Lecture II:

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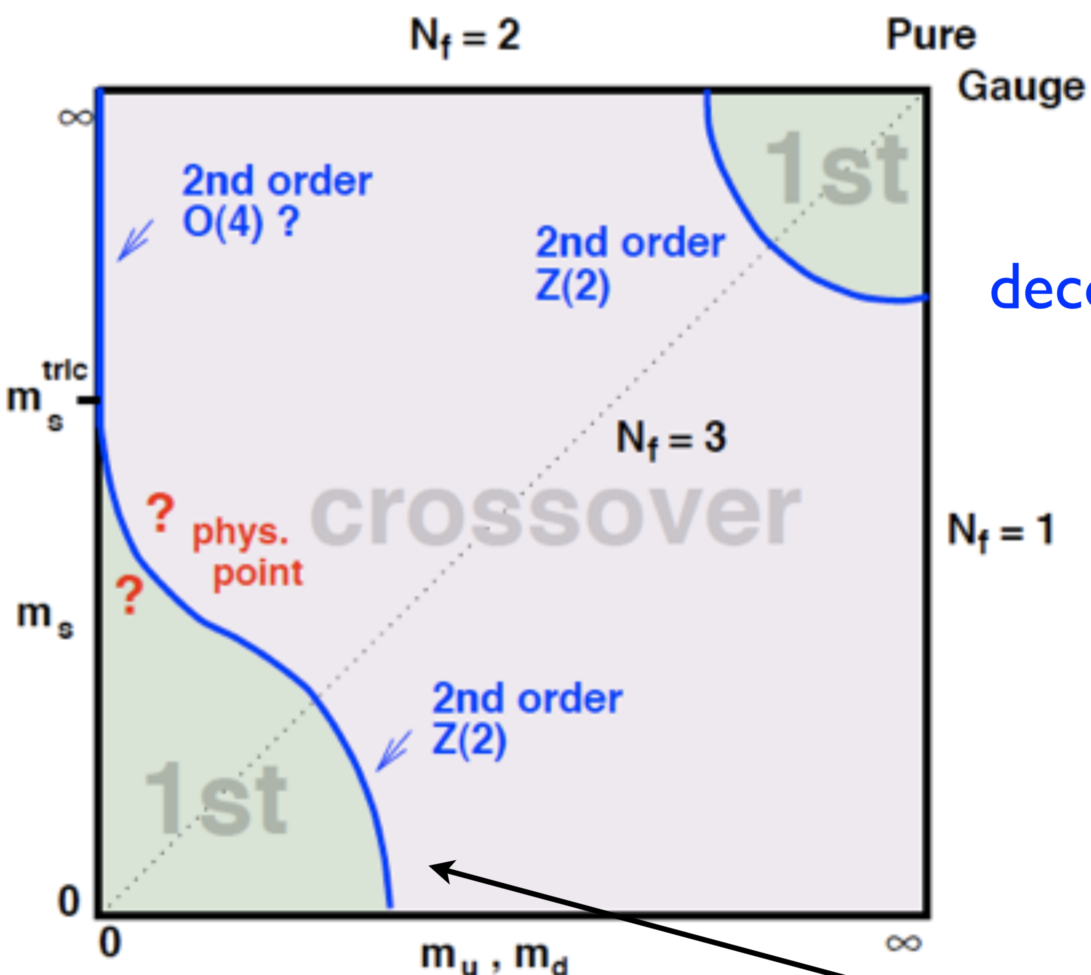
- The QCD phase transition at zero density
- Lattice QCD at finite temperature and density
- Towards the QCD phase diagram

The order of the QCD thermal transition, $\mu = 0$

deconfinement p.t.:
breaking of global $Z(3)$



deconfinement critical line

chiral critical line

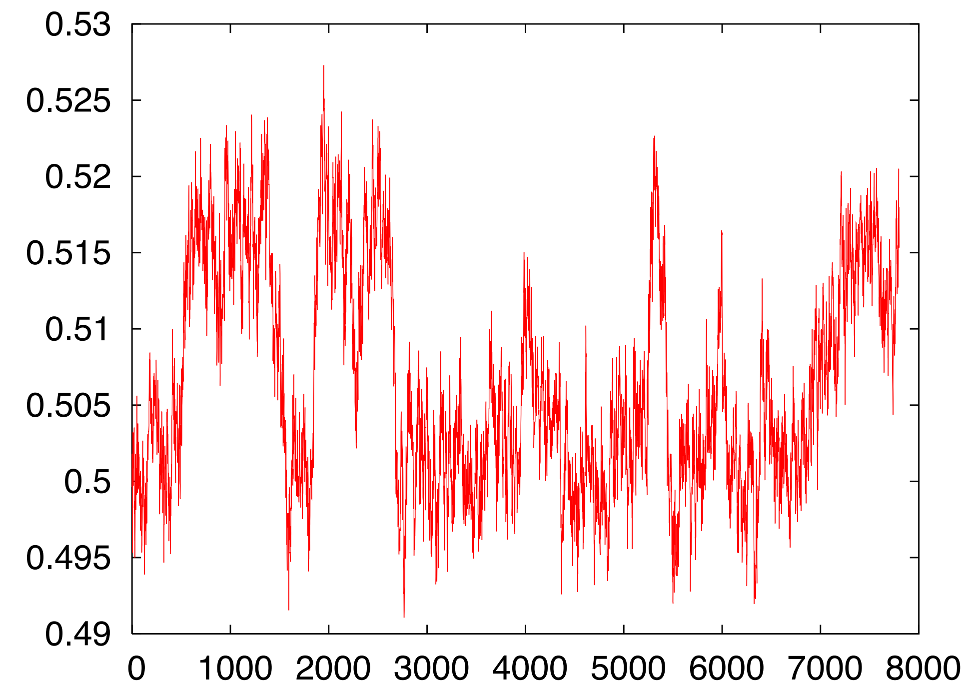
chiral p.t.
restoration of global
$SU(2)_L \times SU(2)_R \times U(1)_A$

anomalous

Finding a phase transition in QCD: fluctuations

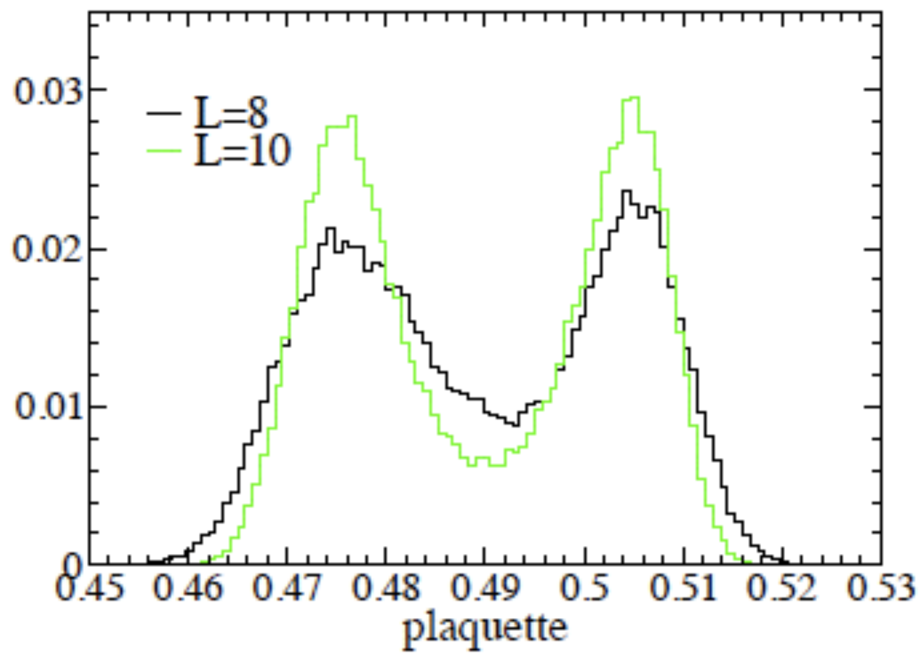
Very difficult!

Monte Carlo history,
plaquette near phase boundary

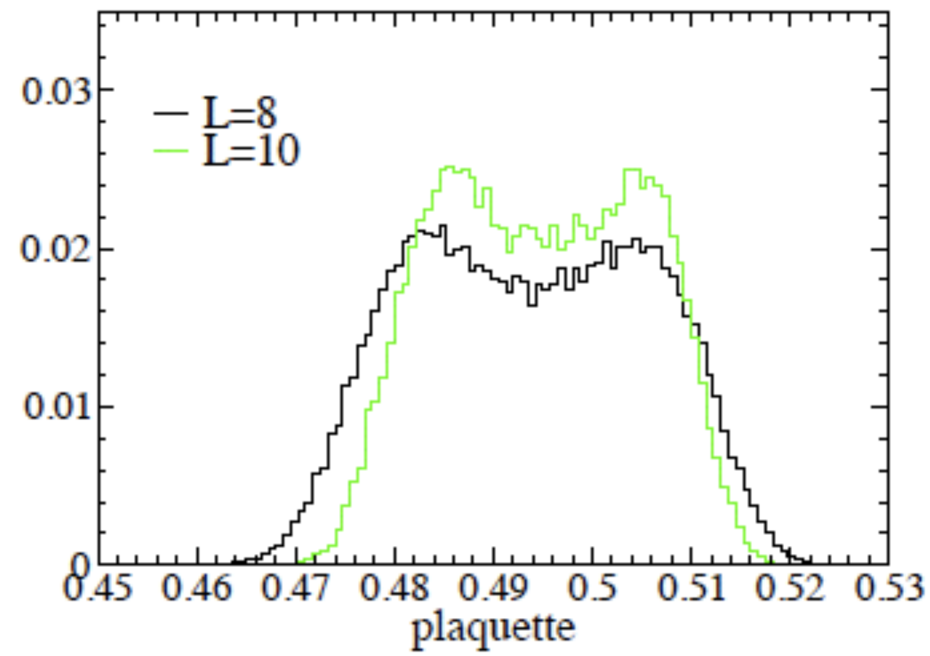


Distribution:

first-order



crossover



Finding a phase transition in QCD: fluctuations

Fluctuations visible in any observable, but largest in "order parameter":

$$O \in \{\mathrm{Tr}L, \bar{\psi}\psi, \mathrm{Tr}U_p, \ldots\}$$

Generalised susceptibilities:

$$\chi_O = \int d^3x \, (\langle O(\mathbf{x})O(0)\rangle - \langle O(\mathbf{x})\rangle\langle O(0)\rangle)$$

(Note: can be generalised to 4d, but the QCD equilibrium system is 3d!)

Volume averages (intensive variables):

$$\bar{O} = \frac{1}{V}\int d^3x \; O(\mathbf{x})$$

$$\chi_{\bar{O}} = N_s^3(\langle \bar{O}^2\rangle - \langle \bar{O}\rangle^2) = N_s^3\langle(\delta\bar{O})^2\rangle$$

fluctuation: $\delta\bar{O} = \bar{O} - \langle\bar{O}\rangle$

Pseudo-critical couplings (finite V!):

$$\chi(\beta_c, m_f) = \chi_{\max} \Rightarrow \beta_c(m_f)$$

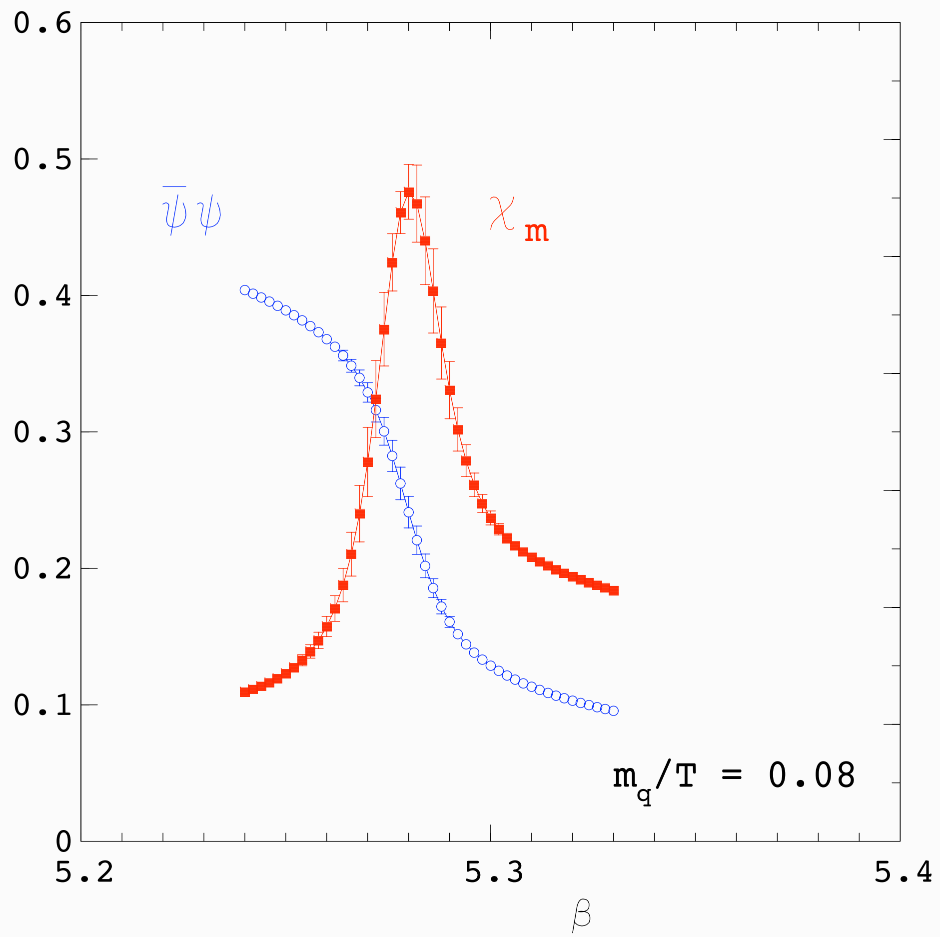
- fluctuations maximal but finite!
- pseudo-critical parameters not unique!

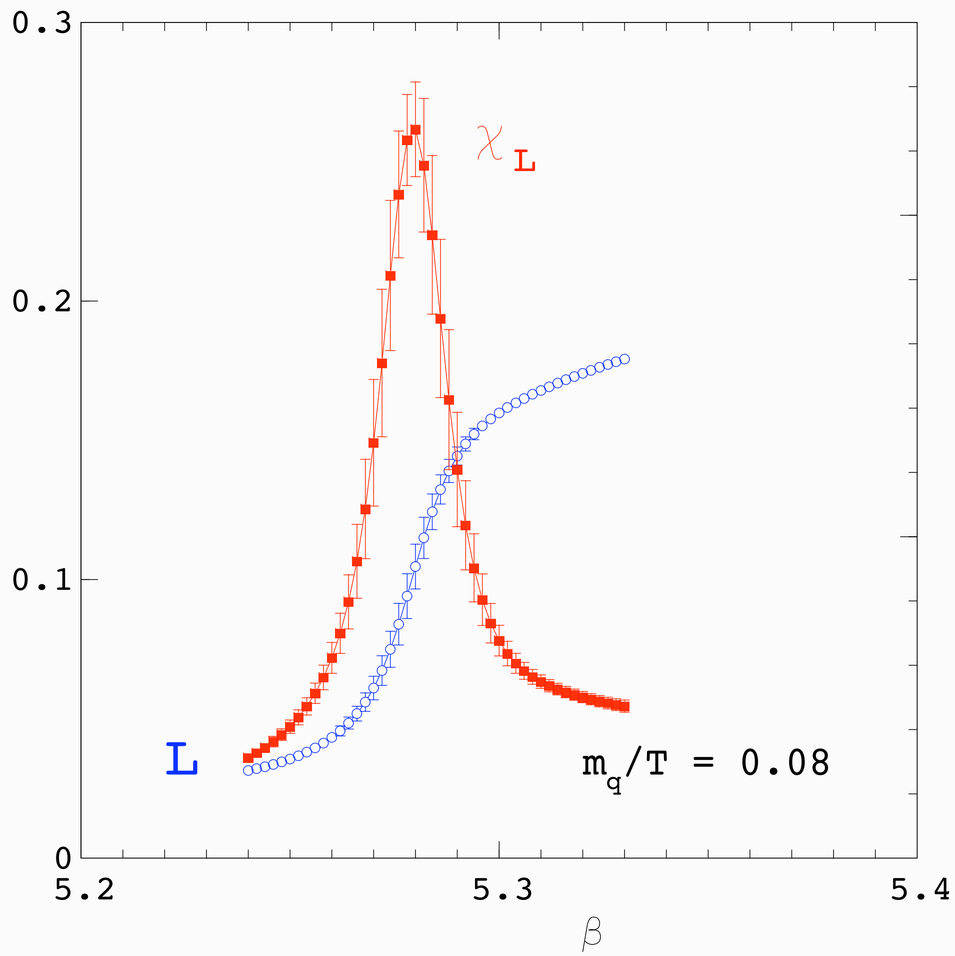
Finding the phase transition: the critical temperature

Measuring the `order parameter' as function of lattice coupling (viz. T)

$$\beta = \frac{2N_c}{g^2(a)} \qquad T = \frac{1}{aN_t}$$

here: $N_f = 2$





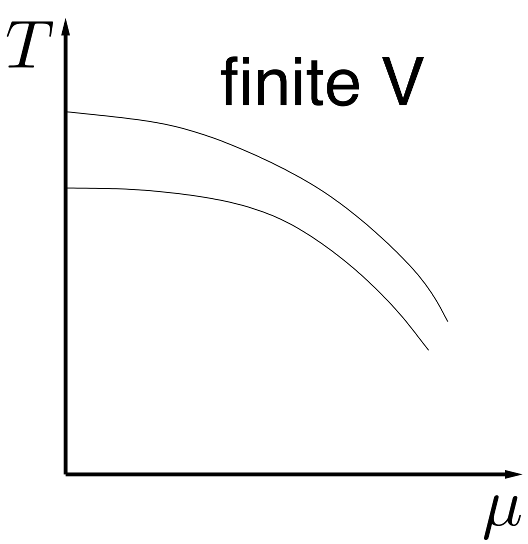
Susceptibilities: $\chi = VN_t(\langle\bar{\mathcal{O}}^2\rangle - \langle\bar{\mathcal{O}}\rangle^2) \quad \Rightarrow \chi_{max} = \chi(\beta_0) \quad \Rightarrow T_0$

$$T_{deconf} \approx T_{chiral}$$

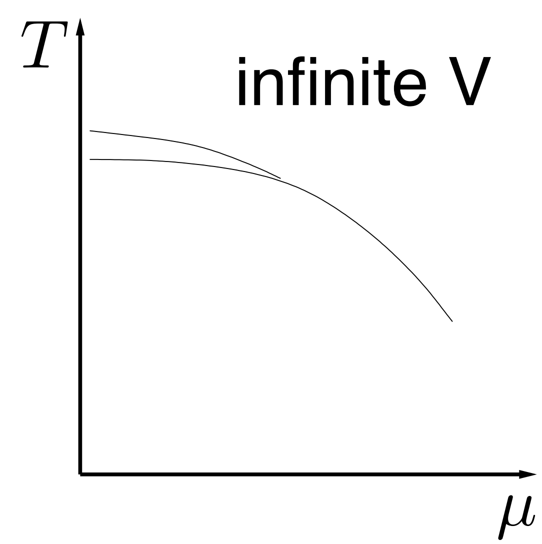
Approaching the thermodynamic limit

different definitions (e.g. scanning in different directions, different observables etc.)

