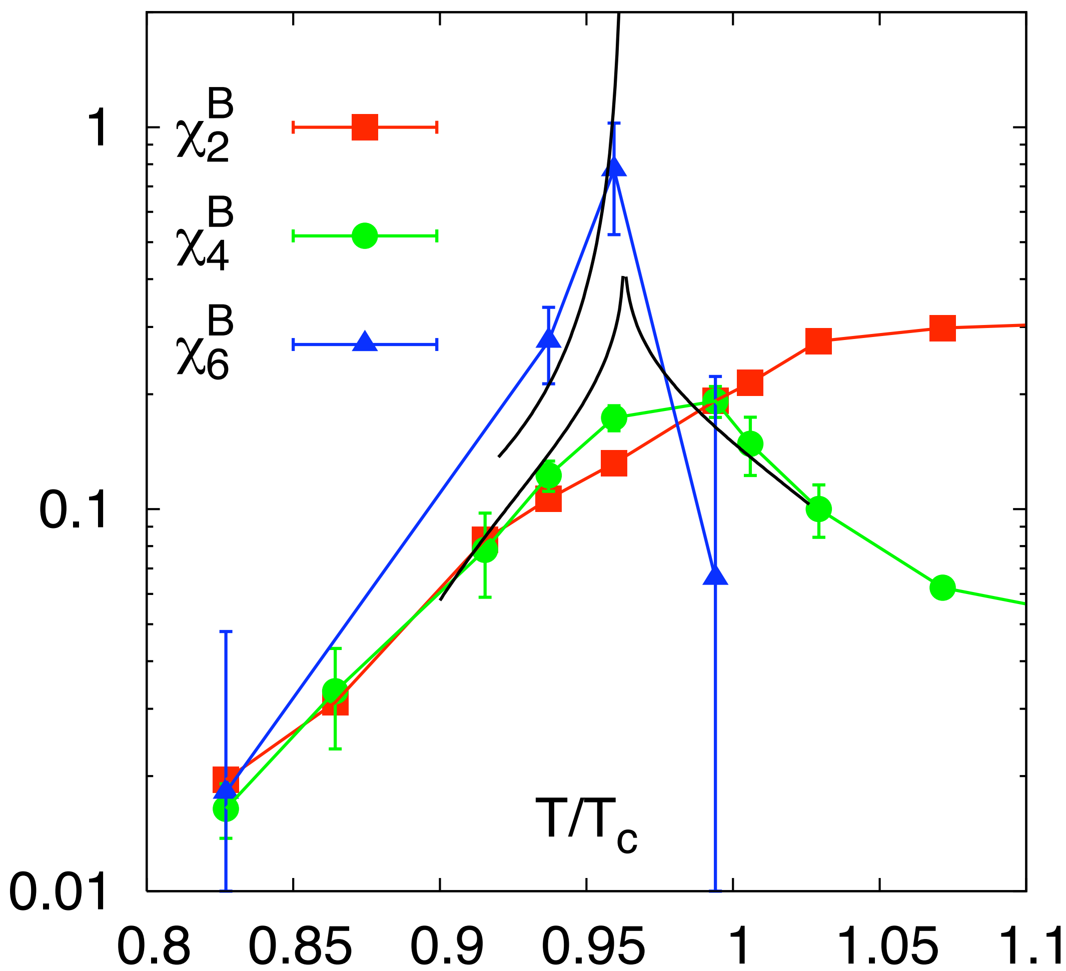

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Hadronic fluctuations

- putting things together:

pressure

$$\frac{p}{T^4} = c_0 + c_2 \left(\frac{\mu}{T}\right)^2 + c_4 \left(\frac{\mu}{T}\right)^4 + c_6 \left(\frac{\mu}{T}\right)^6 + \cdots$$

density

$$\frac{n}{T^3} = 2c_2 \left(\frac{\mu}{T}\right) + 4c_4 \left(\frac{\mu}{T}\right)^3 + 6c_6 \left(\frac{\mu}{T}\right)^5 + \cdots$$

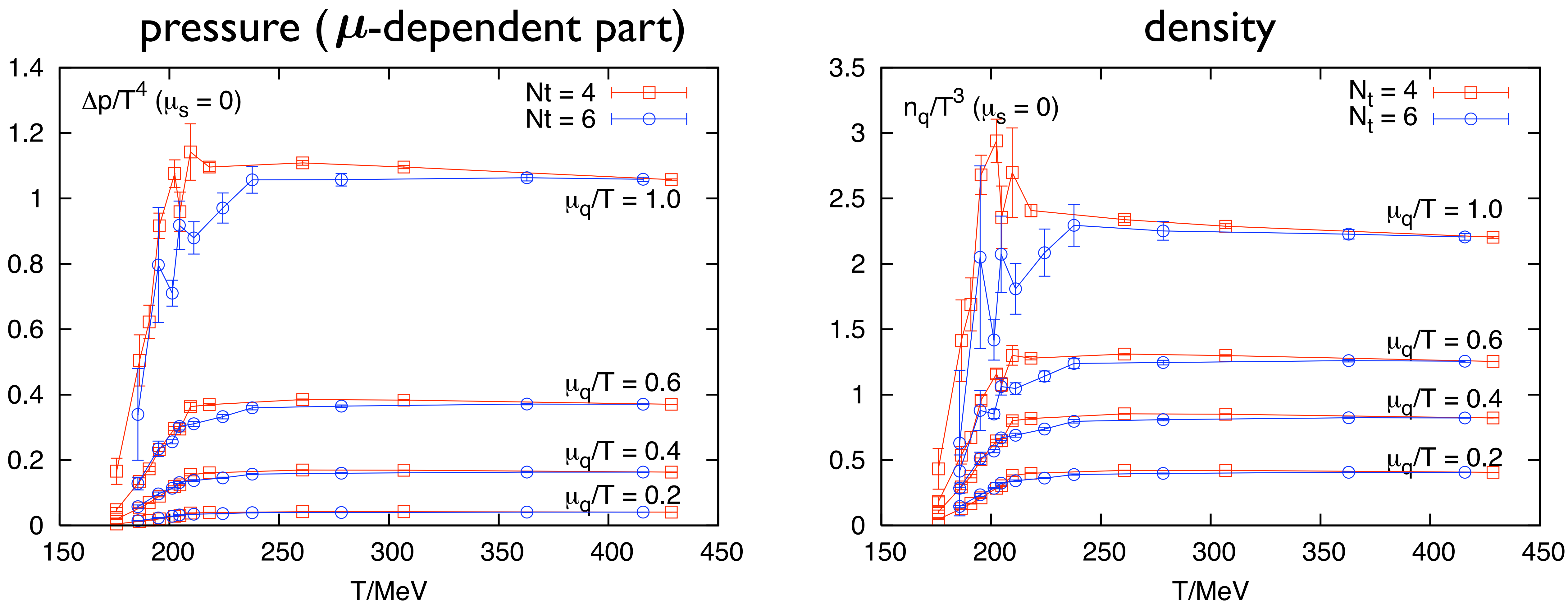
density fluctuations

$$\frac{\chi}{T^2} = 2c_2 + 12c_4 \left(\frac{\mu}{T}\right)^2 + 30c_6 \left(\frac{\mu}{T}\right)^4 + \cdots$$

$\longrightarrow$ obtain all kinds of thermodynamic observables in terms of the coefficients $c_{i,j,k}^{u,d,s}$ at non zero density

Hadronic fluctuations

- putting things together:



⟶ nonzero density contribution is $\leq (10-15)\%$ for $\mu_q/T \leq 1$

⟶ obtain energy density from temperature derivative

⟶ important input for hydrodynamic models of heavy ion collisions: isentropic equation of state

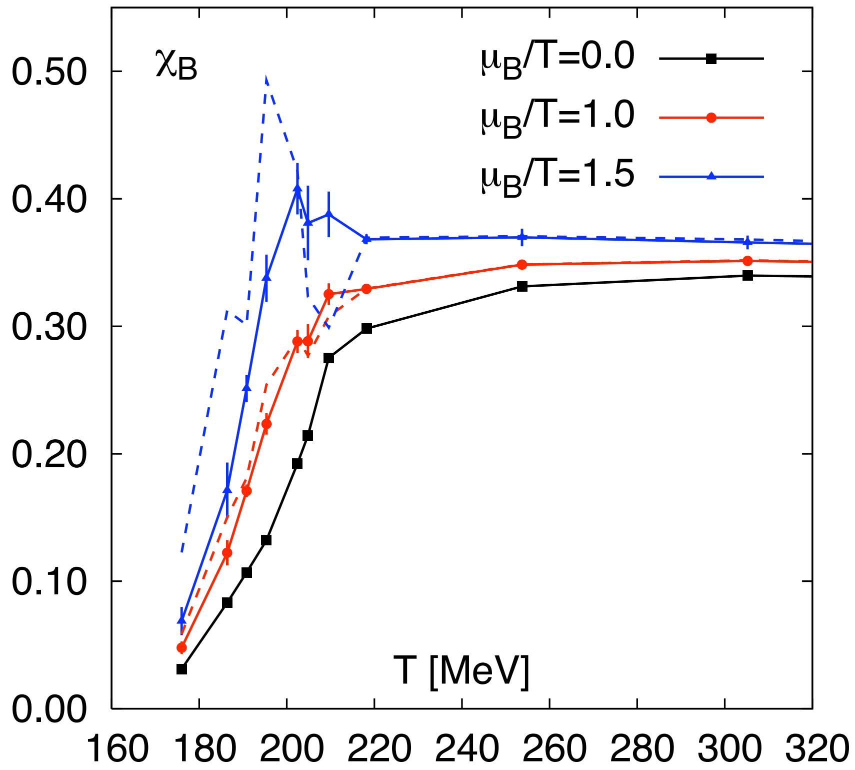
Ejiri *et al.*, PRD73 (2006) 054506; Miao, CS, PoS LATTICE2008 (2008) 172.

