Lecture IV:

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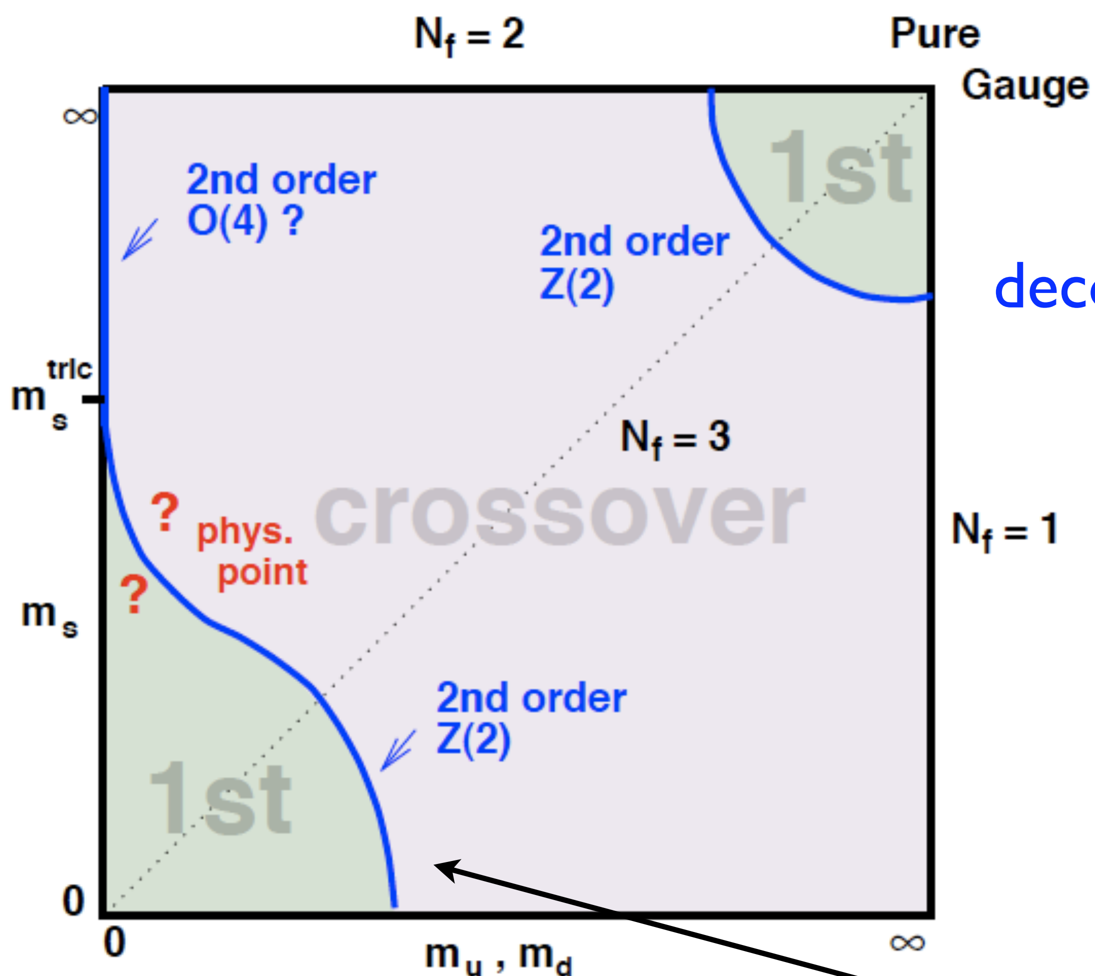
- The thermal phase transition at zero density
- Lattice QCD at finite temperature and density
- Towards the QCD phase diagram

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

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



deconfinement critical line

chiral critical line

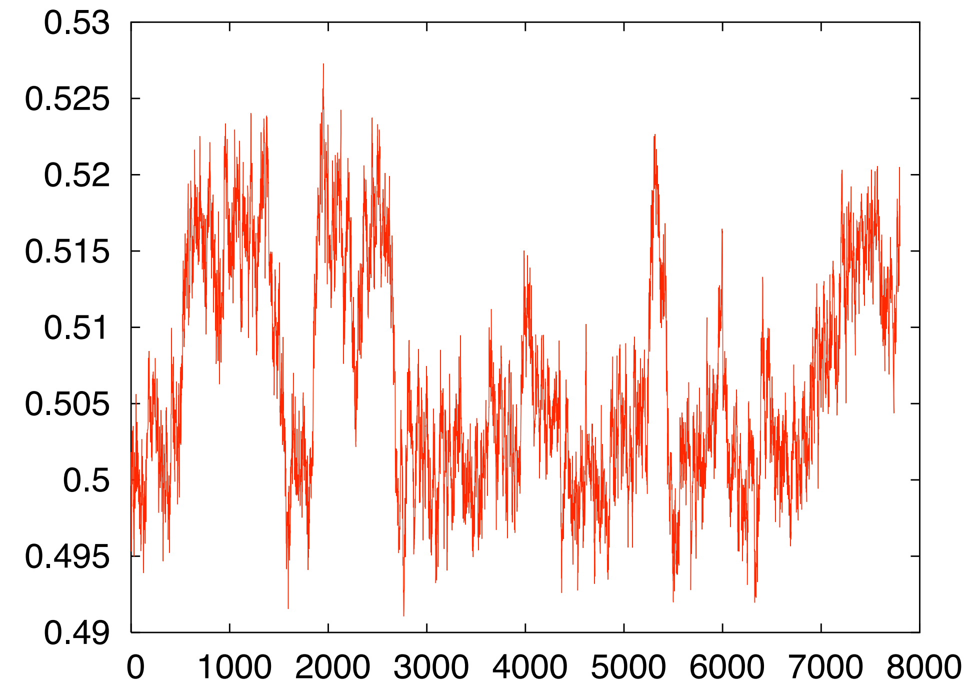
chiral p.t.
restoration of global

$$SU(2)_L \times SU(2)_R \times U(1)_A$$

anomalous

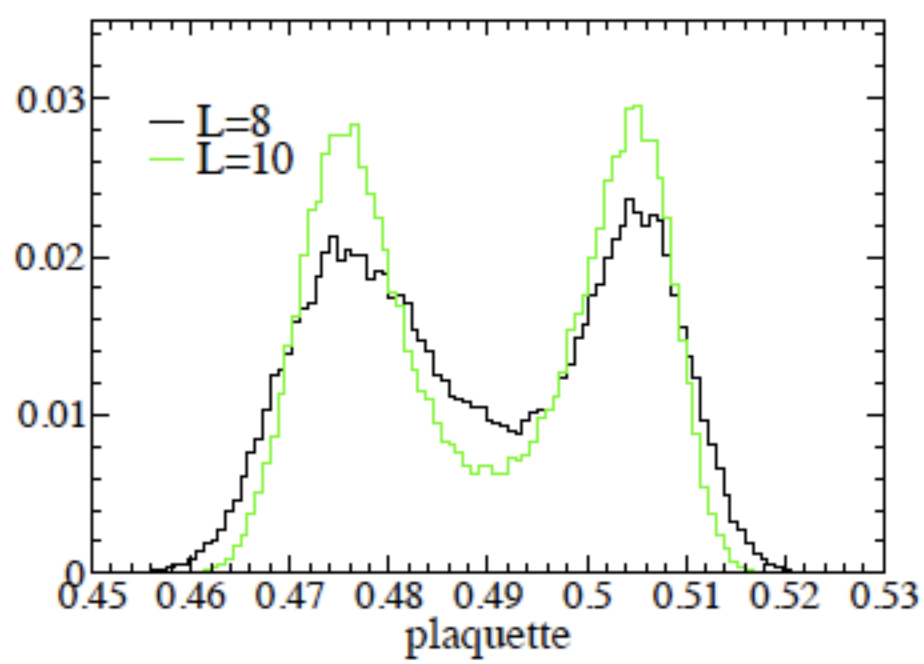
Very difficult!

Monte Carlo history,
plaquette near phase boundary

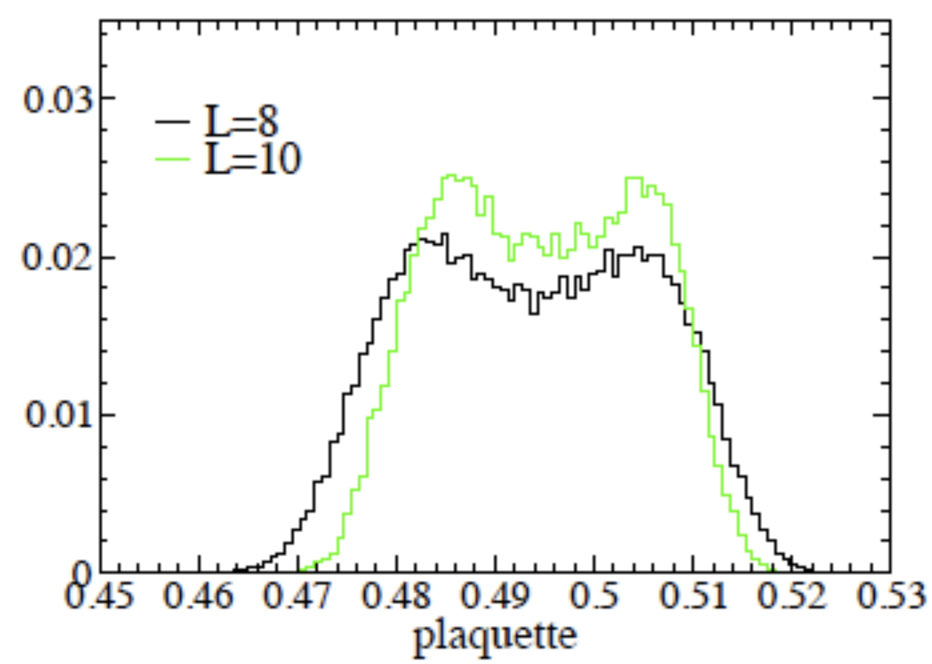


Distribution:

first-order



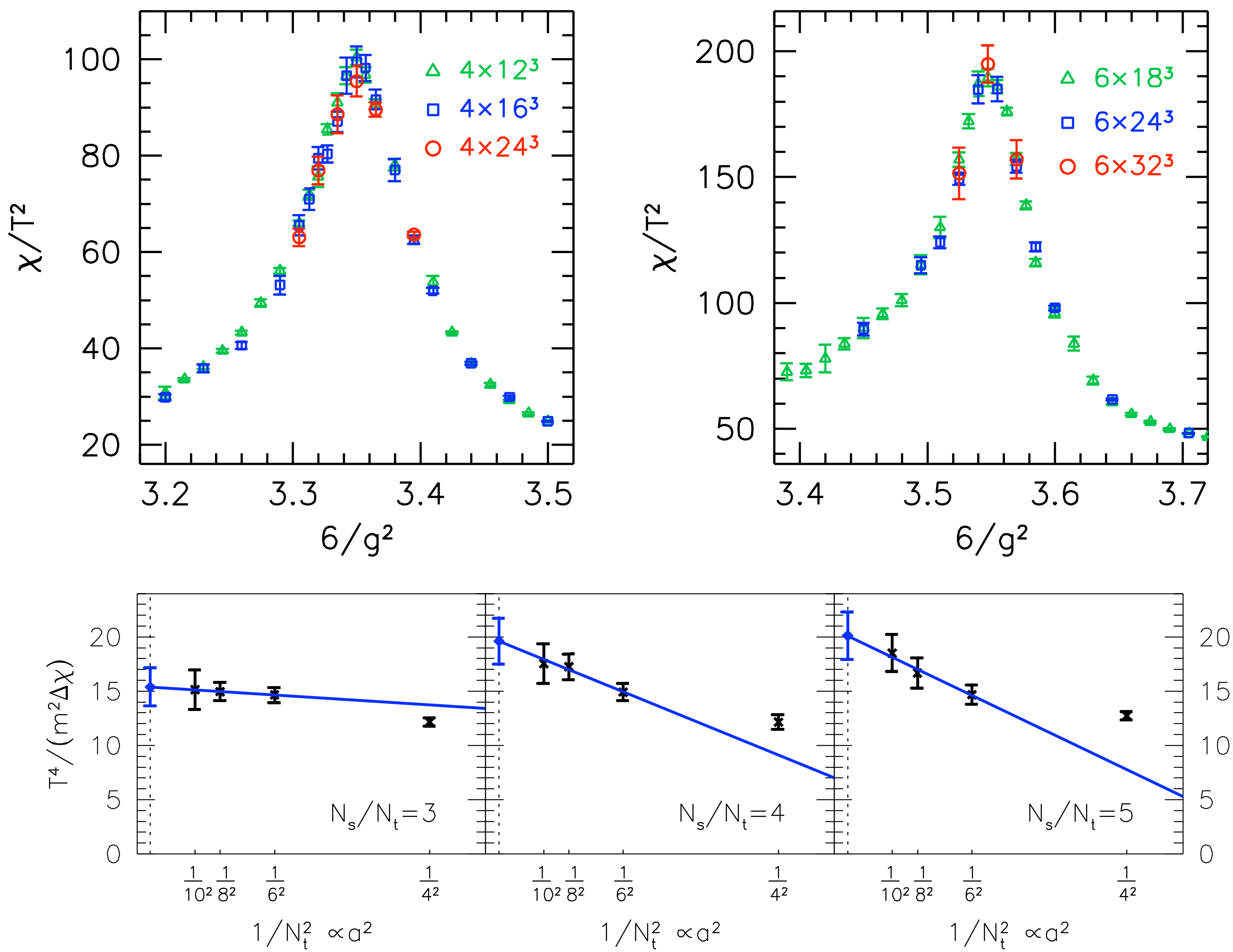
crossover



The nature of the transition for phys. masses

Aoki et al. 06

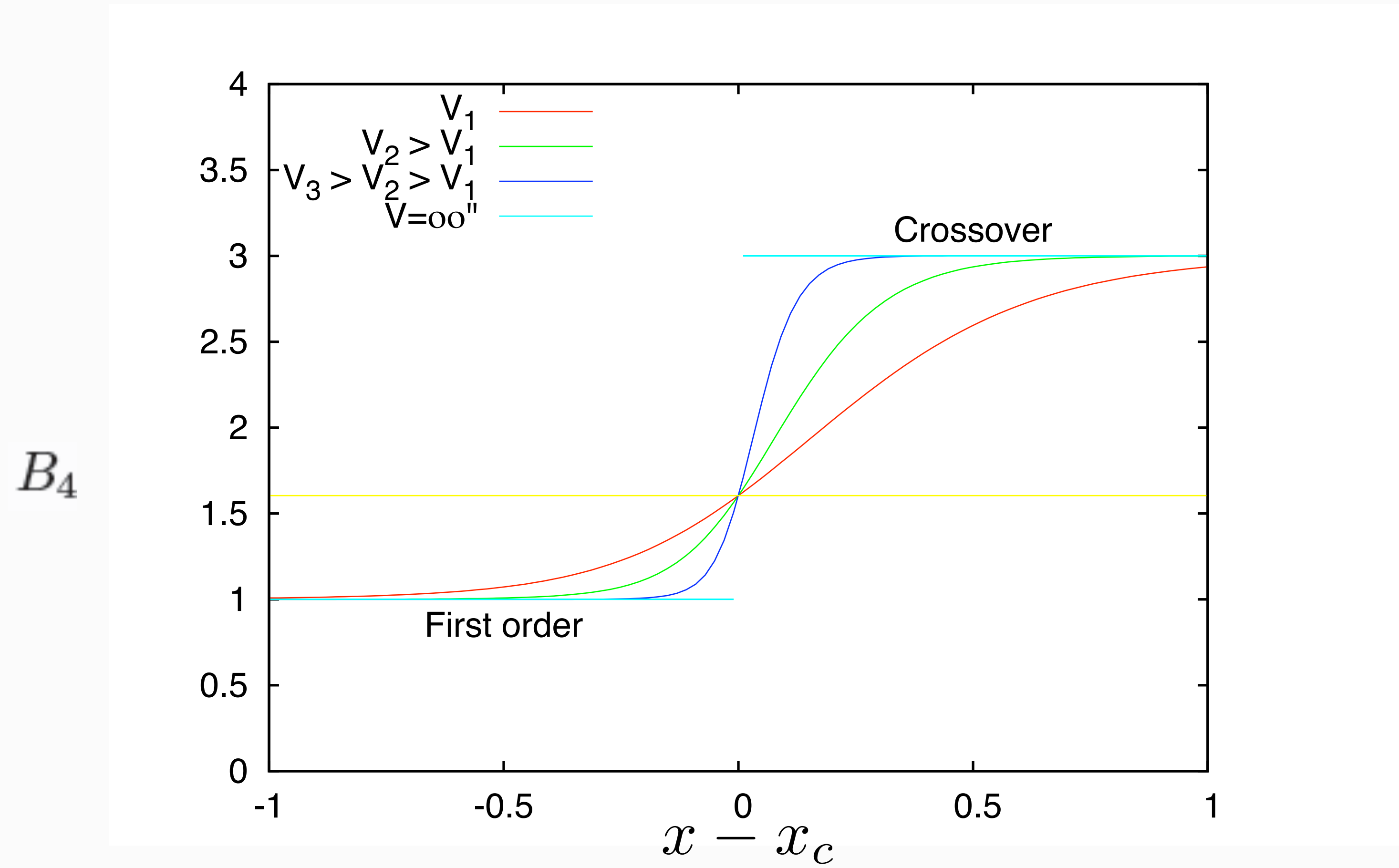
...in the staggered approximation...in the continuum...is a crossover!