$\beta_0(\mu)$ not unique



$\beta_c(\mu)$ unique for p.t., not for crossover



Critical line unique in thermodynamic limit!

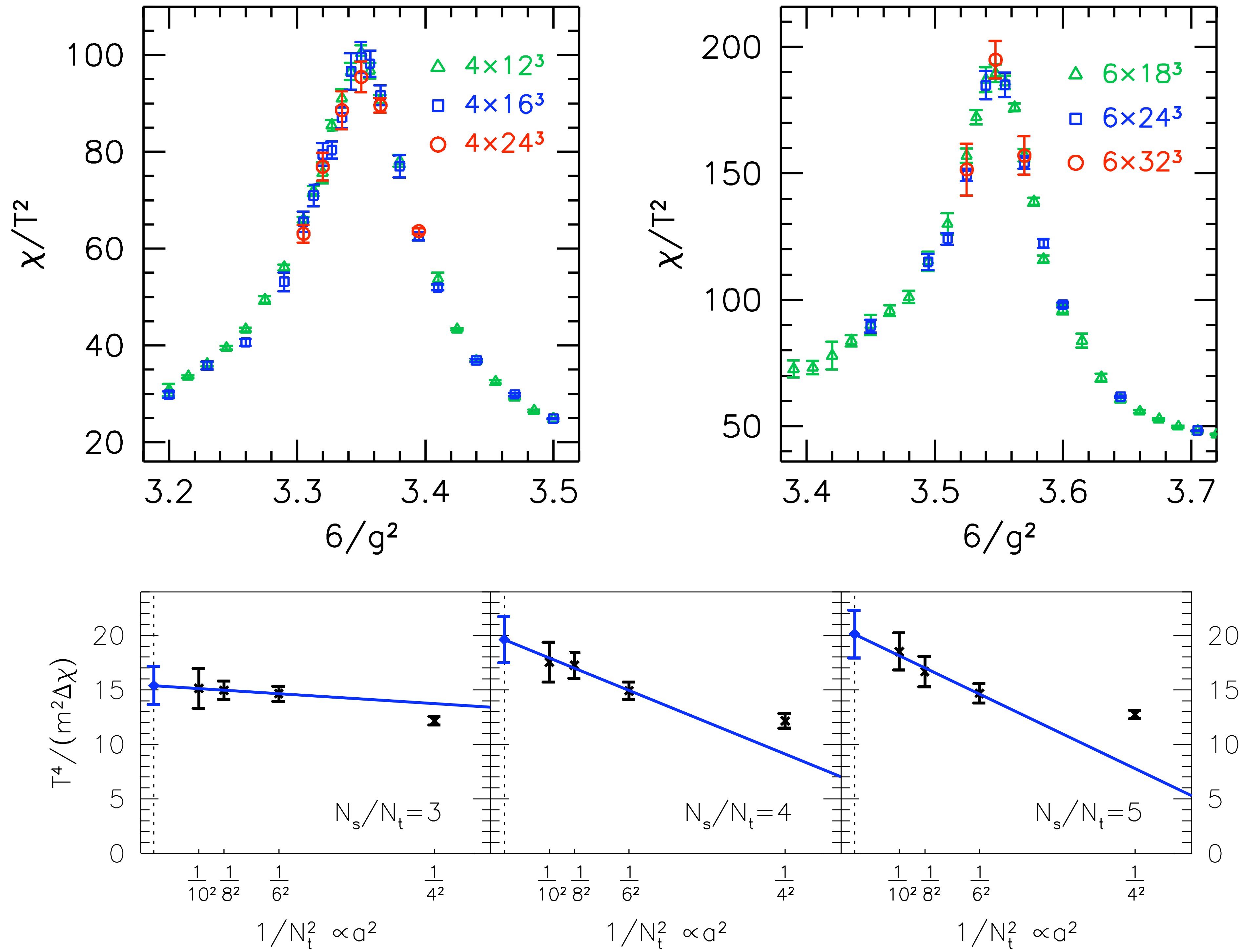
Order of transition: finite volume scaling $(\beta_0(V) - \beta_0(\infty)) \sim V^{-\sigma}$

$\sigma = 1$	1st order
$\sigma < 1$	2nd order
$\sigma = 0$	crossover

The nature of the transition for phys. masses

Aoki et al. 06

...in the staggered approximation...in the continuum...is a crossover!

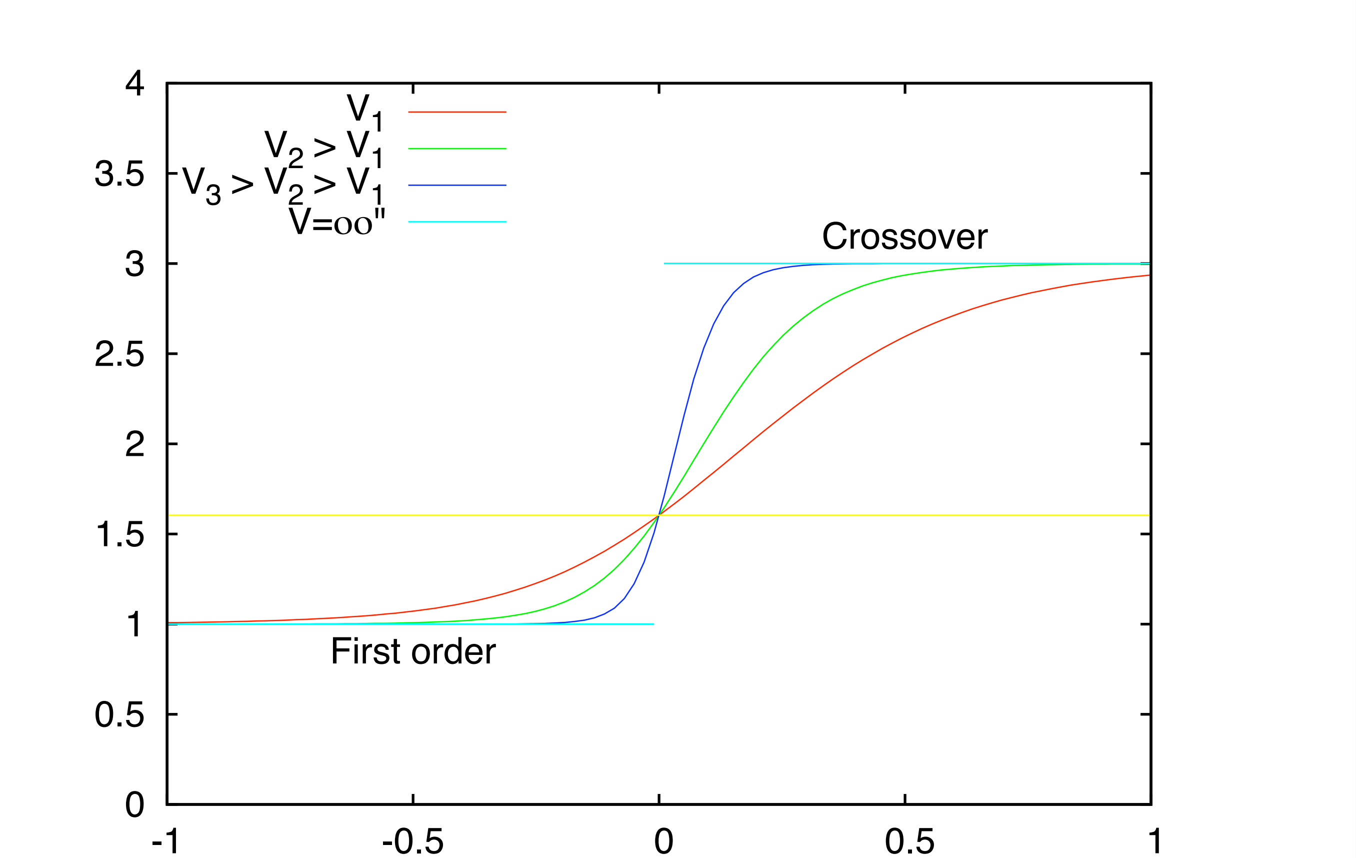


How to identify the order of the phase transition

$$B_4(\bar\psi\psi) \equiv \frac{\langle(\delta\bar\psi\psi)^4\rangle}{\langle(\delta\bar\psi\psi)^2\rangle^2} \xrightarrow{V\to\infty} \begin{cases} 1.604 & \text{3d Ising} \\ 1 & \text{first}-\text{order} \\ 3 & \text{crossover} \end{cases}$$

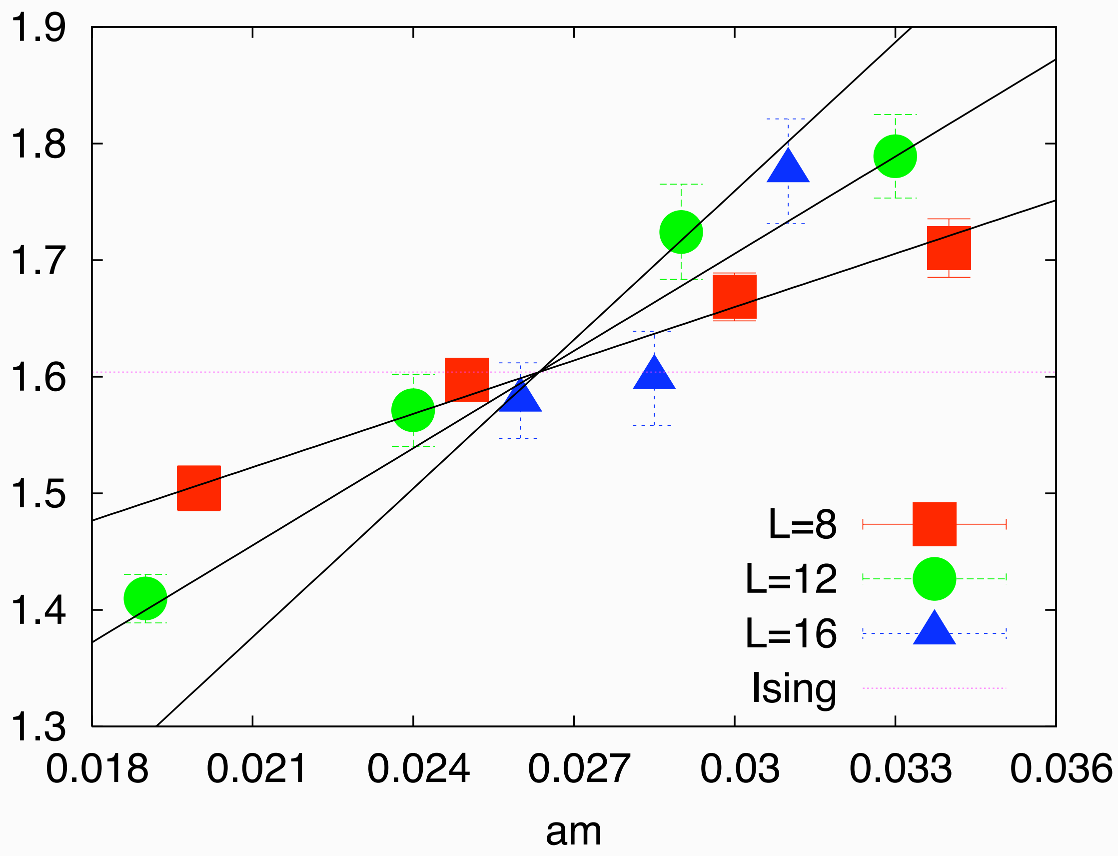
$\mu = 0:$ $\quad B_4(m,L) = 1.604 + bL^{1/\nu}(m - m_0^c), \quad \nu = 0.63$

