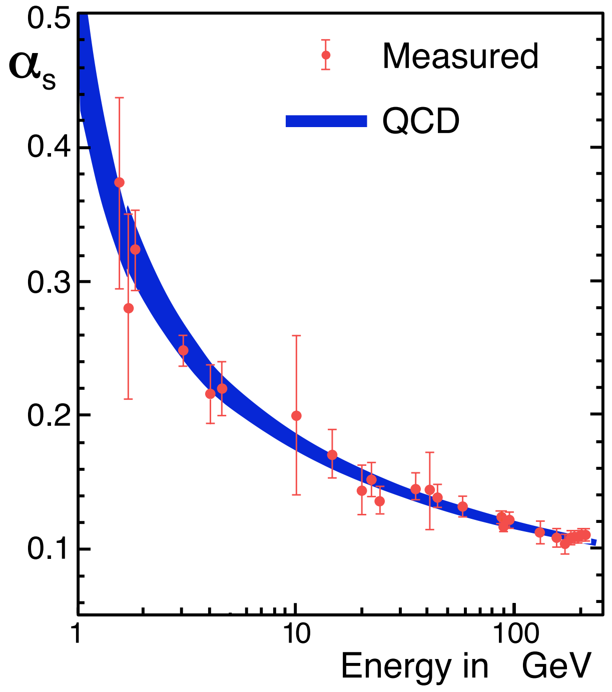
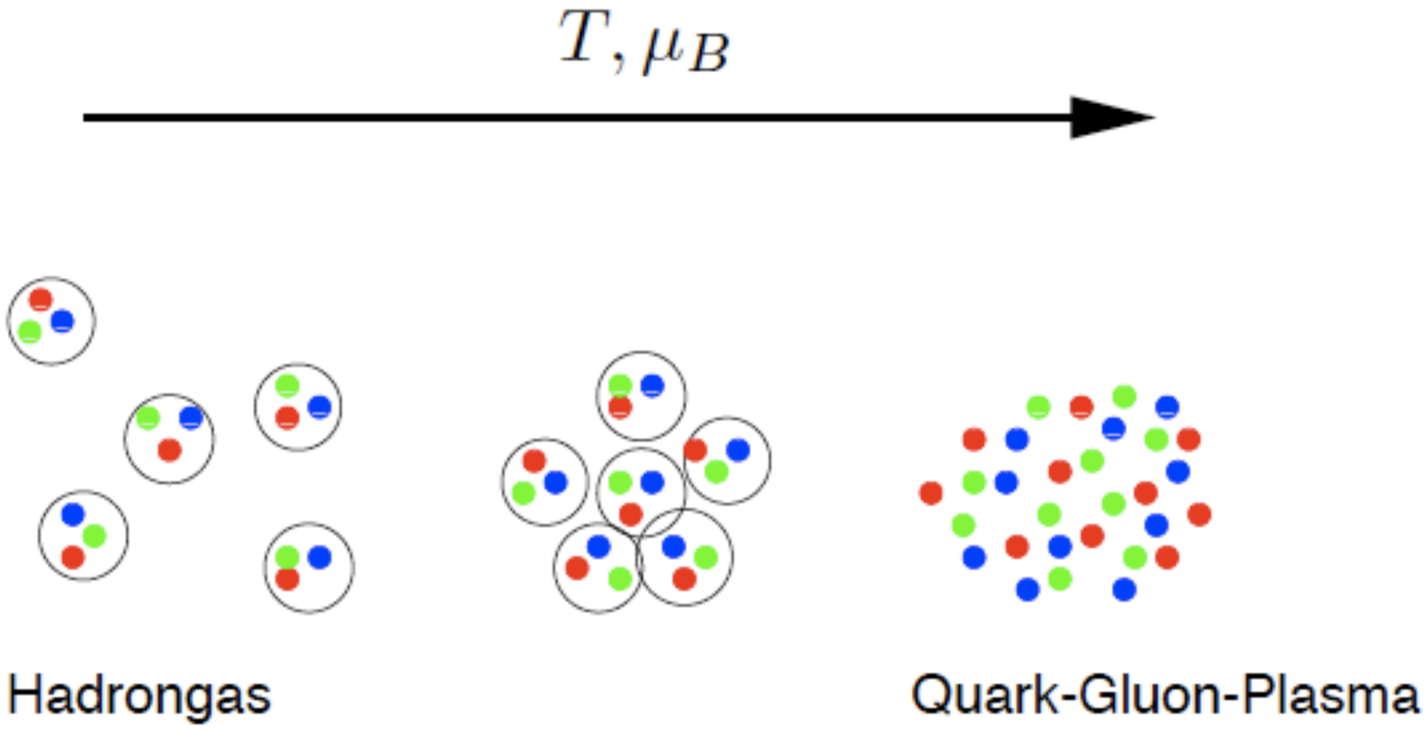
Lecture IV

- Introduction: QCD at finite temperature and density
- Deconfinement vs. chiral symmetry breaking
- Equation of state
- The phase diagram

Why thermal QCD?



asymptotic freedom $\alpha_s(p \to \infty) \to 0$



Chiral symmetry: broken (nearly) restored

Order parameters: $\langle \bar{\psi}\psi \rangle, \langle \psi\psi \rangle$

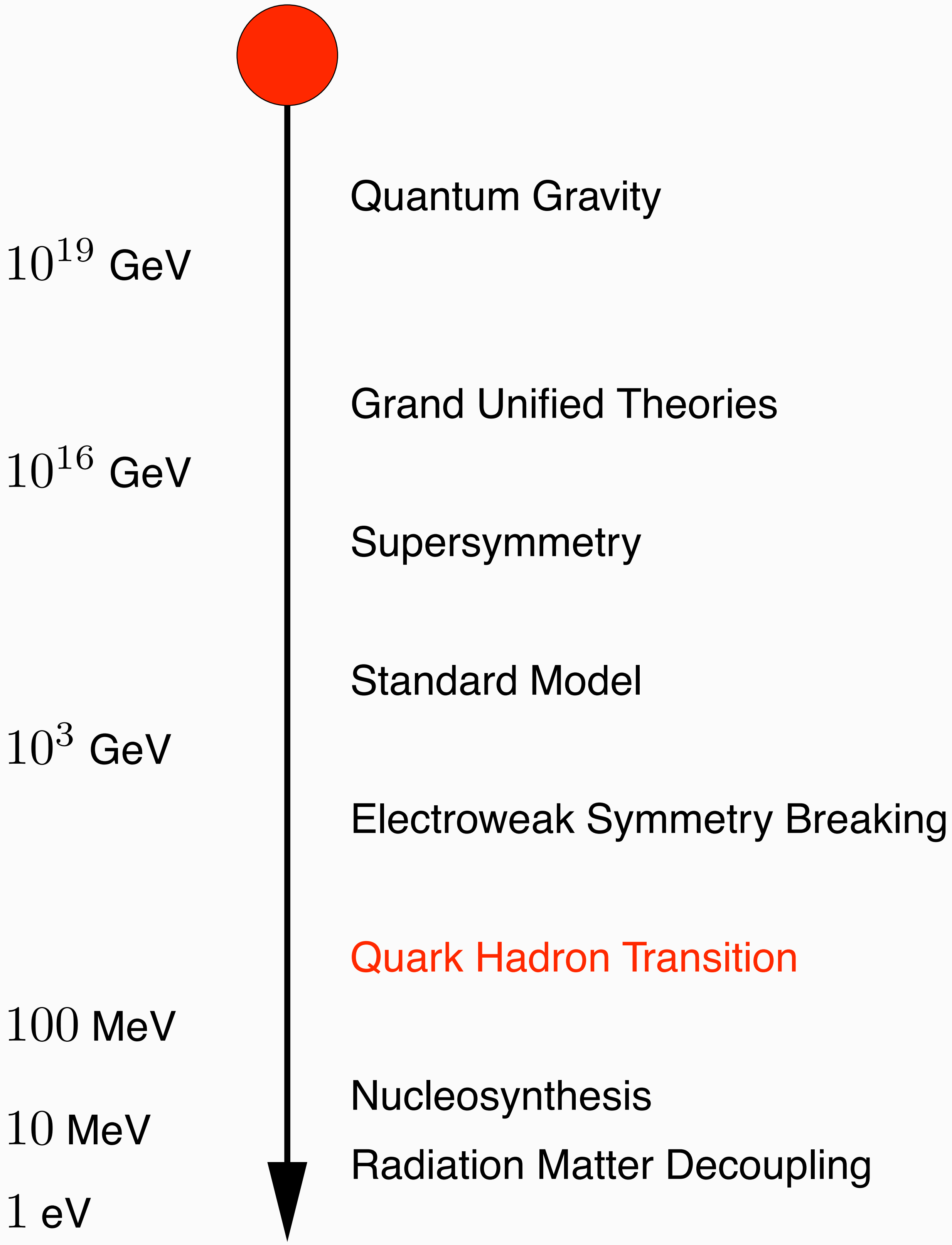
chiral condensate , Cooper pairs

Thermal QCD in nature

Physics of early universe:

non-abelian plasma physics
$(\mu_B \approx 0)$

➡ QCD is prototype



Quantum Gravity

10^{19} GeV

Grand Unified Theories

10^{16} GeV

Supersymmetry

Standard Model

10^{3} GeV

Electroweak Symmetry Breaking

Quark Hadron Transition

100 MeV

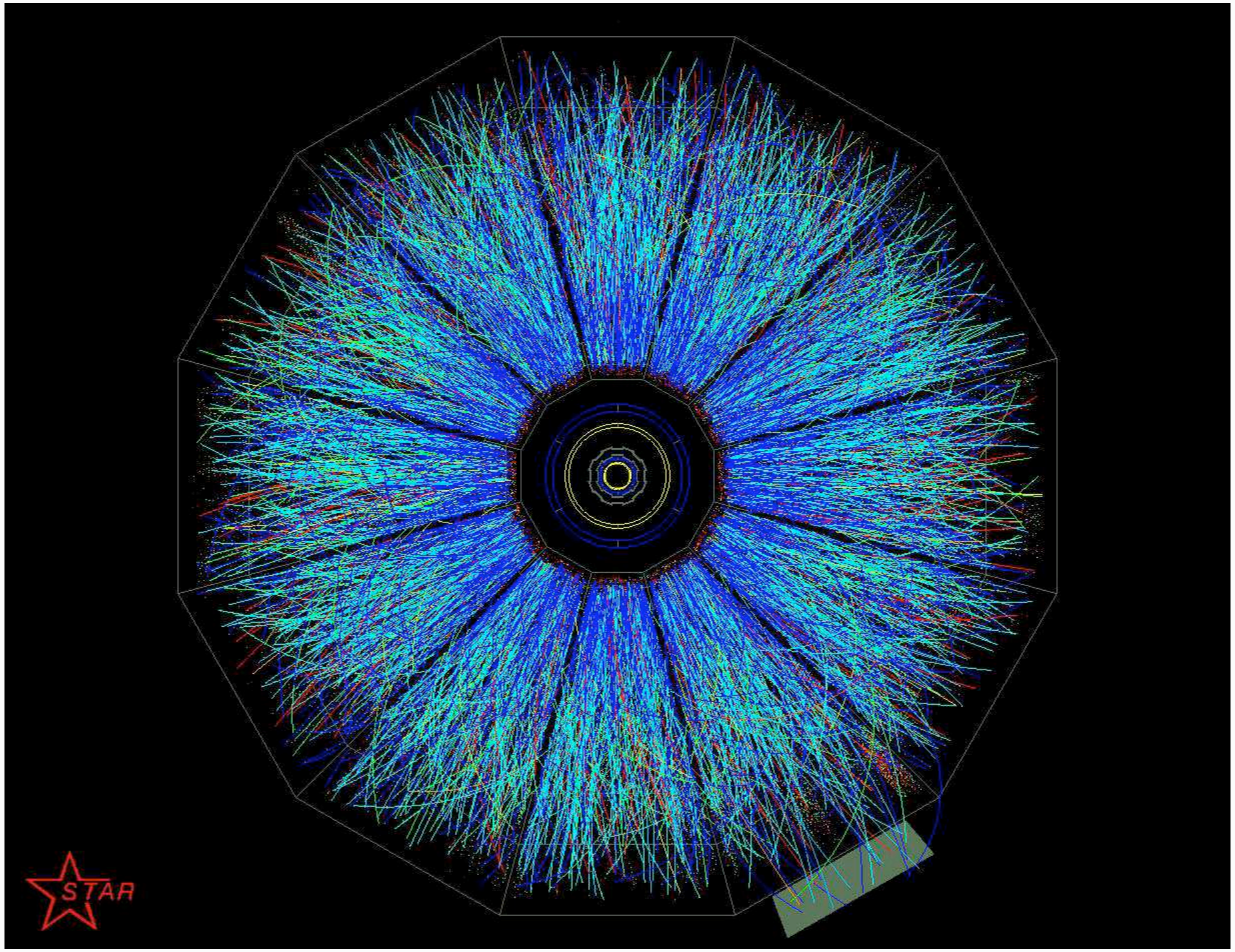
Nucleosynthesis

10 MeV

Radiation Matter Decoupling

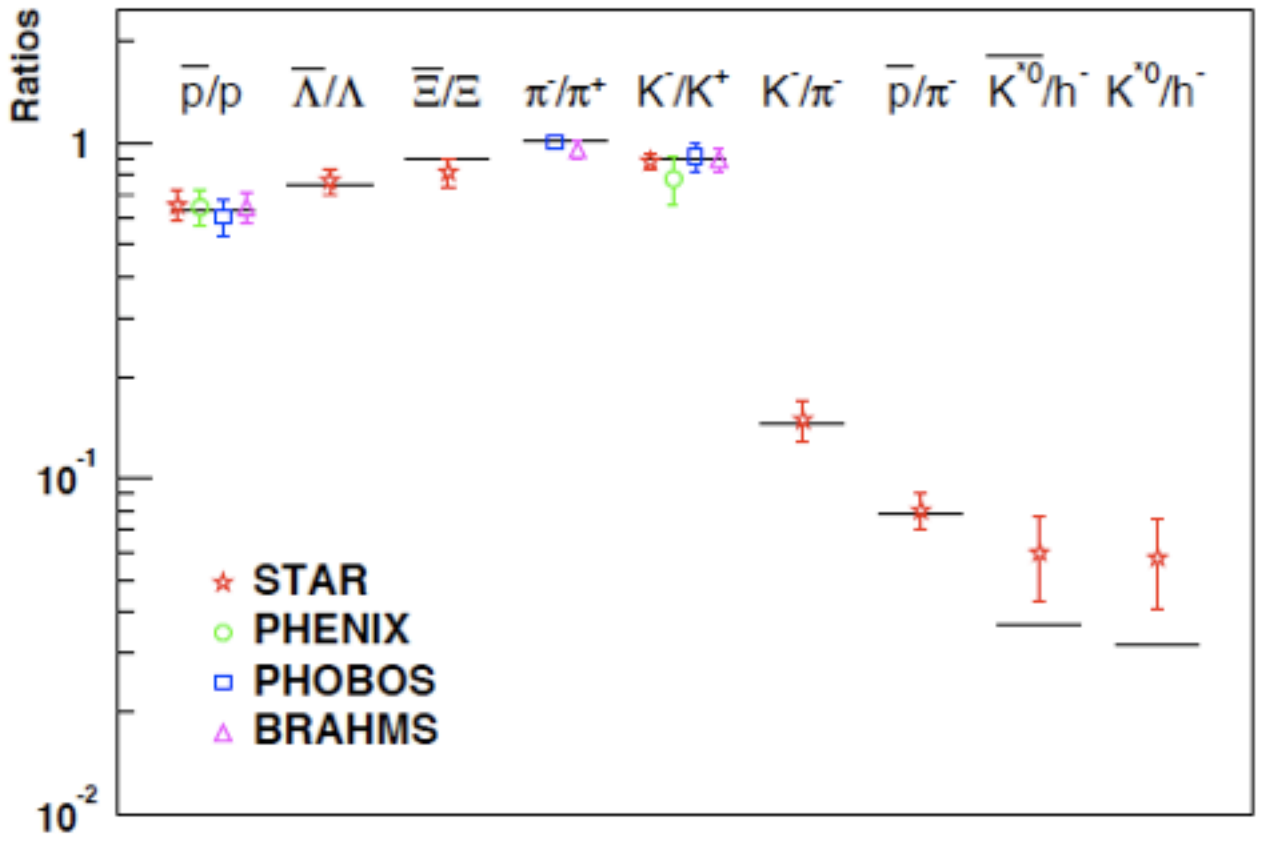
1 eV

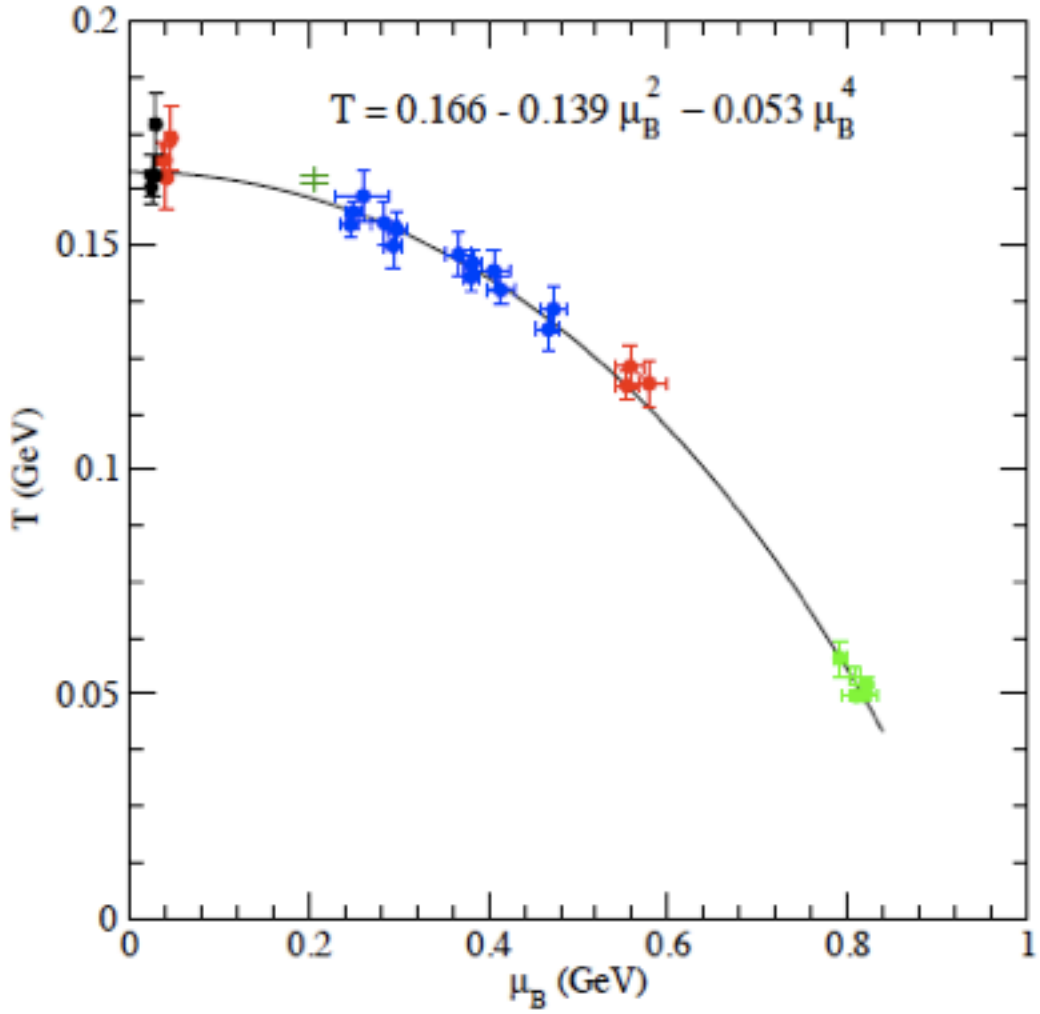
Thermal QCD in experiment



heavy ion collision experiments at RHIC, LHC, GSI....