Hadronic fluctuations

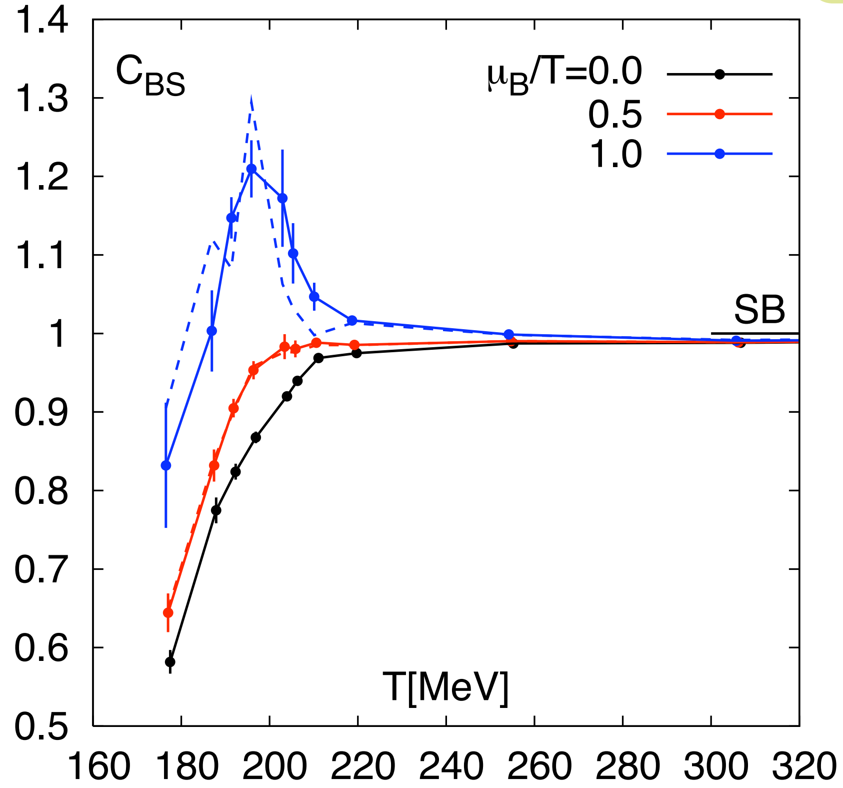
at $\mu_B > 0$ $(\mu_S = \mu_Q = 0)$

baryon number fluctuations

$$\chi_B = 2c_2^B + 12c_4^B \left(\frac{\mu_B}{T}\right)^2 + \cdots$$

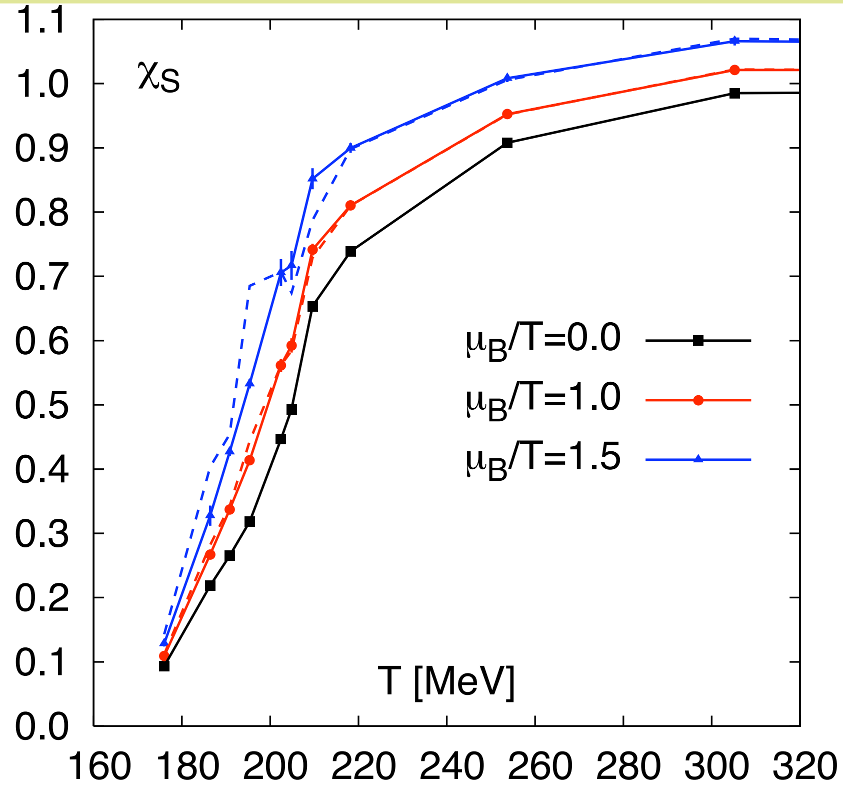


baryon number - strangeness correlations



strangeness fluctuations

$$\chi_S = 2c_{0,2}^{B,S} + 2c_{2,2}^{B,S} \left(\frac{\mu_B}{T}\right)^2 + \cdots$$



$$C_{BS} = \frac{c_{1,1}^{B,S} + 3c_{3,1}^{B,S}\left(\frac{\mu_B}{T}\right)^2 + \cdots}{\chi_S\left(\frac{\mu_B}{T}\right)}$$

→ LO introduces a peak in the fluctuations/correlations, NLO shifts the peak towards smaller temperatures

→ truncation errors become large at $\mu_B/T \gtrsim 1.5$

curvature of the phase boundary

- How to obtain the μ-dependence of the crossover temperature?

follow the peak position of a susceptibility (χ_2^B)

$\longrightarrow$ μ-dependence only introduce at the 6th order, noisy signal

better:
make use of the determination of the non universal parameters (T_c, t_0, h_0)
from mapping QCD to the $O(4)$-chiral critical behavior

recall: (lecture by F. Karsch)

$$t = \frac{1}{t_0}\frac{T - T_c}{T_c}$$
(reduced temperature)

$$h = \frac{H}{h_0}$$
(external field)

QCD:

$H \sim m_q$

(quark mass)

our choice:
$H = m_l/m_s$

$$M_0 = m_s \left\langle \bar{\psi}\psi \right\rangle_l / T^4 = h^{1/\delta} f_G(z)$$

(order parameter) (scaling function)

curvature of the phase boundary

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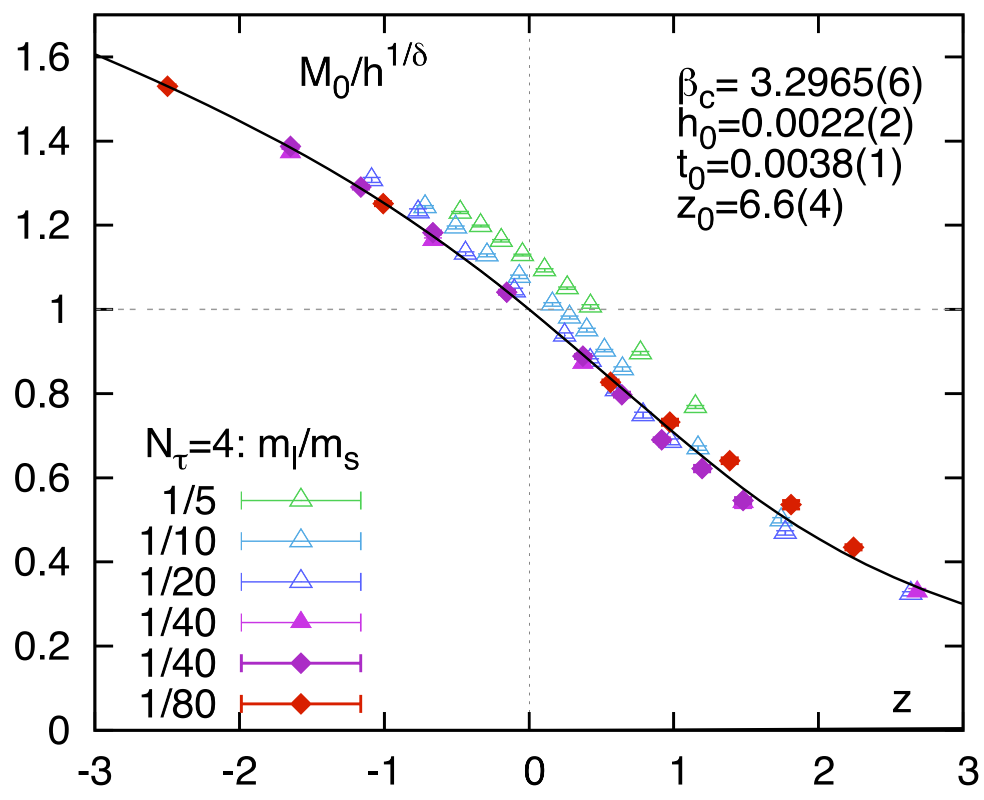

curvature of the phase boundary

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follow the peak position of a susceptibility (χ_2^B)

$\longrightarrow$ μ-dependence only introduce at the 6th order, noisy signal

better:

make use of the determination of the non universal parameters (T_c, t_0, h_0) from mapping QCD to the $O(4)$-chiral critical behavior

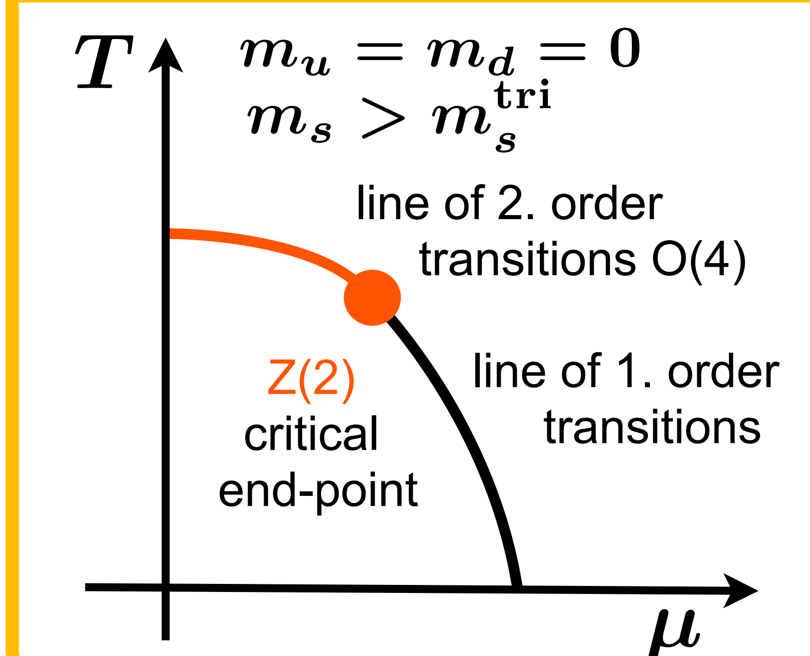
$\longrightarrow$ introduce chemical potential

$$t = \frac{1}{t_0}\left(\left(\frac{T}{T_c} - 1\right) + \kappa_q \left(\frac{\mu_q}{T}\right)^2\right) = 0$$

$$\Rightarrow \frac{T_c(\mu_q)}{T_c} = 1 - \kappa_q \left(\frac{\mu_q}{T}\right)^2$$