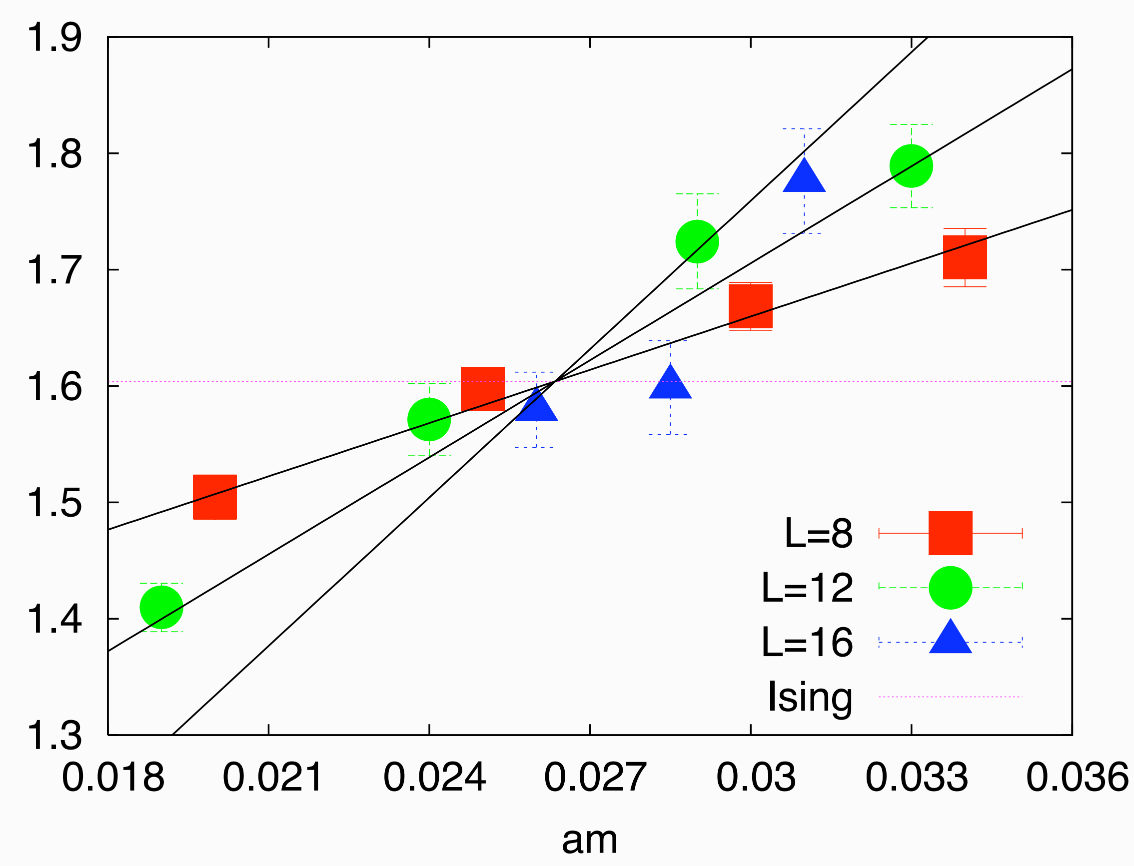
How to identify the order of the phase transition

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

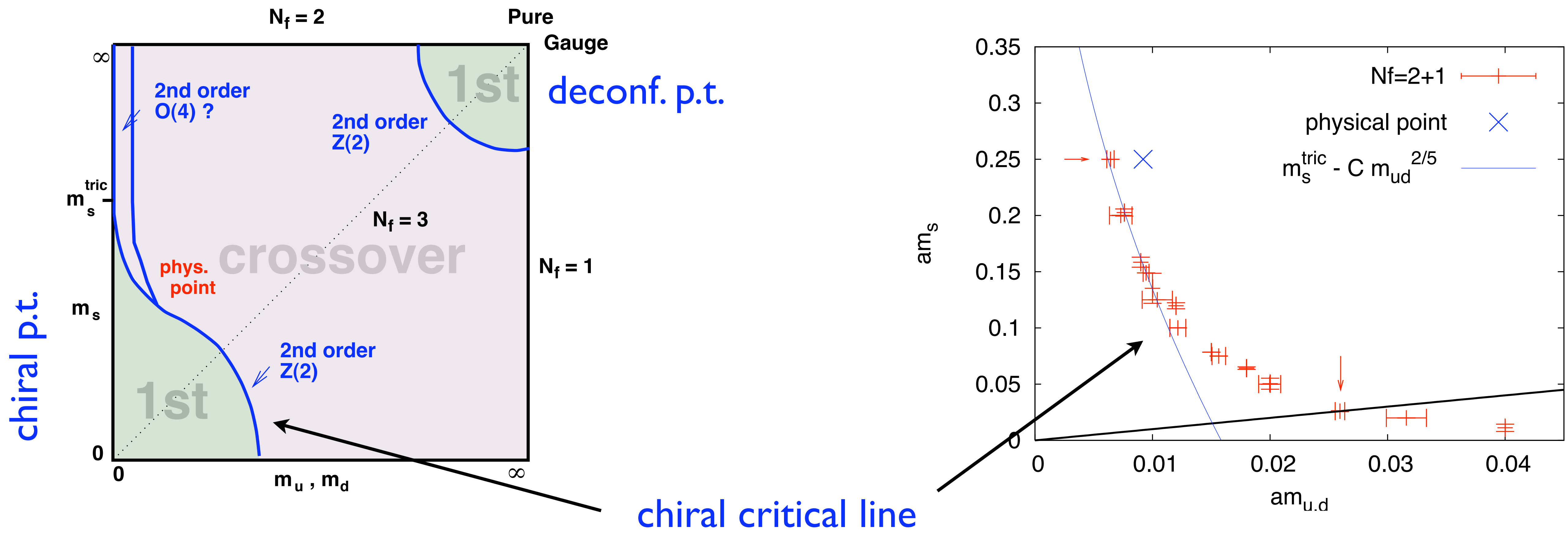
$\mu = 0$: $$B_4(m,L) = 1.604 + bL^{1/\nu}(m - m_0^c), \quad \nu = 0.63$$



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

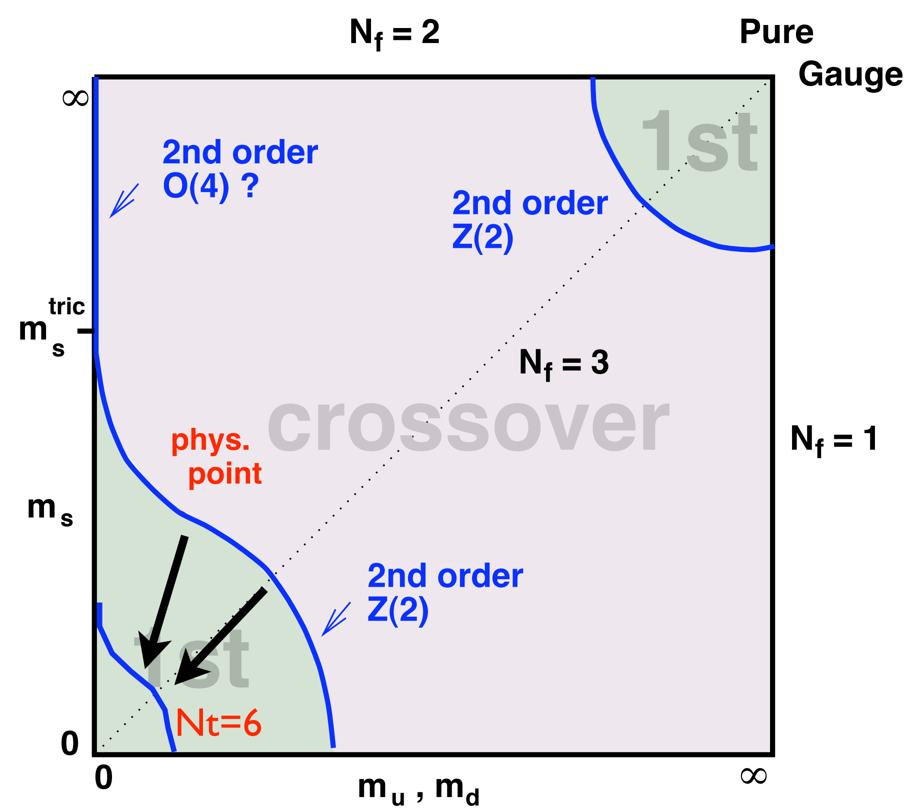


Order of p.t., arbitrary quark masses $\mu = 0$



- 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 $m_{u,d} = 0, m_s^{\mathrm{tric}} \sim 2.8T$
- But: $N_f = 2$ chiral O(4) vs. 1st still open
  $U_A(1)$ anomaly! — Di Giacomo et al 05, Kogut, Sinclair 07
  Chandrasekharan, Mehta 07
  Cossu et al. 12, Aoki et al. 12

Towards the continuum: $N_t = 6, a \sim 0.2$ fm



$$\frac{m_\pi^c(N_t = 4)}{m_\pi^c(N_t = 6)} \approx 1.77 \qquad N_f = 3$$

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

First order region shrinks drastically, continuum limit not yet known...

N.B.: for fixed masses in physical units the order of the p.t. depends on the cut-off!

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!

$\Rightarrow$

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

Exact symmetry of the continuum grand canonical partition function:

$$Z(\mu) = \int DA^C\, D\bar{\psi}^C D\psi^C\; \exp -\left[S_g^C + S_f^C(\mu=0) - \mu \int_0^{1/T} dx_0\, Q^C\right]$$
$$= \int DA\, D\bar{\psi} D\psi\; \exp -\left[S_g + S_f(\mu=0) + \mu \int_0^{1/T} dx_0\, Q\right] \;= Z(-\mu)$$

Lattice implementation, naive: $S_f[M(\mu)] = S_f[M(0)] + a\mu \sum_x \psi(x)\gamma_0\psi(x)$

Introduces divergence, which is absent at zero density: failure! $\epsilon = \frac{1}{V}\frac{\partial}{\partial(\frac{1}{T})}\ln Z \stackrel{a\to 0}{\longrightarrow} \infty$

Another symmetry broken by the discretisation!

Continuum fermion number like current coupling to (imaginary) gauge field:

$$j^0 = \bar{\psi}\gamma^0\psi \qquad\qquad \mu Q = -ig\int d^3x\, A_0 j_0 \quad \text{with} \quad A_0 = i\frac{\mu}{g}$$

Effectively part of covariant derivative, "gauged" U(1), protects against renormalisation

Lattice implementation: lattice covariant derivative with external gauge field

$$U_{0,\mathrm{ext}} = \mathrm{e}^{iagA_0} = \mathrm{e}^{-a\mu}$$

Wilson fermions:

$$S_f^W = a^3 \sum_x \Big(\bar\psi(x)\psi(x) - \kappa \left[\mathrm{e}^{a\mu}\bar\psi(x)(r-\gamma_0)U_0(x)\psi(x-\hat{0}) + \mathrm{e}^{-a\mu}\bar\psi(x+\hat{0})(r+\gamma_0)U_0^\dagger(x)\psi(x) \right] \\ - \kappa \sum_{j=1}^{3} \left[\bar\psi(x)(r-\gamma_j)U_j(x)\psi(x+\hat{j}) + \bar\psi(x+\hat{j})(r+\gamma_j)U_j^\dagger(x)\psi(x) \right] \Big)$$

(Discretisation not unique, only continuum limit)

Now use $\det(\not{D}(U^\dagger) + m + \gamma_0\mu) = \det(\not{D}(U) + m - \gamma_0\mu)$ $\qquad S_g[U^\dagger] = S_g[U]$

$\Rightarrow$ $$Z(\mu) = Z(-\mu)$$

The sign problem

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

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

With complex chemical potential:

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

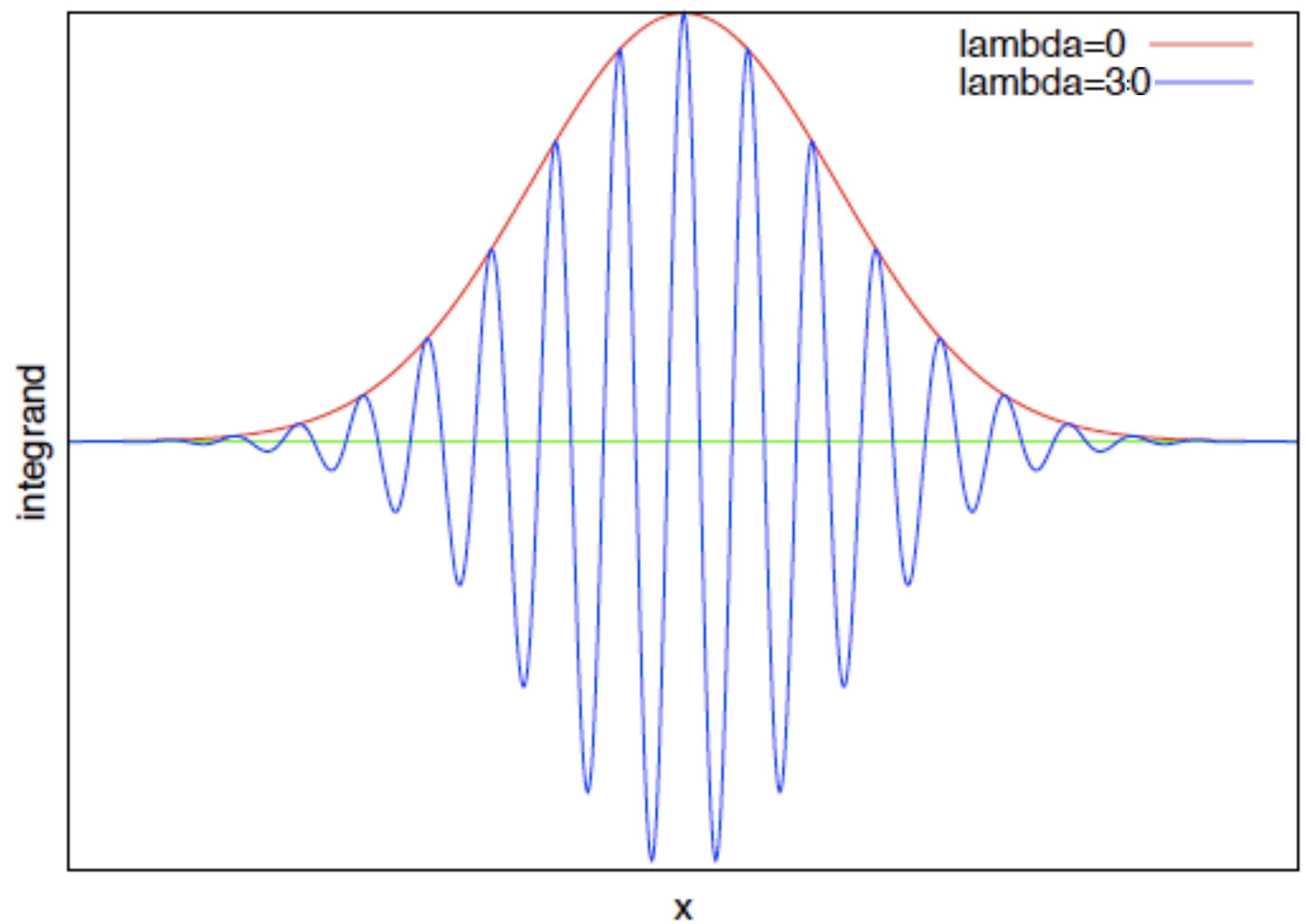
$$\det(\not{D}+m-\gamma_0\mu) = \det{}^*(\not{D}+m+\gamma_0\mu^*)$$

"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

Example: Polyakov loop

$$\langle \ldots \rangle_g = \int DU \ldots \exp -S_g[U]$$

$$\langle \mathrm{Tr} L \rangle = \mathrm{e}^{-\frac{F_Q}{T}} = \langle \mathrm{Re}\mathrm{Tr} L \; \mathrm{Re} \det M \; - \mathrm{Im}\mathrm{Tr} L \; \mathrm{Im} \det M \rangle_g$$
$$\langle (\mathrm{Tr} L)^* \rangle = \mathrm{e}^{-\frac{F_{\bar{Q}}}{T}} = \langle \mathrm{Re}\mathrm{Tr} L \; \mathrm{Re} \det M \; + \mathrm{Im}\mathrm{Tr} L \; \mathrm{Im} \det M \rangle_g$$

Static quarks and anti-quarks must have different free energy at finite density!