B_4

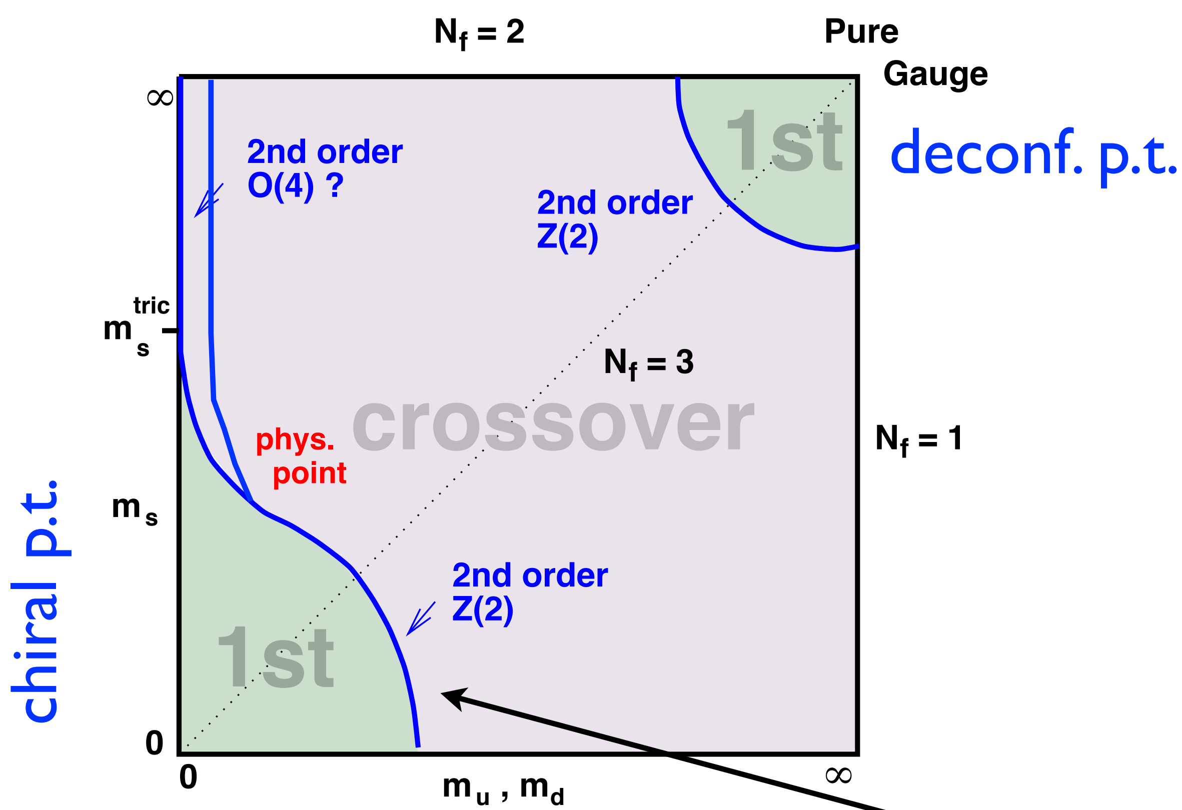


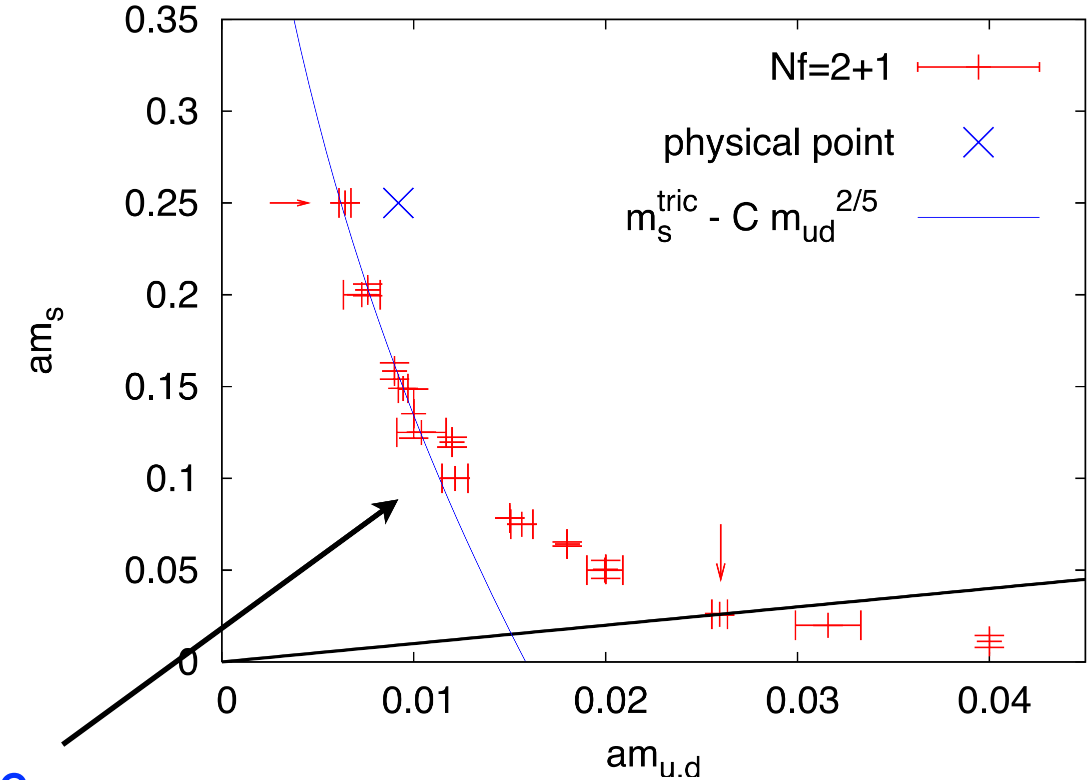
$x - x_c$

parameter along phase boundary, $T = T_c(x)$



Order of p.t., arbitrary quark masses $\mu = 0$

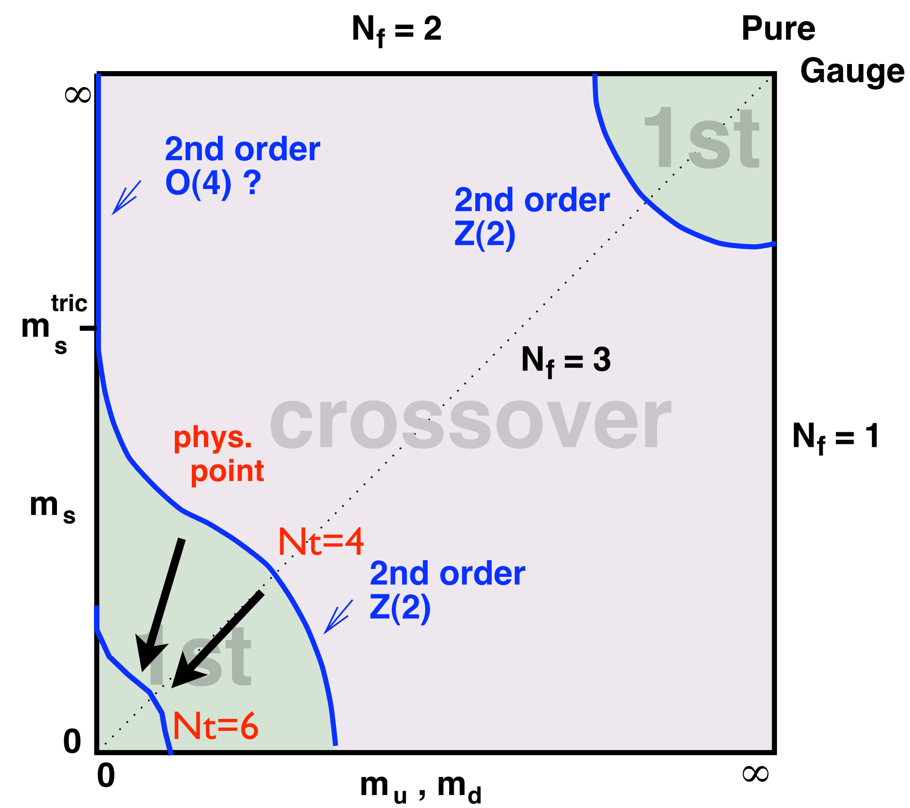




chiral critical line

- physical point: crossover in the continuum — Aoki et al 06
- chiral critical line on $N_t = 4, a \sim 0.3$ fm — de Forcrand, O.P. 07
- consistent with tri-critical point at $m_{u,d} = 0, m_s^{\rm tric} \sim 2.8T$
- But: $N_f = 2$ chiral O(4) vs. 1st still open — Di Giacomo et al 05, Kogut, Sinclair 07
  $U_A(1)$ anomaly! — Chandrasekharan, Mehta 07
  Cossu et al. 12, Aoki et al. 12

Large cut-off effects on critical lines!

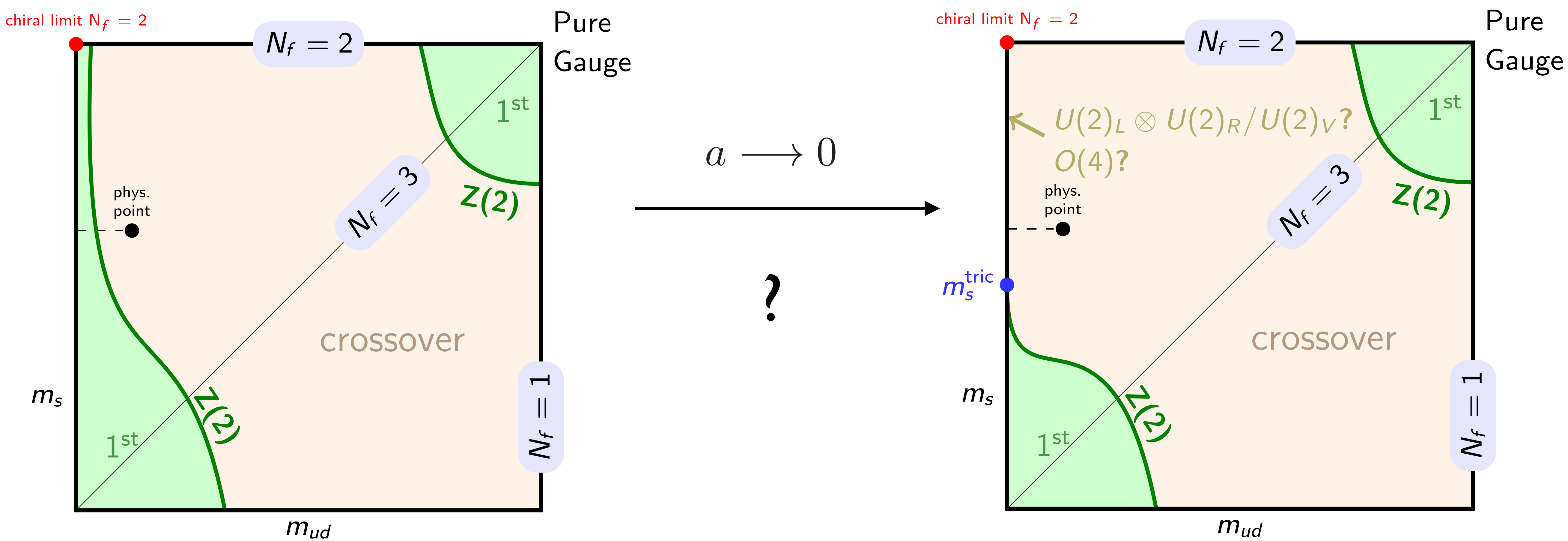


de Forcrand, Kim, O.P. 07
Endrodi et al 07

- Physical point deeper in crossover region as $a \to 0$

critical pion mass shrinks by factor ~1.8 from a=0.3 fm to a=0.2 fm!
no continuum limit yet!

Order of the transition in the chiral limit is not yet settled!



Coarse lattices:
chiral limit is first order!

Unimproved staggered: Bonati et al. 14
Unimproved Wilson: Pinke, O.P. 14

Lattice QCD at finite baryon density

$$Z = \hat{\mathrm{Tr}}\, \mathrm{e}^{-(H-\mu Q)}, \quad Q = \int d^3x\, \bar{\psi}(x)\gamma_0\psi(x) = \int d^3x\, \psi^\dagger(x)\psi(x)$$

Quark number and chemical potential: $Q = B/3, \mu = \mu_B/3$

Necessary for real world applications: heavy ion collisions, nuclear matter, compact stars,...

Behaviour under charge conjugation: $C = \gamma_0\gamma_2 \qquad \gamma_\mu = \gamma_\mu^\dagger, \{\gamma_5, \gamma_\mu\} = 0$

$$A_\mu^C = -A_\mu^*, \quad \psi^C = \gamma_0\gamma_2\bar{\psi}^T, \quad \bar{\psi}^C\gamma_0\psi^C = -\bar{\psi}\gamma_0\psi$$

sign flip in Q!

$\Rightarrow$

$$\begin{aligned} \mu > 0 &: \quad \text{net baryon number} \\ \mu < 0 &: \quad \text{net anti-baryon number} \end{aligned}$$

The sign problem

Dirac operators satisfy
(continuum, Wilson, staggered,...)

$$(\not{D} + m)^\dagger = \gamma_5(\not{D} + m)\gamma_5$$

With complex chemical potential:

$$\gamma_5(\not{D} + m - \gamma_0\mu)\gamma_5 = (-\not{D} + m + \gamma_0\mu) = (\not{D} + m + \gamma_0\mu^*)^\dagger$$

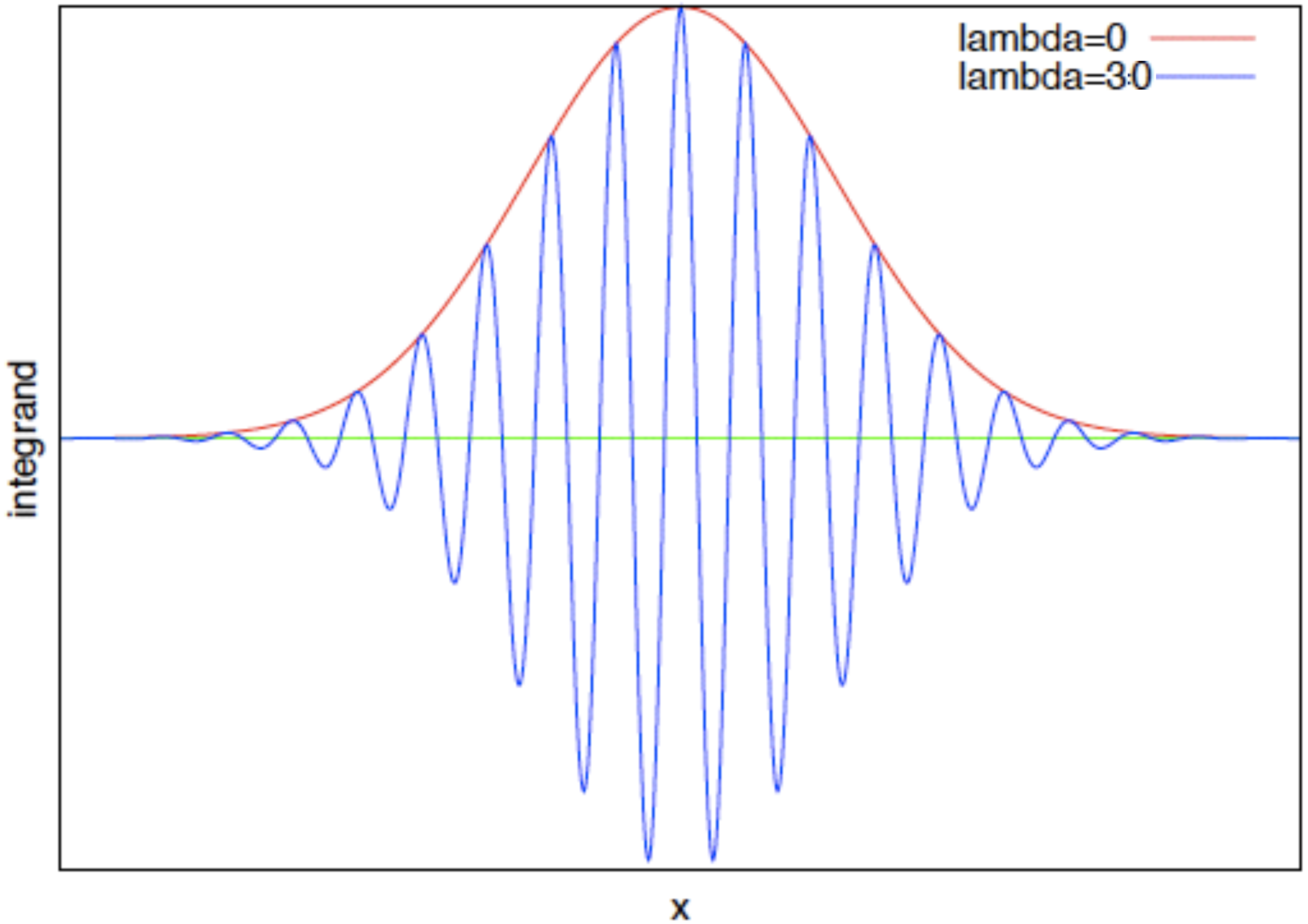
$$\det(\not{D} + m - \gamma_0\mu) = \det{}^*(\not{D} + m + \gamma_0\mu^*)$$

"Sign problem" of QCD

- Complex measure cannot be used for MC importance sampling
- After integration over gauge fields the partition function is real!
- Generic for systems with anti-particles, necessary for physics!

1 dim. illustration

- Example: $Z(\lambda) = \int dx \exp(-x^2 + \mathbf{i}\lambda\mathbf{x})$



- $Z(\lambda)/Z(0) = \exp(-\lambda^2/4)$: exponential cancellations

Approximate methods to evade the sign problem: Reweighting

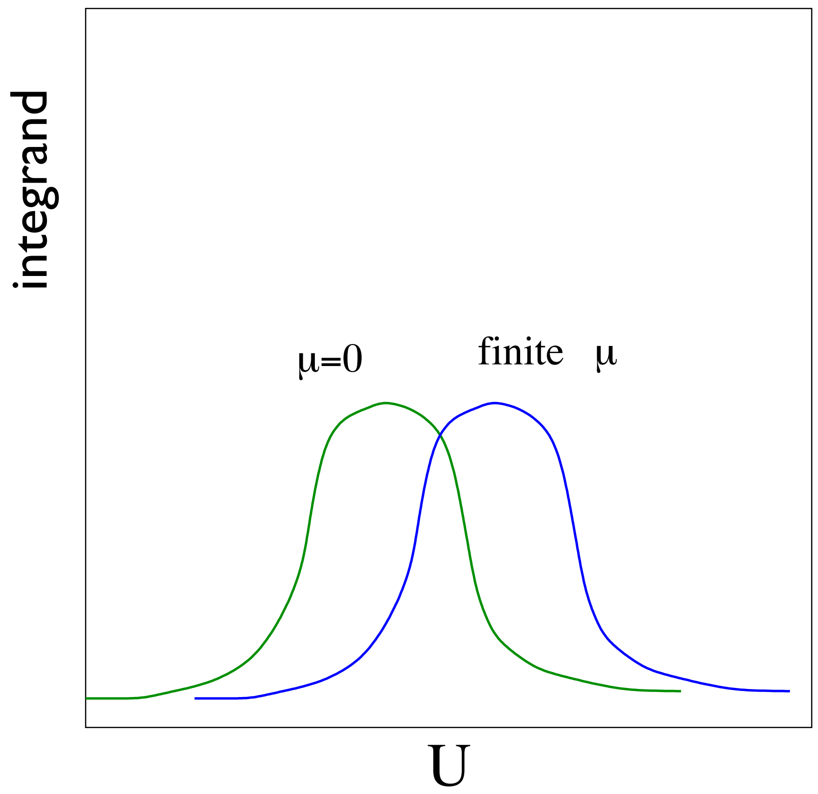
Based on exact relation:

$$Z(\mu) = \int DU \ \det M(\mu) \, \mathrm{e}^{-S_g[U]} = \int DU \ \det M(0) \, \frac{\det M(\mu)}{\det M(0)} \, \mathrm{e}^{-S_g[U]}$$

$$= Z(0) \left\langle \frac{\det M(\mu)}{\det M(0)} \right\rangle_{\mu=0} .$$

I. Numerically difficult, signal exponentially suppressed with volume

$$\frac{Z(\mu)}{Z(0)} = \exp - \frac{F(\mu) - F(0)}{T} = \exp - \frac{V}{T} \left(f(\mu) - f(0) \right)$$



II. Overlap problem, because of importance sampling

With increasing difference the most frequent configs. are increasingly unimportant

Finite density by Taylor expansion

Taylor expansion of the pressure around zero density:

$$\frac{p}{T^4} = \sum_{n=0}^{\infty} c_{2n}(T) \left(\frac{\mu}{T}\right)^{2n} \equiv \Omega(T,\mu)$$

$$c_0(T) = \frac{p}{T^4}(T,\mu=0), \quad c_{2n}(T) = \frac{1}{(2n)!} \left.\frac{\partial^{2n}\Omega}{\partial(\frac{\mu}{T})^{2n}}\right|_{\mu=0}$$

The coefficients can be computed at zero density!

Other physical quantities follow:

$$\frac{n}{T} = \frac{\partial\Omega}{\partial(\frac{\mu}{T})} = 2c_2\frac{\mu}{T} + 4c_4\left(\frac{\mu}{T}\right)^3 + \ldots,$$

$$\frac{\chi_q}{T^2} = \frac{\partial^2\Omega}{\partial(\frac{\mu}{T})^2} = 2c_2 + 12c_4\left(\frac{\mu}{T}\right)^2 + 30c_6\left(\frac{\mu}{T}\right)^4 + \ldots$$

No sign problem, but need small μ/T

Higher coeffs. increasingly difficult:

$$\frac{\partial\langle O\rangle}{\partial\mu} = \left\langle\frac{\partial O}{\partial\mu}\right\rangle + N_f\left(\left\langle O\frac{\partial \ln\det M}{\partial\mu}\right\rangle - \langle O\rangle\left\langle\frac{\partial \ln\det M}{\partial\mu}\right\rangle\right)$$

QCD at imaginary chemical potential

No sign problem; general idea:

Observables have definite symmetry, even or odd in chemical potential

$$\langle O \rangle (\mu_i) = \sum_{k=1}^{N} c_k \left(\frac{\mu_i}{T}\right)^{2k}$$

- Simulate left side without further systematic error
- Check if fit to low order polynomial is possible $\mu/T < 1$
- Analytic continuation trivial (in the absence of singularities) $\mu_i \to -i\mu_i$

General considerations:

Partition function is periodic $Z = \hat{\mathrm{T}}\mathrm{r}\, e^{-\frac{(H - i\mu_i Q)}{T}}$

Is this a healthy theory?

Yes! Recall $\mu Q = -ig \int d^3x\, A_0 j_0 \quad \text{with} \quad A_0 = i\frac{\mu}{g}$

Equivalent to theory in real external field!