$\Rightarrow$ **scaling laws control curvature of the critical line**

expected phase diagram



curvature of the phase boundary

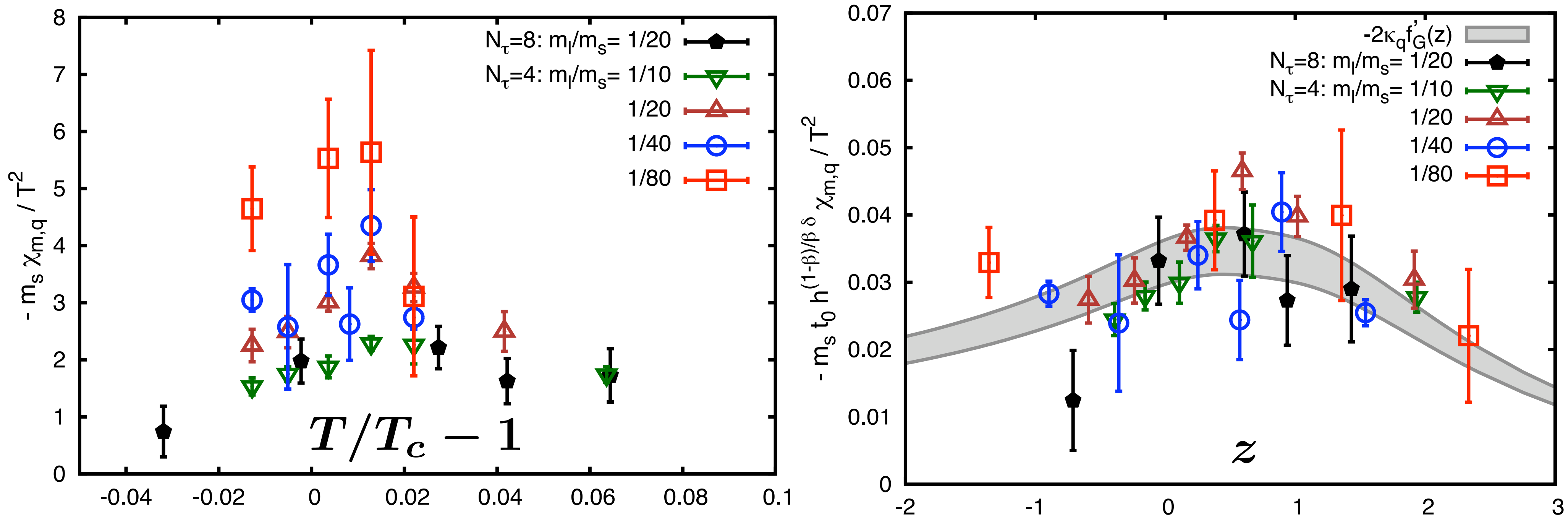
- How to obtain the μ-dependence of the crossover temperature?

> the critical line provides an upper bound to the curvature of the crossover temperature

- determine κ_q by a scaling analysis of the mixed susceptibility

$$\chi_m = \frac{\partial^2 M}{(\partial \mu / T)^2} = \frac{2\kappa_q}{t_0 T_c} h^{(\beta-1)/\beta\delta} f'_G(z) \propto \chi_t$$

$\Rightarrow$ **one fit parameter:** κ_q



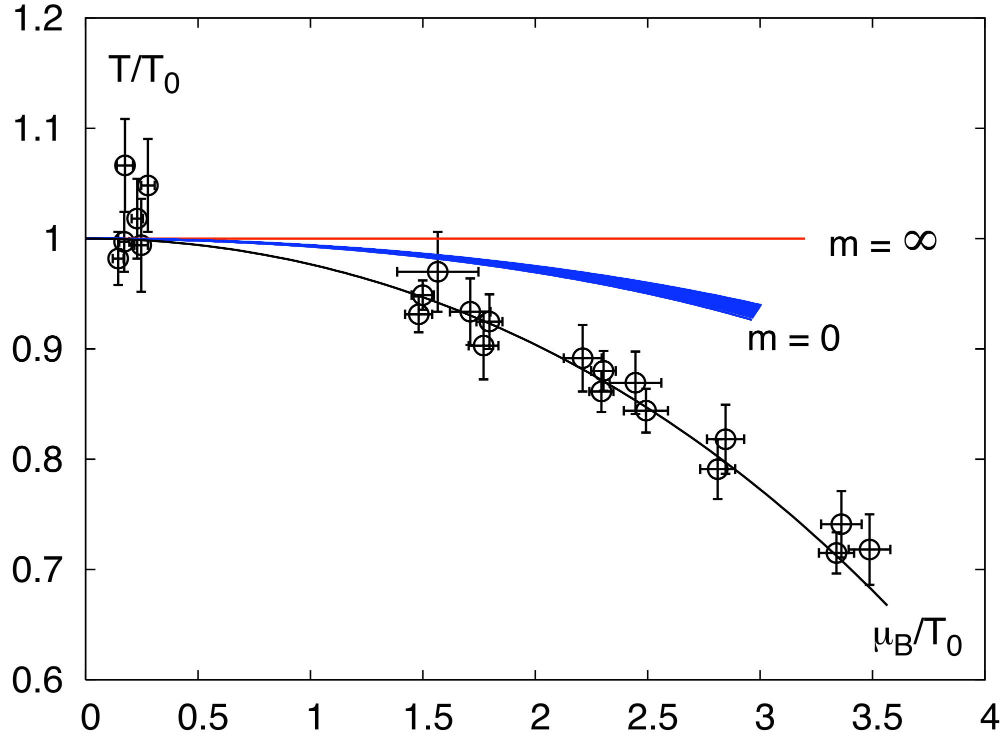
$\Rightarrow$ **obtain from p4-action,** $N_\tau = 8, 4: \kappa_q = 0.059(6)$

Kaczmarek *et al*, PRD 83 (2011) 014504.

curvature of the phase boundary

- comparison with freeze-out line

  - Statistical models are very successful in describing particle abundances observed in heavy ion collision; use a parametrization of the freeze-out curve



statistical model:

$$\frac{T_c}{T} = 1 - 0.023\left(\frac{\mu_B}{T}\right)^2 - d\left(\frac{\mu_B}{T}\right)^4$$

Cleymans, *et al.*, PRC 73 (2006) 034905

lattice:

$$\frac{T_c}{T} = 1 - 0.0066(7)\left(\frac{\mu_B}{T}\right)^2$$

Kaczmarek *et al*, PRD 83 (2011) 014504.

$\Rightarrow$ **curvature of the freeze-out curve seems to be larger**

- **open issues**: continuum limit, strangeness conservation, nonzero electric charge

Baryonic fluctuations

hadron resonance gas

$$\ln Z(T,V,\mu_B,\mu_S,\mu_Q) = \sum_{i\in hadrons} \ln Z_{m_i}(T,V,\mu_B,\mu_S,\mu_Q)$$

$$\sum_{i\in mesons} \ln Z^B_{m_i}(T,V,\mu_S,\mu_Q) + \sum_{i\in baryons} \ln Z^F_{m_i}(T,V,\mu_B,\mu_S,\mu_Q)$$

mesons:

$$\frac{p_i}{T^4} = \frac{d_i}{\pi^2}\left(\frac{m_i}{T}\right)^2 \sum_{l=1}^{\infty} (+1)^{l+1} l^{-2} K_2(lm_i/T) \cosh(lS_i\mu_S/T + lQ_i\mu_Q/T)$$

baryons:

$$\frac{p_i}{T^4} = \frac{d_i}{\pi^2}\left(\frac{m_i}{T}\right)^2 \sum_{l=1}^{\infty} (-1)^{l+1} l^{-2} K_2(lm_i/T) \cosh(lB_i\mu_B/T + lS_i\mu_S/T + lQ_i\mu_Q/T)$$

Boltzmann approximation

ratios are independent of spectrum and volume

$\longrightarrow$ possibly large parts of cut-off effects cancel

3 ratios:

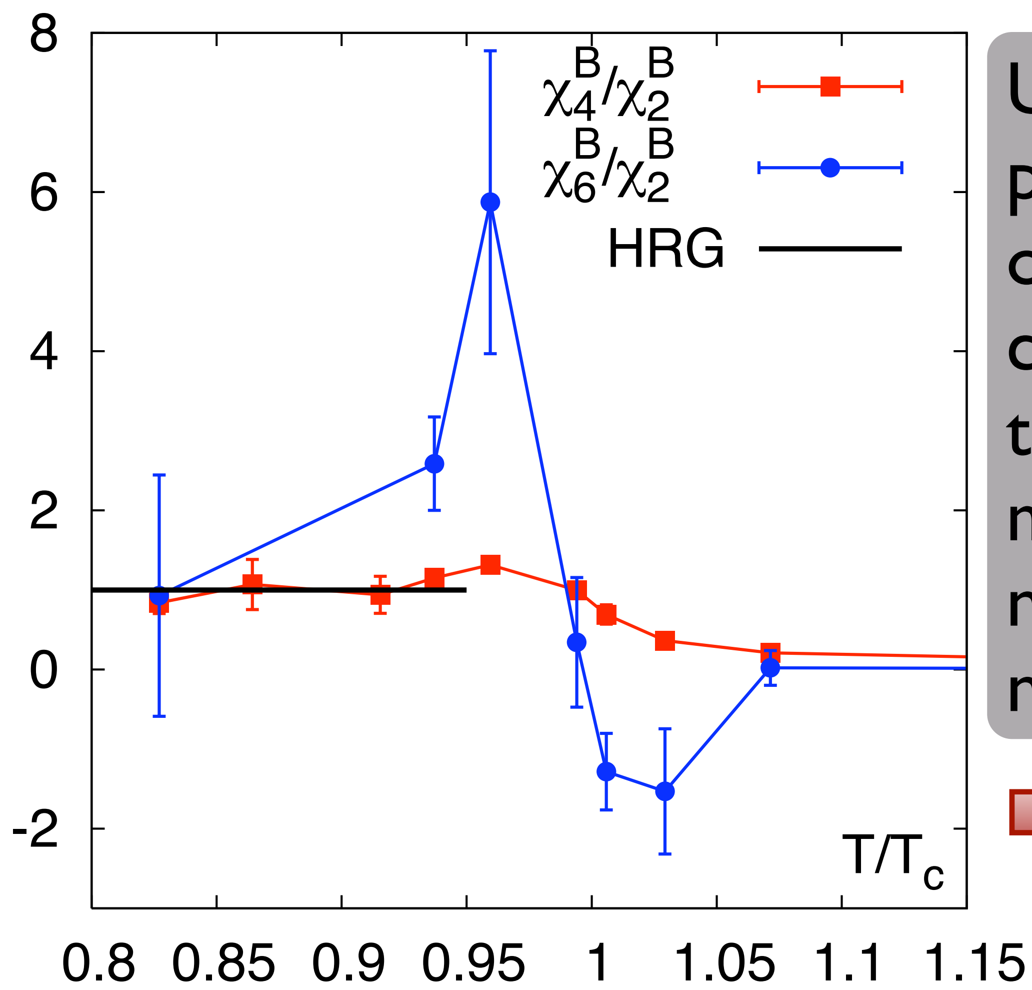
$$\frac{\chi_4^B}{\chi_2^B} = \kappa\sigma^2 = \frac{B^4}{B^2} = 1$$

$$\frac{\chi_3^B}{\chi_2^B} = S\sigma = \frac{B^3}{B^2}\tanh(\mu_B/T)$$

$$\frac{\chi_2^B}{\chi_1^B} = \sigma^2/N_B = \frac{B^2}{B^1}\coth(\mu_B/T)$$

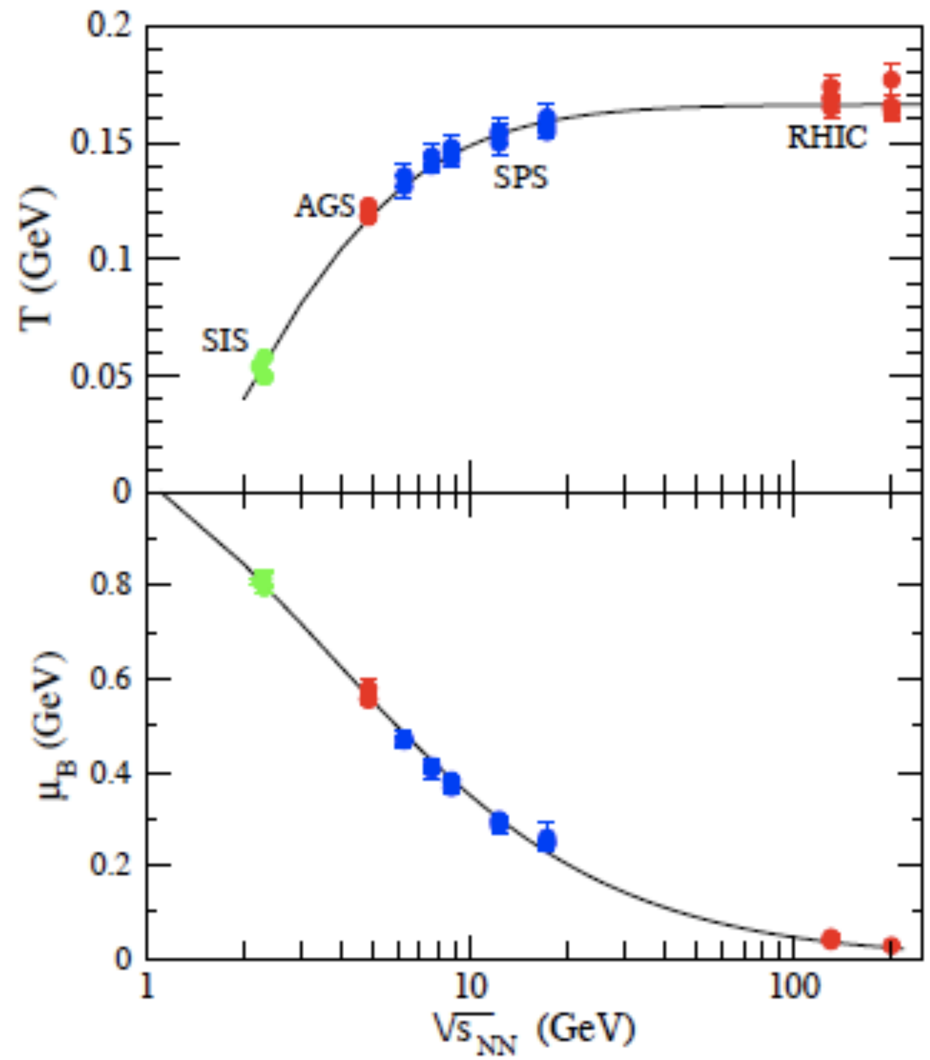
Baryonic fluctuations

- sixth order fluctuations



CS, Theor. Phys. Suppl.186, 563 (2010)

Use parametrization of freeze-out curve to connect to STAR measurements of net-proton number



$$T(\mu_B) = 0.166\ \mathrm{GeV} - 0.139\ \mathrm{GeV}^{-1}\mu_B^2 - 0.053\ \mathrm{GeV}^{-3}\mu_B^4$$

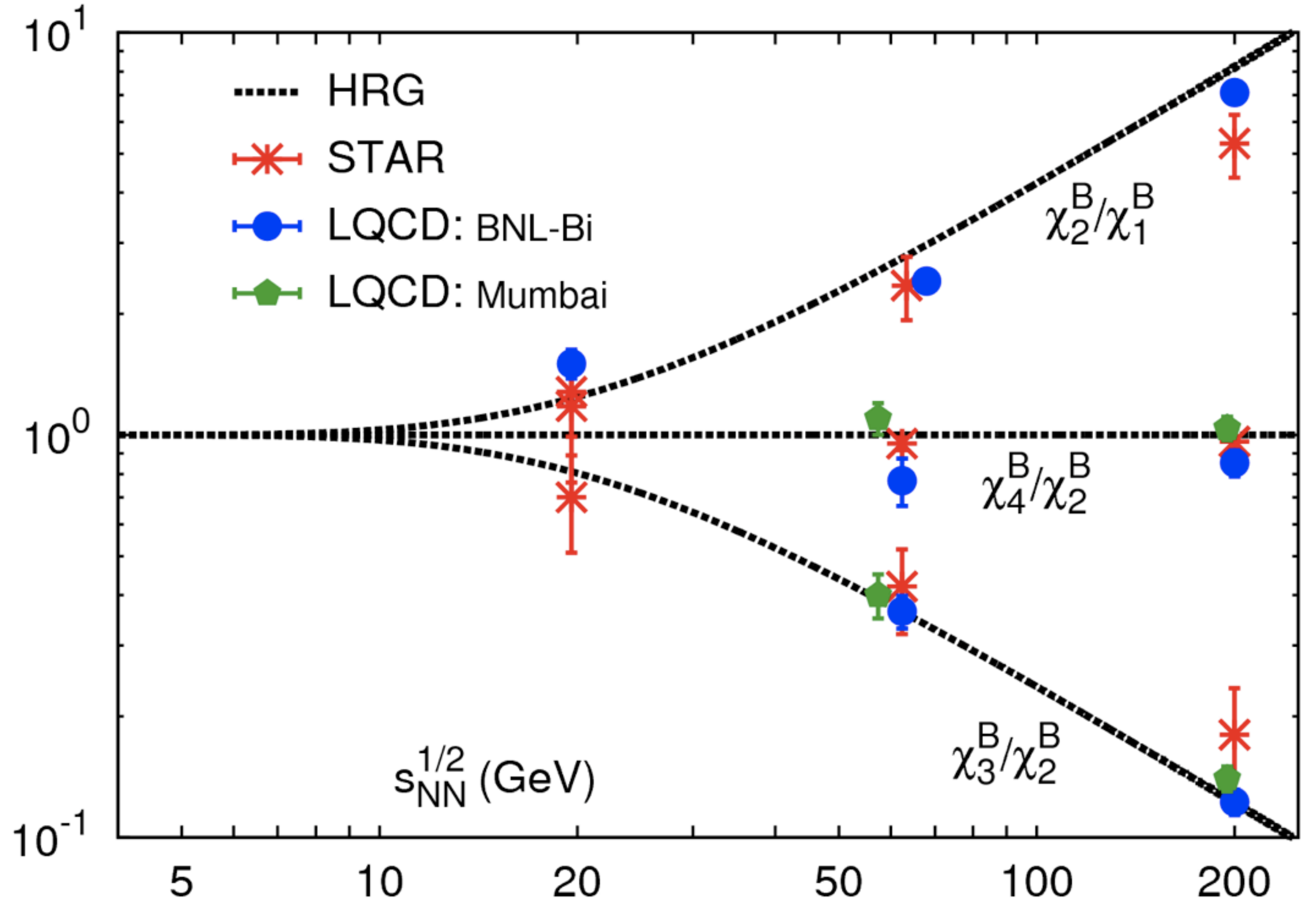
$$\mu_B(\sqrt{s}) = \frac{1.308\ \mathrm{GeV}}{1 + 0.273\ GeV^{-1}\sqrt{s}}$$

- sensitive to relevant quantum numbers in the medium
- divergent at the critical point

[Cleymans et al., Phys. Rev. C 63 (2006) 034905]