Sign problem expresses
property under C-conjugation!

$$\det(\not{D} + m - \gamma_0 \mu) \xrightarrow{C} \det(\not{D} + m + \gamma_0 \mu)$$

Fixes:

- Cluster algorithms find configs. with conjugate determinant
works for particular Hamiltonians, but not QCD

- Simulation with Langevin algorithms (no importance sampling)
Only proven to work for real actions, but work for some ranges of coupling constants

Special cases without sign problem

Imaginary chemical potential:

$$\det(\not{D} + m - \gamma_0\mu) = \det{}^*(\not{D} + m + \gamma_0\mu^*)$$ real for $\mu = i\mu_i, \mu_i \in \mathbb{R}$

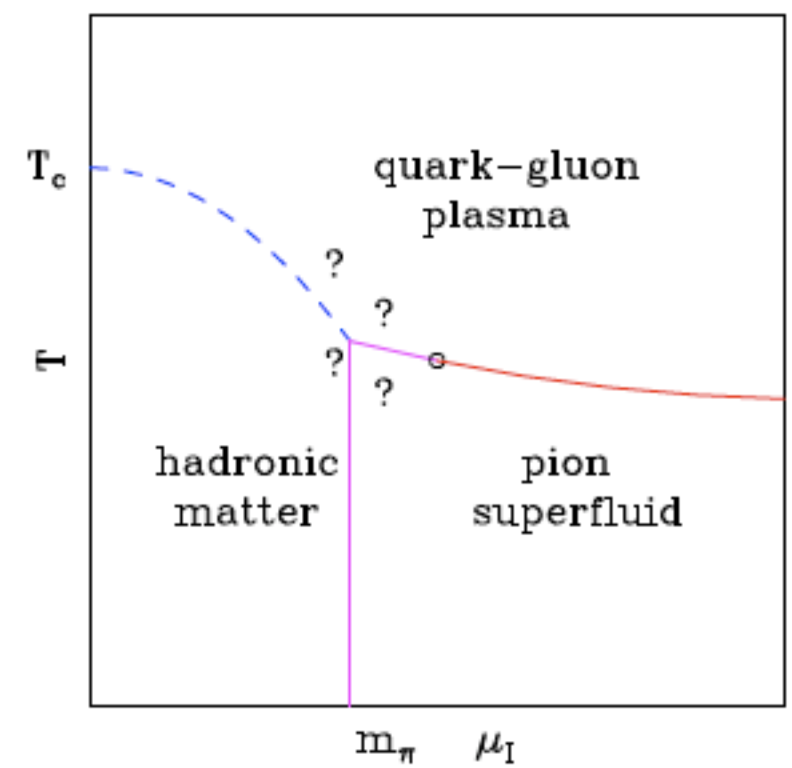
Two flavours, finite isospin chemical potential:

$$\mu_u = -\mu_d \equiv \mu_I$$

$$\det(\not{D} + m - \gamma_0\mu_I)\det(\not{D} + m + \gamma_0\mu_I)$$

$$= |\det(\not{D} + m - \gamma_0\mu_I)|^2 \geq 0$$

$N_f=2$ QCD at finite isospin density



Two colours, SU(2) QCD:

$$S[\not{D} + m - \gamma_0\mu]S^{-1} = [\not{D} + m - \gamma_0\mu^*]^*$$

$$S = C\gamma_5\sigma^2 \qquad ST^aS^{-1} = -T^{a*}$$

real reps.

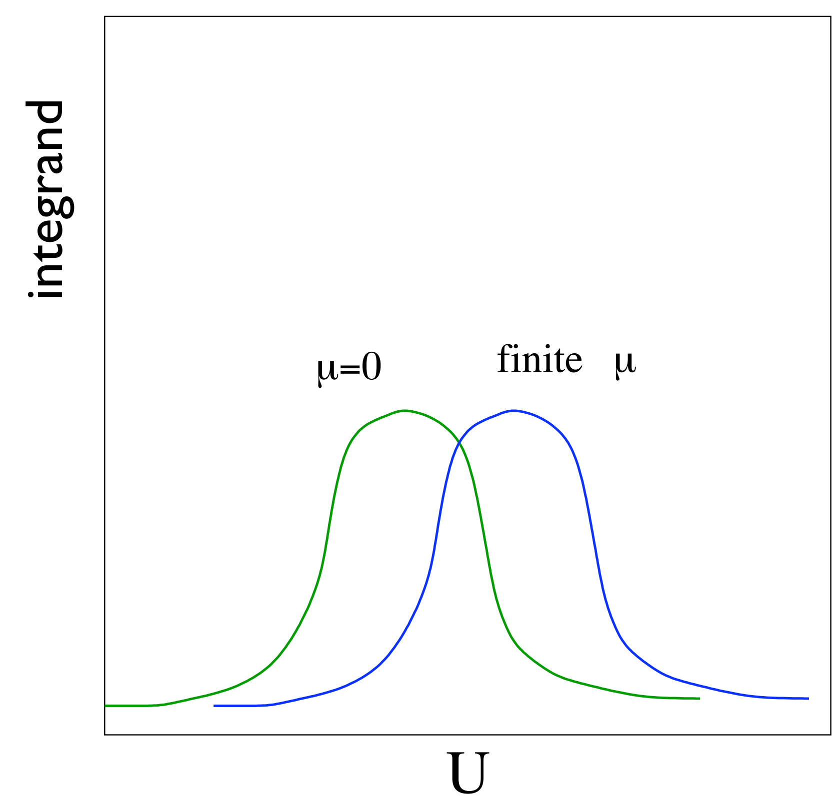
Approximate methods to evade the sign problem: Reweighting

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 $Z = \hat{\mathrm{Tr}}\, e^{-\frac{(H - i\mu_i Q)}{T}}$

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

Measure and action are invariant, hence

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

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

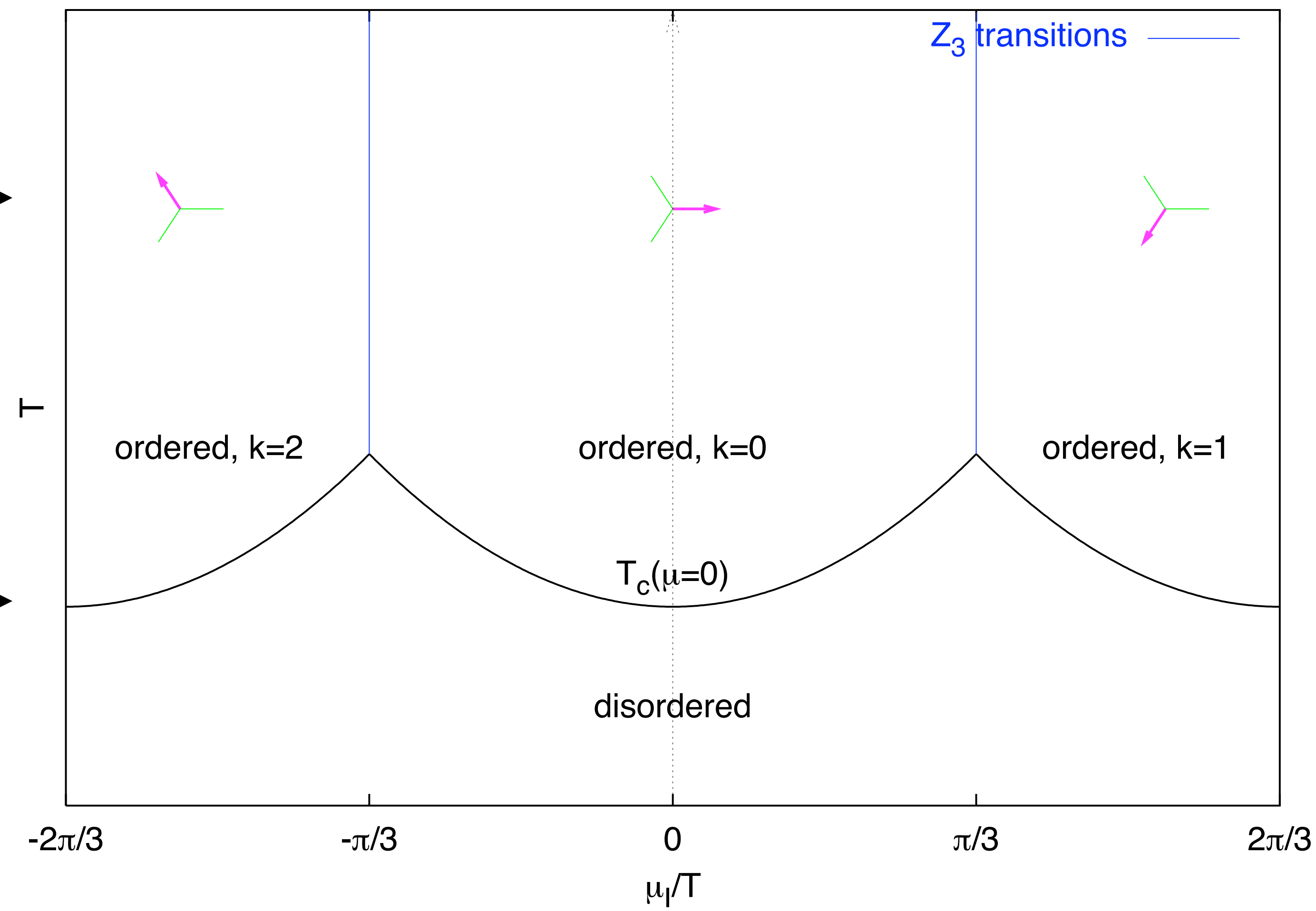
Both partition fcns. related by gauge trafo, identical!

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

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:

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

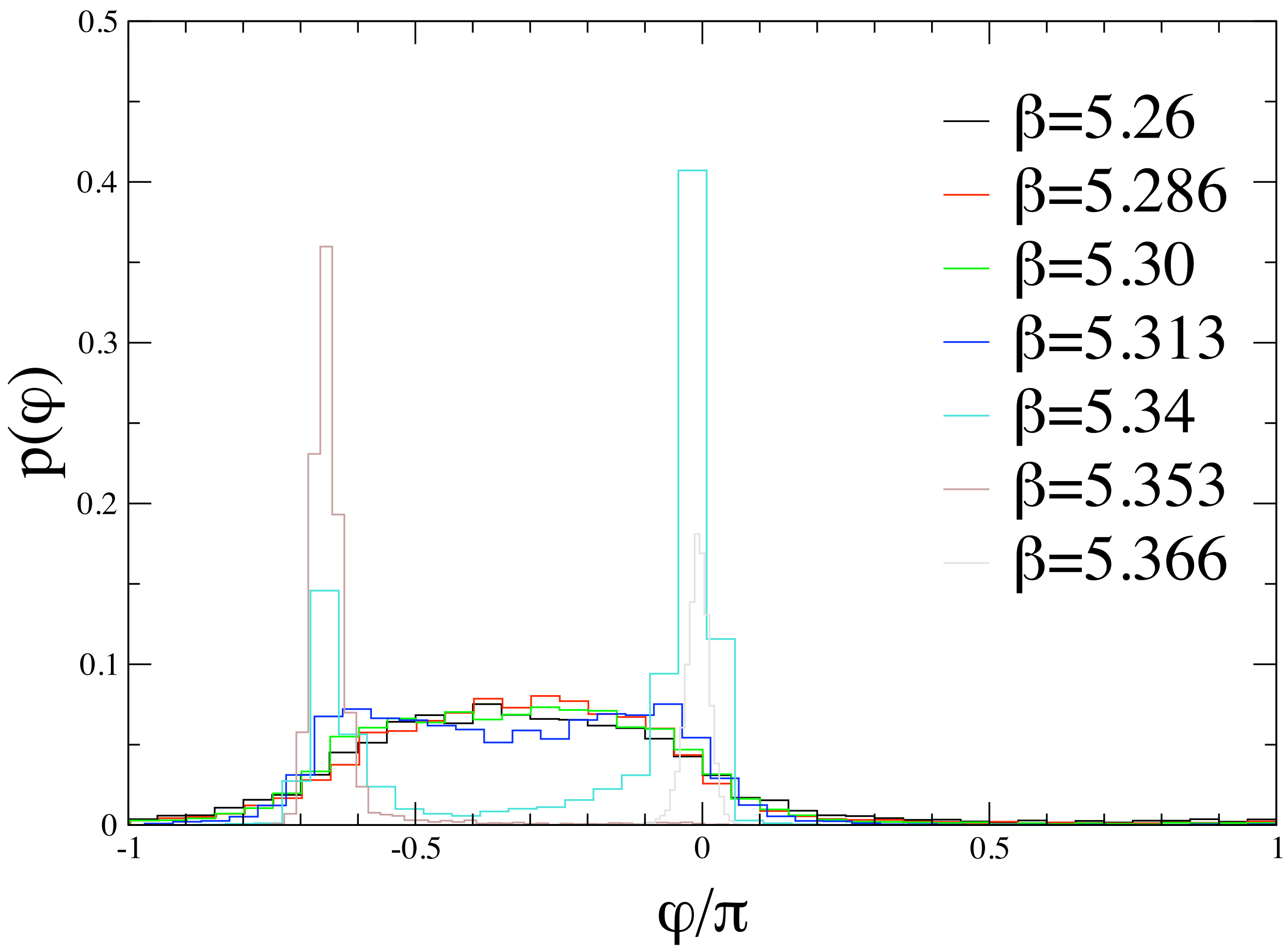
Limited by singularity (phase transition) closest to $\mu = 0$

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: $\langle L(x) \rangle = |\langle L(x) \rangle| \, \mathrm{e}^{i\varphi}$