Periodicity non-trivial:

Chemical potential can be absorbed by boundary conditions

$$Z^{(1)}(i\mu_i) = \int DU \det M(0) \mathrm{e}^{-S_g}, \quad \text{b.c.:} \quad \psi(\tau + N_\tau, \mathbf{x}) = -\mathrm{e}^{i\frac{\mu_i}{T}} \psi(\tau, \mathbf{x})$$

Consider the topological gauge trafo $g'(\tau + N_\tau, x) = \mathrm{e}^{-i\frac{2\pi n}{N}} g'(\tau, \mathbf{x})$

Measure and action are invariant, hence

$$Z^{(2)}(i\mu_i) = \int DU \det M(0) \mathrm{e}^{-S_g}, \quad \text{b.c.:} \quad \psi(\tau + N_\tau, \mathbf{x}) = -\mathrm{e}^{-i\frac{2\pi n}{N}} \mathrm{e}^{i\frac{\mu_i}{T}} \psi(\tau, \mathbf{x})$$

$$Z^{(2)}\left(i\frac{\mu_i}{T} + i\frac{2\pi n}{N}\right) = Z^{(1)}\left(i\frac{\mu_i}{T}\right)$$

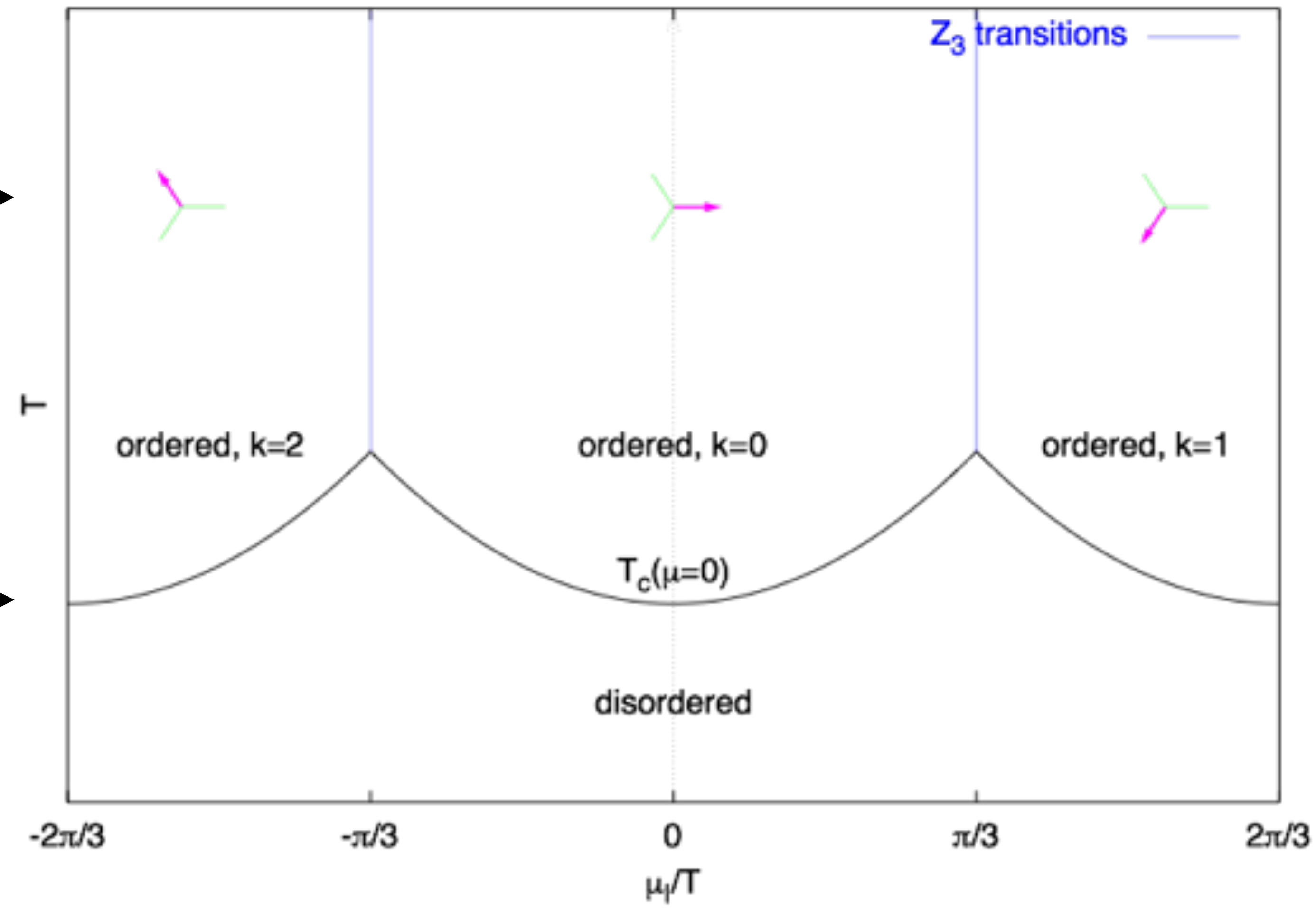
Both partition fcns. related by gauge trafo, identical!

Roberge-Weiss symmetry: $$Z\left(i\frac{\mu_i}{T} + i\frac{2\pi n}{N}\right) = Z\left(i\frac{\mu_i}{T}\right)$$

The phase diagram at imaginary chemical potential

Phase of Polyakov loop →

Analytic continuation of chiral/deconfinement transition, depends on Nf, quark masses →



Roberge-Weiss: Z(3) transitions are first order for large T (perturbation theory)
crossover for small T (strong coupling limit)

analytic continuation within:

$|\mu|/T \leq \pi/3 \Rightarrow \mu_B \lesssim 550\mathrm{MeV}$

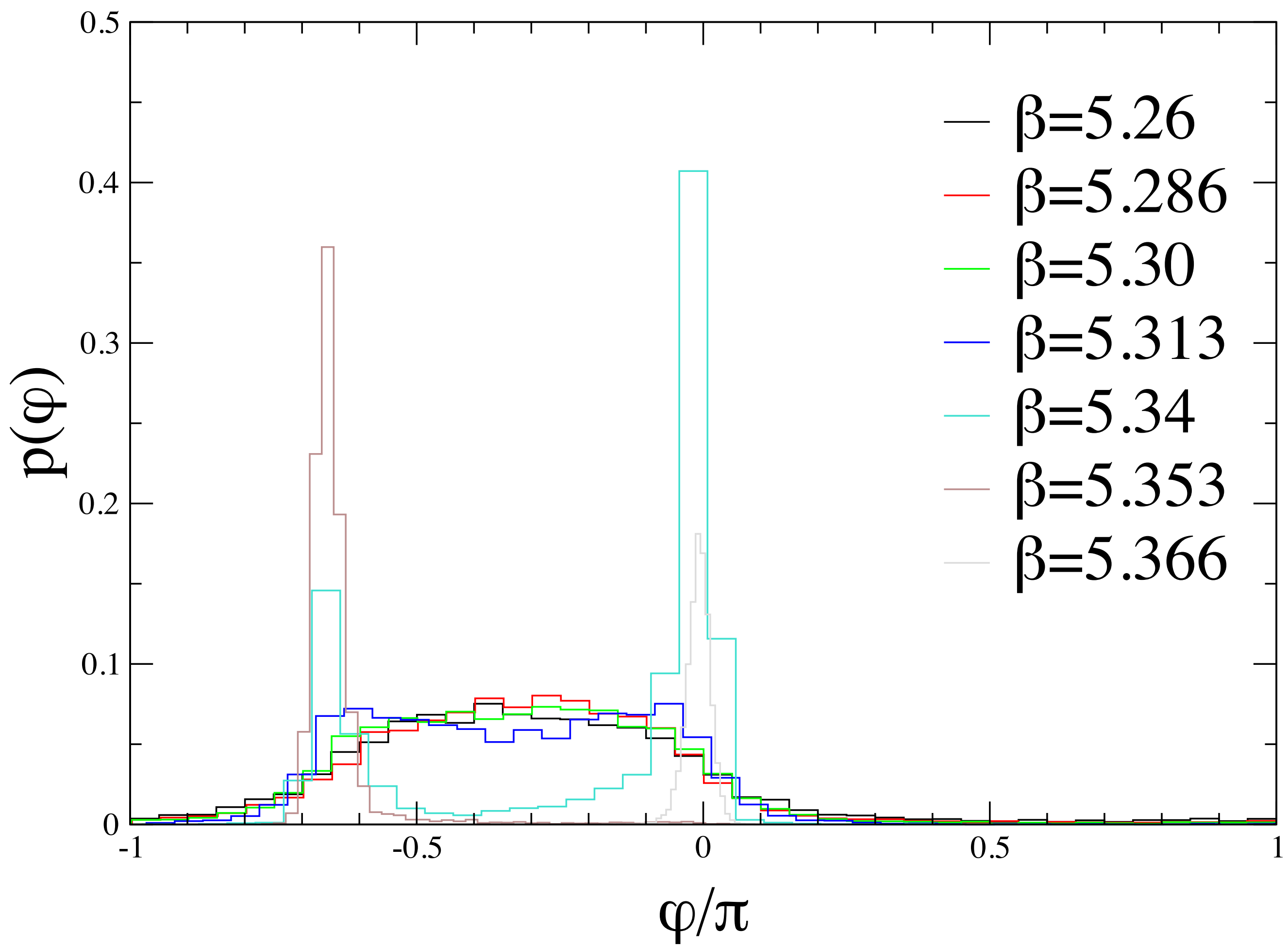
Limited by singularity (phase transition) closest to $\mu = 0$

The Z(3) transition numerically

Nf=2: de Forcrand, O.P. 02

Nf=4: D'Elia, Lombardo 03

Sectors characterised by phase of Polyakov loop: $\langle L(x) \rangle = |\langle L(x) \rangle| \, \mathrm{e}^{i\varphi}$



Low T: crossover High T: first order p.t.

Towards the QCD phase diagram

Analyticity of the (pseudo-)critical line

Recall definition by peak of susceptibilities: $\chi_{max} = \chi(\beta_c, m_f, \mu)$

Implicit definition of pseudo-critical line $\beta_c(m_f, \mu)$

Implicit function theorem:

For analytic susceptibility, also the implicitly defined pseudo-critical coupling is analytic (always true on finite V!)

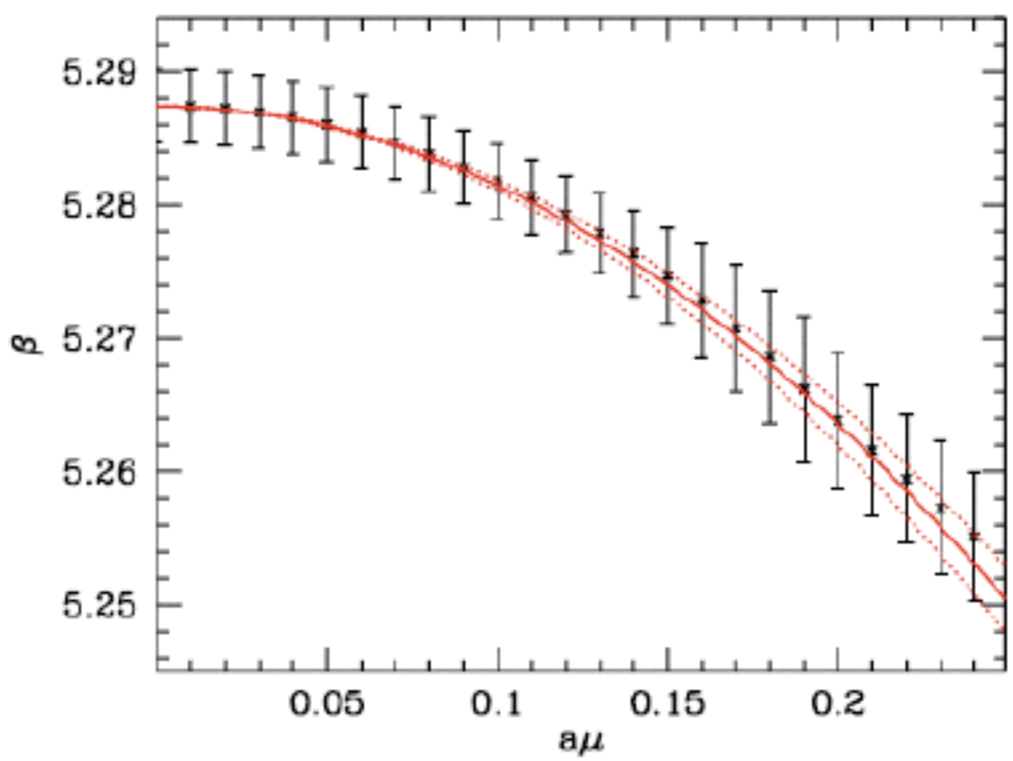
$$\beta_c(m_f, \frac{\mu}{T}) = \sum_n b_{2n}(m_f) \left(\frac{\mu}{T}\right)^{2n}$$

$$\Rightarrow \quad \frac{T_c(m_f,\mu)}{T_c(m_f,0)} = 1 + t_2(m_f)\left(\frac{\mu}{T}\right)^2 + t_4(m_f)\left(\frac{\mu}{T}\right)^4 + \ldots$$

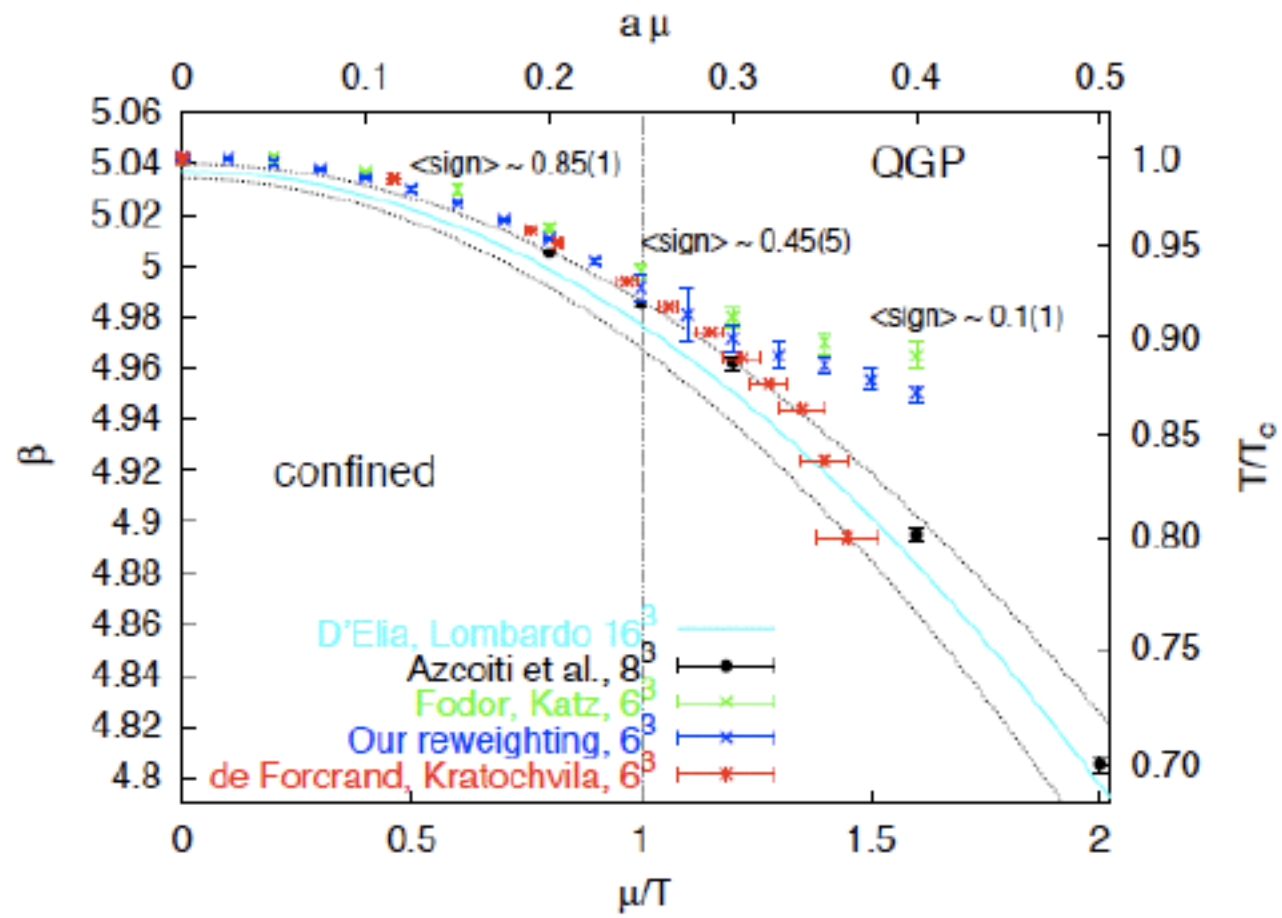
- Accessible to all methods discussed for sufficiently small chemical potential
- Crosscheck, in particular between Taylor coefficients and imaginary chem. pot.

Test of methods: comparing $T_c(\mu)$

Reweighting vs. imag. μ (FK, FP)



Rew., imag. μ, canonical ensemble ...