Phase boundary from hadron freeze-out?





- At fixed collision energy $\sqrt{s}$, abundances well fitted by Boltzmann distribution (T, μ_B)
- T(freeze-out) $\leq\ T_c$ but very close ?

Braun-Munzinger et al

Statistical mechanics reminder

System of particles with conserved number operators $N_i, i = 1, 2, ...$
in contact with heat bath at temperature T

canonical ensemble: exchange of energy with bath, volume V, numbers N_i fixed

grand canonical ensemble: exchange of energy and particles with bath

density matrix and partition function → thermodynamic properties

$$\begin{aligned} \rho &= \mathrm{e}^{-\frac{1}{\mathrm{T}}(\mathrm{H}-\mu_{\mathrm{i}}\mathrm{N}_{\mathrm{i}})} \\ Z &= \mathrm{Tr}\,\rho = Z(V, T, \mu_1, \mu_2, ...; \text{particle props.}) \end{aligned}$$

observables: $\langle O \rangle = Z^{-1}\,\mathrm{Tr}(\rho O)$

$$\begin{aligned} F &= -T \ln Z \\ P &= \frac{\partial (T \ln Z)}{\partial V} \\ N_i &= \frac{\partial (T \ln Z)}{\partial \mu_i} \\ S &= \frac{\partial (T \ln Z)}{\partial T} \end{aligned}$$

QCD at finite temperature and density

Grand canonical partition function

$$Z(V,T,\mu;g,N_f,m_f) = \mathrm{Tr}(\mathrm{e}^{-(\mathrm{H}-\mu\mathrm{Q})/\mathrm{T}}) = \int \mathrm{DA}\,\mathrm{D}\bar{\psi}\,\mathrm{D}\psi\;\mathrm{e}^{-\mathrm{S_g}[\mathrm{A}_\mu]}\mathrm{e}^{-\mathrm{S_f}[\bar{\psi},\psi.\mathrm{A}_\mu]}$$

Action

$$S_g[A_\mu] \quad = \quad \int\limits_0^{1/T} dx_0 \int\limits_V d^3\mathbf{x}\;\frac{1}{2}\mathrm{Tr}\;F_{\mu\nu}F_{\mu\nu}$$

$$S_f[\bar{\psi},\psi,A_\mu] \quad = \quad \int\limits_0^{1/T} dx_0 \int\limits_V d^3\mathbf{x}\;\sum_{f=1}^{N_f}\bar{\psi}_f\left(\gamma_\mu D_\mu + m_q^f - \mu\gamma_0\right)\psi_f$$

quark number $\quad N_q^f = \bar{\psi}_f\gamma_0\psi_f$

Parameters

$$g^2, m_u \sim 3\mathrm{MeV}, m_d \sim 6\mathrm{MeV}, m_s \sim 120\mathrm{MeV}, V, T, \mu = \mu_B/3$$

$$N_f = 2+1$$

Two problems of perturbation theory

- strong coupling $g(300\mathrm{MeV}) \sim 1$
- finite T infrared problem for non-abelian theories: Linde

gauge boson self-coupling: $\frac{g^2}{e^{E/T}-1} \overset{E,p\ll T}{\sim} \frac{g^2 T}{m}$

at finite T

➡ infrared divergent for $m = 0$,

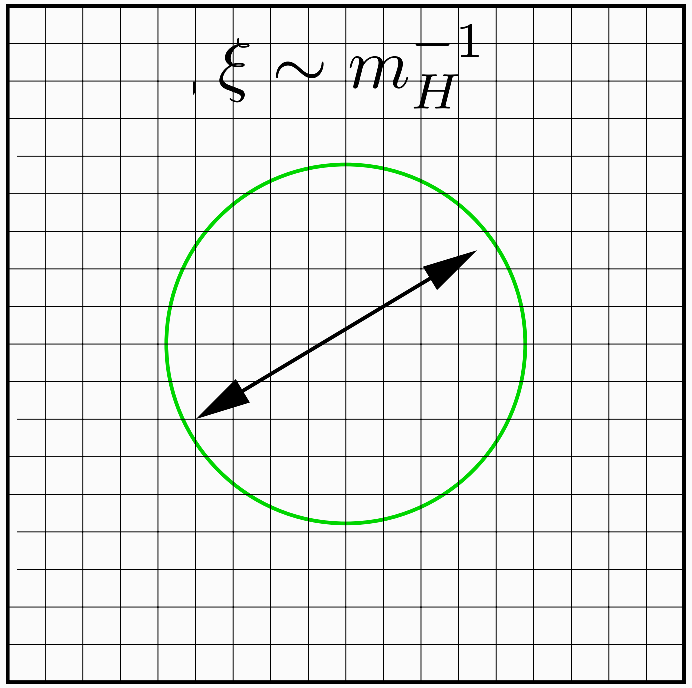
e.g. QCD, symmetric phase electroweak theory

resummation generates magnetic mass scale $m \sim g^2 T$ ➡ convergence??

finite T QFT has no solid perturbative definition, even for weak coupling!

Requirements for and constraints from the lattice:

correlation length ξ : lightest gauge invariant (hadronic?) mass scale



$$a \ll \xi \ll aL \text{ !}$$

scale of interest: $T_c \sim 200\text{MeV} \sim (1\text{fm})^{-1}$

feasible lattices: $32^3 \times 4, 16^3 \times 8$

$T = \frac{1}{aN_t}$ ➡ $a \sim 0.1 - 0.3\text{fm}$

➡ $aL \sim 1.5 - 3\text{fm}$

low T (confined) phase: $m_\pi \gtrsim 250\text{MeV}$ lighter just beginning...

high T (deconfined) phase: $m_\pi \sim T, \xi \sim 1/T$ ➡ $\frac{1}{N_t} \ll 1 \ll \frac{L}{N_t}$

➡ $T \lesssim 5T_c$

QCD in two important limits: I. the quenched limit

I. infinitely heavy quarks: ➡ pure gauge theory with static sources

static quark propagator: Polyakov loop $L_{\mathbf{x}} = \prod_{x_0=1}^{N_t} U_{n,0} \quad , \quad n \equiv (x_0, \mathbf{x})$

global Z(3) symmetry:

$S_g[U]$ invariant under $U_0(\mathbf{x},t) \rightarrow z_n U_0(\mathbf{x},t), \quad z_n = \mathrm{e}^{\mathrm{i}2\pi \mathrm{n}/3} \in \mathrm{Z}(3)$

static sources transform non-trivially: $L_{\mathbf{x}} \rightarrow z_n L_{\mathbf{x}}$

free energy of a static quark in a plasma:

$$\langle \mathrm{Tr}\, L_{\mathbf{x}} \rangle \sim \mathrm{e}^{-F_q/T}$$

McLerran, Svetitsky

➡ order parameter for confinement: $\langle L \rangle \begin{cases} = 0 \Leftrightarrow \text{confined phase}, & T < T_c \\ > 0 \Leftrightarrow \text{deconfined phase}, & T > T_c \end{cases}$

free energy of static quark anti-quark pair:

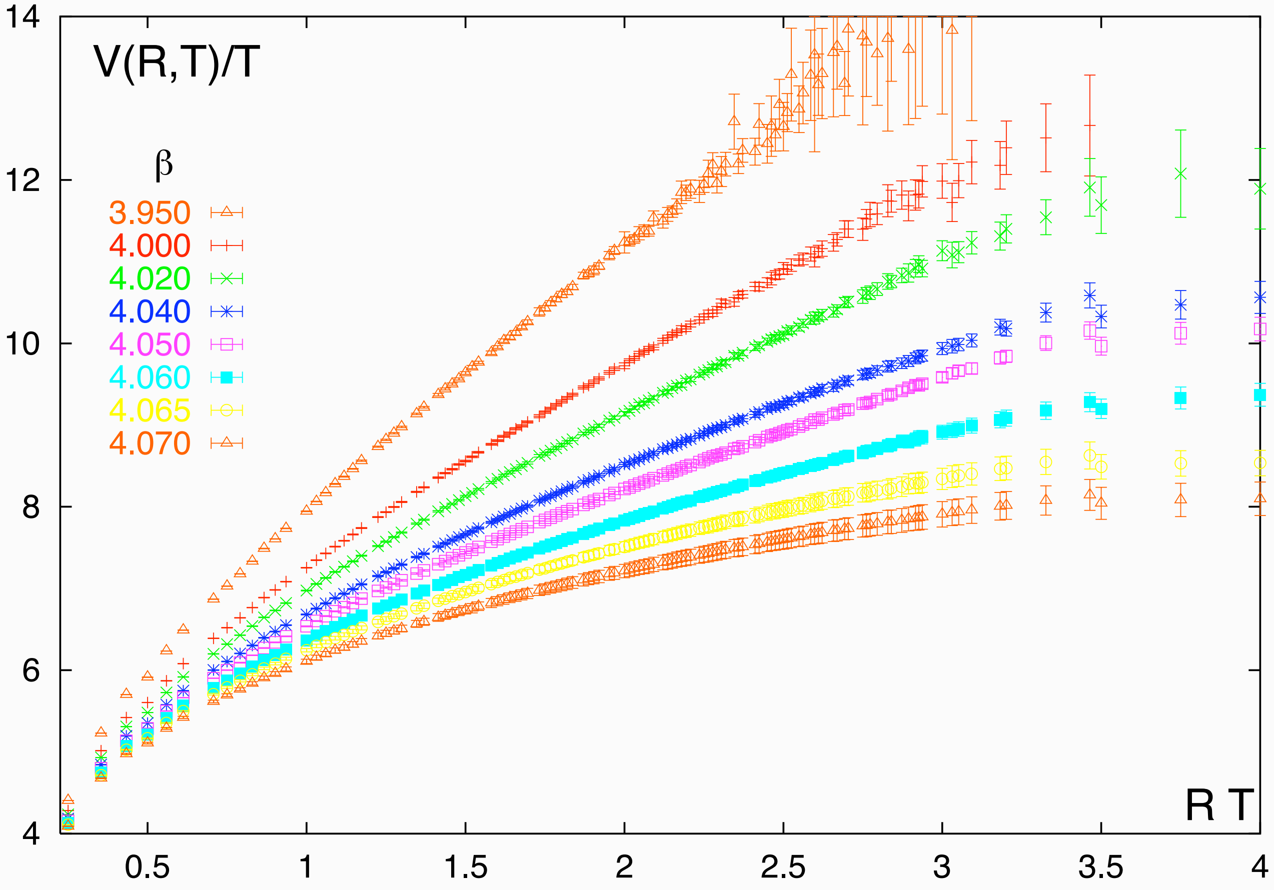
(= static potential + Boltzmann weighted thermal excitations)

$$\exp\left(-\frac{F_{\bar{q}q}(r,T)}{T}\right) = \langle \mathrm{Tr} L_{\mathbf{x}} \mathrm{Tr} L_{\mathbf{y}}^{\dagger} \rangle \quad , \quad r = |\mathbf{x} - \mathbf{y}|$$

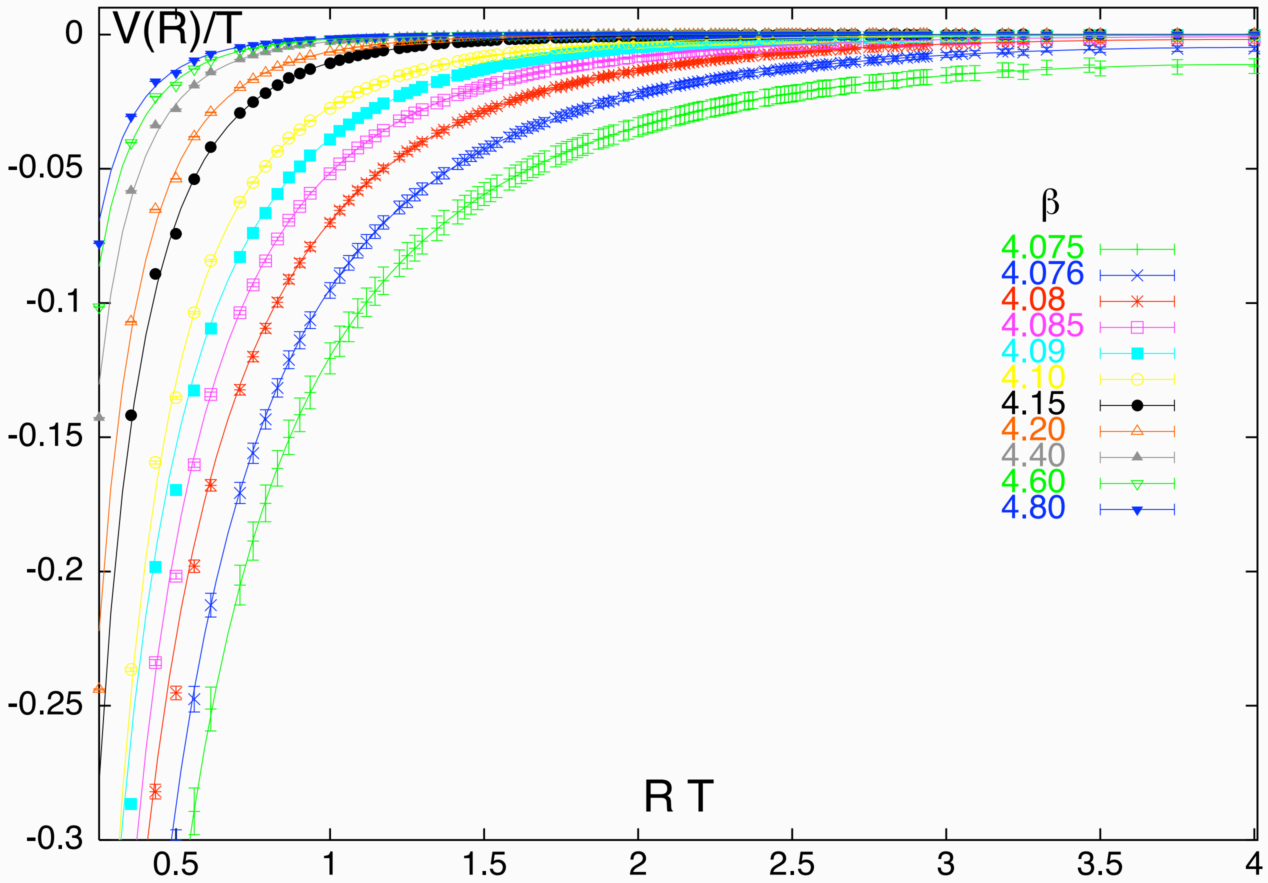
deconfinement transition: spontaneous breaking of global Z(3) symmetry at high T

The static quark free energy in the quenched limit

Bielefeld



$$T < T_c$$



$$T > T_c$$

$$\frac{\sigma(T)}{\sigma(0)} = a\sqrt{1 - b\frac{T^2}{T_c^2}}$$

$$\frac{F_{q\bar{q}}(r,T)}{T} = -\frac{c(T)}{(rT)^d}\mathrm{e}^{-\mu(T)r}$$

II. The chiral limit of QCD

massless quarks:

S_f invariant under global chiral transformations $U_A(1) \times SU(N_f)_L \times SU(N_f)_R$

spontaneous symmetry breaking: $SU(N_f)_L \times SU(N_f)_R \rightarrow SU(N_f)_V$

➡ $N_f^2 - 1$ massless Goldstone bosons, pions

order parameter: chiral condensate $\langle\bar{\psi}\psi\rangle = \frac{1}{L^3 N_t} \frac{\partial}{\partial m_q} \ln Z$

$$\langle\bar{\psi}\psi\rangle \begin{cases} > \ 0 \ \Leftrightarrow \ \text{symmetry broken phase,} & T \ < \ T_c \\ = \ 0 \ \Leftrightarrow \ \text{symmetric phase,} & T \ > \ T_c \end{cases}$$

chiral transition: spontaneous restoration of global $SU(N_f)_L \times SU(N_f)_R$ at high T

But: chiral limit cannot be simulated!!

Physical QCD

.....breaks both chiral and Z(3) symmetry explicitly

.....but displays confinement and very light pions

- no order parameter → no phase transition necessary!
- if there is a p.t.: are there two distinct transitions?
- if there is just one p.t.: is it related to chiral or Z(3) dynamics?
- if there is no phase transition: how do the properties of matter change?

Equation of state: ideal (non-interacting) gases

partition fcn. for one relativistic bosonic/fermionic d.o.f.:

$$\ln Z = V \int \frac{d^3p}{(2\pi)^3} \ln\left(1 \pm \mathrm{e}^{-(E(p)-\mu)/T}\right)^{\pm 1}, \qquad E(p) = \sqrt{\mathbf{p}^2 + m^2}$$

equation of state for g d.o.f., two relevant limits:

Stefan-Boltzmann

$\mathit{Relativistic\ Boson},\ m \ll T$	$\times\ (\mathit{Fermion})$	$\mathit{Non\text{-}relativistic},\ m \gg T$
$p_r = g\frac{\pi^2}{90}T^4$	$\left(\frac{7}{8}\right)$	$p_{nr} = gT\left(\frac{mT}{2\pi}\right)^{\frac{3}{2}}\exp(-m/T)$
$\epsilon_r = g\frac{\pi^2}{30}T^4$	$\left(\frac{7}{8}\right)$	$\epsilon_{nr} = \frac{m}{T}p_{nr} \gg p_{nr}$

➡ $p_r = \epsilon_r/3, \qquad p_{nr} \simeq 0$

The QCD equation of state

Task: compute free energy density or pressure density

$$f = -\frac{T}{V} \ln Z(T,V)$$

➡ all bulk thermodynamic properties follow:

$$p = -f, \qquad \frac{\epsilon - 3p}{T^4} = T \frac{\mathrm{d}}{\mathrm{d}T} \left(\frac{p}{T^4} \right), \qquad \frac{s}{T^3} = \frac{\epsilon + p}{T^4}, \qquad c_s^2 = \frac{\mathrm{d}p}{\mathrm{d}\epsilon}$$

Technical problem: partition function in Monte Carlo normalized to 1.