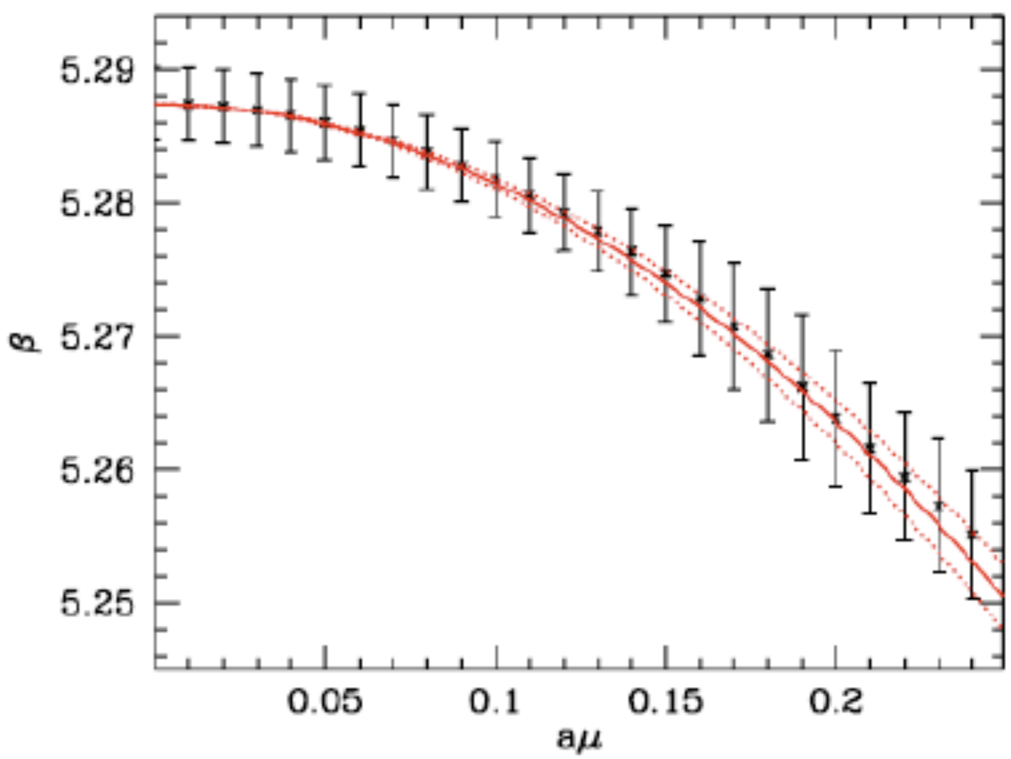


Low T: crossover

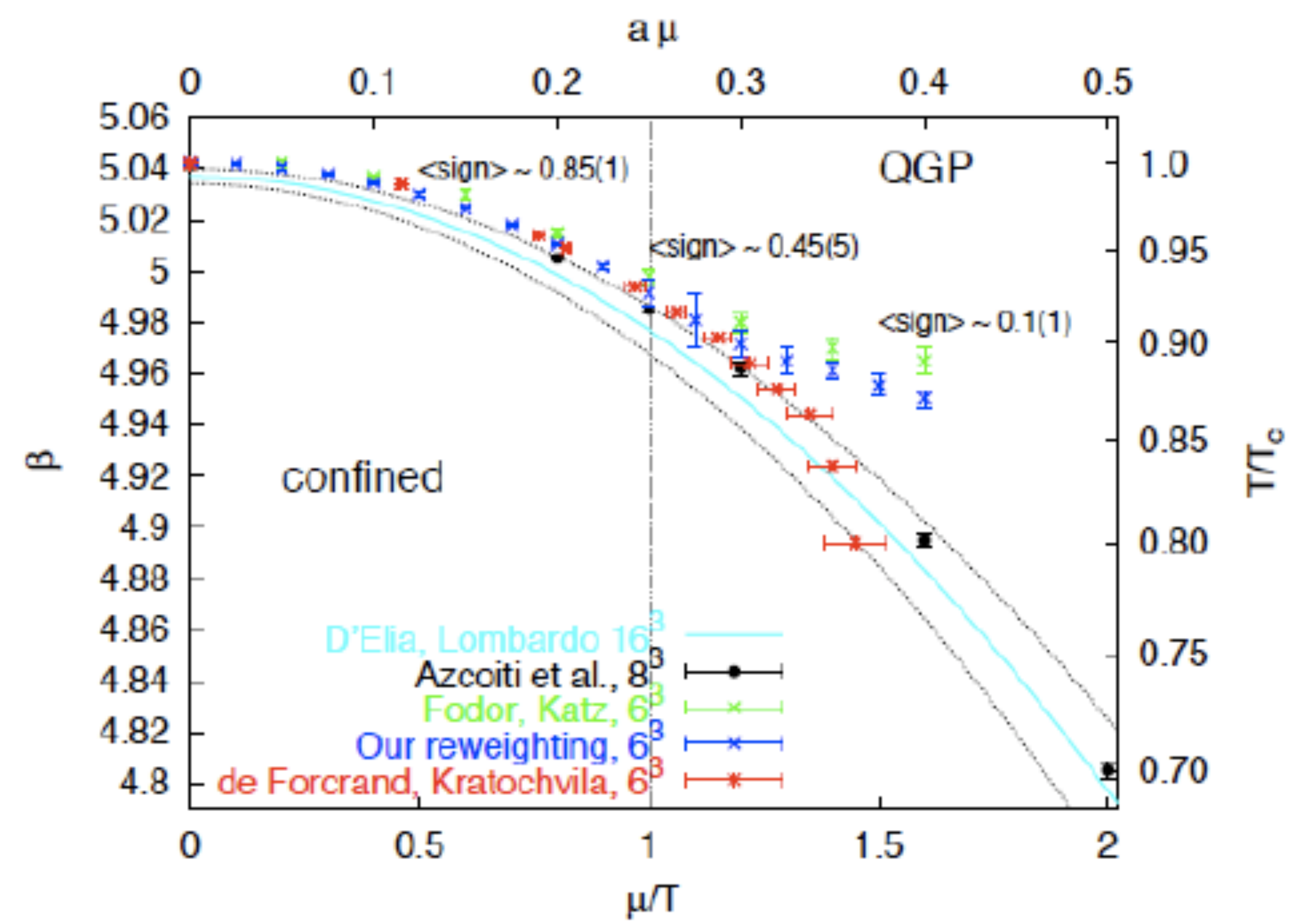
High T: first order p.t.

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

Reweighting vs. imag. μ (FK, FP)

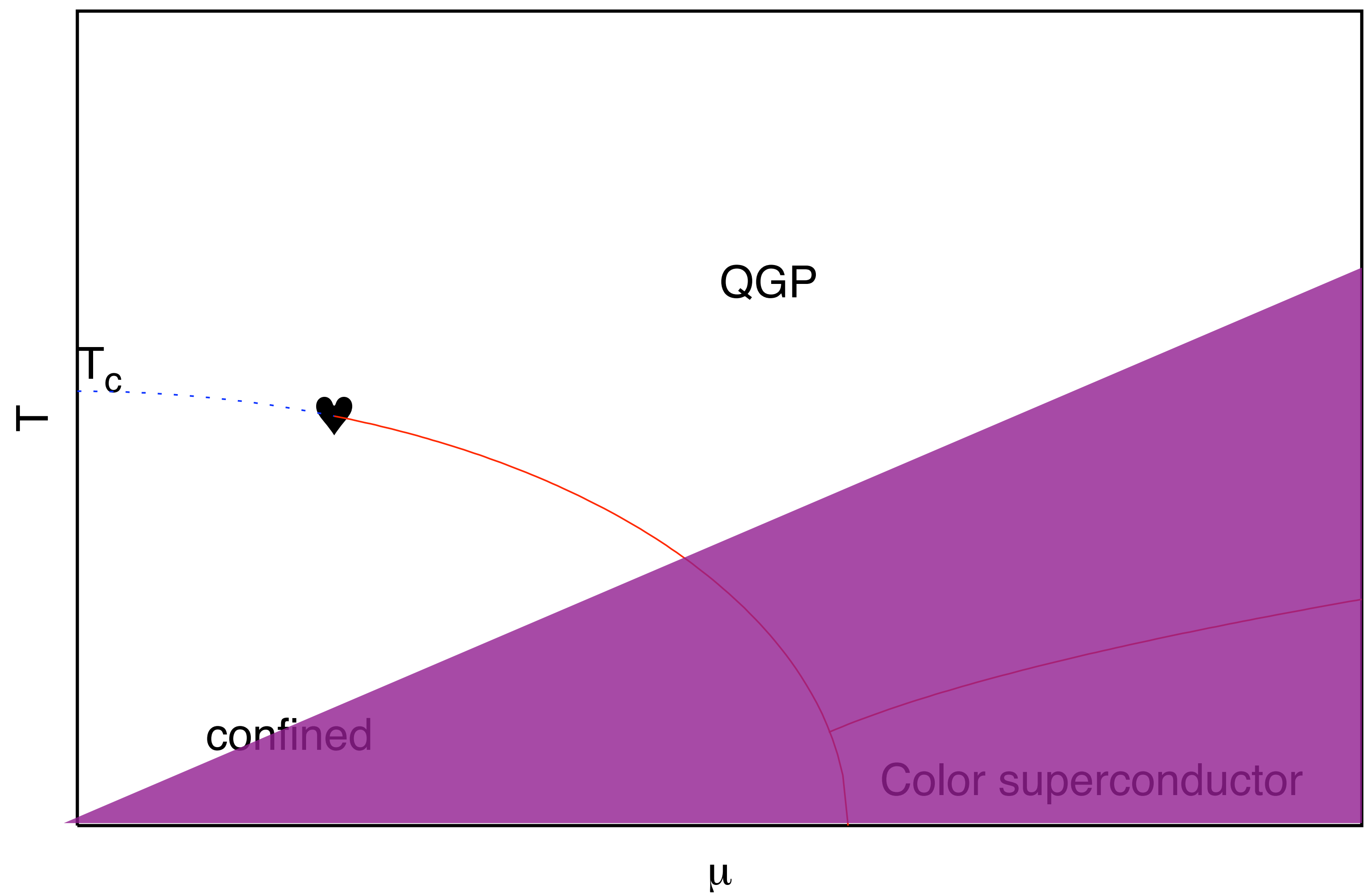


Rew., imag. μ, canonical ensemble ...



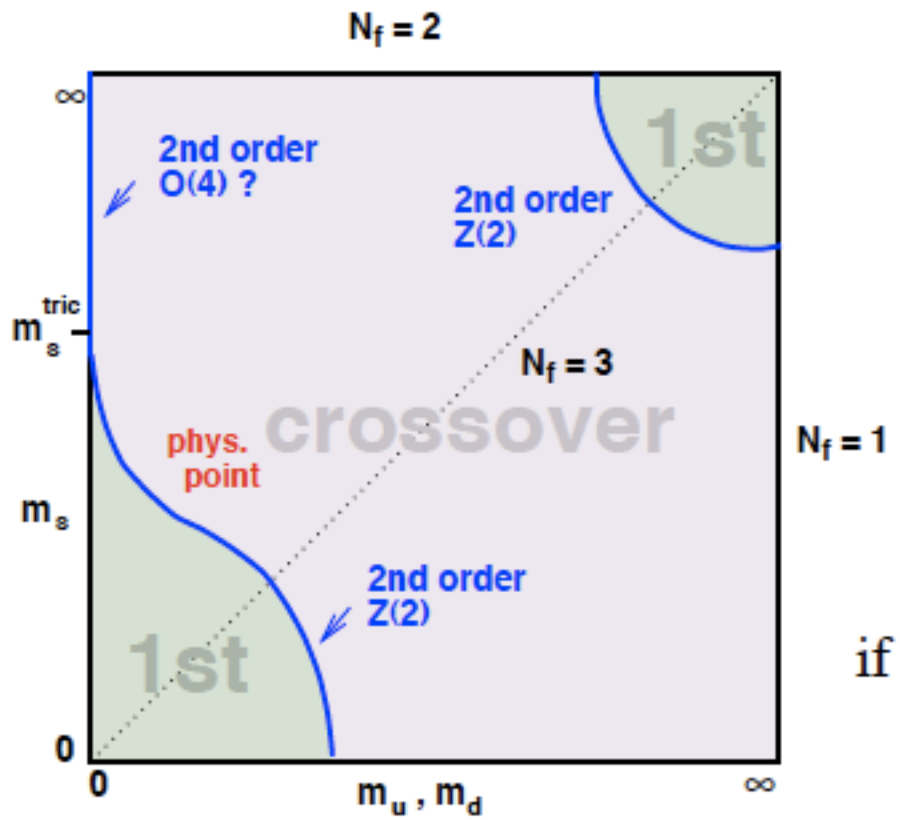
All agree on $T_0(m,\mu)$!!! $(\mu/T \lesssim 1)$

The calculable region of the phase diagram

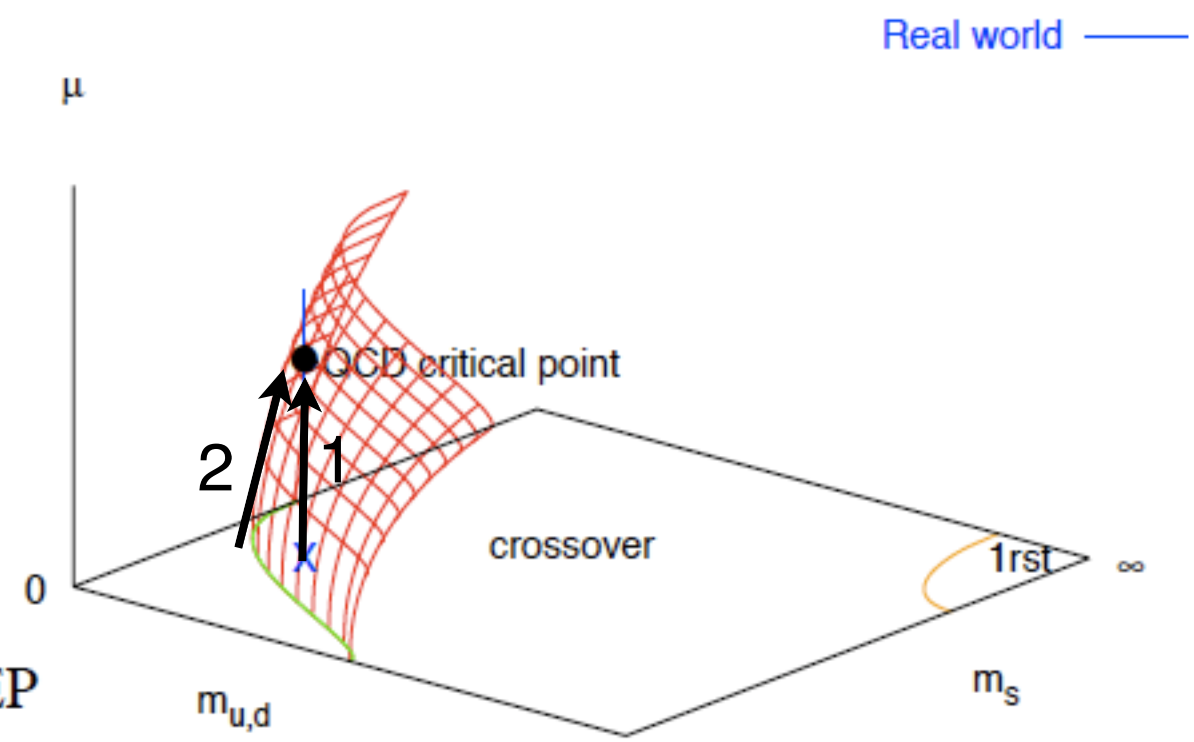


- need $\mu/T \lesssim 1 \quad (\mu = \mu_B/3)$
- Upper region: equation of state, screening masses, quark number susceptibilities etc. under control

Much harder: is there a QCD critical point?