Baryonic fluctuations

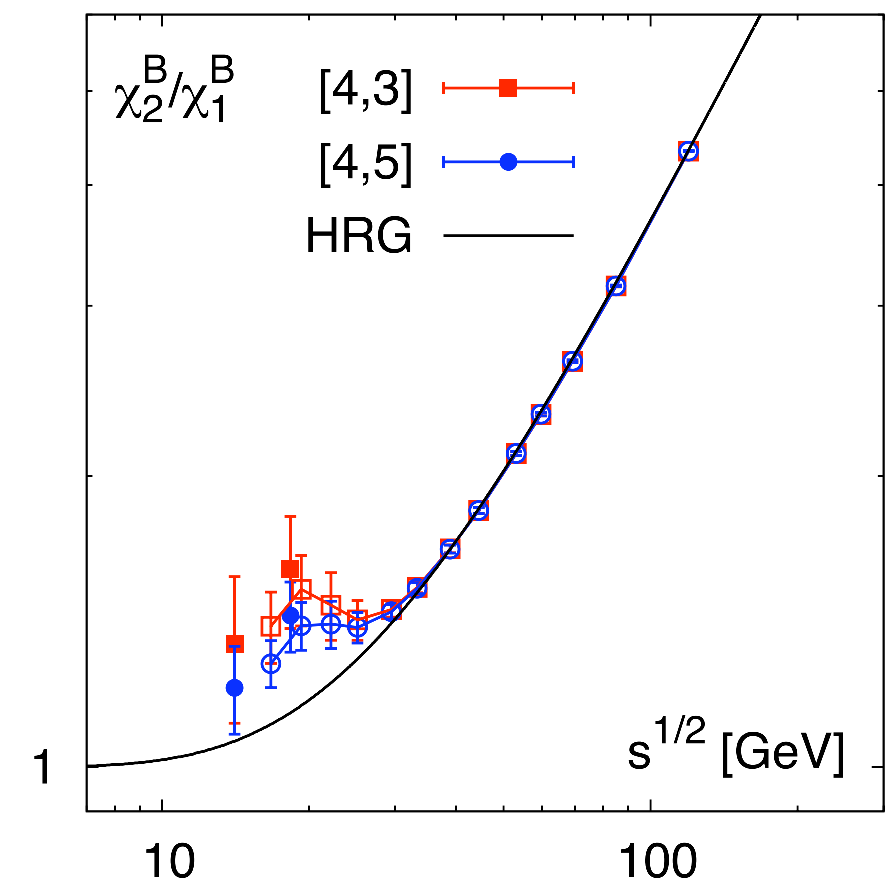
Lattice vs. Experiment:



Mukherjee, QM 2011

[HRG: Karsch, Redlich, PLB 695 (2011)]

[STAR data: Aggarwal et al, PRL (2010) 022302]



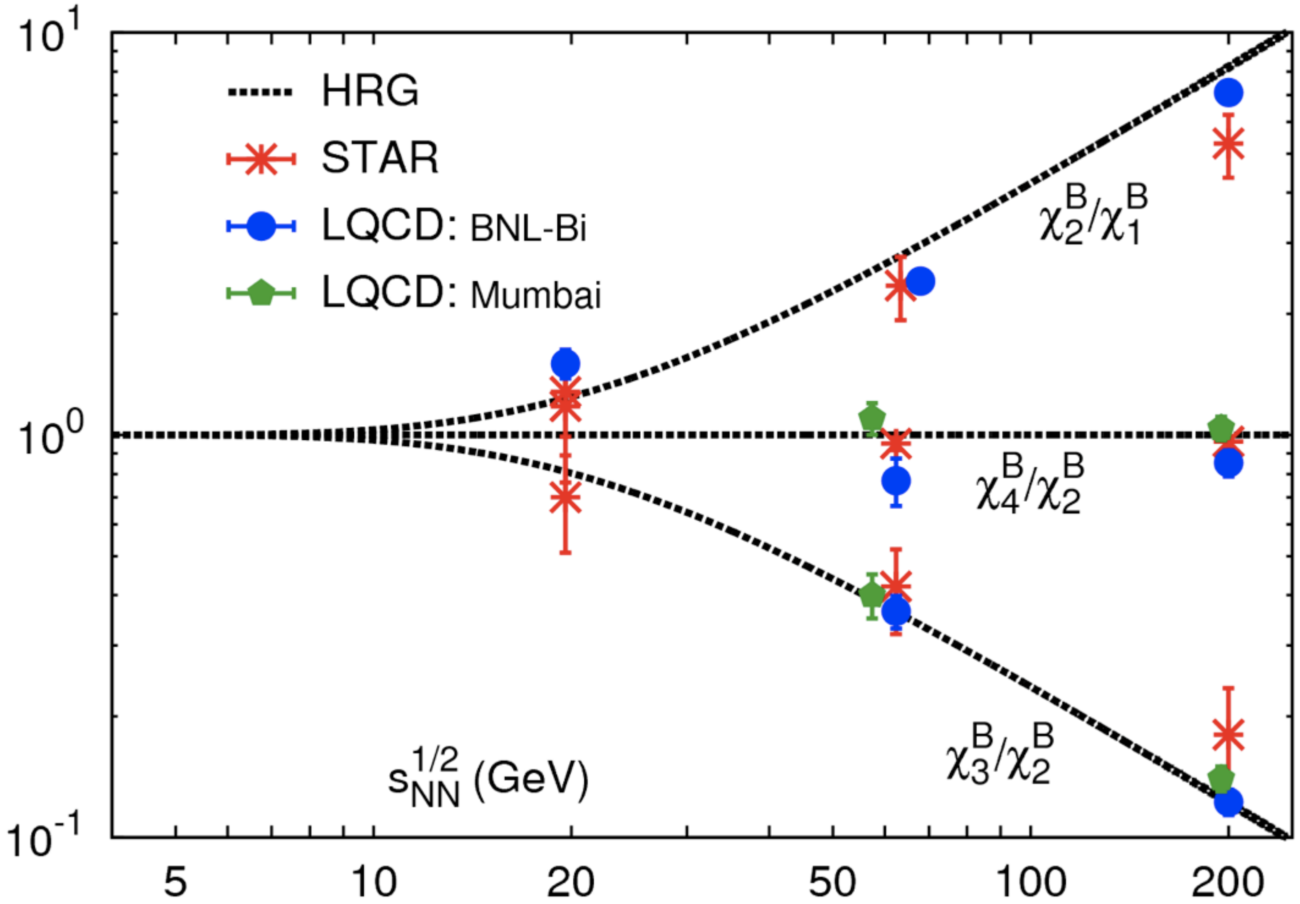
CS, *Theor. Phys. Suppl. 186, 563 (2010)*

- net-proton number fluctuations can be described by the HRG
  solid lines: $\mu_Q \neq 0, \mu_S \neq 0$
  dashed lines: $\mu_Q = 0, \mu_S = 0$

- fluctuations increase for small $\sqrt{s}$
- sensitive to truncation of the series due to close radius of convergence

Baryonic fluctuations

Lattice vs. Experiment:



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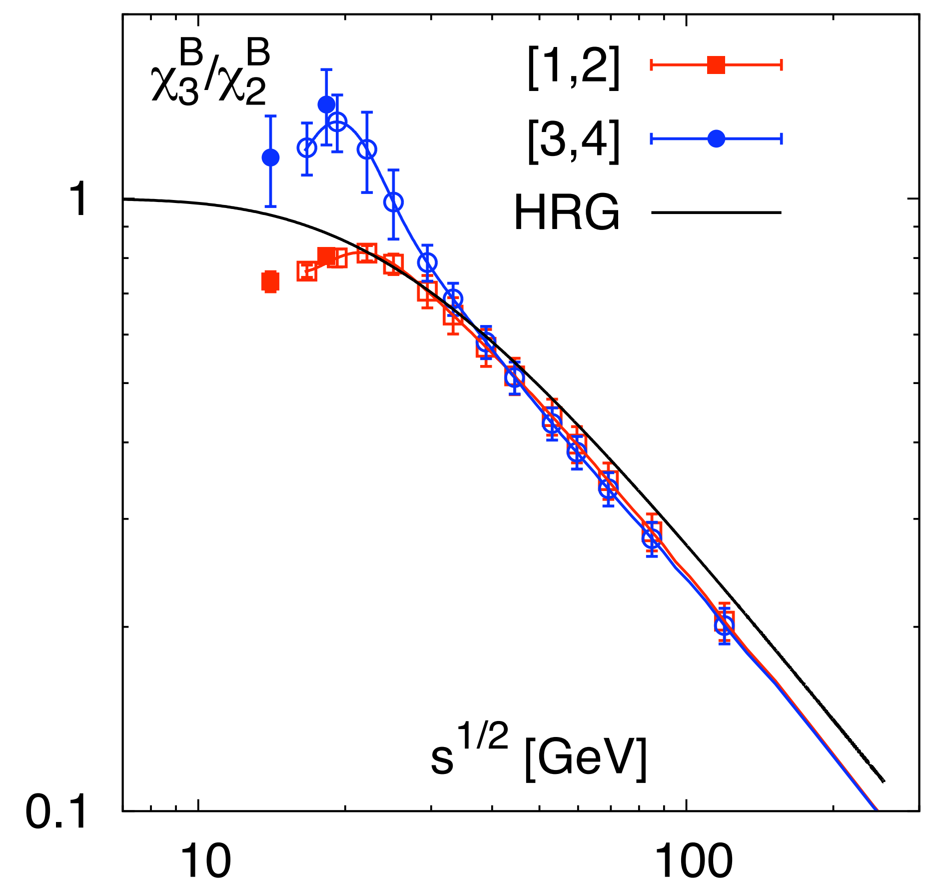