➡ Z, p, f not directly calculable, only $\langle O \rangle = Z^{-1}\,\mathrm{Tr}(\rho O)$

➡ Integral method:

$$\left. \frac{f}{T^4} \right|_{T_o}^{T} = -\frac{1}{V} \int_{T_o}^{T} \mathrm{d}x \, \frac{\partial x^{-3} \ln Z(x,V)}{\partial x}$$

modify for lattice action:

$$\left.\frac{f}{T^4}\right|_{\beta_o}^{\beta} = -\frac{N_\tau^3}{L^3}\int_{\beta_o}^{\beta} \mathrm{d}\beta' \left(\left\langle \frac{\partial \ln Z}{\partial \beta} \right\rangle - \left\langle \frac{\partial \ln Z}{\partial \beta} \right\rangle_{T=0} \right)$$

N.B.: lower integration constant not rigorously defined,
but exponentially suppressed

$$\frac{f}{T^4}(\beta_0) \sim \mathrm{e}^{-\mathrm{m_{glueball}/T}} \approx 0$$

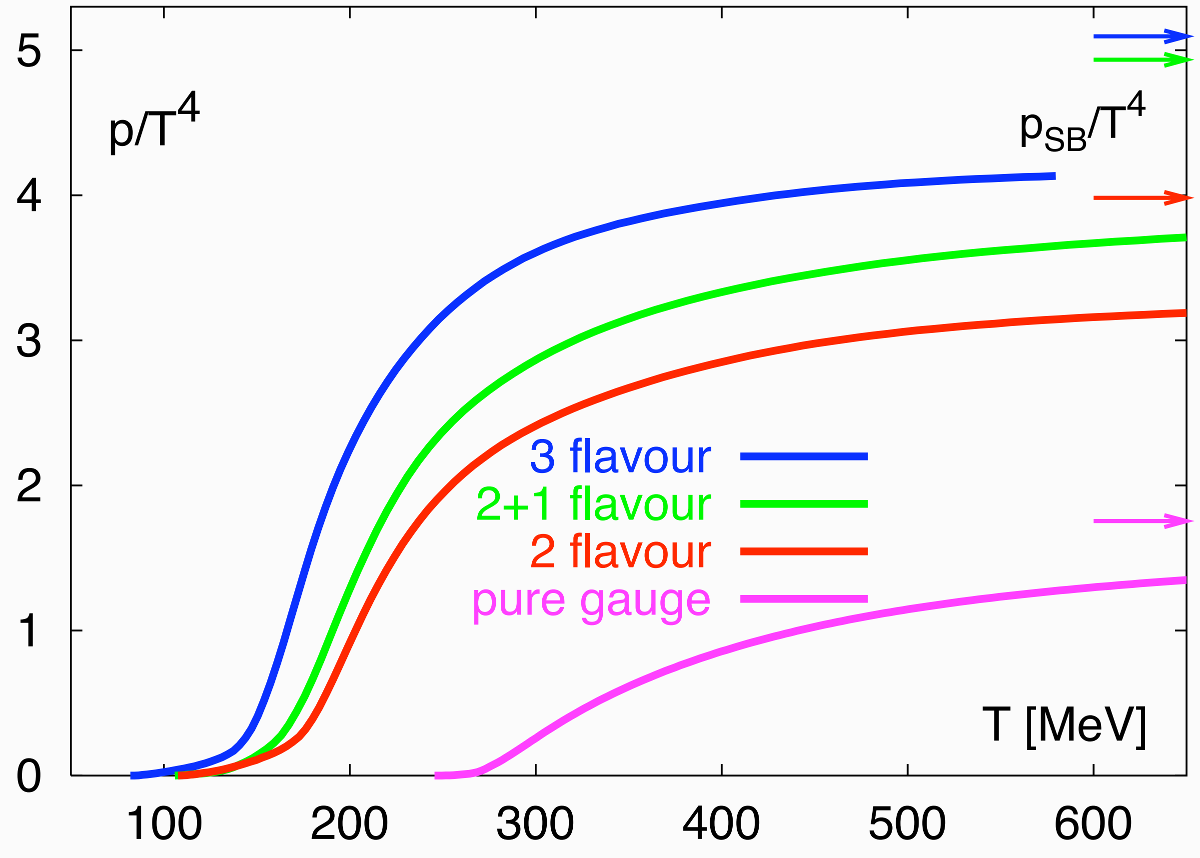
cut-off effects in the high temperature, ideal gas limit: momenta $\sim T \sim \frac{1}{a}$

$$\left.\frac{p}{T^4}\right|_{N\tau} = \left.\frac{p}{T^4}\right|_{\infty} + \frac{c}{N_\tau^2} + \mathcal{O}(N_\tau^{-4})$$ (staggered)

Numerical results on the equation of state

staggered p4-improved, $N_\tau = 4$

Bielefeld



compare with ideal gas:

$$\frac{\epsilon_{SB}}{T^4} = \frac{3p_{SB}}{T^4} = \begin{cases} 3\frac{\pi^2}{30} & , T < T_c \\ (16 + \frac{21}{2} N_f)\frac{\pi^2}{30} & , T > T_c \end{cases}$$

$T > T_c$: more degrees of freedom, but significant interaction!

➡ sQGP or `almost ideal' gas....?

Equation of state for physical quark masses

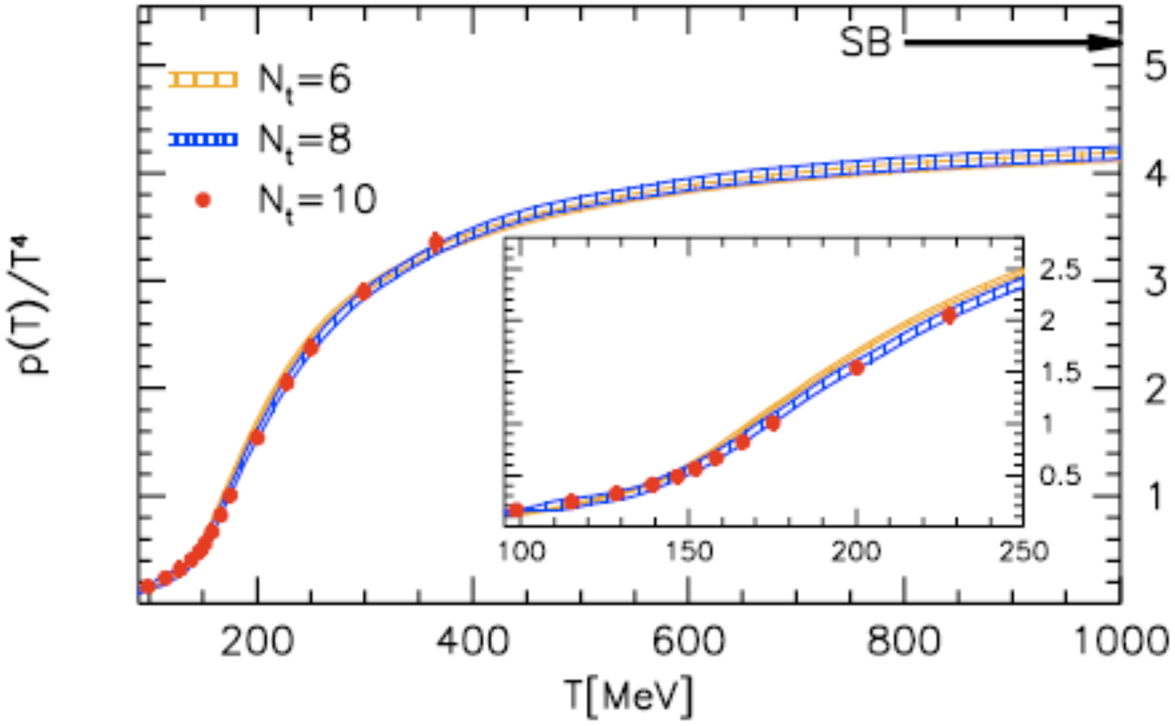


Figure 10: The pressure normalized by T^4 as a function of the temperature on $N_t = 6, 8$ and 1 lattices. The Stefan-Boltzmann limit $p_{SB}(T) \approx 5.209 \cdot T^4$ is indicated by an arrow. For our highest temperature $T = 1000$ MeV the pressure is almost 20% below this limit.