$\underbrace{\longrightarrow}_{}$ if *chiral* CEP



Two strategies:

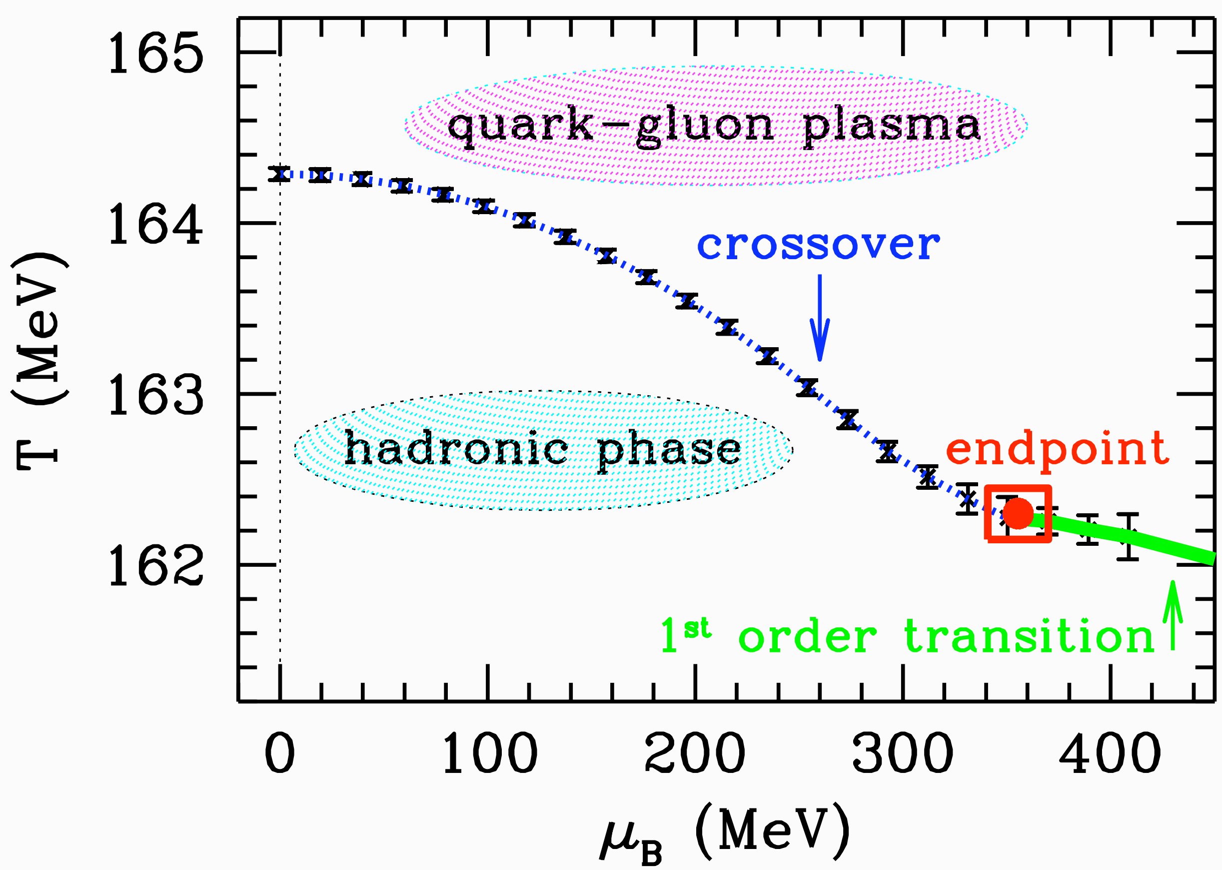
1 follow vertical line: $m = m_{\text{phys}}$, turn on μ

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

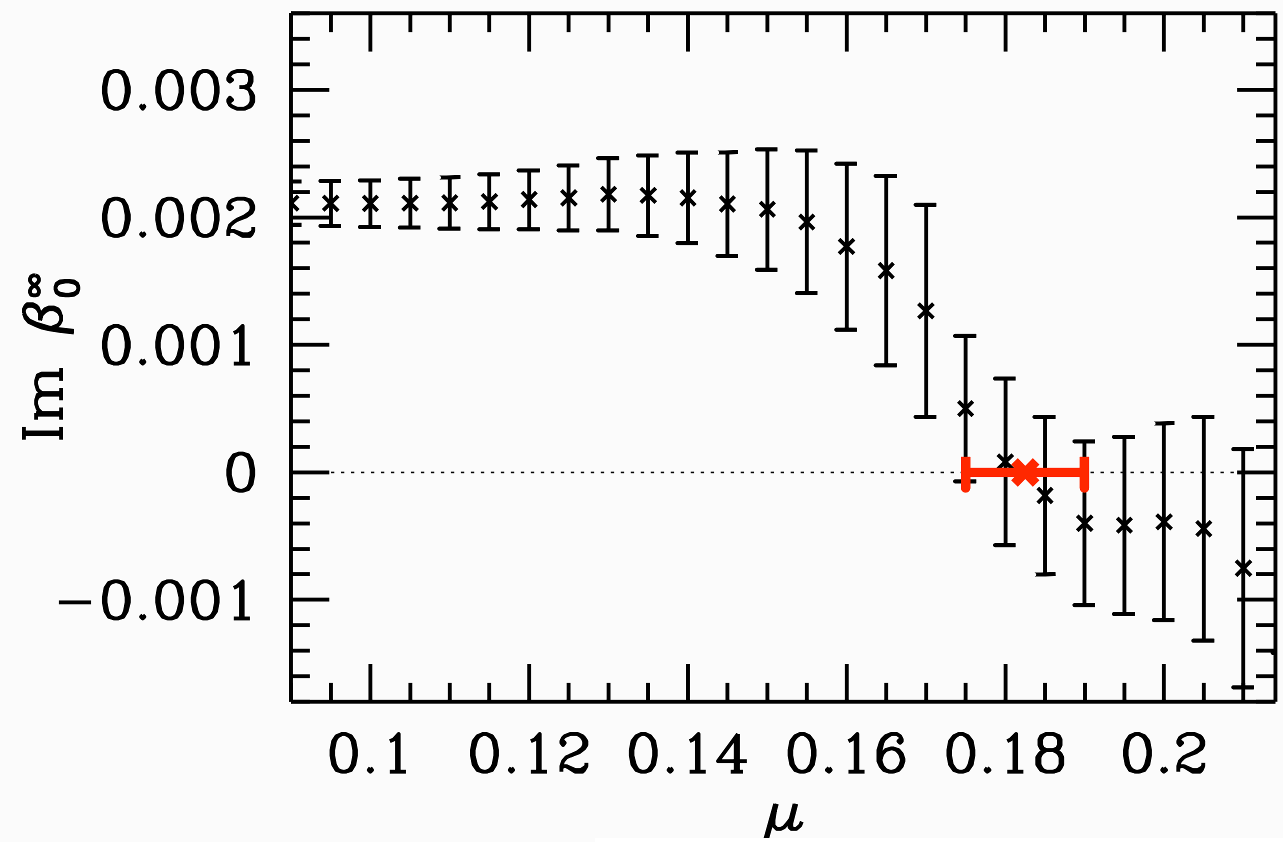
Approach 1a: CEP from reweighting

Fodor, Katz 04

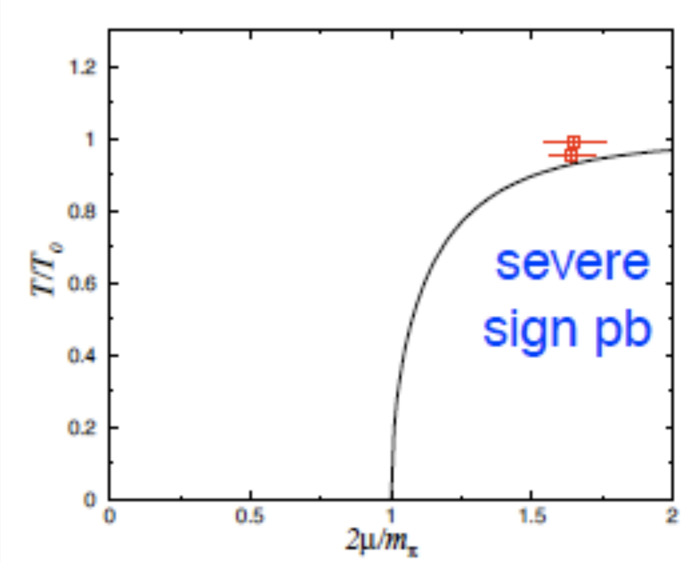
$N_t = 4, N_f = 2+1$ physical quark masses, unimproved staggered fermions



Lee-Yang zero:



$$(\mu_E^q, T_E) = (120(13), 162(2))\ \text{MeV}$$



abrupt change: caused by baryon or pion condensation?

Splittorf 05, Stephanov 08

Approach 1b: CEP from Taylor expansion

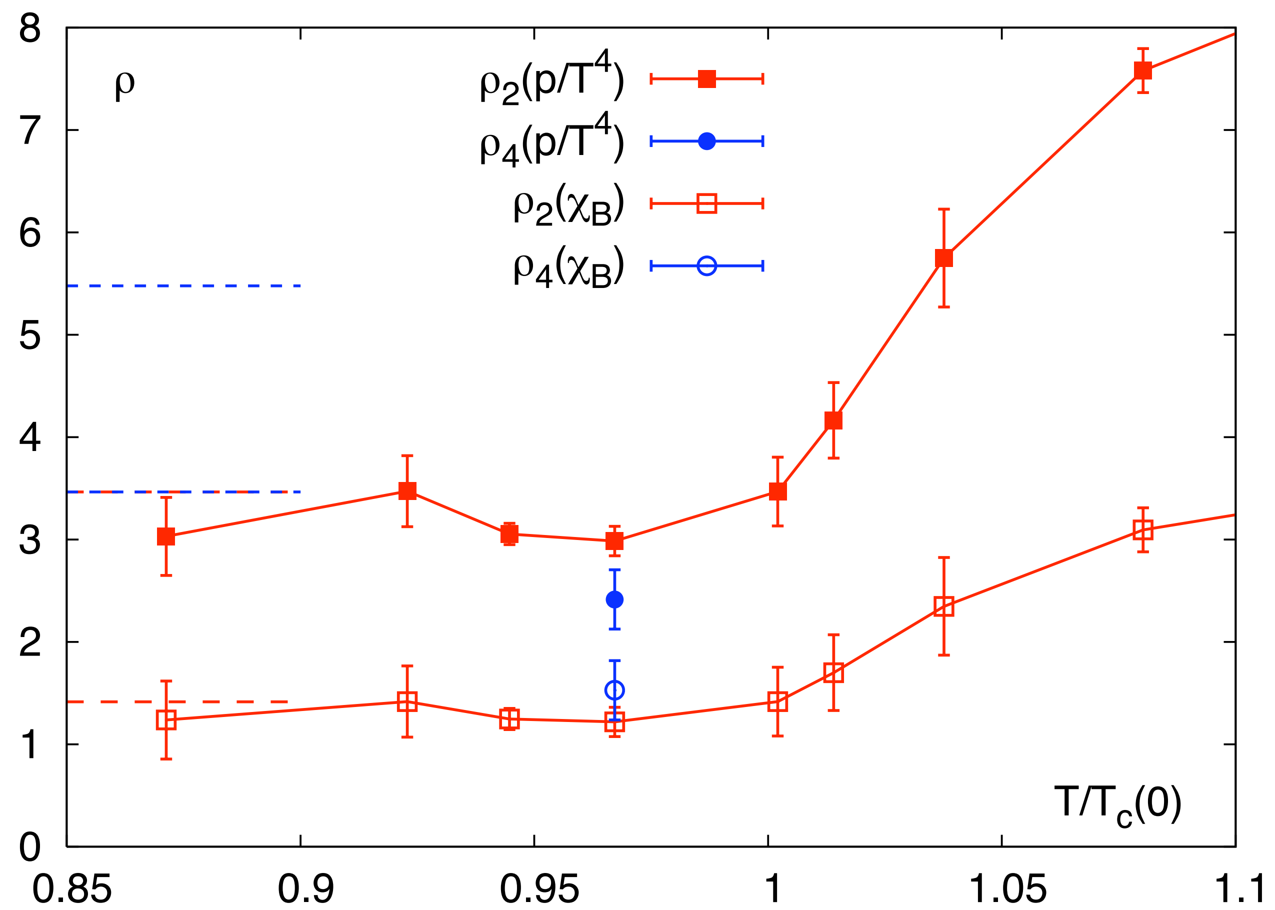
$$\frac{p}{T^4} = \sum_{n=0}^{\infty} c_{2n}(T) \left(\frac{\mu}{T}\right)^{2n}$$

Nearest singularity=radius of convergence $\quad \frac{\mu_E}{T_E} = \lim_{n\to\infty} \sqrt{\left|\frac{c_{2n}}{c_{2n+2}}\right|}, \quad \lim_{n\to\infty} \left|\frac{c_0}{c_{2n}}\right|^{\frac{1}{2n}}$

Different definitions agree only for $n \to \infty$
not n=1,2,3,...
control of systematics?

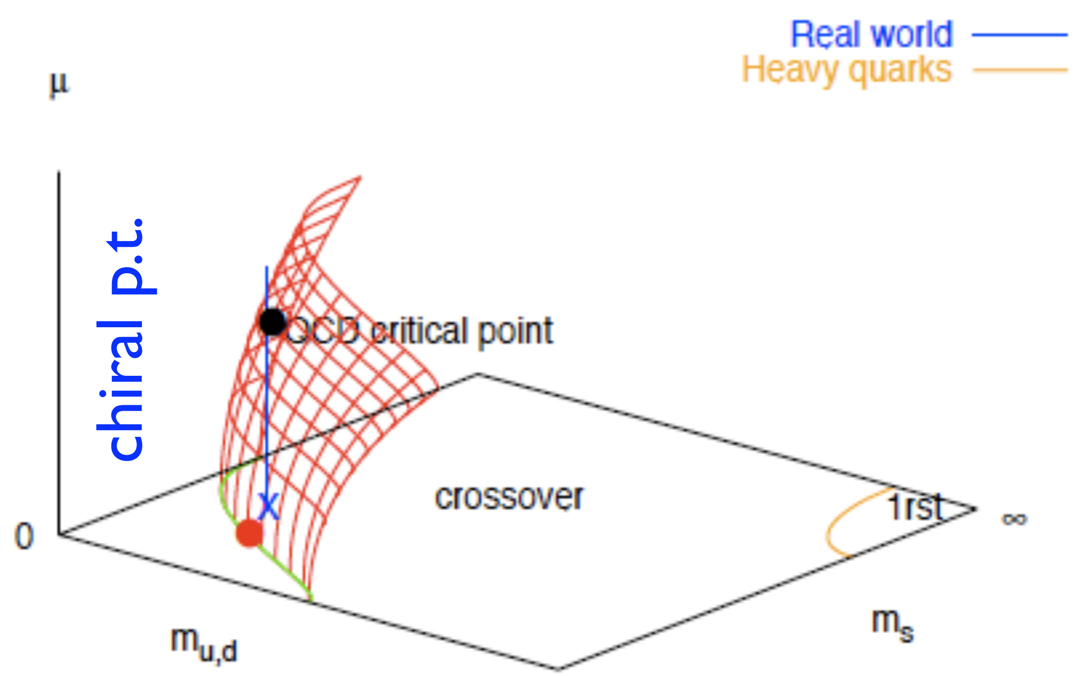
Hadron resonance gas

C.Schmidt, hotQCD 09

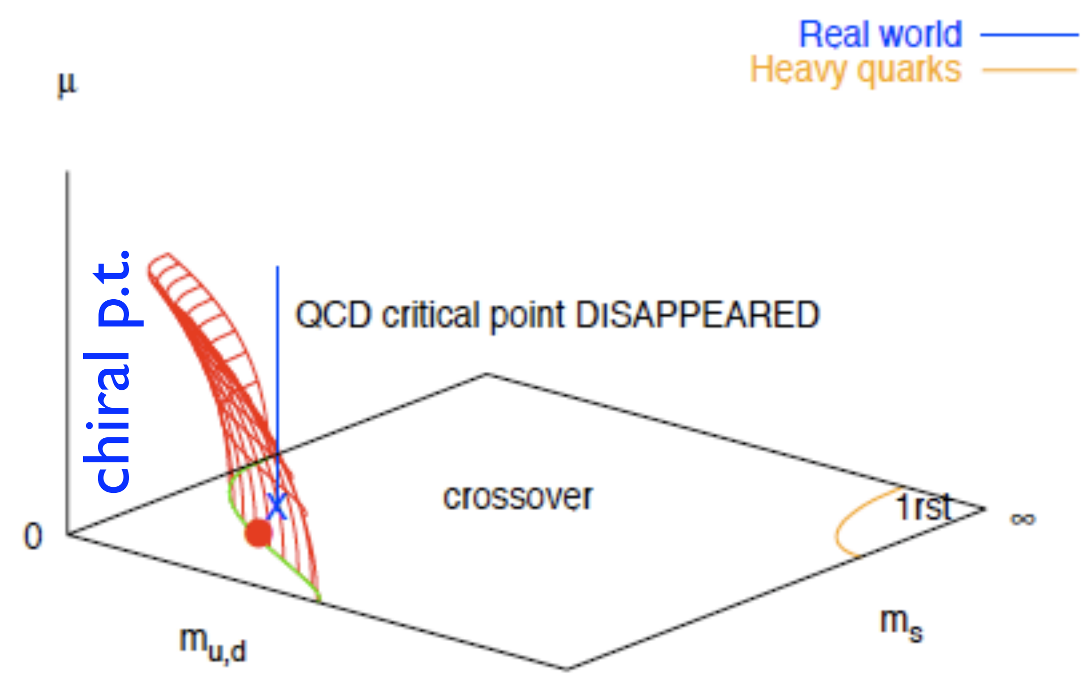


Radius of convergence necessary condition for CEP, but can it proof its existence?