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Baryonic fluctuations

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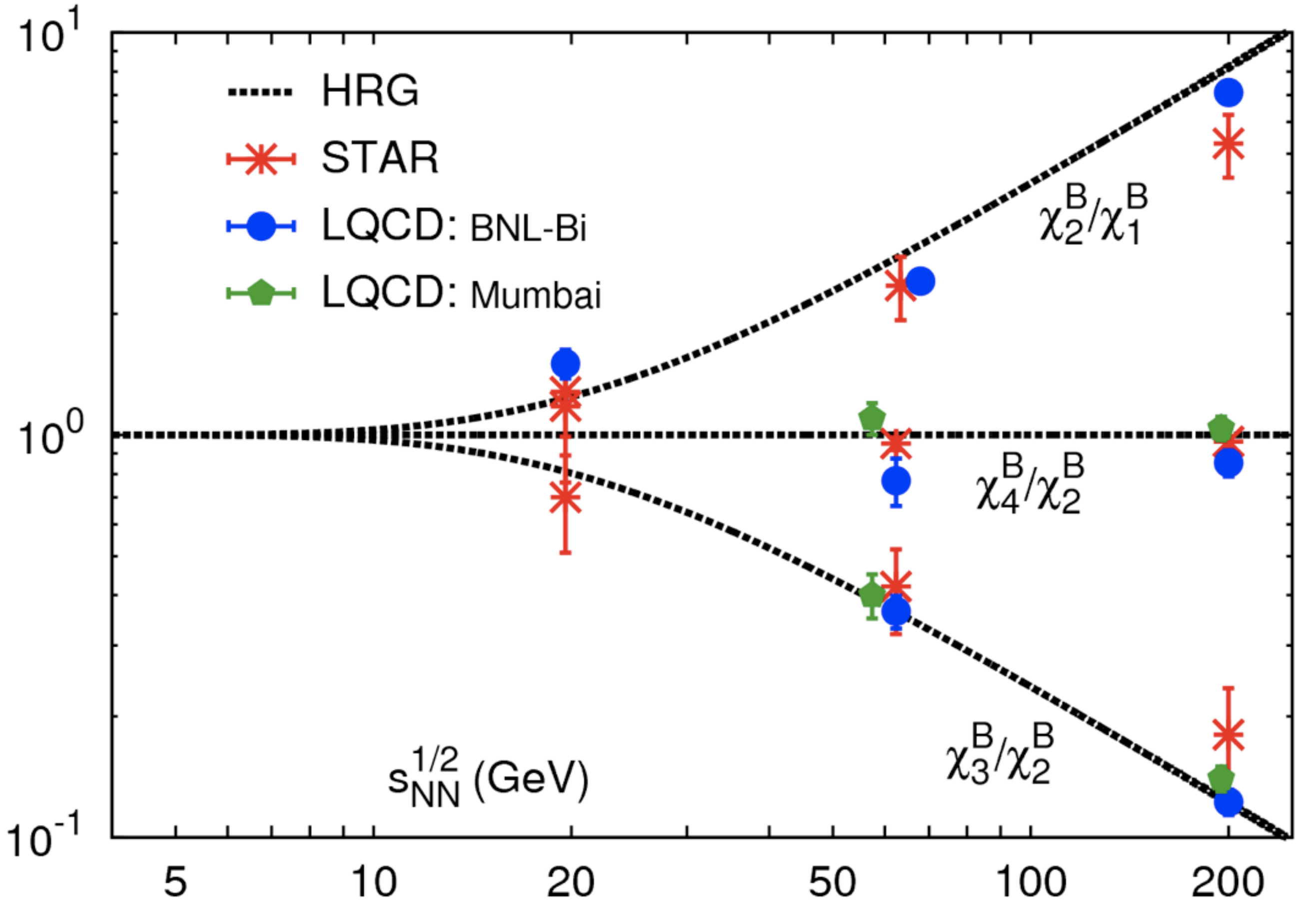

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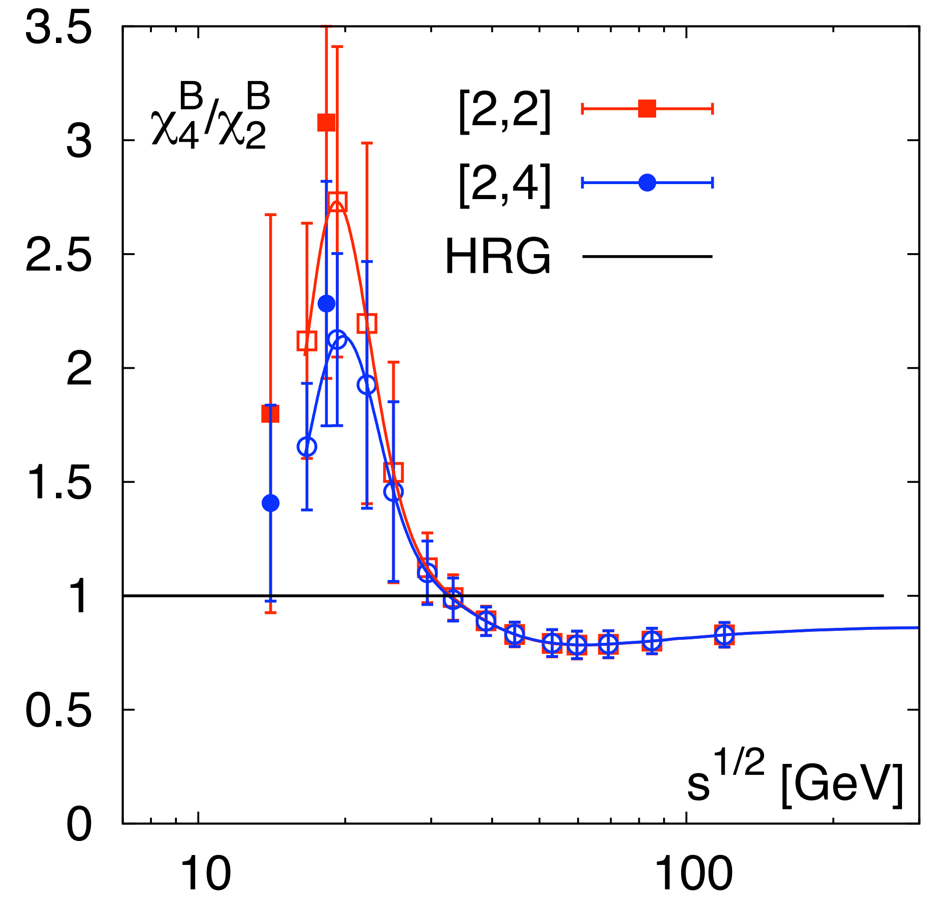

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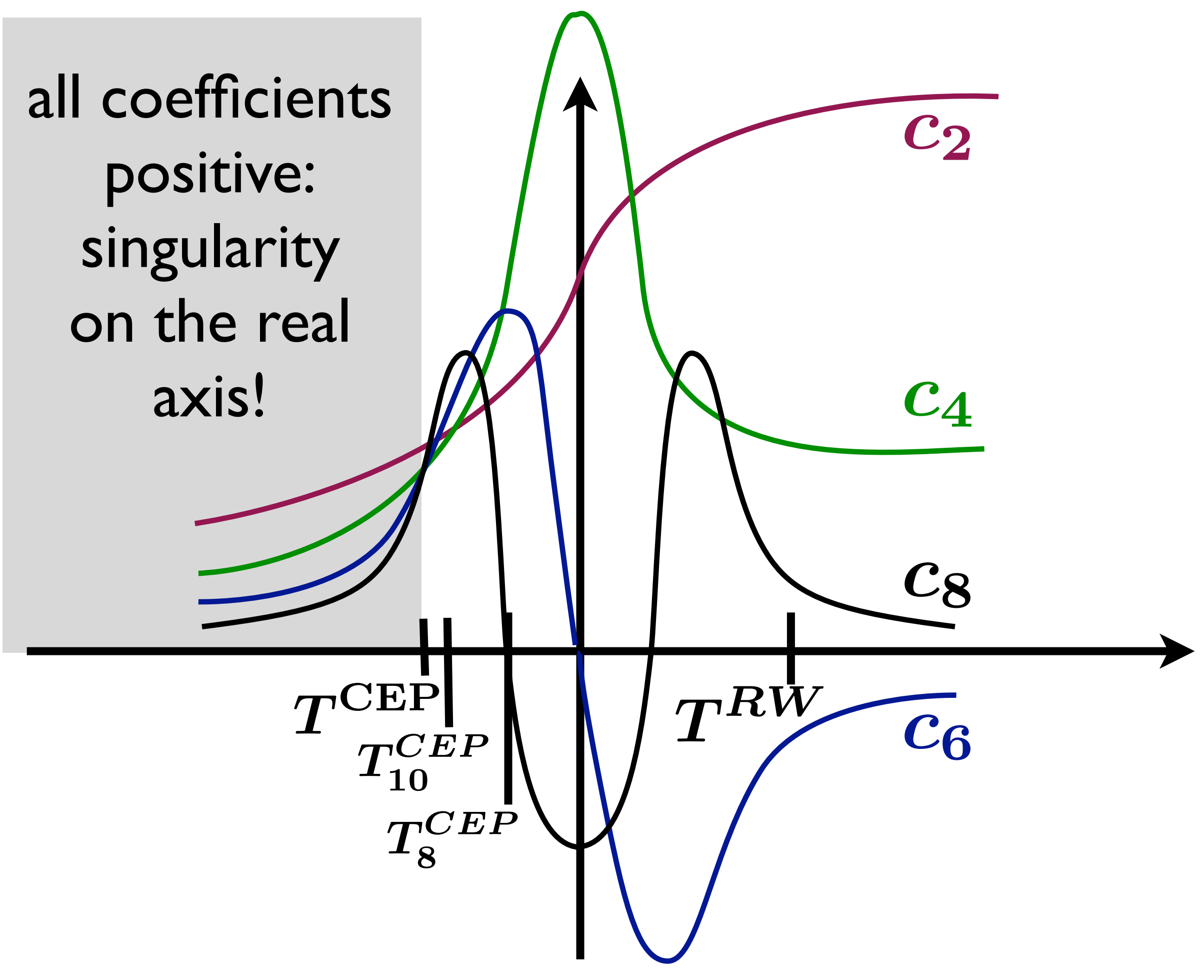
The critical endpoint