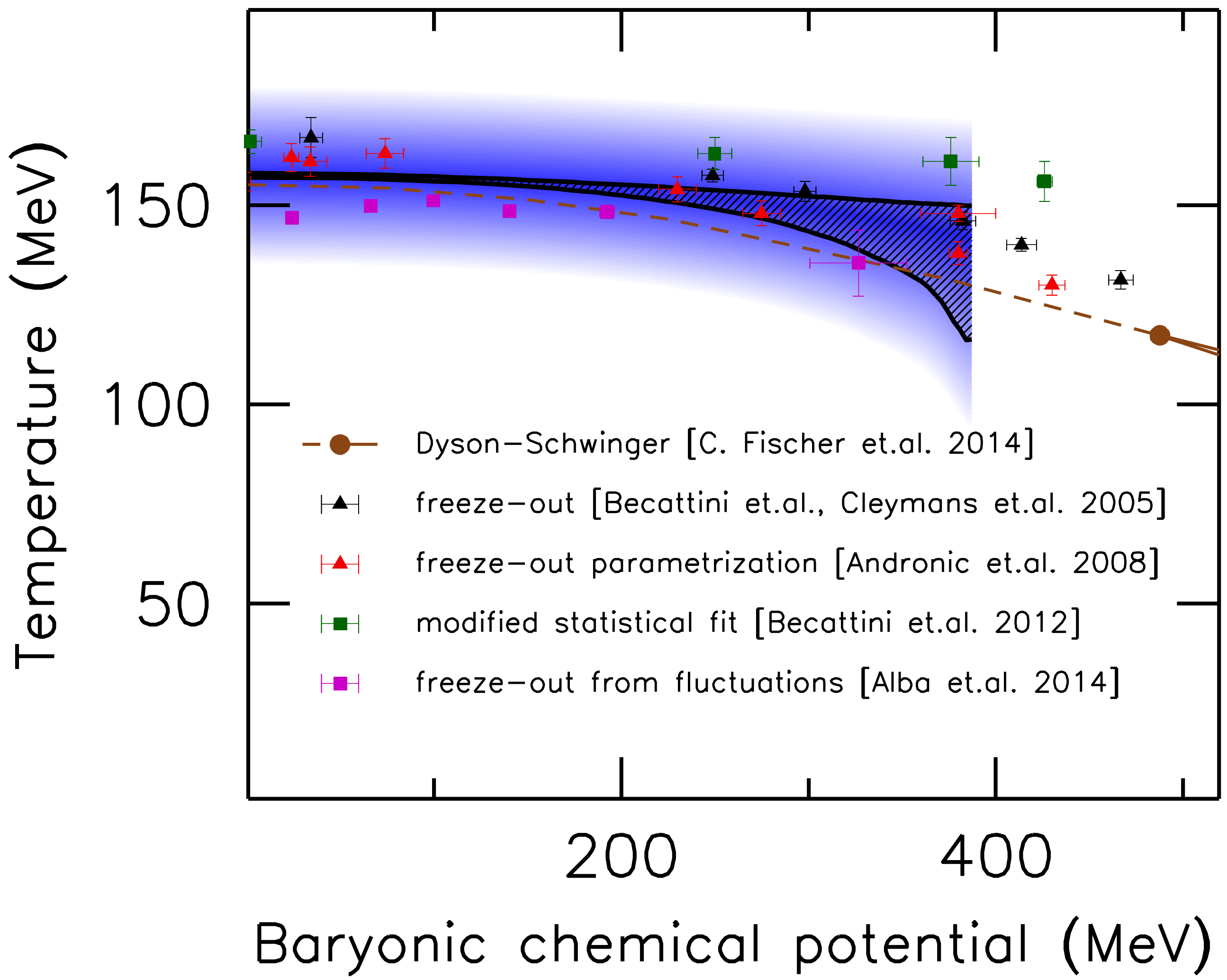
All agree on $T_0(m, \mu)$**!!!** $\quad (\mu/T \lesssim 1)$

The crossover for physical masses

In the continuum:

$$\frac{T_c(\mu_B)}{T_c(\mu=0)} = 1 - \kappa\left(\frac{\mu_B}{T_c(\mu_B)}\right)^2 + \mathcal{O}(\mu_B^4)$$

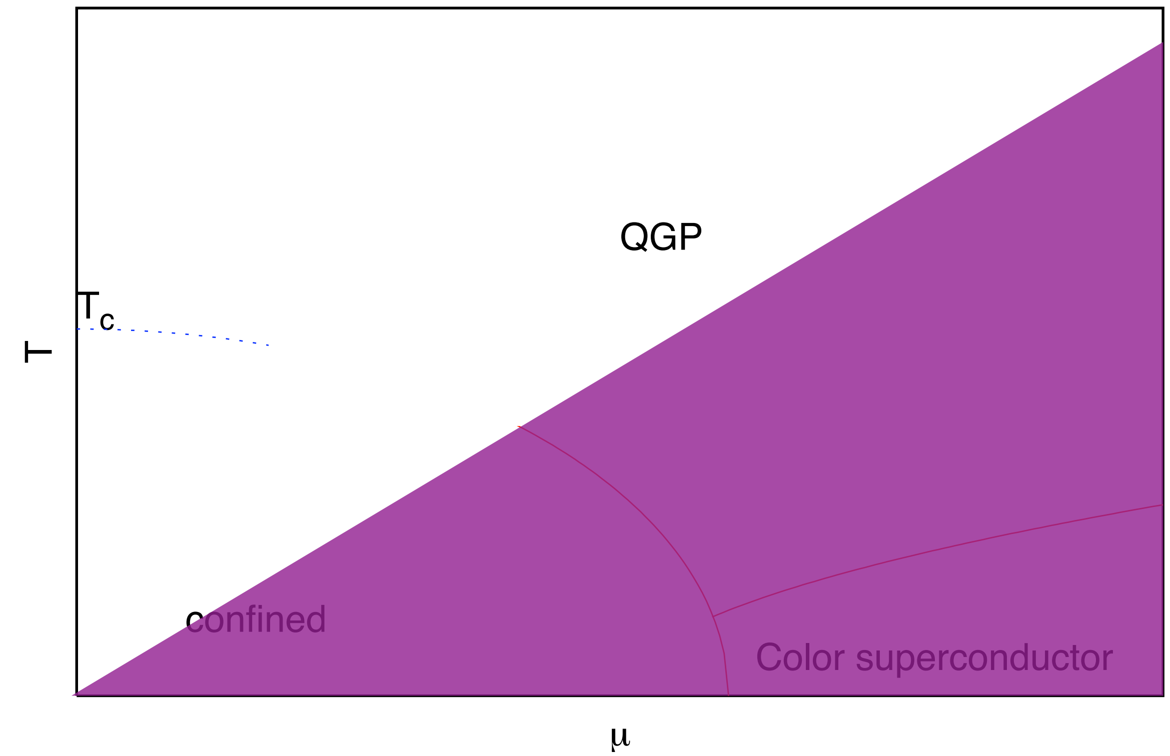
Budapest - Wuppertal 15



Consistent with other simulations and different actions

Bonati et al., 15
Cea et al. 15
Bielefeld-Brookhaven 14

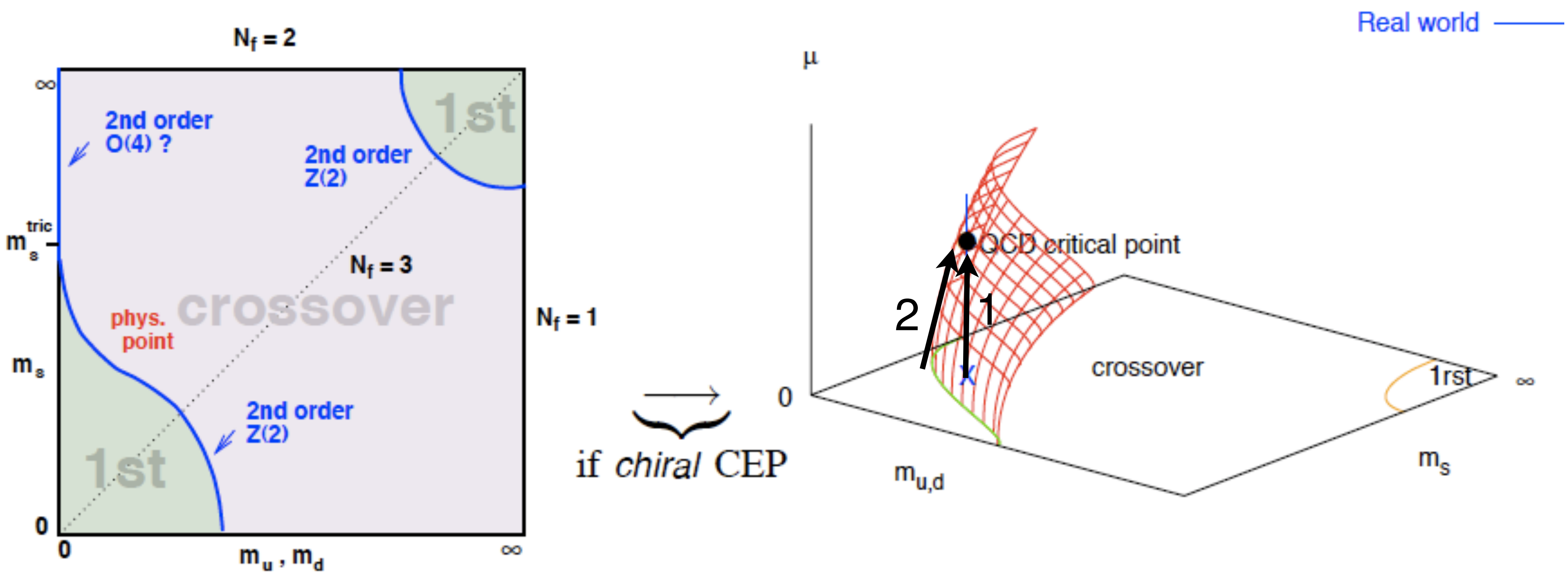
Lattice-calculable region of the QCD phase diagram



- Sign problem prohibits direct simulation, circumvented by approximate methods: reweigthing, Taylor expansion, imaginary chem. pot., need $\mu/T \lesssim 1 \quad (\mu = \mu_B/3)$
- No critical point in the controllable region, some signals beyond
- Complex Langevin: lots of progress, but not in all parameter space, no "guarantees"

So far only "heavy dense QCD", i.e. static quarks Aarts et al. 16
cf. density of states Langfeld et al. 16

Much harder: is there a QCD critical point?



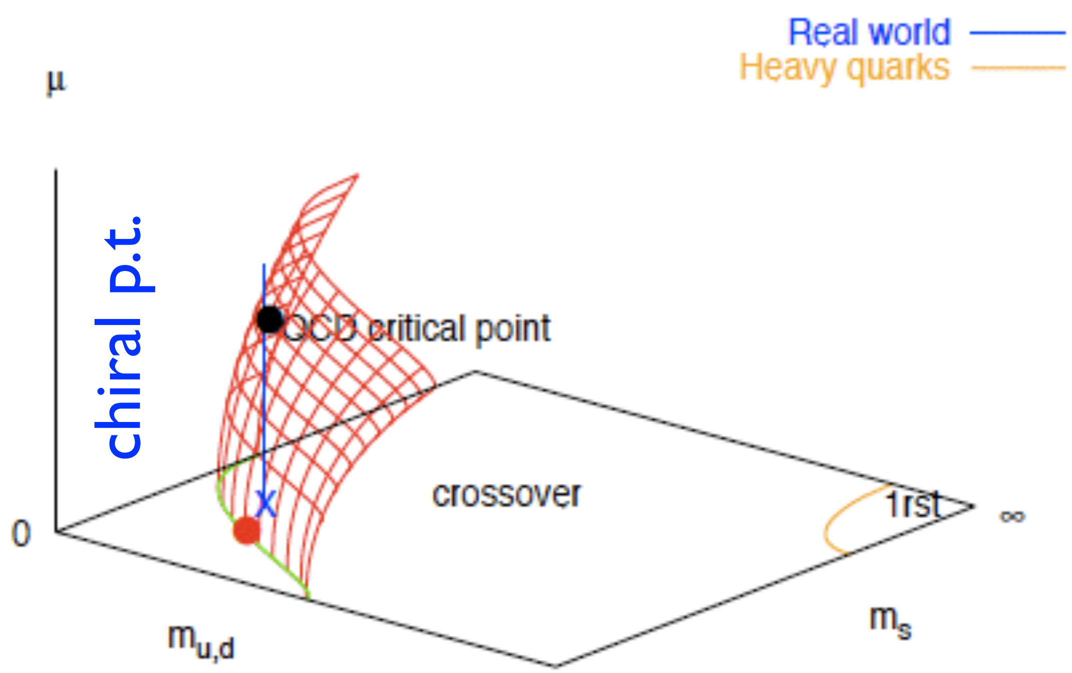
Two strategies:

1 follow vertical line: $m = m_{\rm phys}$, turn on μ

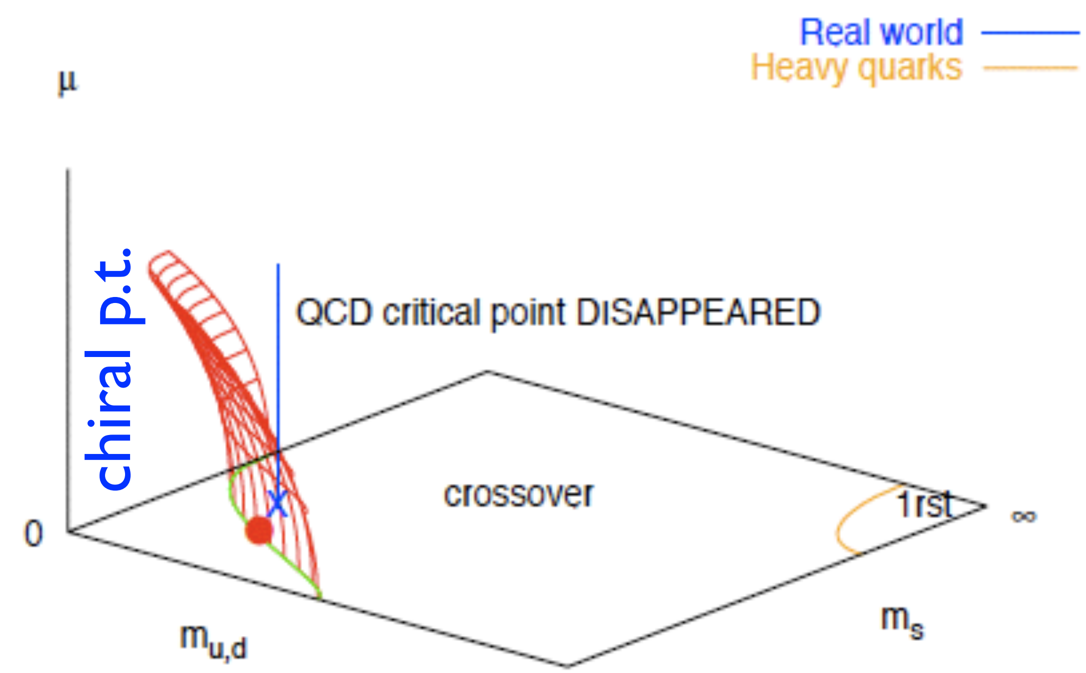
2 follow critical surface: $m = m_{\rm crit}(\mu)$

Some methods trying (1) give indications of critical point, but systematics not yet controlled

Approach 2: follow chiral critical line → surface



$c_1 > 0$



$c_1 < 0$

$$\frac{m_c(\mu)}{m_c(0)} = 1 + \sum_{k=1} c_k \left(\frac{\mu}{\pi T}\right)^{2k}$$

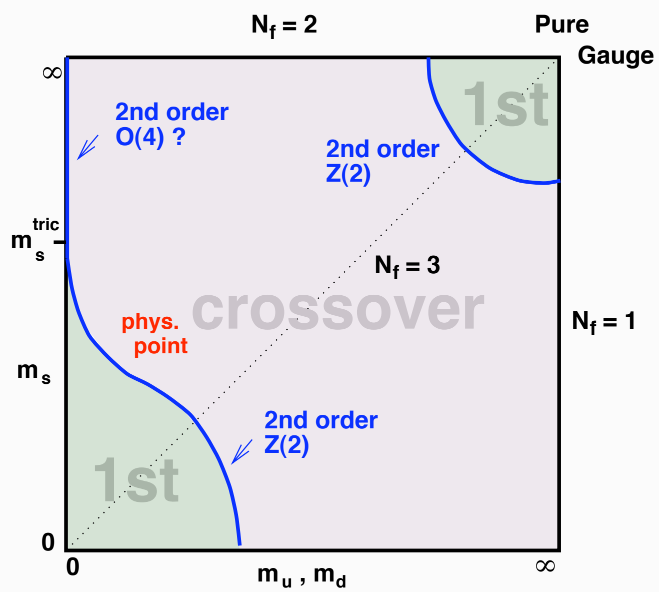
1. Tune quark mass(es) to $m_c(0)$: 2nd order transition at $\mu = 0$, $T = T_c$
   known universality class: $3d$ Ising

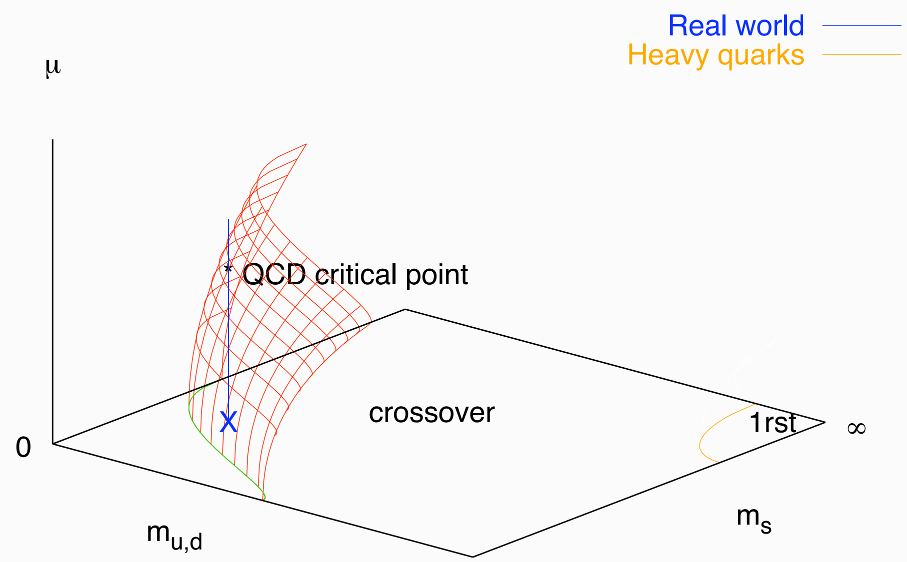
2. Measure derivatives $\frac{d^k m_c}{d\mu^{2k}}|_{\mu=0}$:

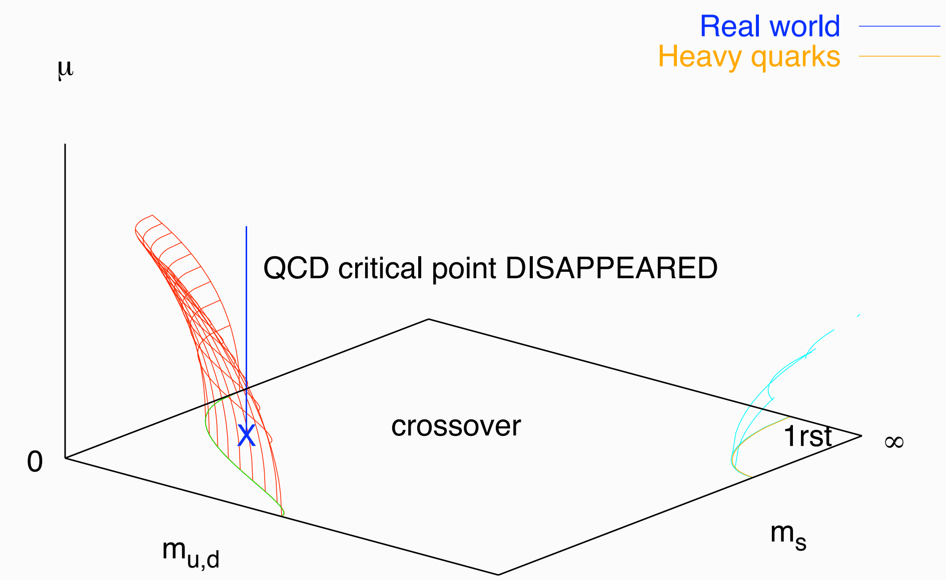
   Turn on imaginary μ and measure $\frac{m_c(\mu)}{m_c(0)}$

de Forcrand, O.P. 08,09

Finite density: chiral critical line ⟶ critical surface





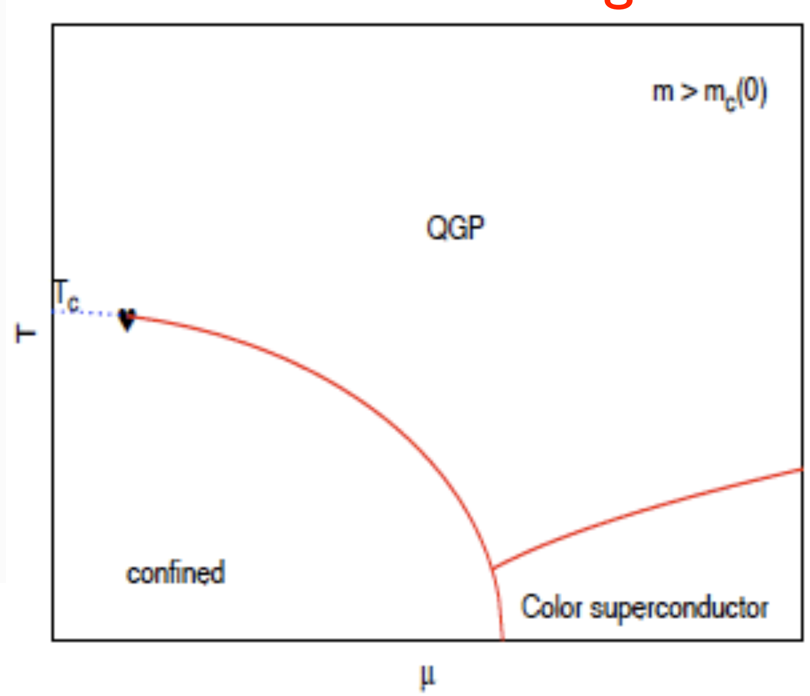


$$\frac{m_c(\mu)}{m_c(0)} = 1 + \sum_{k=1} \mathbf{c_k} \left(\frac{\mu}{\pi T}\right)^{2k}$$

$c_1 > 0$ $c_1 < 0$

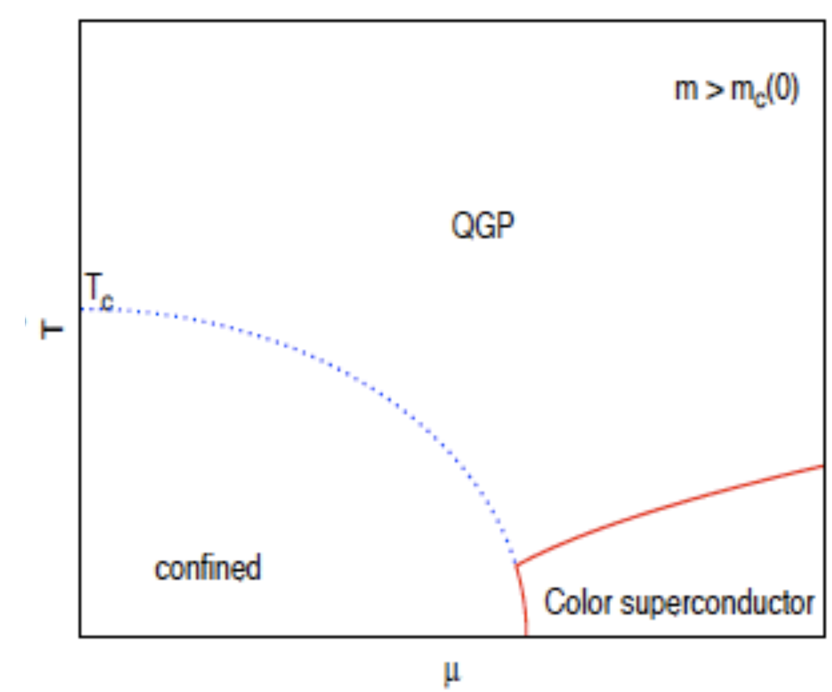
Standard scenario

transition strengthens

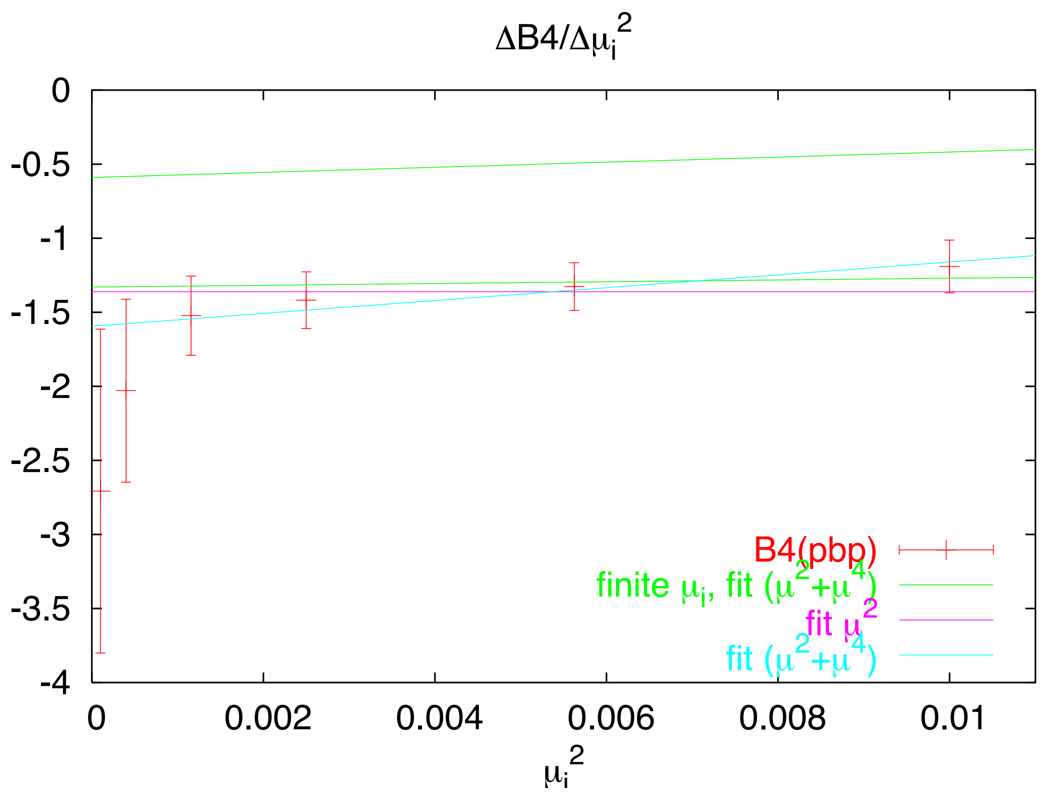


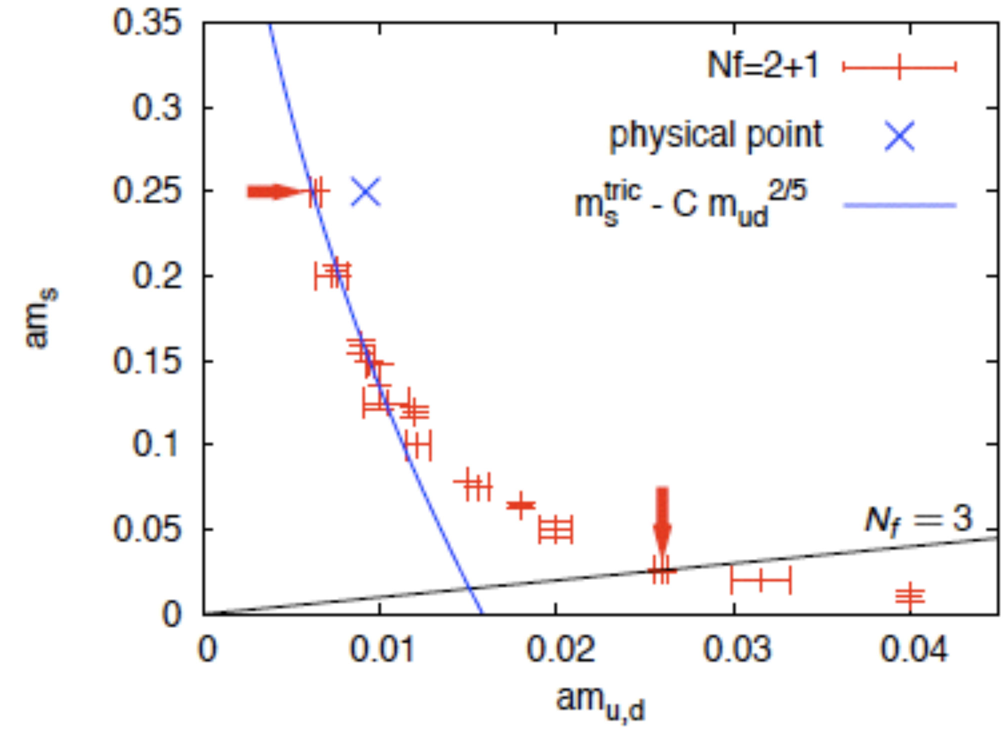
Exotic scenario

transition weakens



Curvature of the chiral critical surface





Nf=3: a) fit to imaginary chemical potential
b) calculation of coefficient by finite differences

consistent $8^3 \times 4$ and $12^3 \times 4$, $\sim 5 \times 10^6$ traj.

$$\frac{m_c(\mu)}{m_c(0)} = 1 - 3.3(3)\left(\frac{\mu}{\pi T}\right)^2 \underbrace{- 47(20)\left(\frac{\mu}{\pi T}\right)^4}_{\text{8th derivative of P}} - \ldots$$

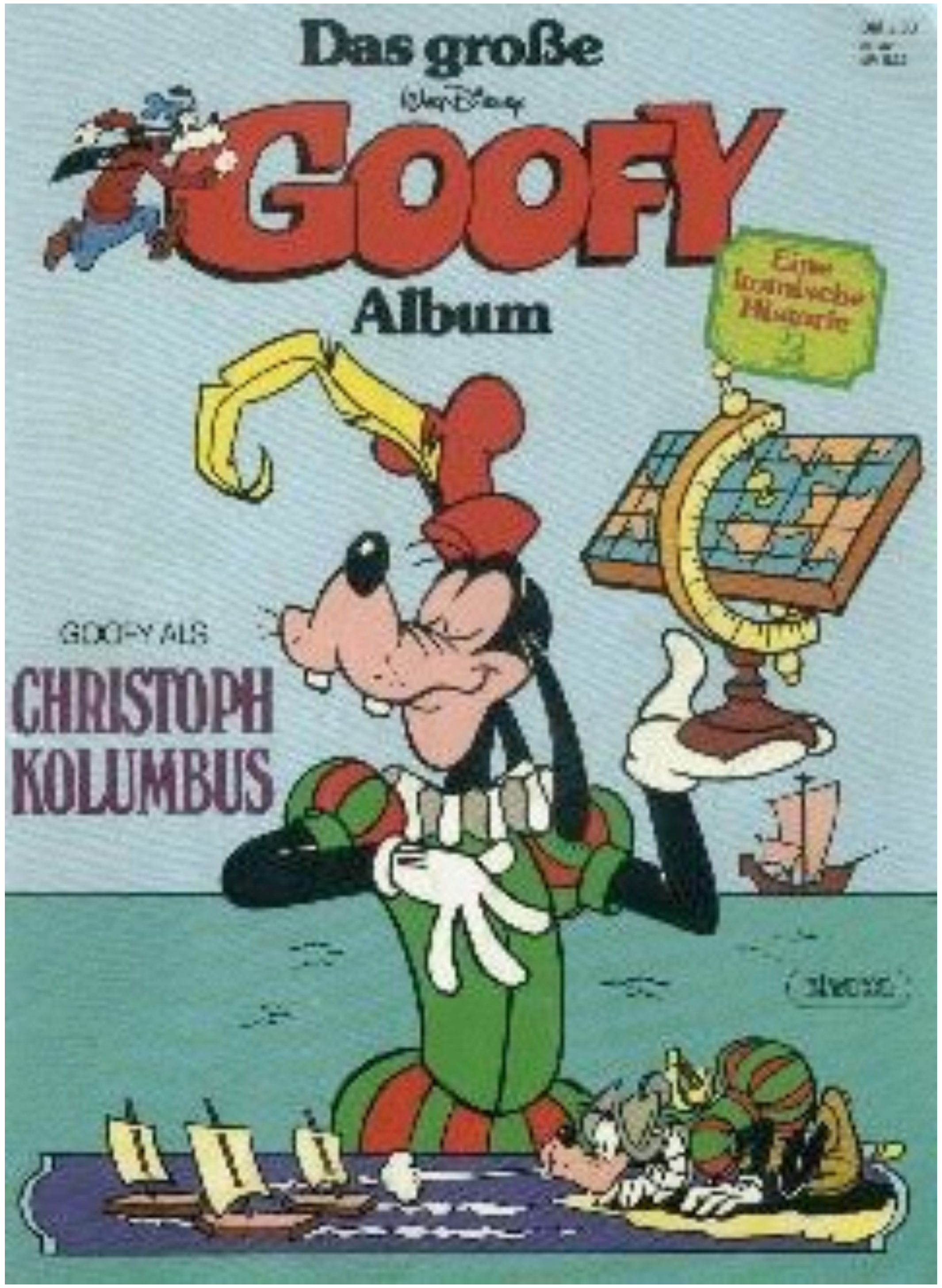
$16^3 \times 4$, Grid computing, $\sim 10^6$ traj.

$$\frac{m_c^{u,d}(\mu)}{m_c^{u,d}(0)} = 1 - 39(8)\left(\frac{\mu}{\pi T}\right)^2 - \ldots$$

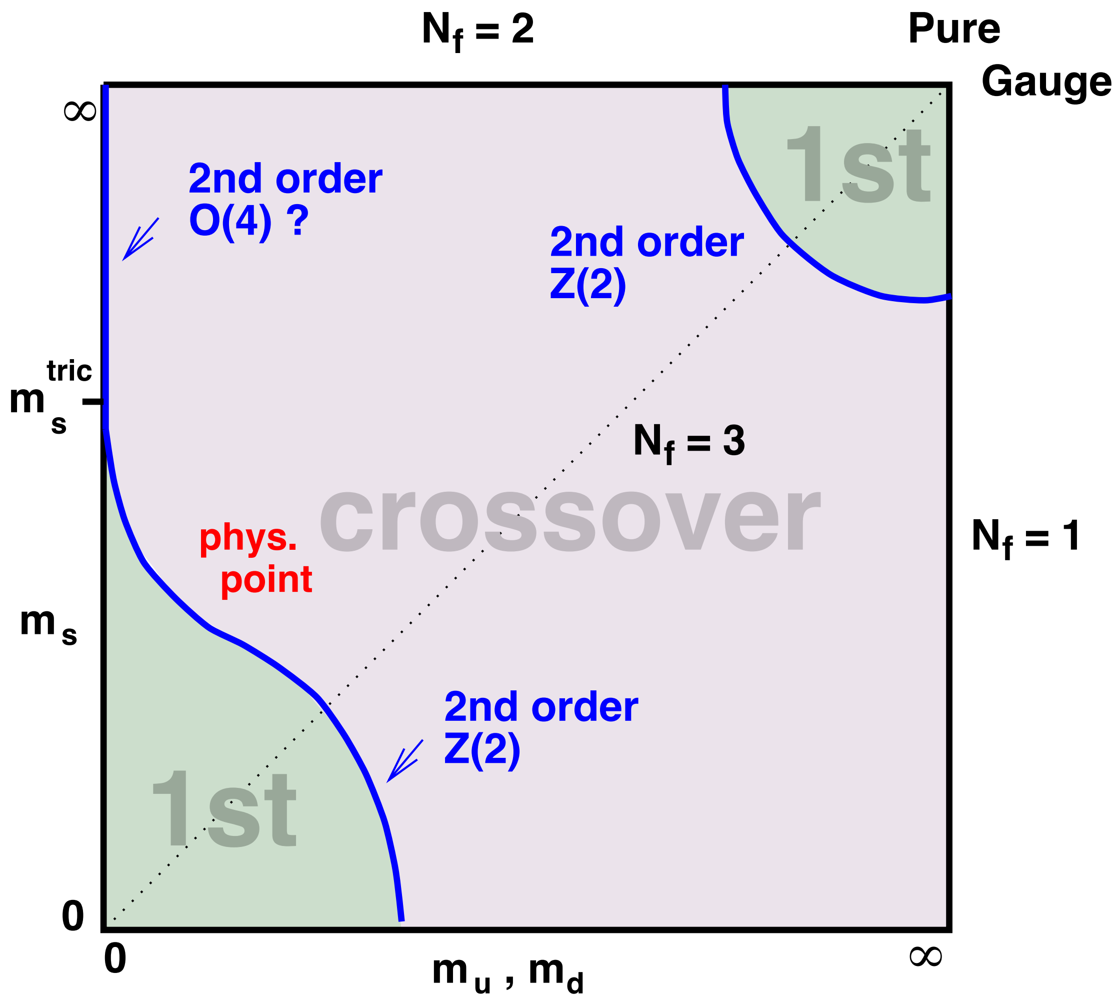
Importance of higher order terms ?