Approach 2: follow chiral critical line ➡ surface



$c_1 > 0$



$c_1 < 0$

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

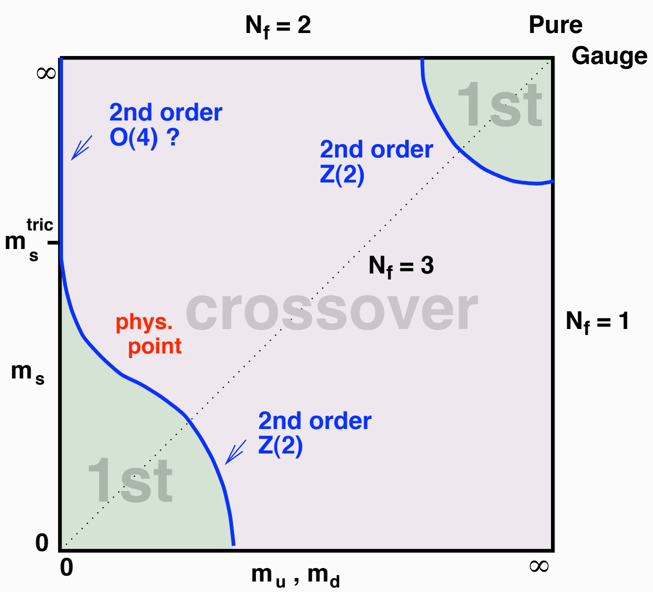
1. Tune quark mass(es) to $m_c(0)$: 2nd order transition at $\mu = 0$, $T = T_c$
   known universality class: $3d$ Ising

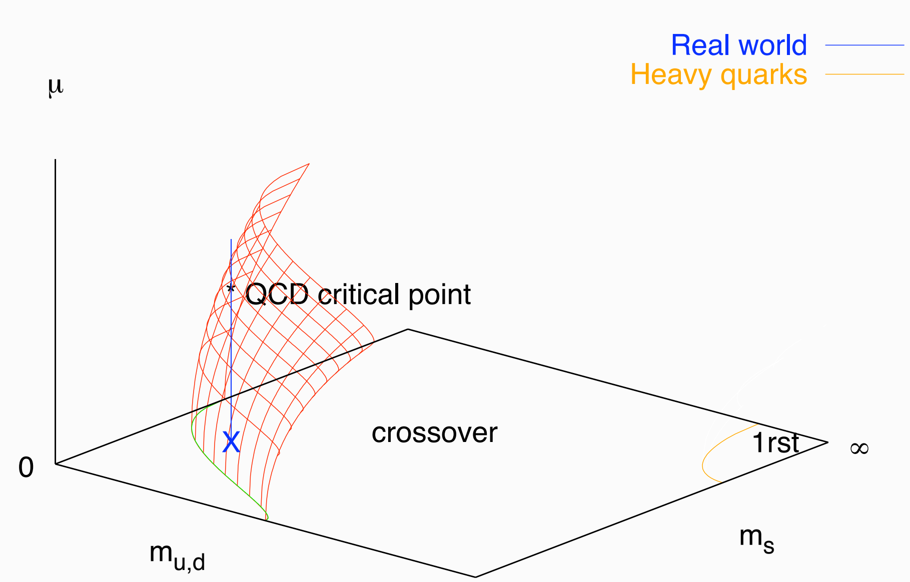
2. Measure derivatives $\frac{d^k m_c}{d\mu^{2k}}|_{\mu=0}$:

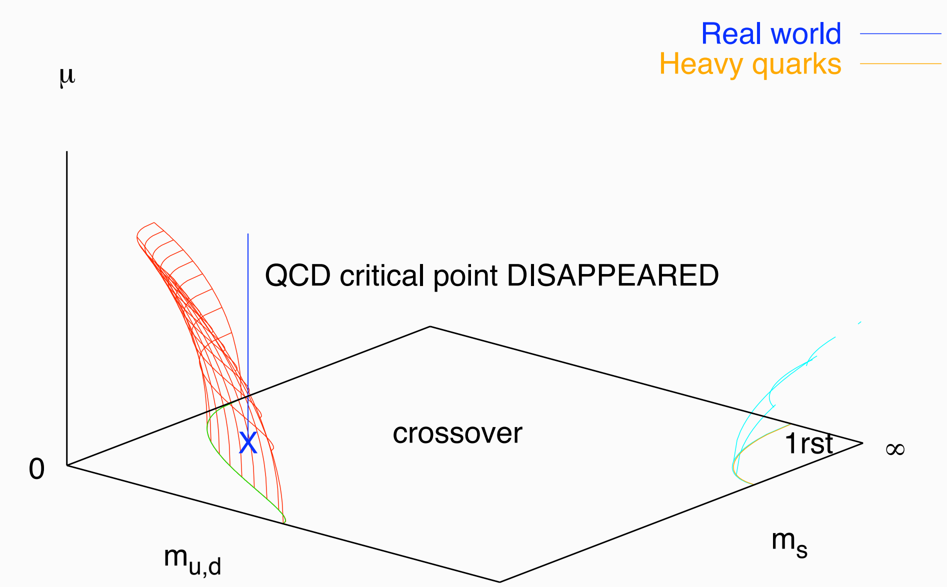
   Turn on imaginary μ and measure $\frac{m_c(\mu)}{m_c(0)}$

de Forcrand, O.P. 08,09

Finite density: chiral critical line ⟶ critical surface





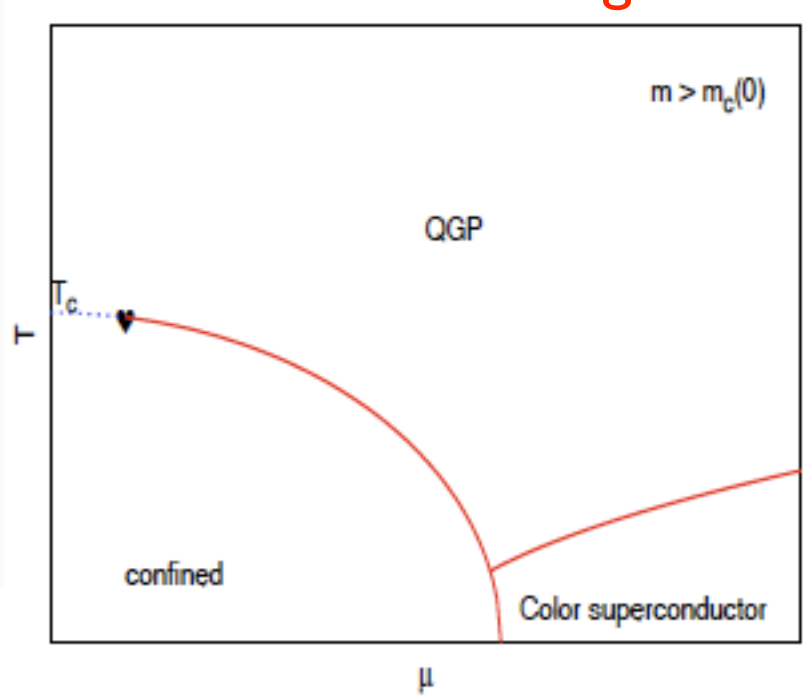


$$\frac{m_c(\mu)}{m_c(0)} = 1 + \sum_{k=1} \mathbf{c_k} \left(\frac{\mu}{\pi T}\right)^{2k}$$

$c_1 > 0$ $c_1 < 0$

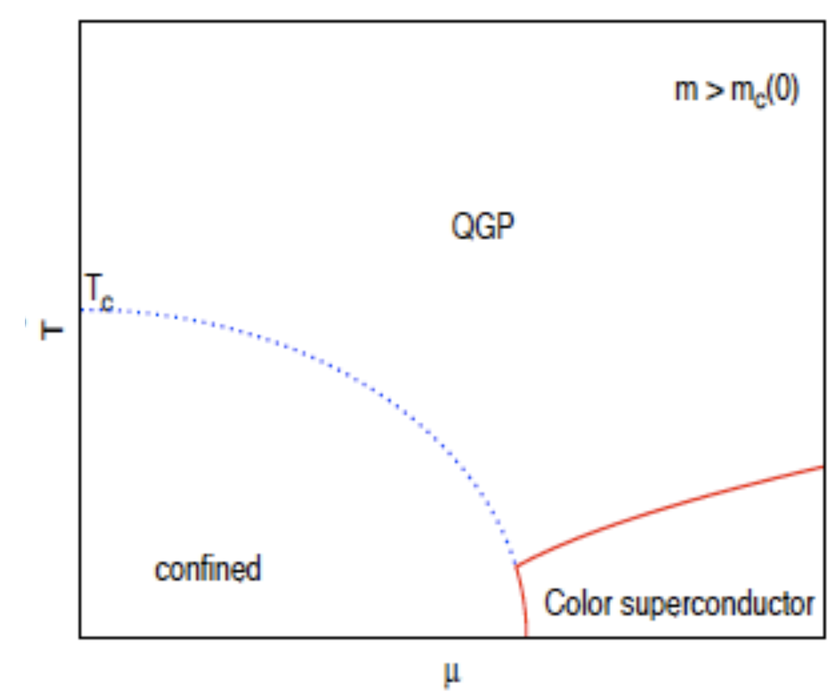
Standard scenario

transition strengthens

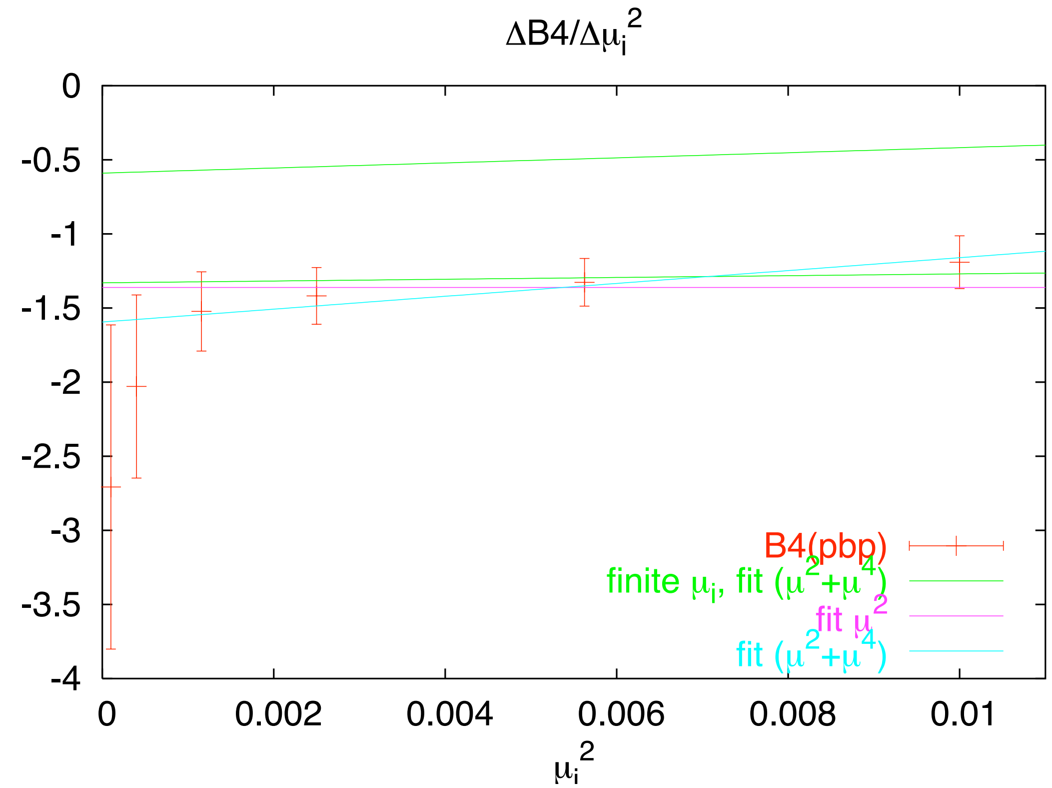


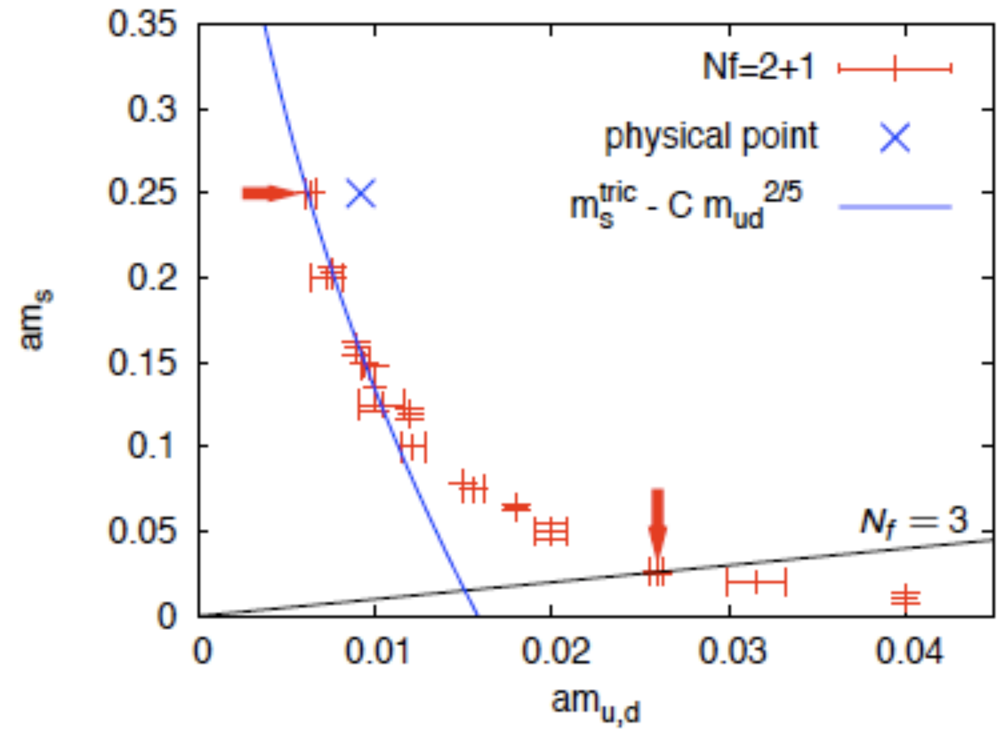
Exotic scenario

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.

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

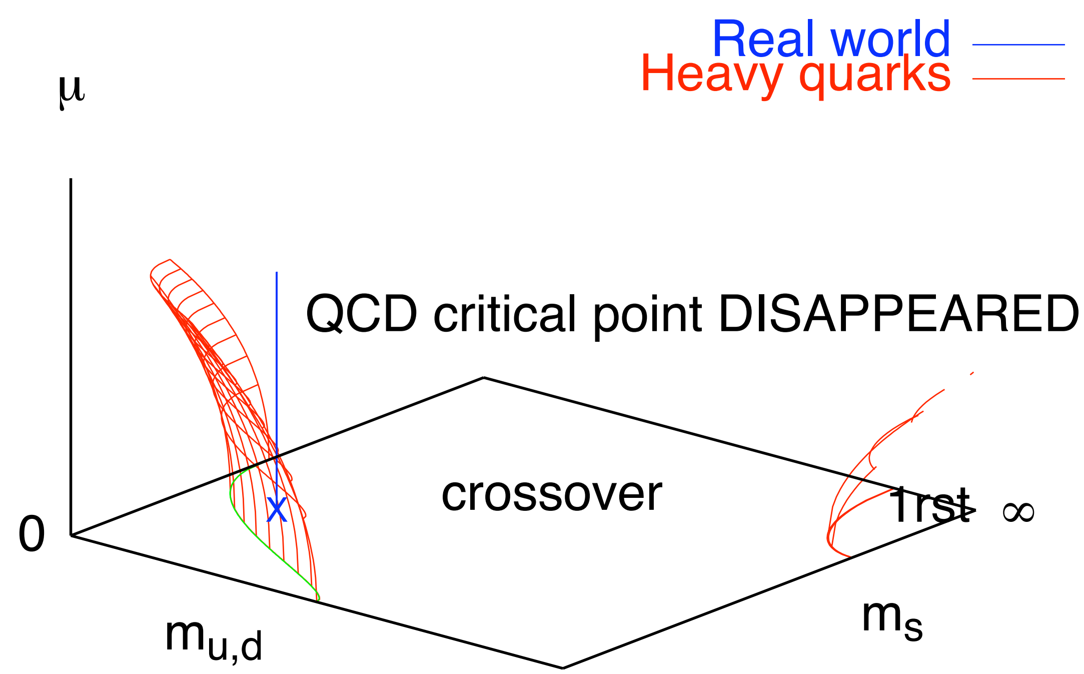
$16^3 \times 4$, Grid computing, $\sim 10^6$ traj.