Hadron resonance gas model

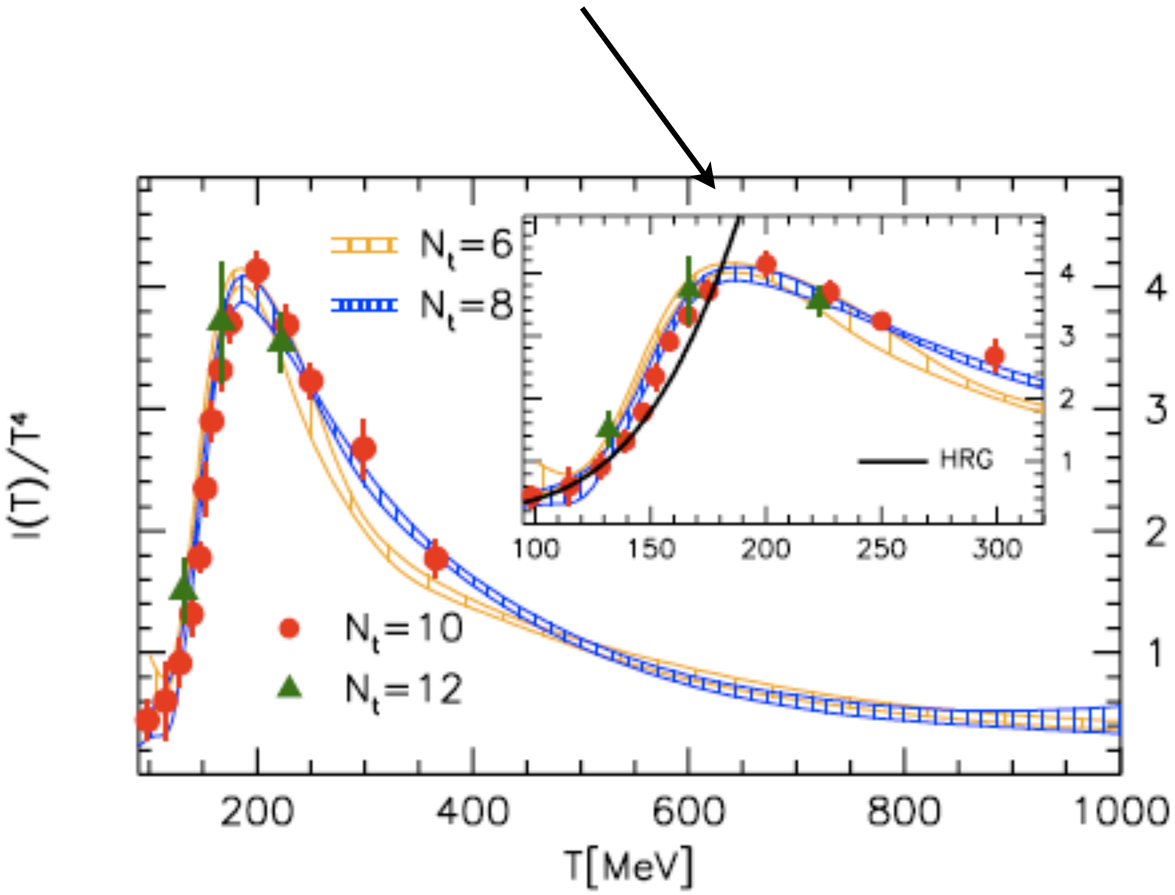


Figure 9: The trace anomaly $I = \epsilon - 3p$ normalized by T^4 as a function of the temperature $N_t = 6, 8, 10$ and 12 lattices.

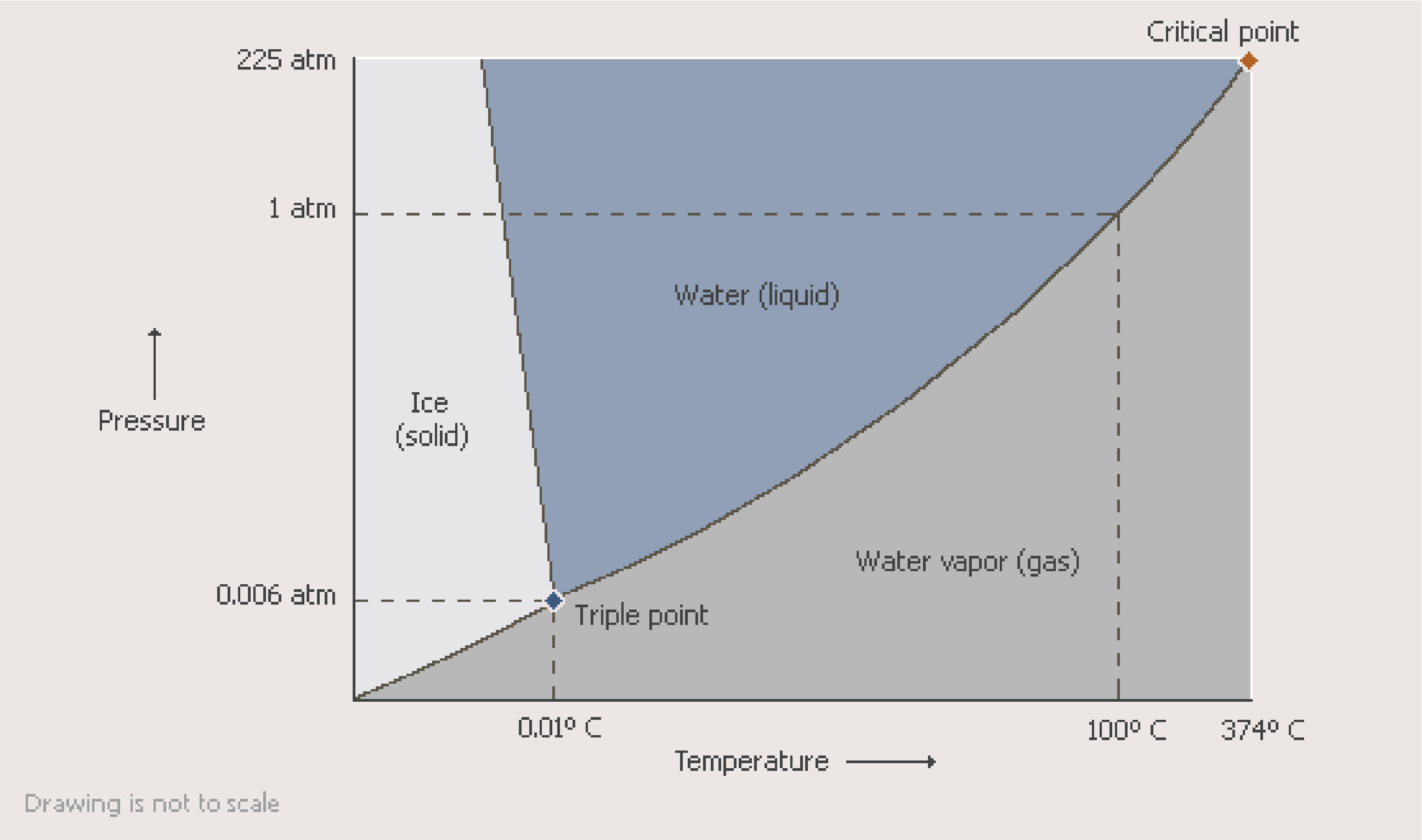
Budapest-Marseille-Wuppertal 10

Phase transitions and phase diagrams

- phase transitions: singularities in free energy F $\Rightarrow$zeroes in partition function Z

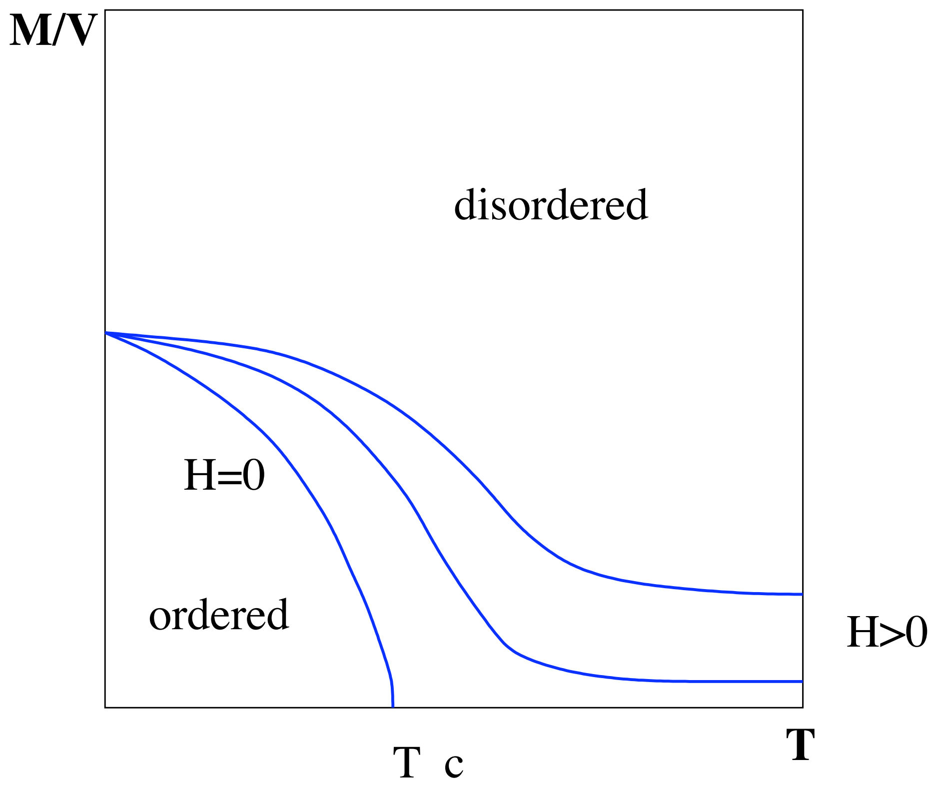
  only in thermodynamic limit! (Lee, Yang)
- first order: jump in order parameter, latent heat, phase coexistence
- second order: diverging correlation length
- crossover smooth, analytic transition

Example 1: water



order parameter: density ρ

Example 2: ferromagnetism



Ising model, Z(2) symmetry

spins with nearest neighbour interaction

$$E = -\sum_{ij} \epsilon_{i,j} s_i s_j - H \sum_i s_i$$

Universality of 2.o. phase transitions, critical exponents:

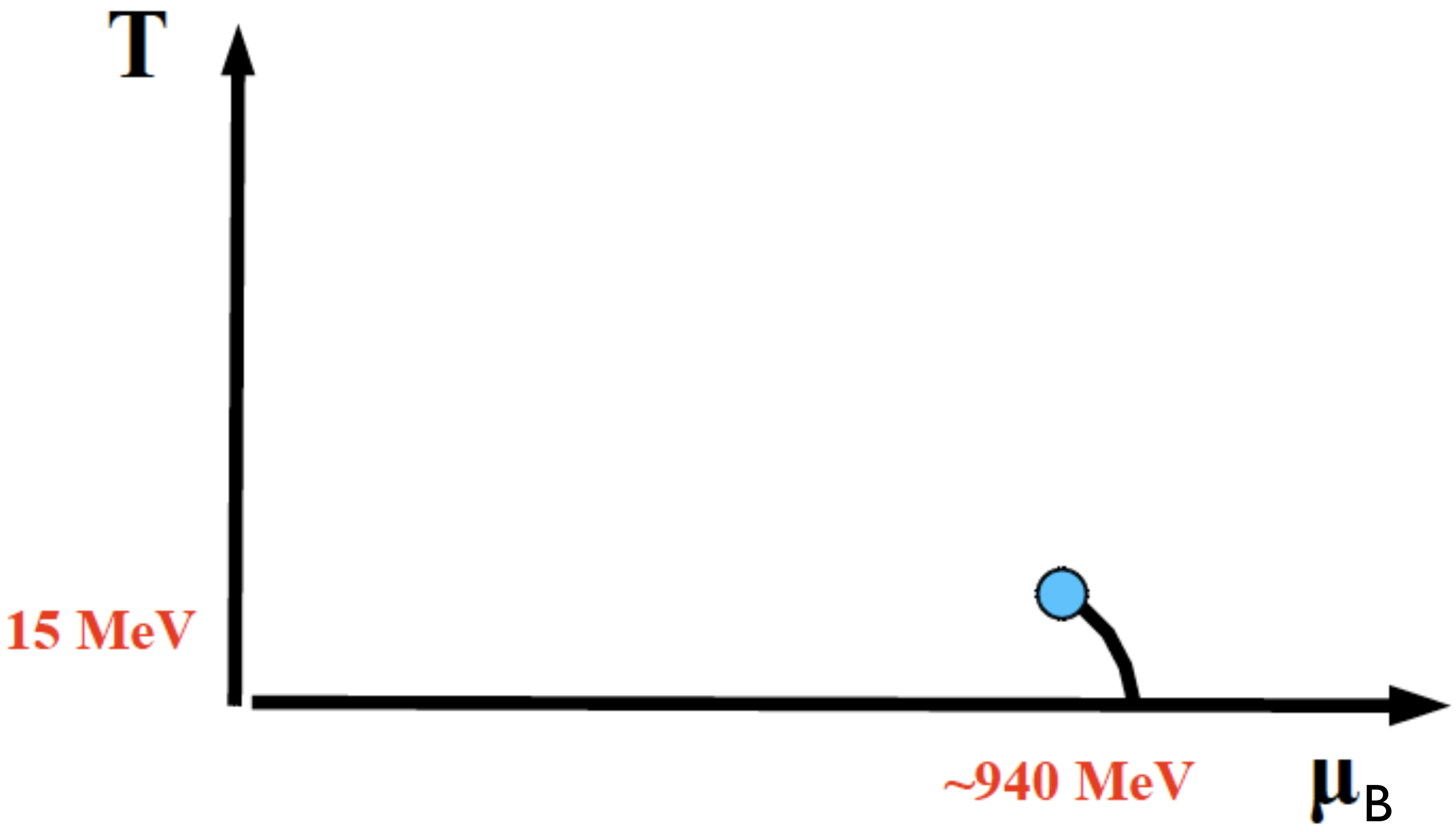
Correlation length diverges: microscopic dynamics unimportant, only global symmetries

specific heat $C \sim |t|^{-\alpha}$, magnetization $M \sim |t|^{\beta}, \ldots$ $t = \frac{T - T_c}{T_c}$

exponents the same for all systems within one universality class!

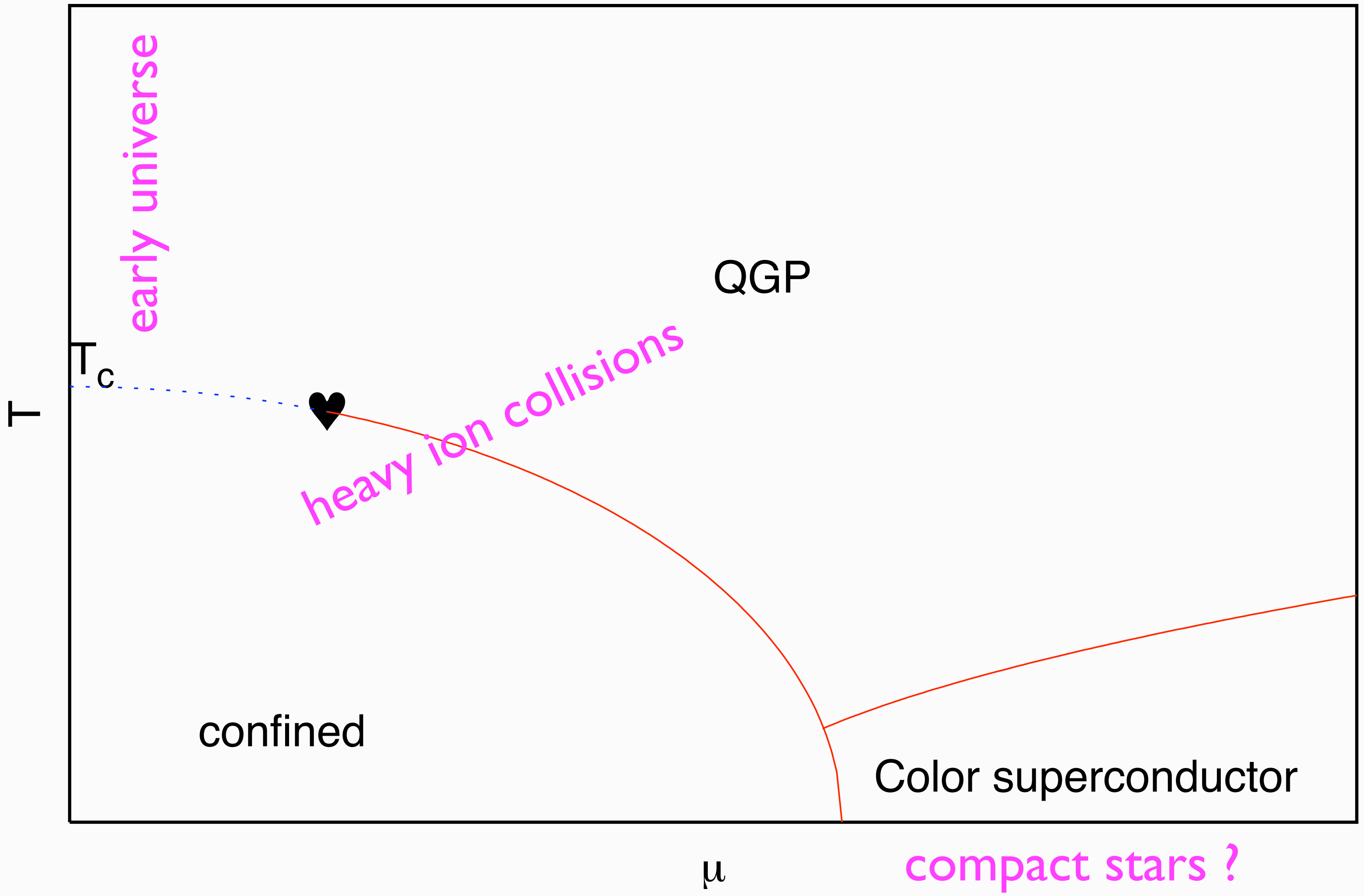
Critical endpoint of water shows 3d Ising universality, Z(2)!

The QCD phase diagram established by experiment:



Nuclear liquid gas transition, Z(2) end point

The conjectured QCD phase diagram



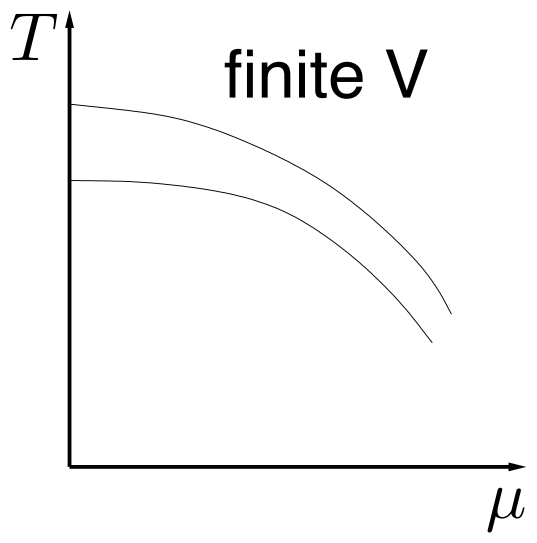
- No first principles calculations before 2001:   sign problem

Expectation based on models: NJL, NJL+Polyakov loop, linear sigma models,
random matrix models, ...