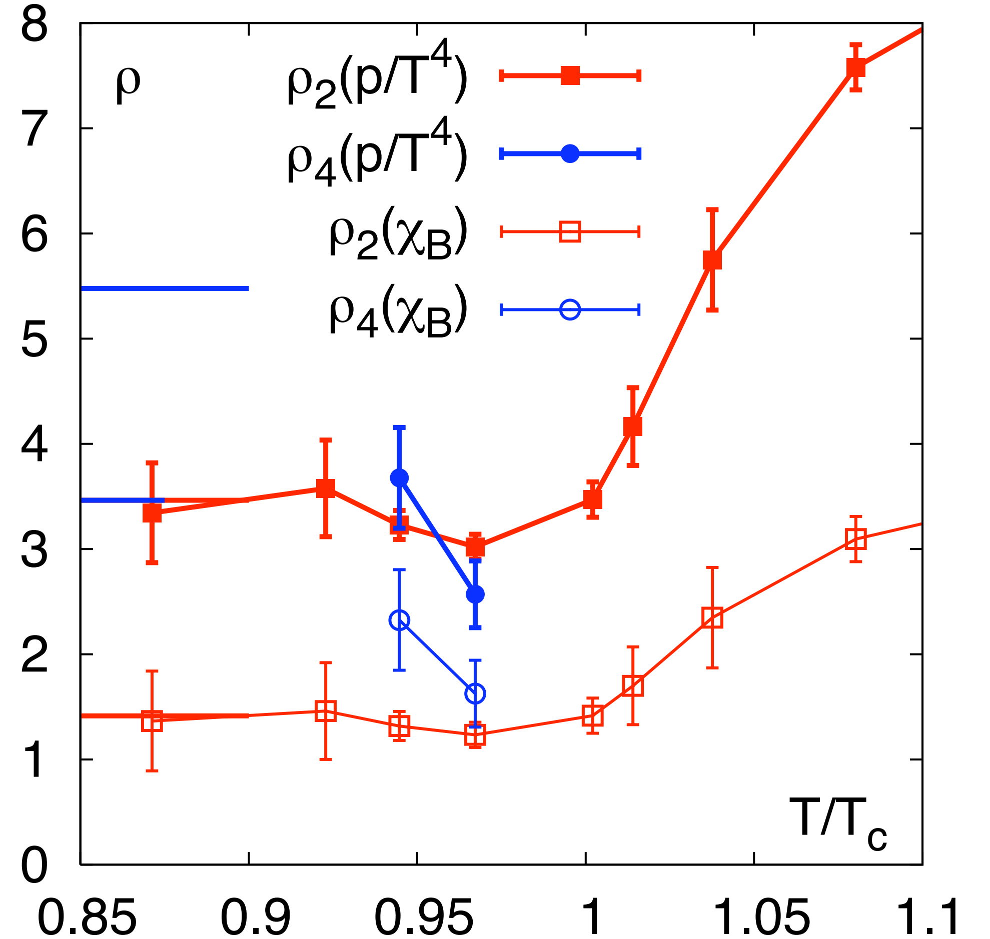
<u>method for locating of the CEP:</u>

- determine largest temperature where all coefficients are positive → $T^{\rm CEP}$
- determine the radius of convergence at this temperature → $\mu^{\rm CEP}$

$$p = c_0 + c_2\,(\mu_B/T)^2 + c_4\,(\mu_B/T)^4 + \cdots$$

$$\chi_B = 2c_2 + 12c_4\,(\mu_B/T)^2 + 30c_6\,(\mu_B/T)^4 + \cdots$$





CS, Theor. Phys. Suppl. 186, 563 (2010)

first non-trivial estimate of $T^{\rm CEP}$ by c_8
second non-trivial estimate of $T^{\rm CEP}$ by c_{10}

$$\rho_n(p) = \sqrt{c_n/c_{n+2}}$$

$$\rho = \lim_{n\to\infty} \rho_n$$

The critical endpoint

method for locating of the CEP:

- determine largest temperature where all coefficients are positive $\rightarrow T^{\mathrm{CEP}}$
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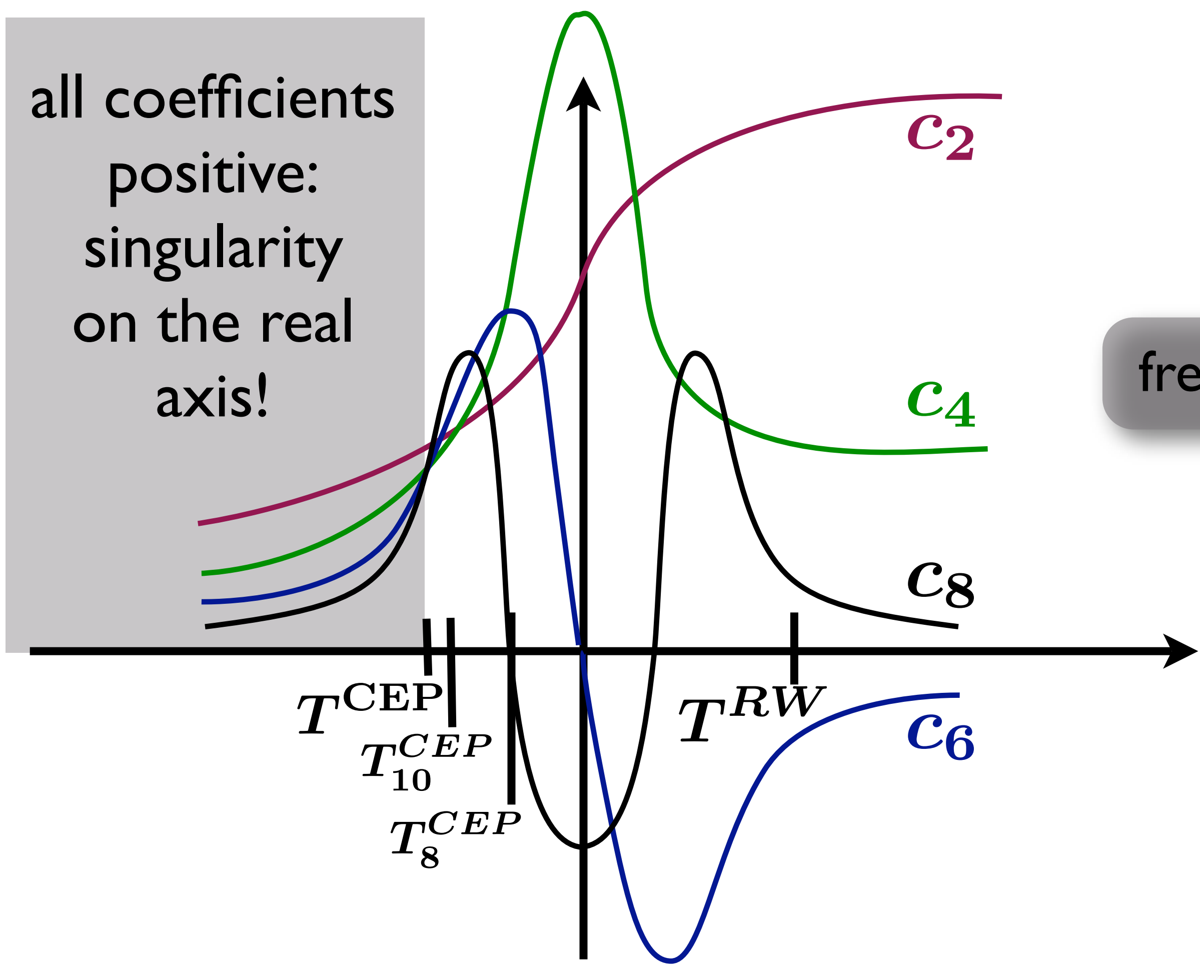

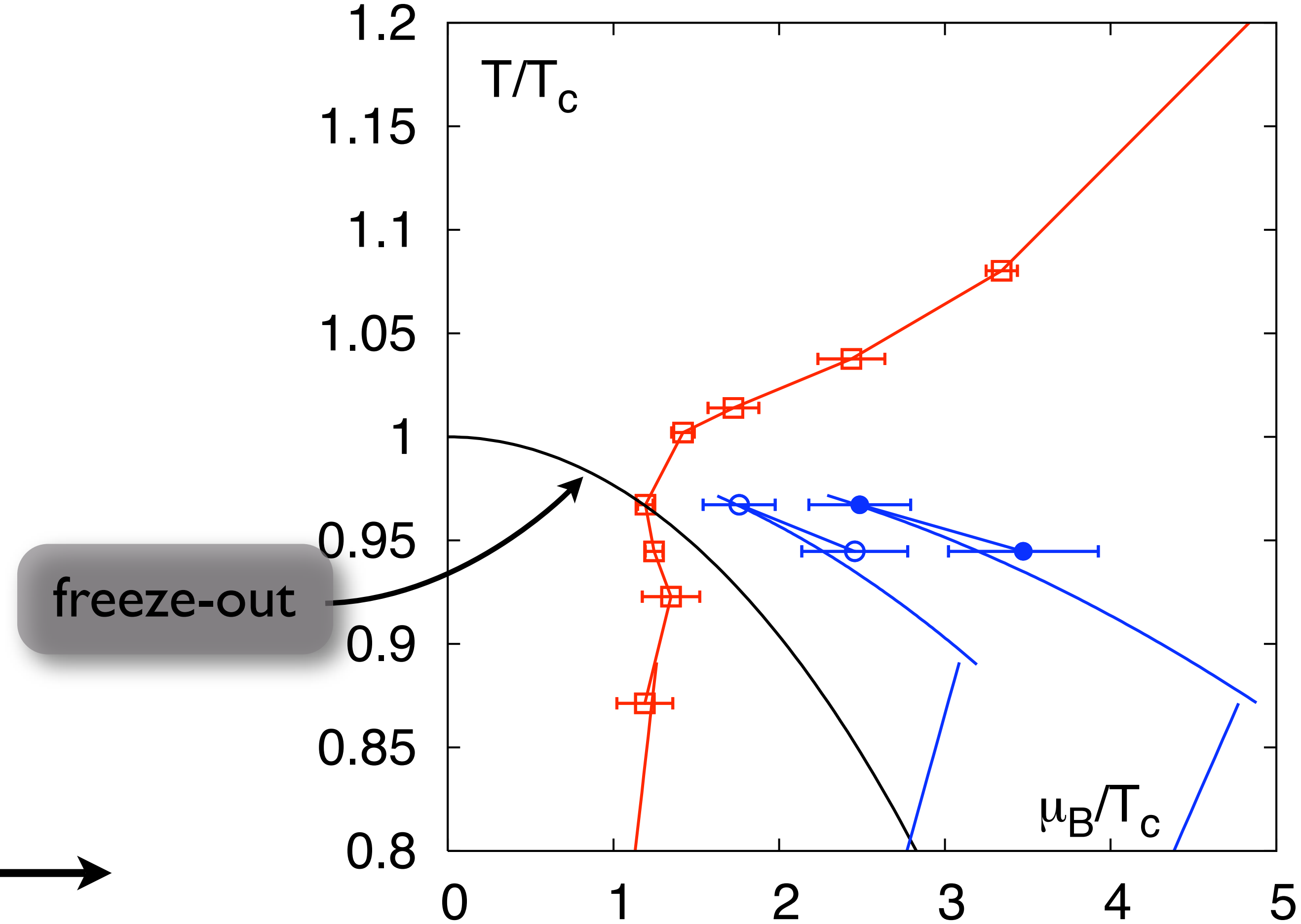

CS, Theor. Phys. Suppl. 186, 563 (2010)