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

Importance of higher order terms ?

de Forcrand, O.P. 08,09

On coarse lattice exotic scenario: no chiral critical point at small density



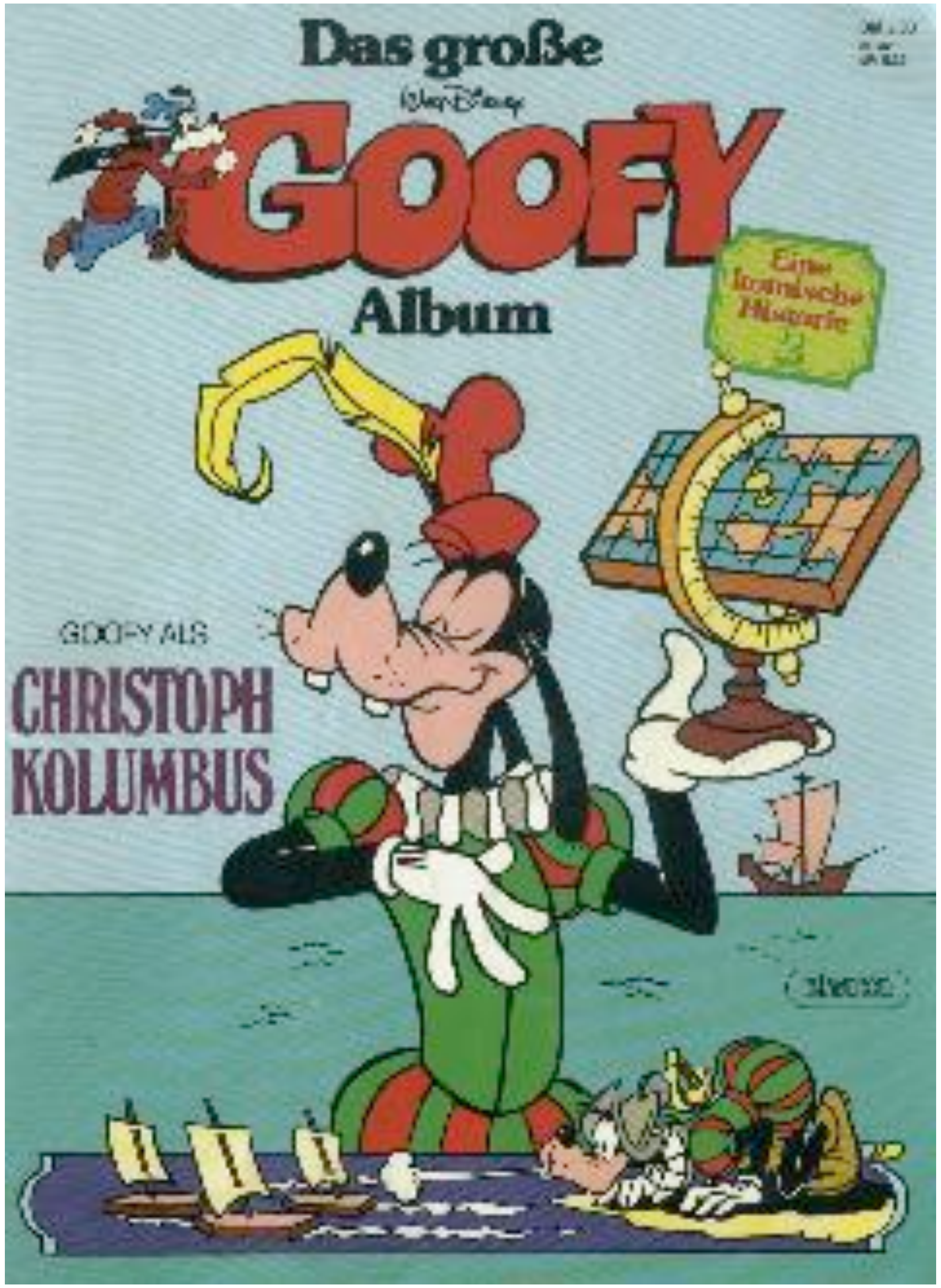
Weakening of p.t. with chemical potential also for:

-Heavy quarks — de Forcrand, Kim, Takaishi 05

-Light quarks with finite isospin density — Kogut, Sinclair 07

-Electroweak phase transition with finite lepton density — Gynther 03

Un-discovering a critical point feels like...

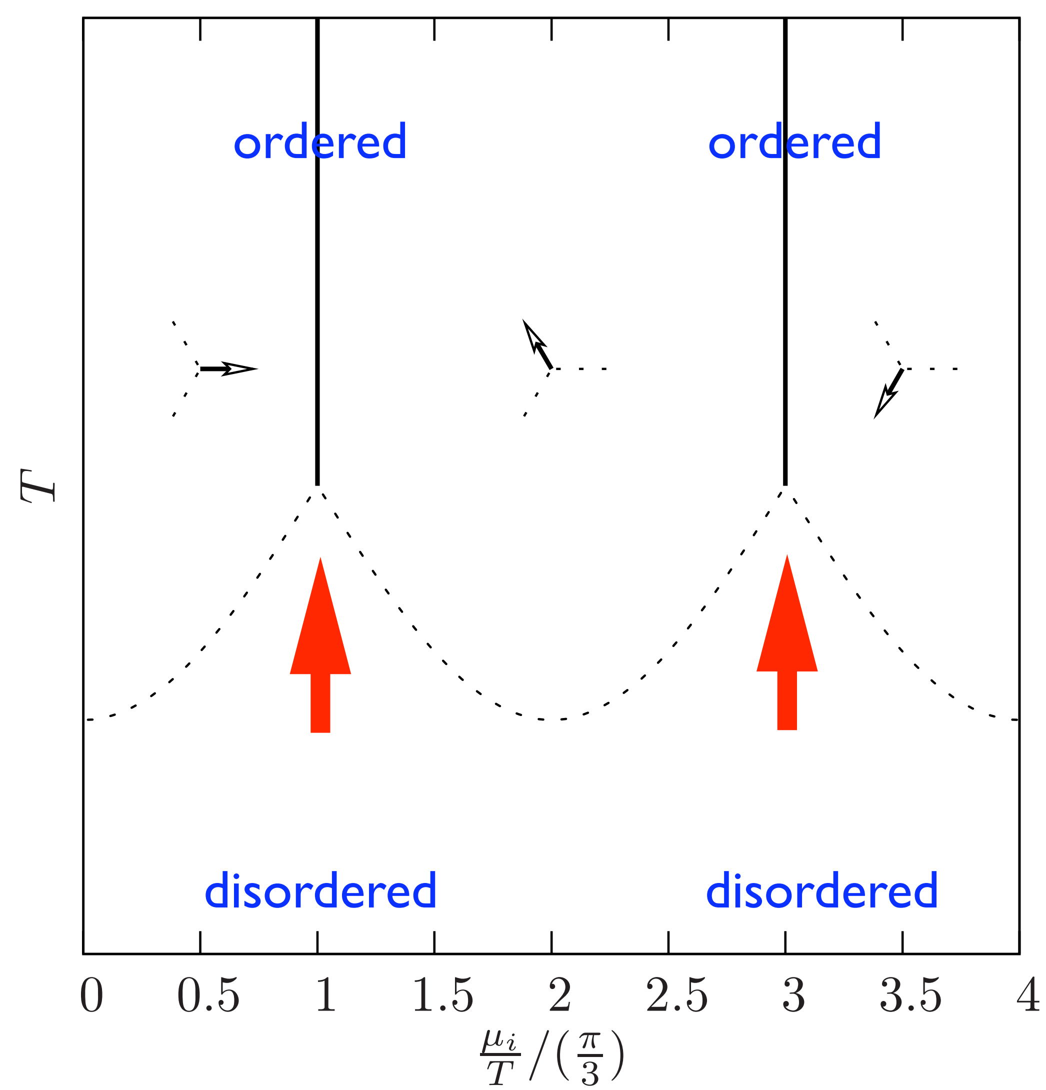


Understanding the curvature from imaginary μ

Nf=4: D'Elia, Di Renzo, Lombardo 07   Nf=2: D'Elia, Sanfilippo 09   Nf=3: de Forcrand, O.P. 10

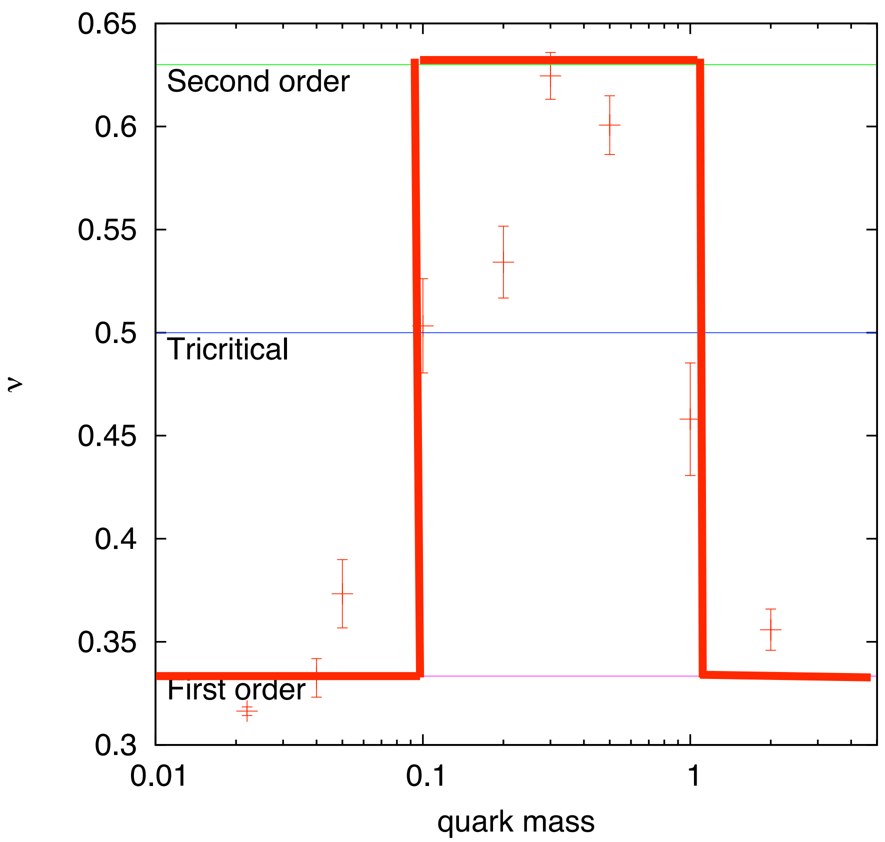
Strategy: fix $\frac{\mu_i}{T} = \frac{\pi}{3}, \pi$, measure Im(L), order parameter at $\frac{\mu_i}{T} = \pi$