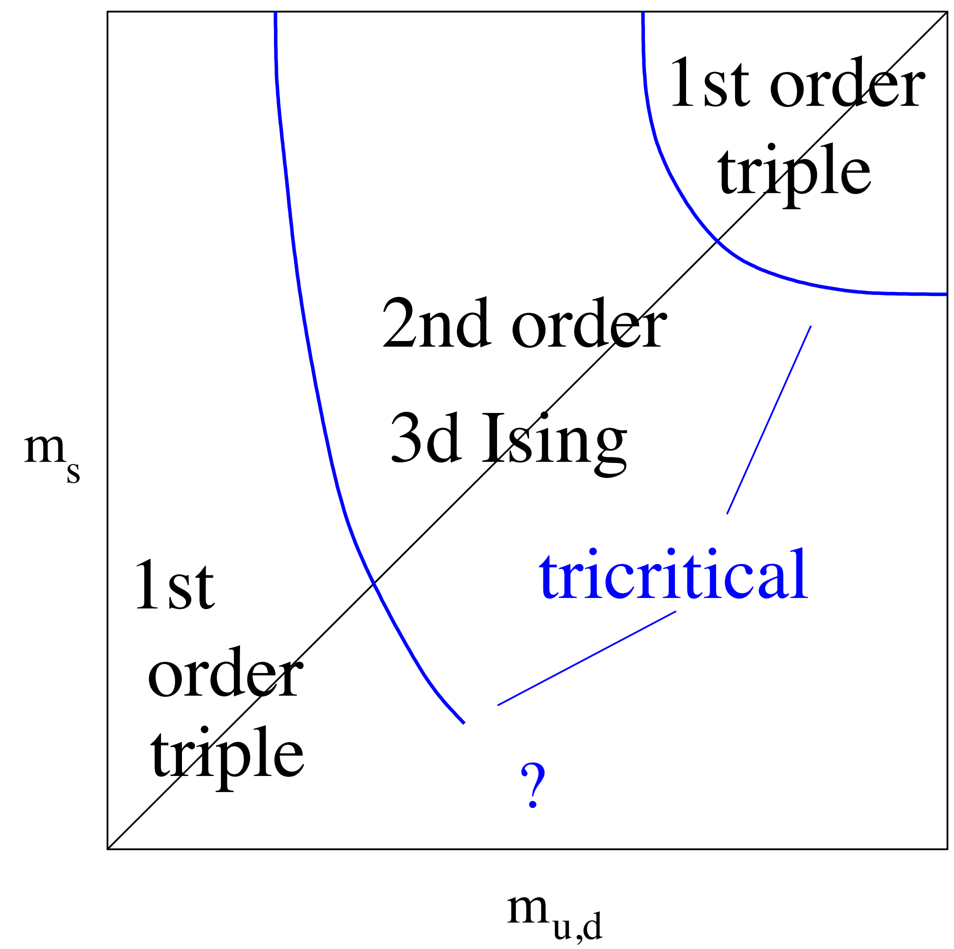
de Forcrand, O.P. 08,09

Un-discovering a critical point feels like...



Critical lines at imaginary μ





$$\mu = 0$$

$$\mu = i\frac{\pi T}{3}$$

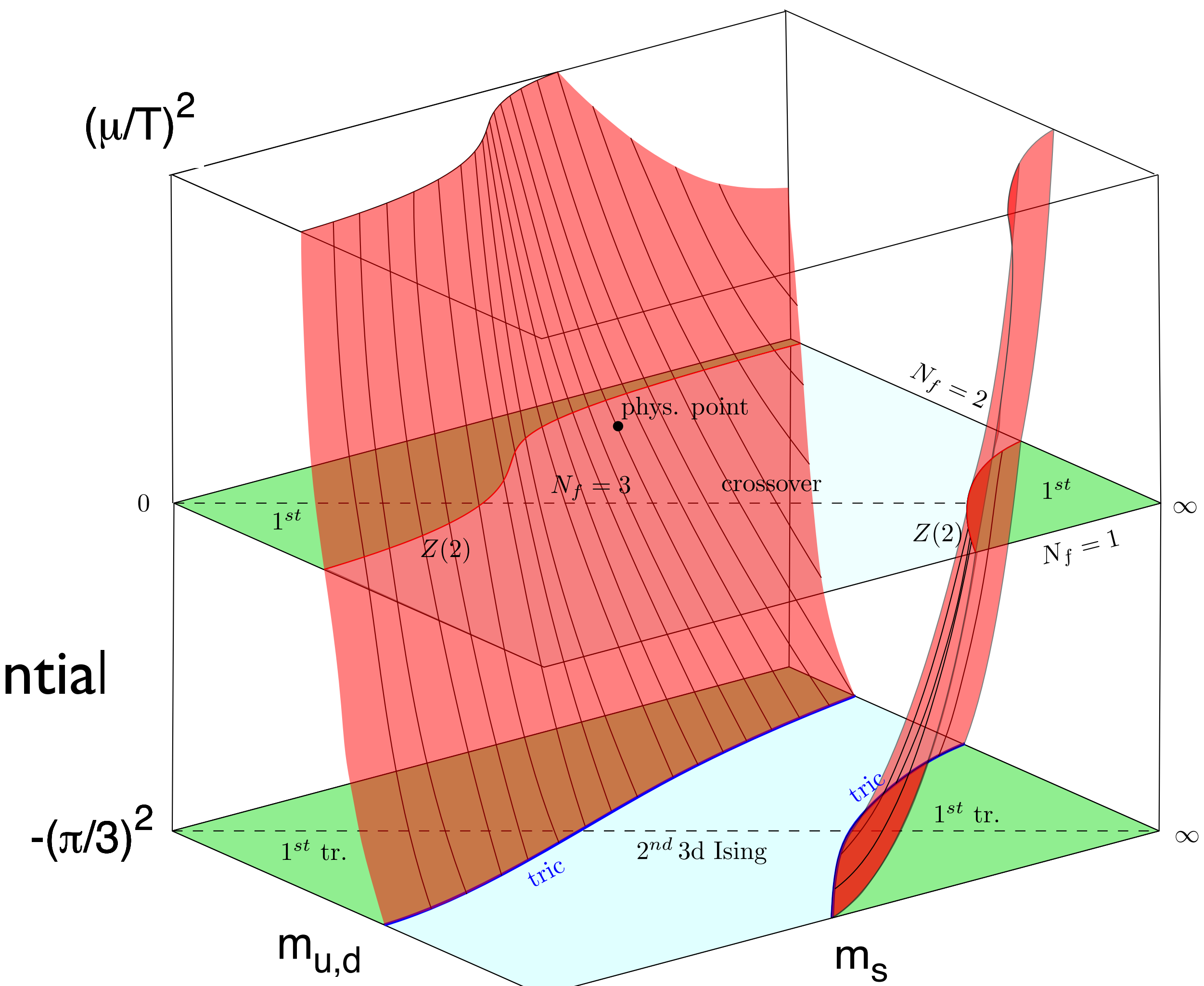
-Connection computable with standard Monte Carlo!

Critical surfaces from imaginary chemical potential

Real and imaginary chemical potential, coarse Nt=4 lattices

Real chemical potential:
sign problem

Imaginary chemical potential
no sign problem



Non-trivial phase structure
Roberge-Weiss Z(3) symmetry!

staggered,Nf=3:
de Forcrand, O.P. 10

staggered,Nf=2:
D'Elia, Sanfillippo 11

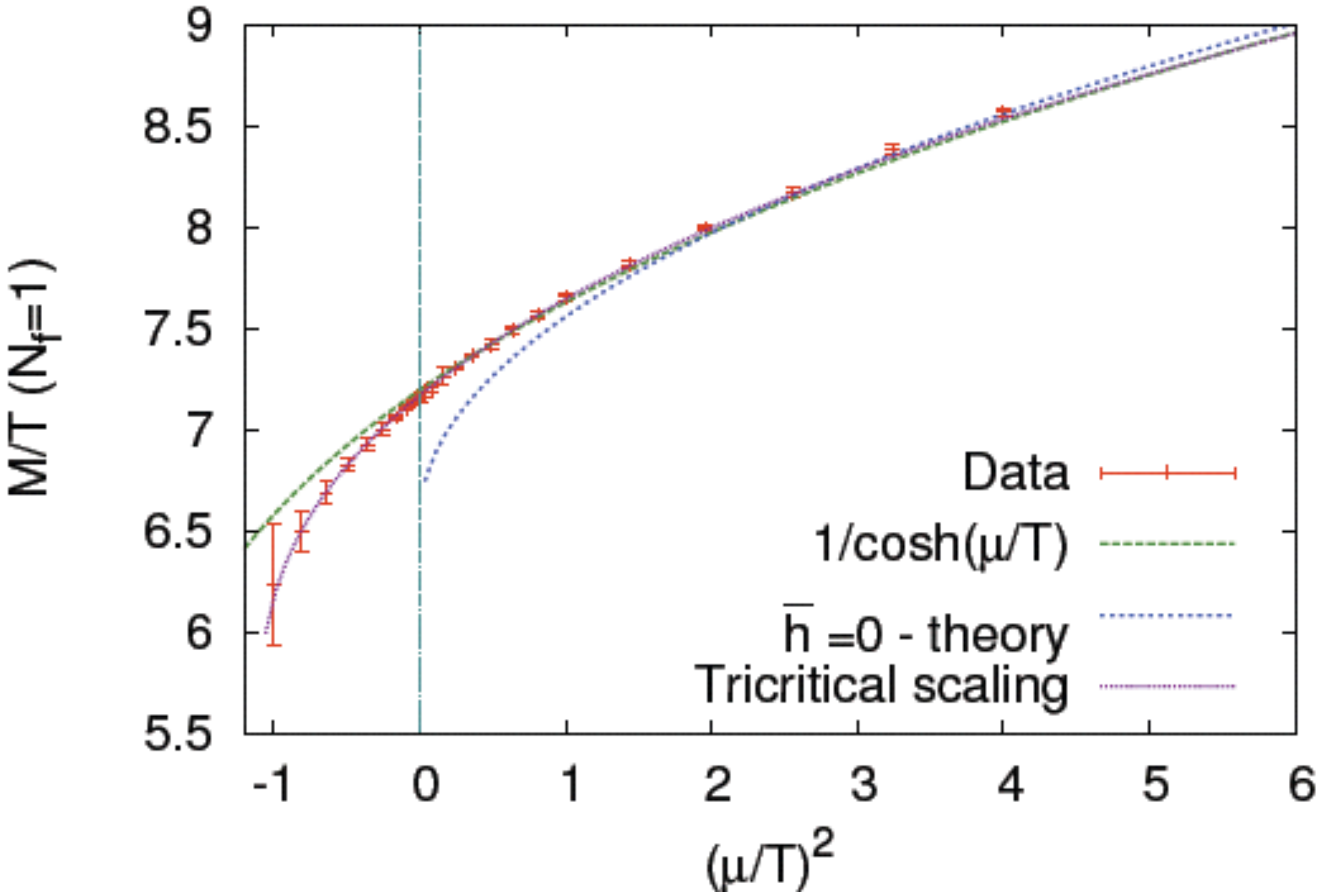
Wilson,Nf=2:
Pinke, O.P. 14

shape, sign of curvatures determined by tricritical scaling!

Heavy quarks

Deconfinement critical line

Fromm, Langelage, Lottini, O.P. 11



tri-critical scaling: $$\frac{m_c}{T}(\mu^2) = \frac{m_{tric}}{T} + K\left[\left(\frac{\pi}{3}\right)^2 + \left(\frac{\mu}{T}\right)^2\right]^{2/5}$$ ← exponent universal

Effective lattice theory for heavy and dense QCD

with M.Fromm, J.Langelage, S.Lottini, M.Neuman, J.Glesaaen

- Two-step treatment:

  I. Calculate effective theory analytically
  II. Simulate effective theory

- Step I.: split temporal and spatial link integrations:

$$Z = \int DU_0 DU_i \, \det Q \, e^{S_g[U]} \equiv \int DU_0 e^{-S_{eff}[U_0]} = \int DL \, e^{-S_{eff}[L]}$$

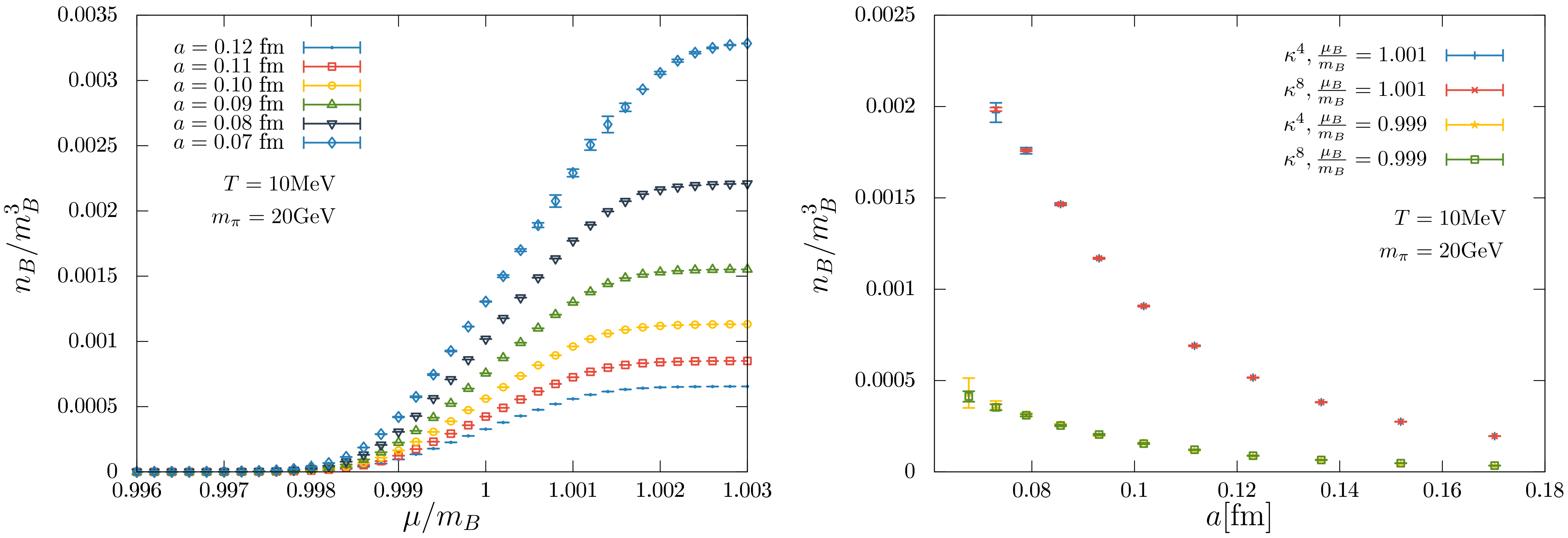
  Spatial integration after analytic strong coupling and hopping expansion $\sim \frac{1}{g^2}, \frac{1}{m_q}$
  (Numerical versions: Greensite et al. ; Bergner et al.)

- Truncation valid for heavy quarks on reasonably fine lattices, a~0.1 fm

- Step II.: Mild sign problem, complex Langevin, Monte Carlo
  Check in SU(2): Scior, von Smekal 15

- New Step II.: Analytic solution by cluster expansion!

Continuum approach

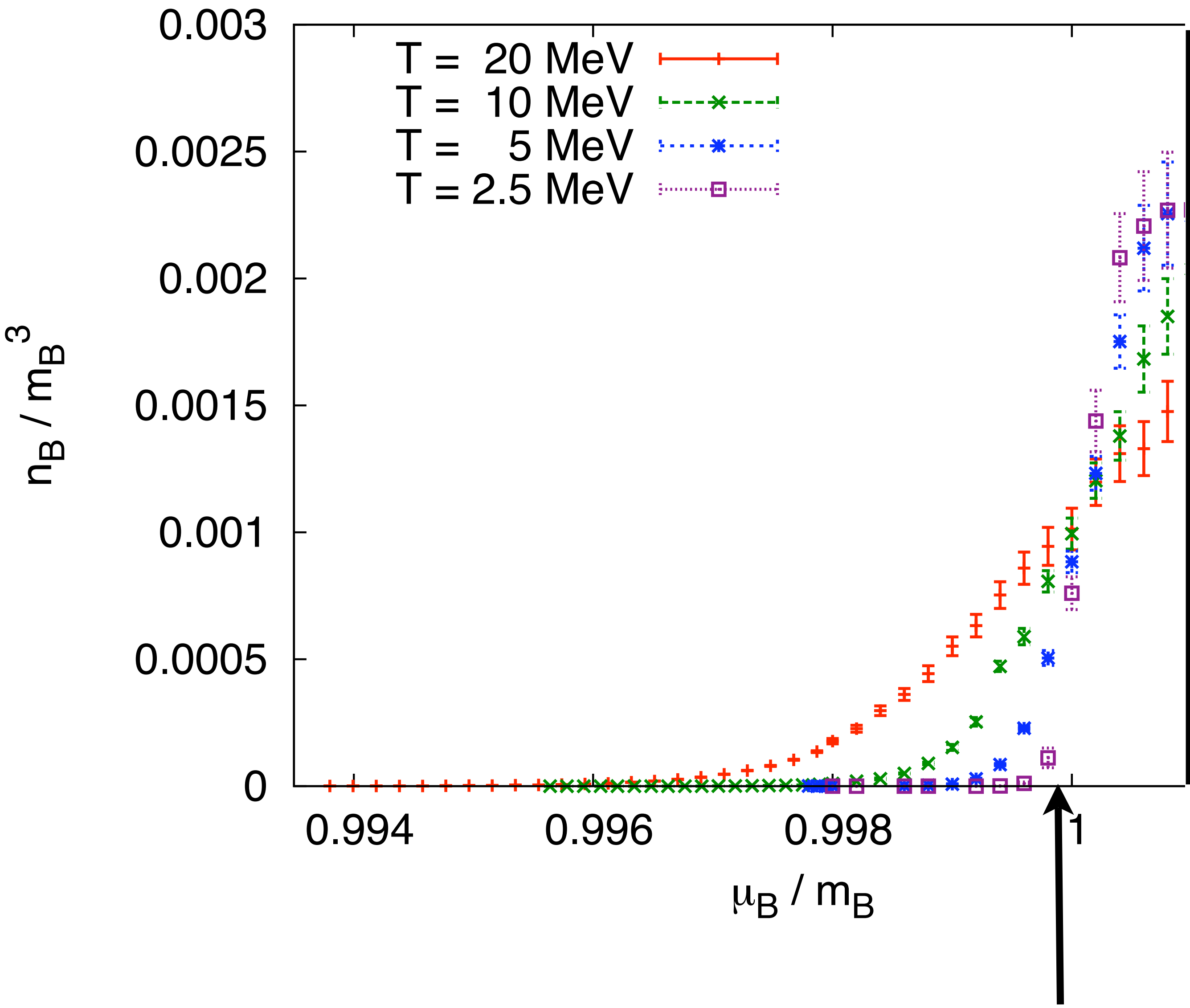


- Continuum approach ~a as expected for Wilson fermions
- Cut-off effects grow rapidly beyond onset transition
- Finer lattice necessary for larger density to avoid saturation