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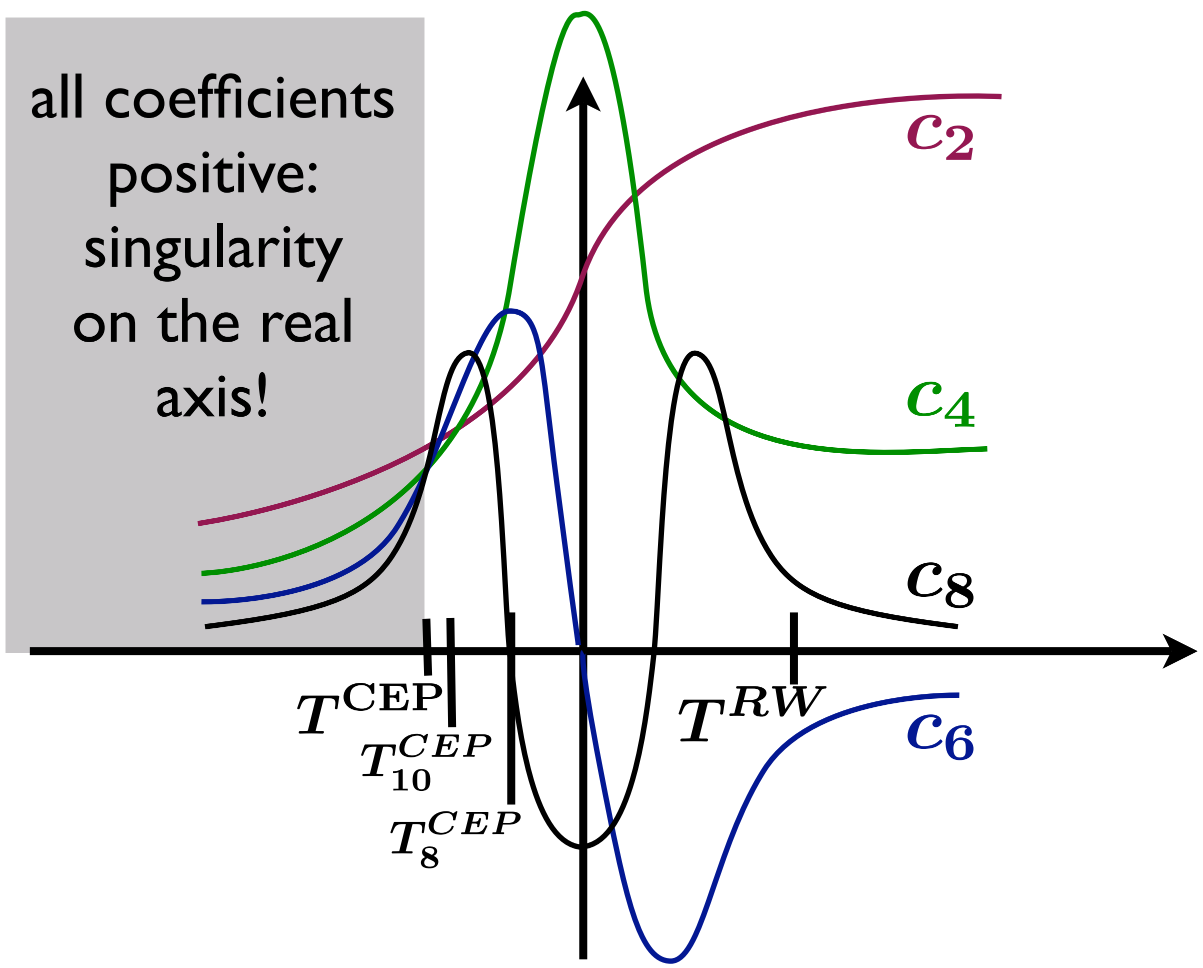

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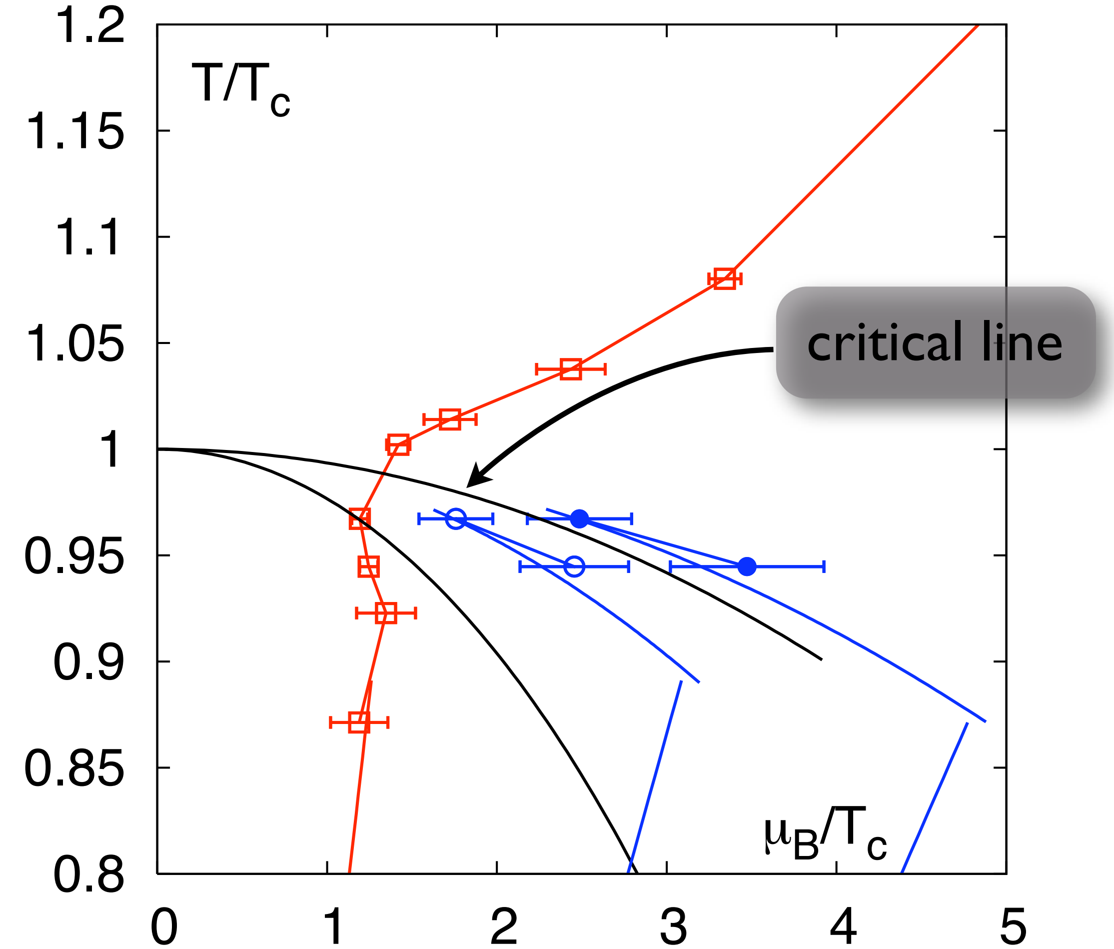

CS, *Theor. Phys. Suppl.186, 563 (2010)*

- radius of convergence is consistent with critical line in the chiral limit

O. Kaczmarek, et al., PRD 83 (2011) 014504

Summary

Part II:

- *Taylor expansion coefficients* of the pressure up to the 6th order have been calculated at zero chemical potential, can be used to obtain bulk thermo-dynamics and fluctuations at nonzero density (p4-action, Nt=4,6). New results from HISQ-action for Nt=6,8,12 are underway.

- The *curvature of the critical line* in the chiral limit was obtained from an analysis of the O(4) ciritcal behavior.

- Ratios of *moments of the baryon number fluctuations* have been computed and compared to the experiment.

- estimates of the *radius of convergence* can possibly be used to estimate a critical end-point at non zero chemical potential

Other directions

- QCD like theories without sign problem:

SU(2)

non compleat list:
- Hands, Montvay, Scorzato, Skullerud, EPJC 22 (2001) 451
- Kogut, Toublan, Sinclair, PRD 68 (2003) 054507
- Hands, Kim, Skullerud, PRD 81 (2010) 091502
- Hands, Kenny, Kim, Skullerud, EPJA 47 (2011) 60

iso-spin chemical potential

non compleat list:
- Kogut, Sinclair, PRD 66 (2002) 034505

- Integrate over gauge links first $\longrightarrow$ no sign problem, feasible at strong couplings Fromm, de Forcrand PRL 104 (2010) 112005; de Forcrand, Unger, arXiv: 1107.1557

- Complexify fields and use complex Langevin algorithm, correct convergence not guaranteed Aarts et al., JEHP 0509 (2009) 052; PLB 687 (2010) 154; PRD 81 (2010) 054508; JHEP 1008 (2010) 017; JHEP 1008 (2010) 020

- Design a model of QCD, calculate parameter to produce all know constrains from lattice QCD and experiment

$\longrightarrow$ see lecture by D. Blaschke