determine order of Z(3) branch/end point as function of m

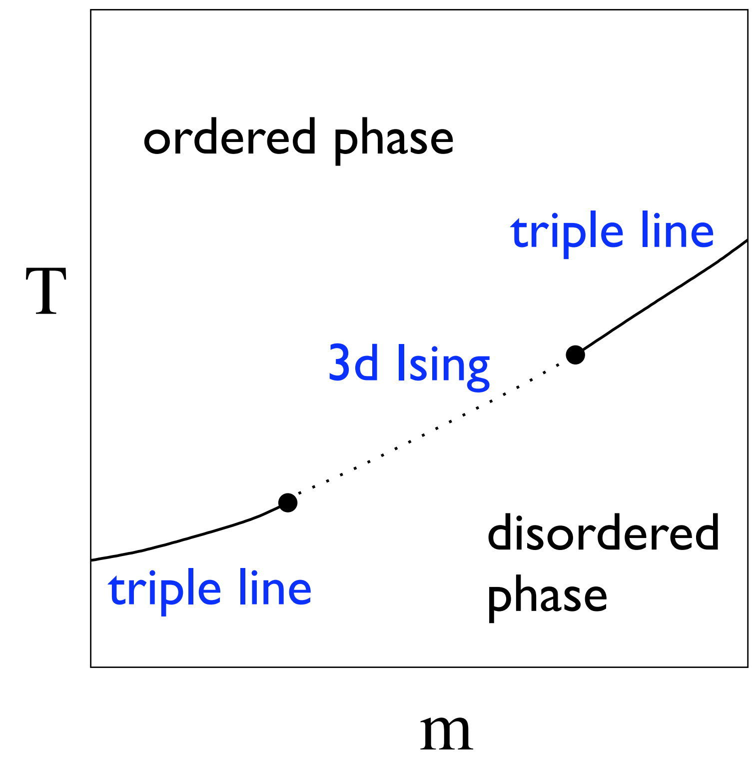


Scaling of Binder cumulant: $\nu = 0.33, 0.5, 0.63$

for 1st order, tri-critical, 3d Ising

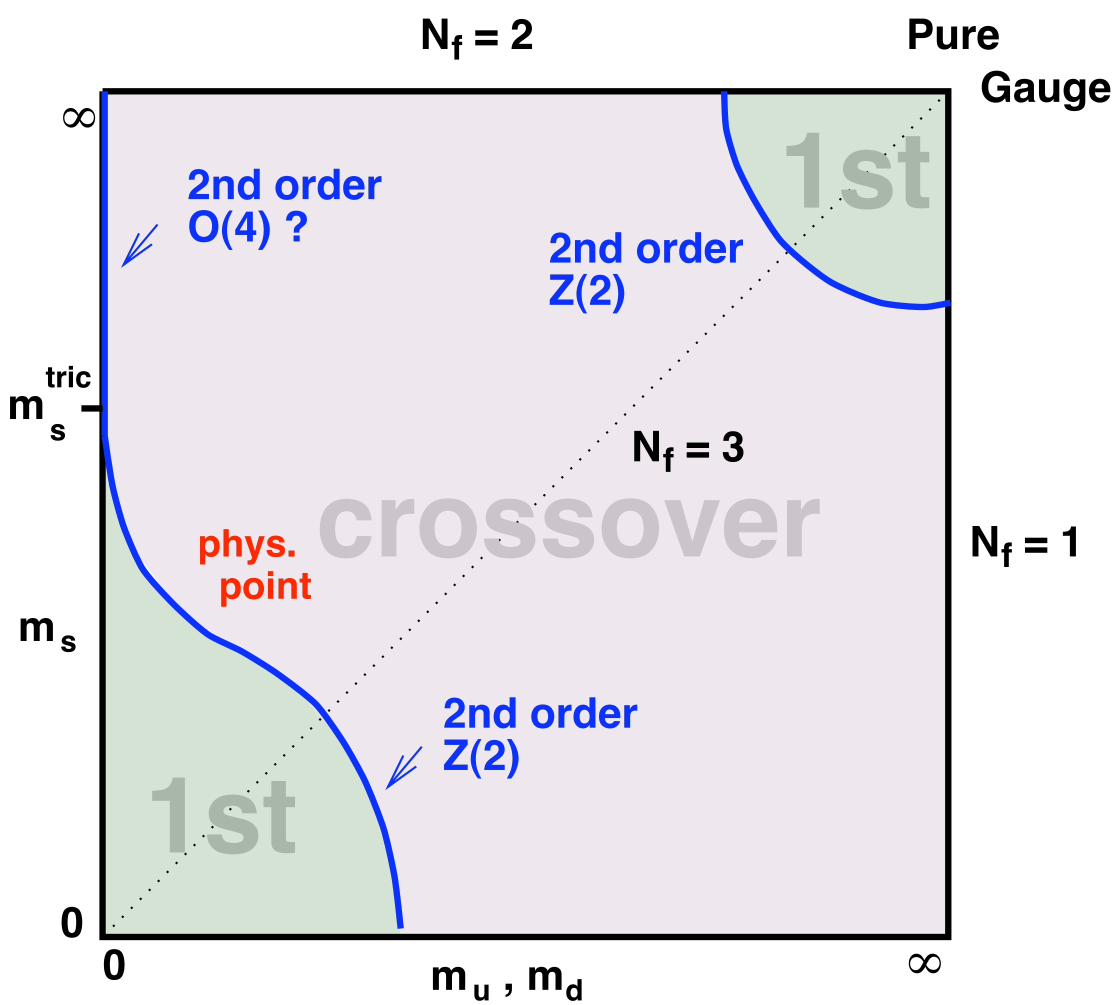


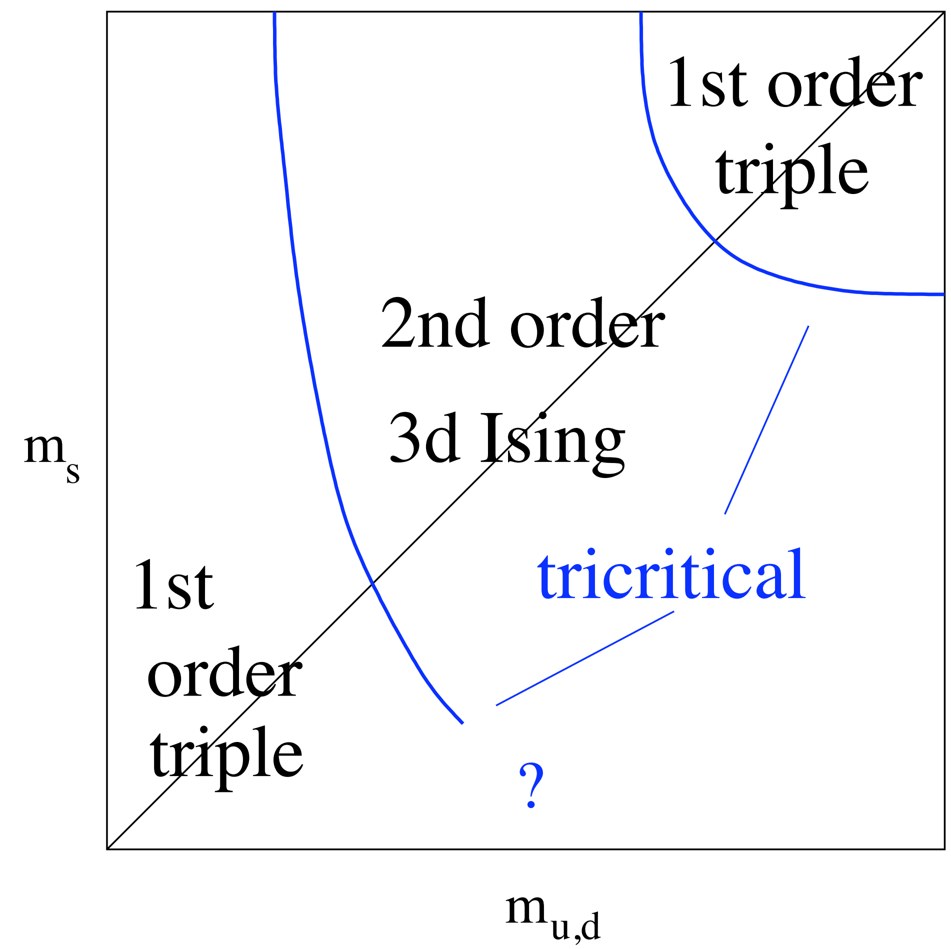
Phase diagram at fixed $\frac{\mu_i}{T} = \frac{\pi}{3}, \pi$



On infinite volume, this becomes a step function, smoothness due to finite L

Critical lines at imaginary μ





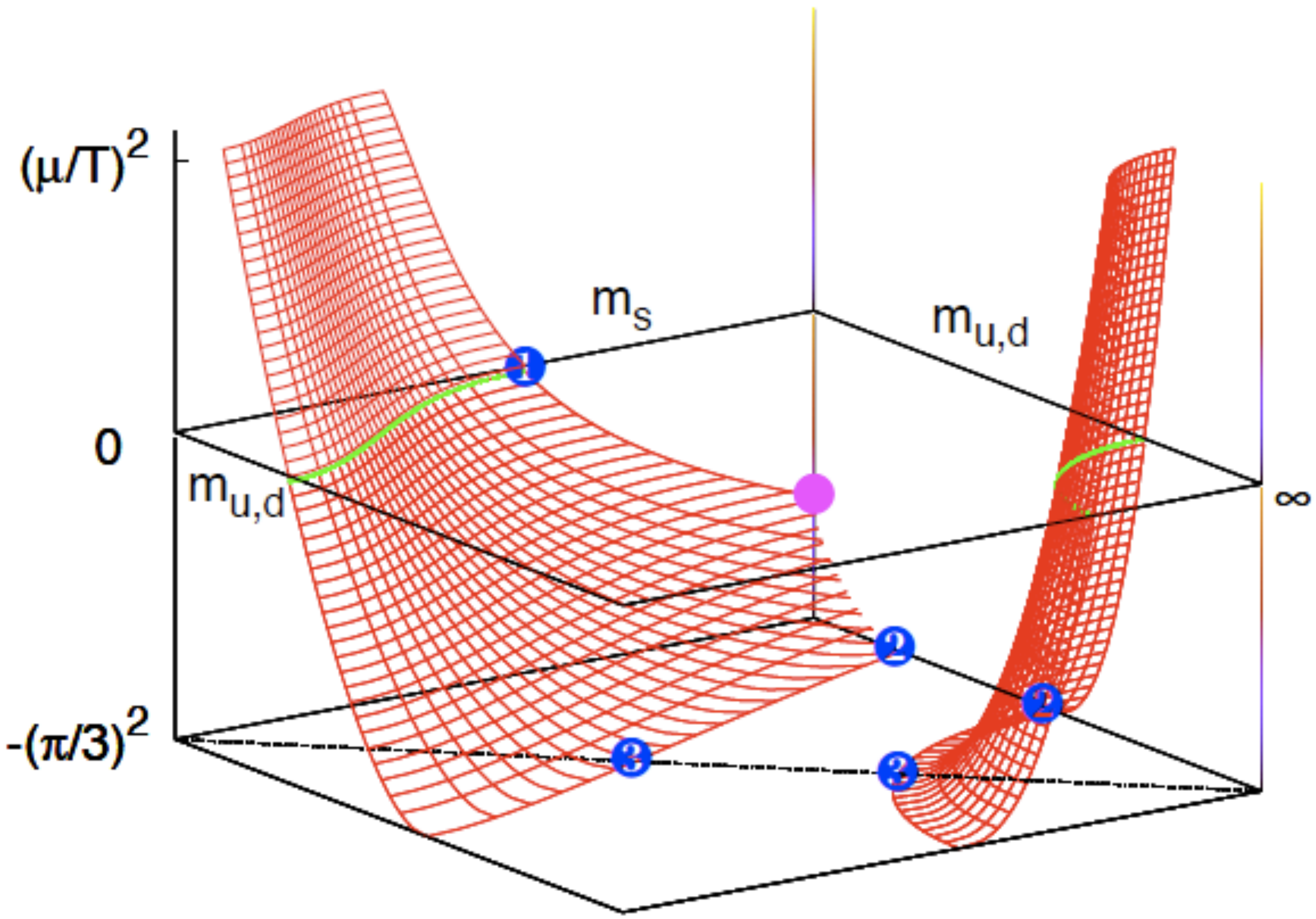
$$\mu = 0$$

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

-Connection computable with standard Monte Carlo!

-Here: heavy quarks in eff. theory

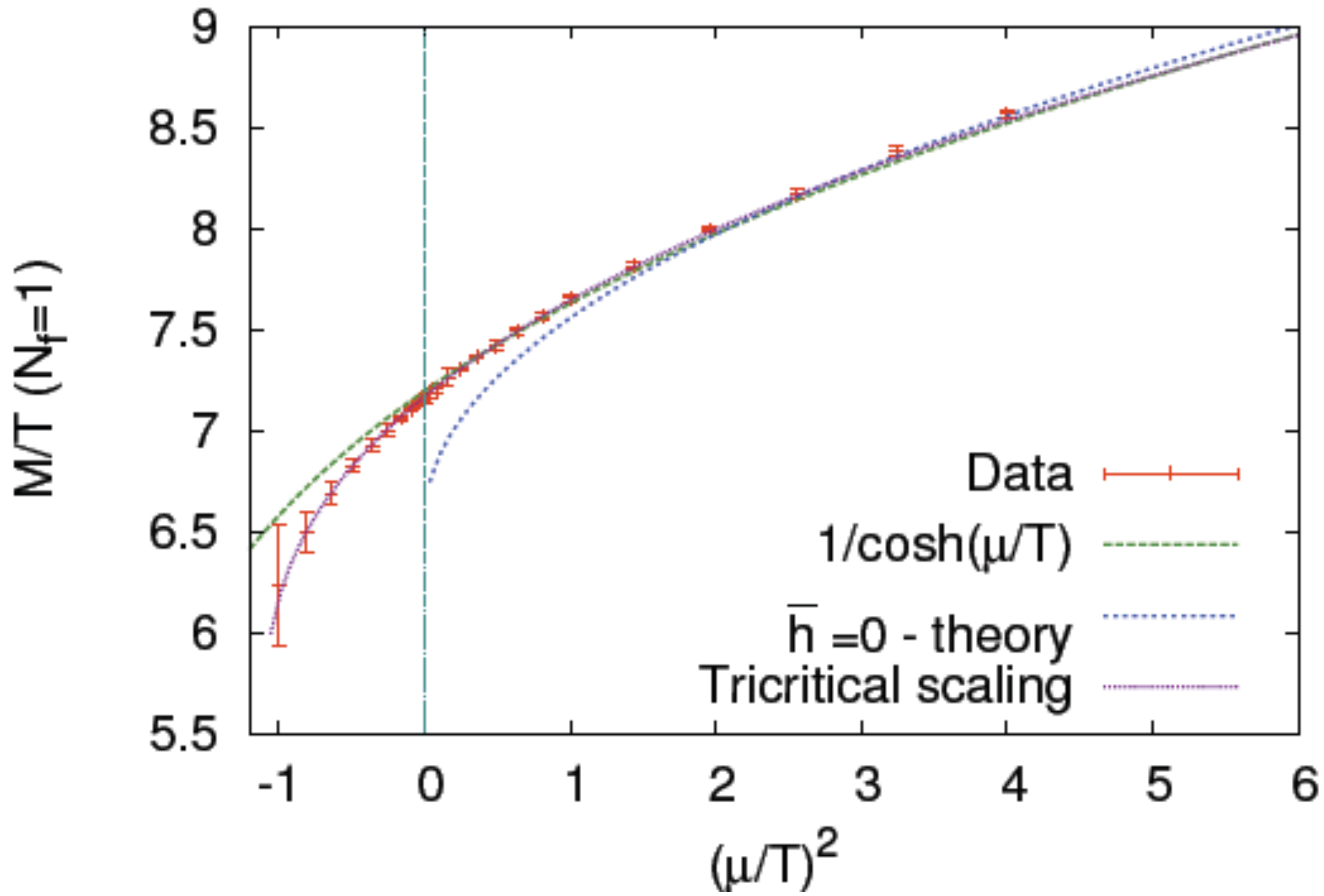
3d, imaginary chemical potential included:



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

Summary Lecture IV

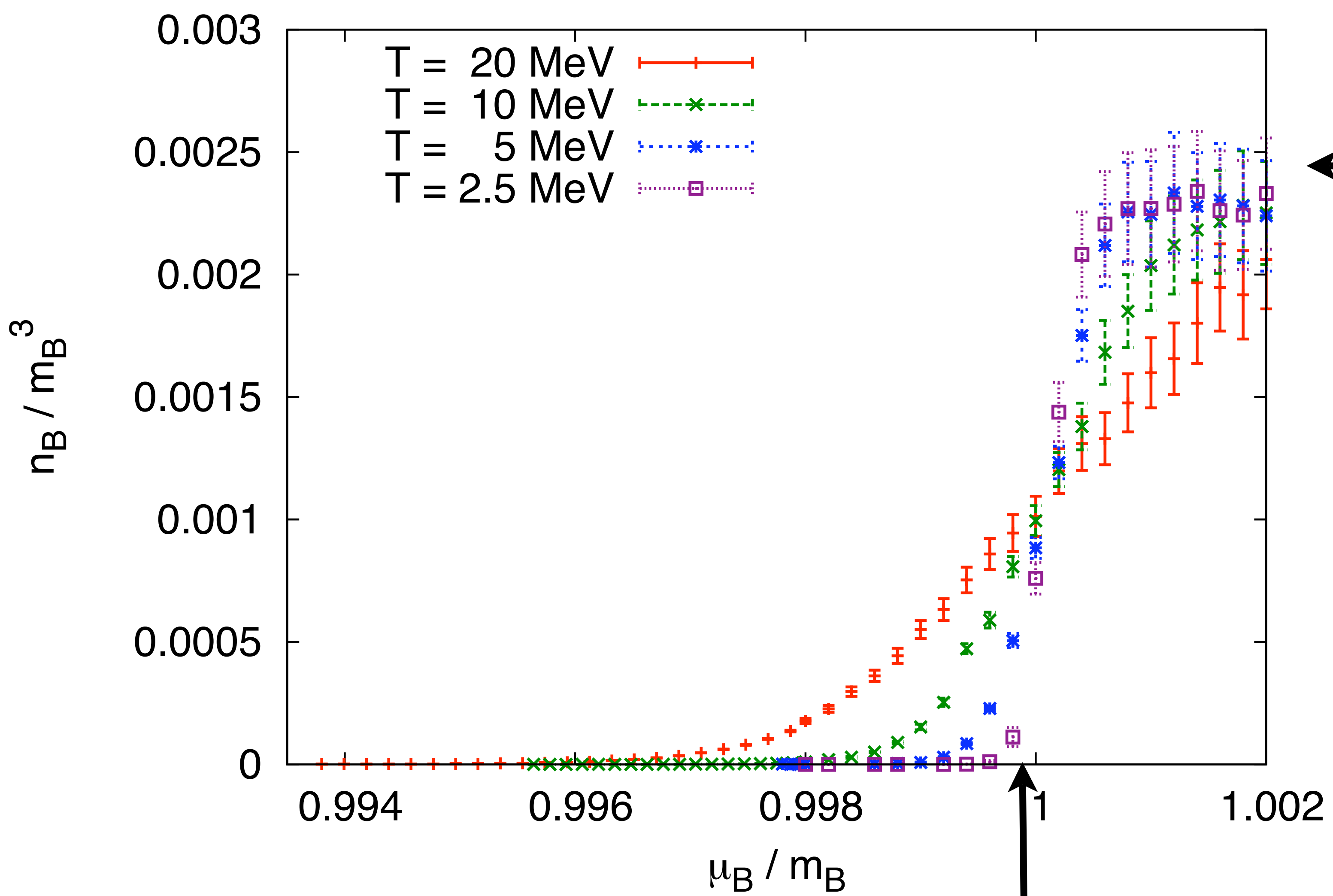
- Thermal transition at zero density is a crossover
- The sign problem is related to C-symmetry
- Direct MC methods to circumvent only at small chemical potential
- In the controlled region there is no evidence for a chiral critical point!
- Langevin algorithms?

New horizon: onset of cold nuclear matter

Based on 3d effective action by strong coupling and hopping exp.

... with very heavy quarks $m_\pi = 20 \text{ GeV}$

continuum limit with 5-7 lattice spacings per point



consistent with physical nuclear density

$$\sim 0.16 \text{ fm}^{-3} \approx 0.15 \cdot 10^{-2}\, m^3_{\text{proton}}$$

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

Frankfurt group, PRL 13

Complex Langevin: no sign problem
convergence criteria satisfied
cf. Seiler, Stamatescu; Aarts, James