Cold and dense, interacting: onset to nuclear matter

continuum extrapolated

$$m_\pi = 20 \text{ GeV}$$



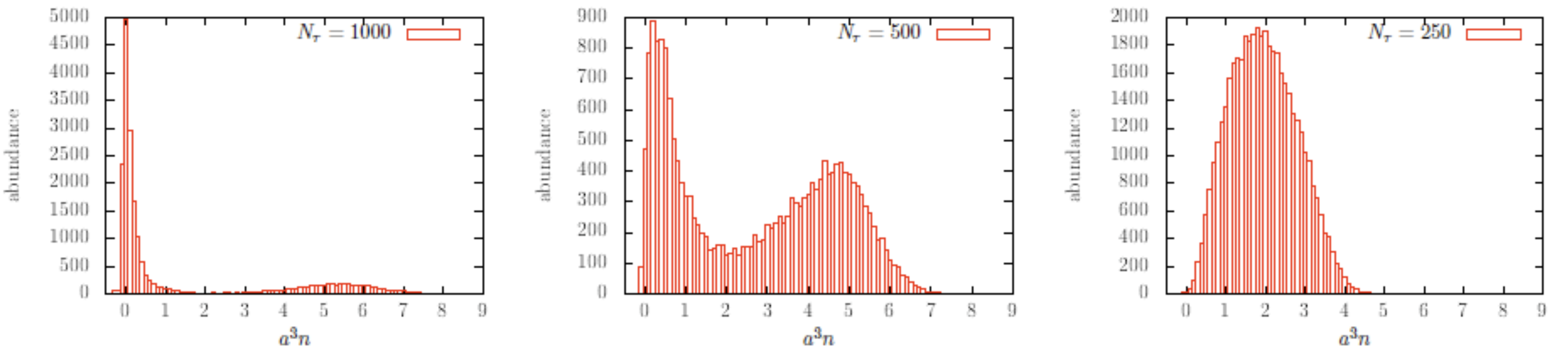
$$\frac{\mu}{T} \sim 4000$$

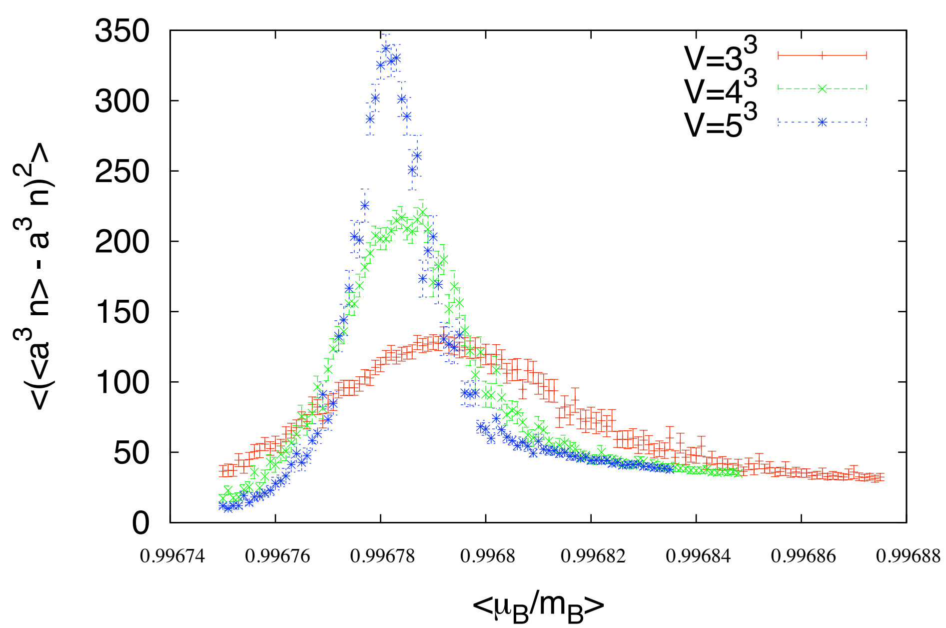
Effect of binding between baryons: $\mu_c < m_B$

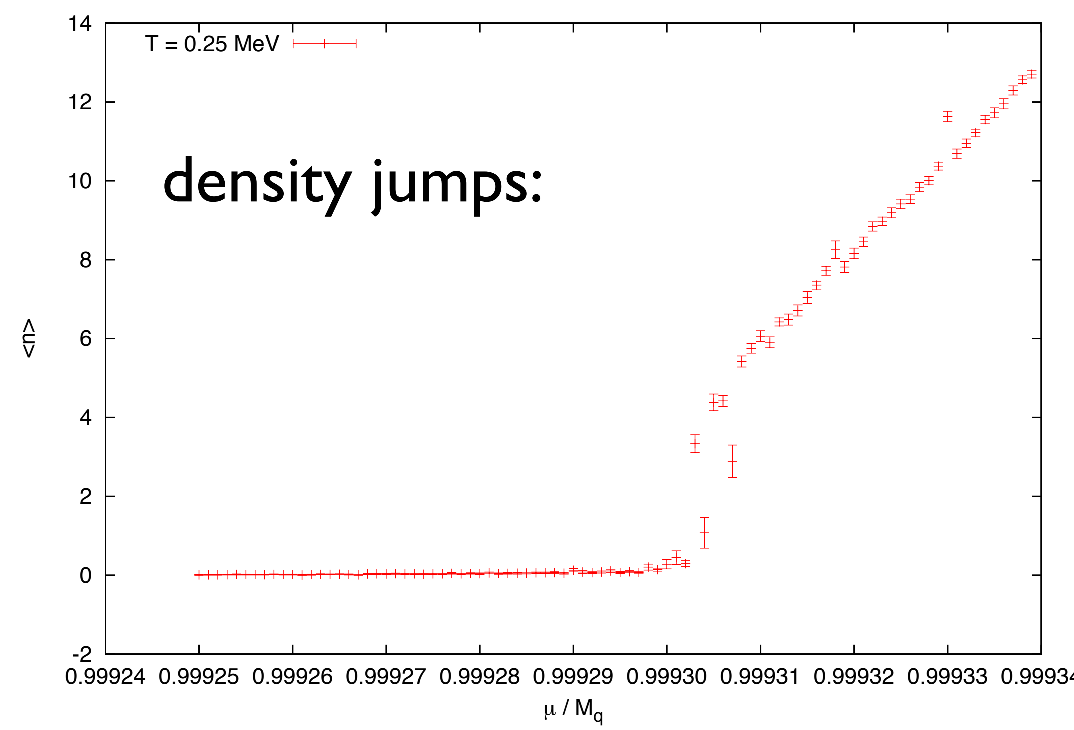
Binding energy per nucleon: $\epsilon = \frac{\mu_c - m_B}{m_B} \sim 10^{-3}$

Transition is smooth crossover: $T > T_c \sim \epsilon\, m_B$

Light quarks: first order transition + endpoint



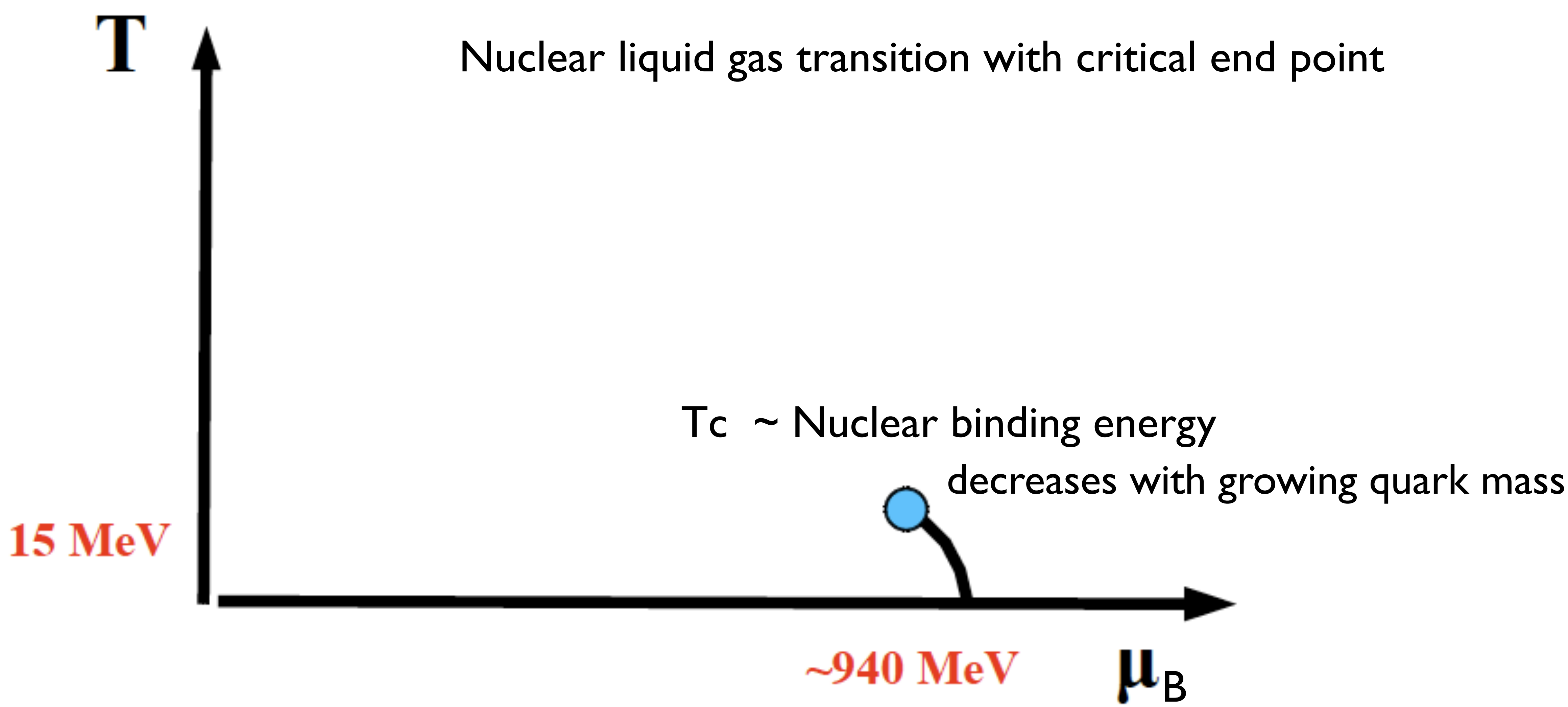




For sufficiently light quarks: $\kappa \sim 0.1$

- Coexistence of vacuum and finite density phase: 1st order
- If the temperature $T = \frac{1}{aN_\tau}$ or the quark mass is raised this changes to a crossover

nuclear liquid gas transition!!!


T
Nuclear liquid gas transition with critical end point
Tc ~ Nuclear binding energy
decreases with growing quark mass
15 MeV
~940 MeV
μB

The effective lattice theory approach II

- Two-step treatment:

  I. Calculate effective theory analytically
  II. Simulate effective theory

- Step I.: integrate over gauge links in strong coupling expansion, leave fermions (staggered)

$$Z_{\rm QCD} = \int d\psi d\bar\psi dU e^{S_F+S_G} = \int d\psi d\bar\psi Z_F \left\langle e^{S_G} \right\rangle_{Z_F}$$

$$\left\langle e^{S_G} \right\rangle_{Z_F} \simeq 1 + \langle S_G \rangle_{Z_F} = 1 + \frac{\beta}{2N_c} \sum_P \left\langle {\rm tr}[U_P + U_P^\dagger] \right\rangle_{Z_F} \qquad Z_F(\psi,\bar\psi) = \int dU e^{S_F}$$

- Result: 4d "polymer" model of QCD (hadronic degrees of freedom!)
  Valid for all quark masses (also m=0!), at strong coupling (very coarse lattices)

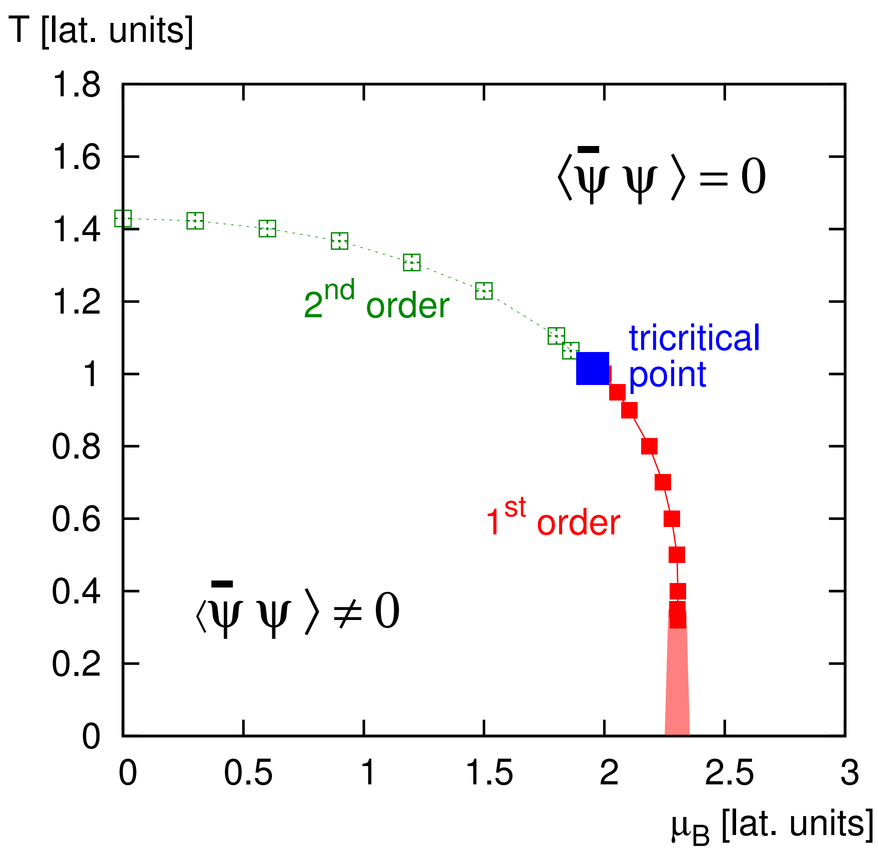
- Step II: sign problem milder: Monte Carlo with worm algorithm

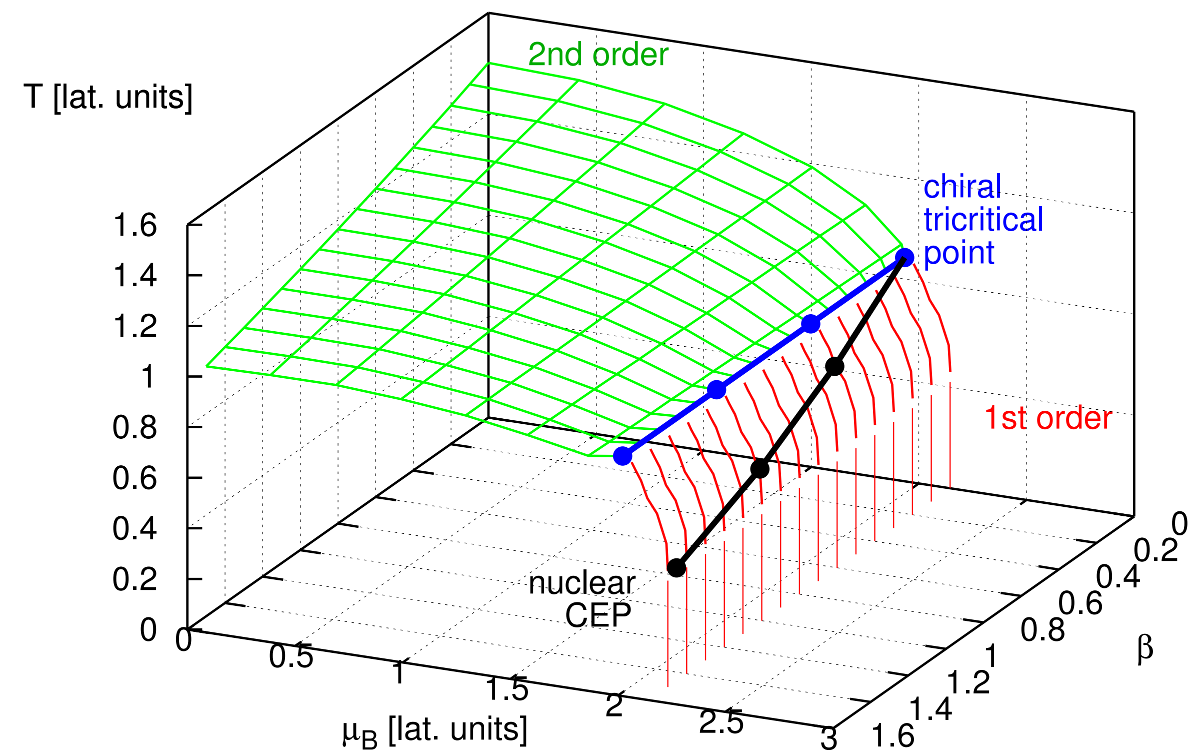
- Numerical simulations without fermion matrix inversion, very cheap!

From strong coupling limit to finite coupling

Unrooted staggered fermions: Nf=4

de Forcrand, Langelage, O.P., Unger 14





Strong coupling limit: $\beta = 0$

Chiral limit: m=0

Including leading gauge corrections

Nucl. and chiral transition coincide!

Summary Lecture II:

- QCD thermal transition at physical point and zero density is crossover
- Order of QCD transition in chiral limit not yet known
- Sign problem prohibits Monte Carlo simulations at finite density
- The QCD crossover gets even softer for small baryon density
- Transition to cold baryon matter seen for:
  effective theory for heavy quarks near continuum,
  effective theory for massless quarks far from the continuum