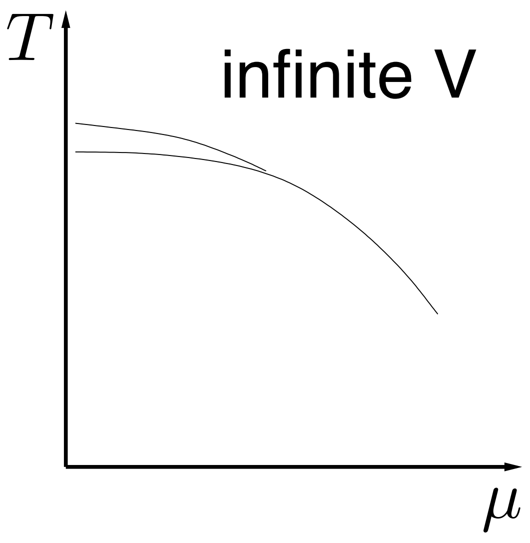
Approaching the thermodynamic limit

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

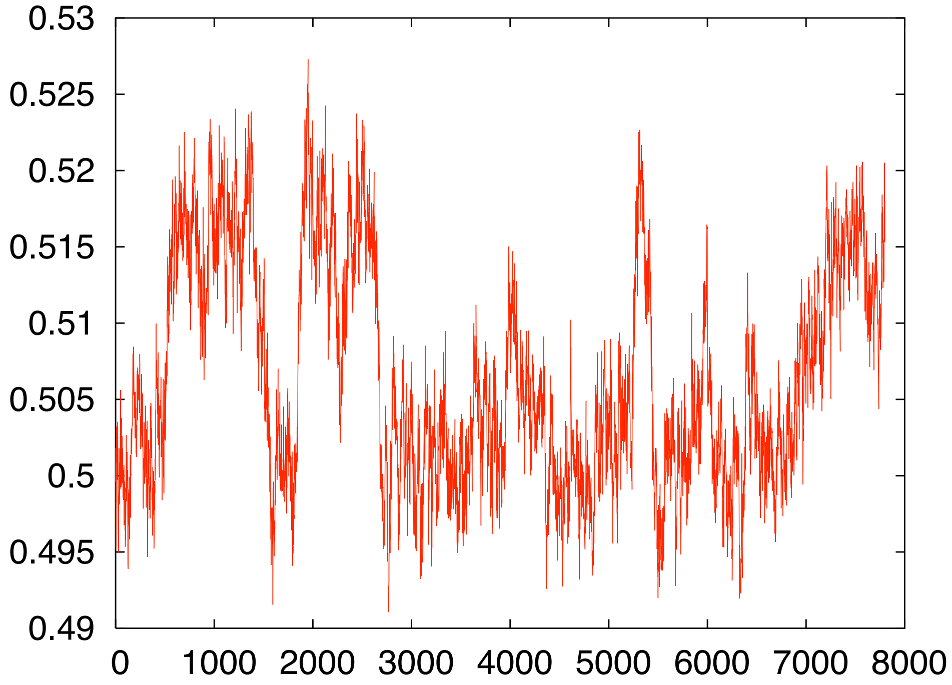


Critical line unique in thermodynamic limit!

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

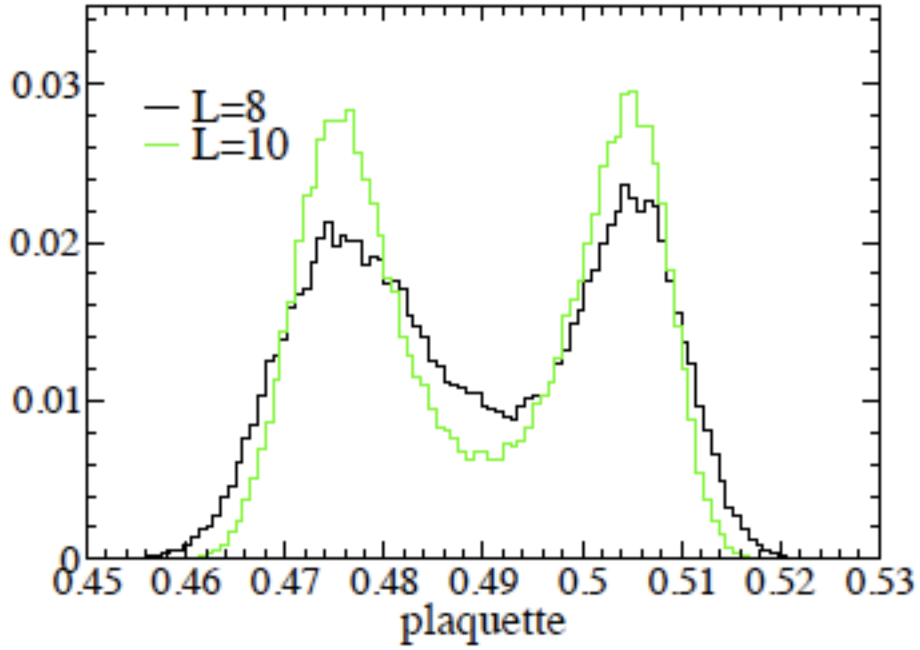
$\sigma = 1$	1st order
$\sigma < 1$	2nd order
$\sigma = 0$	crossover

Monte Carlo history, plaquette

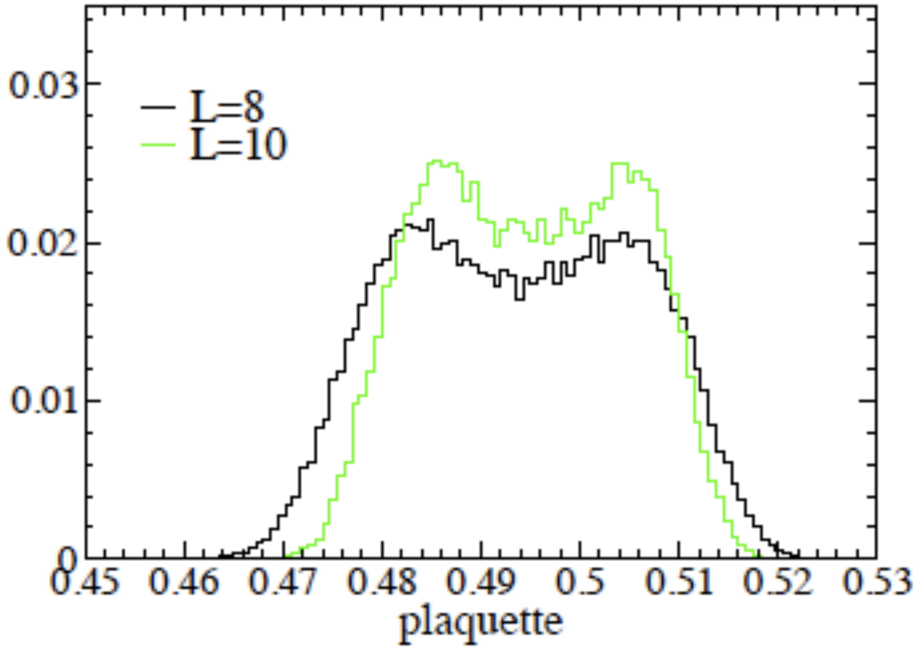


Distribution:

first-order



crossover

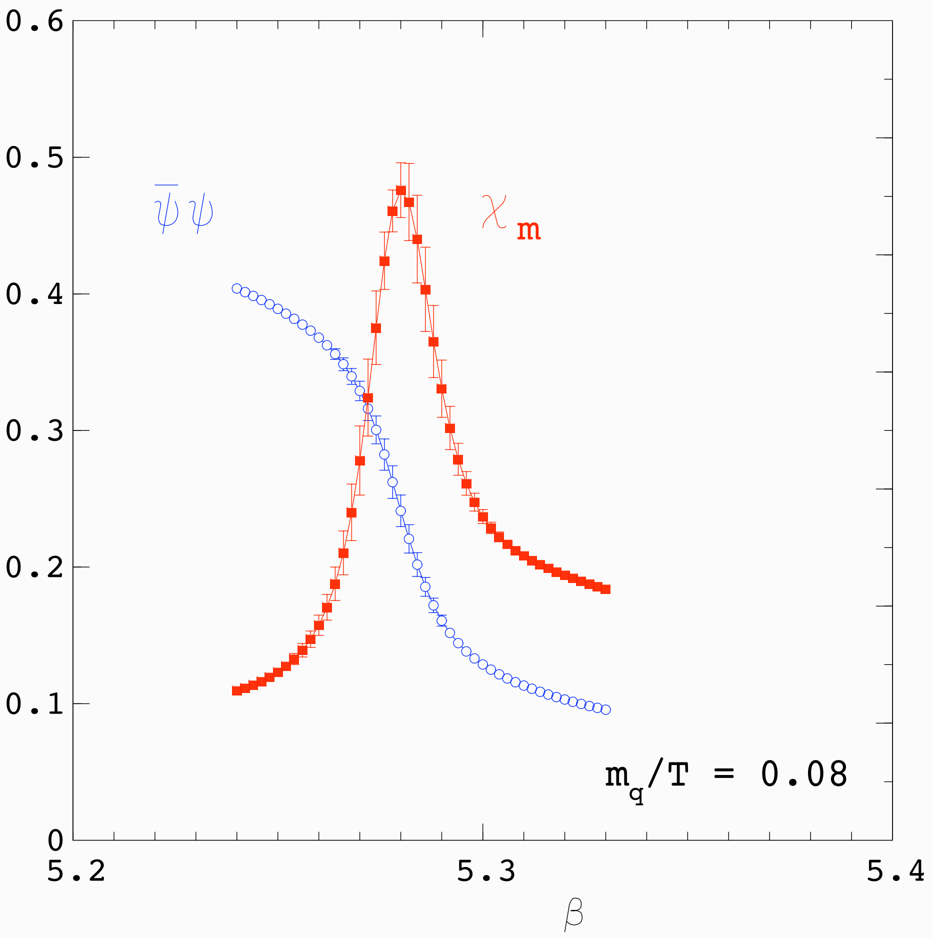


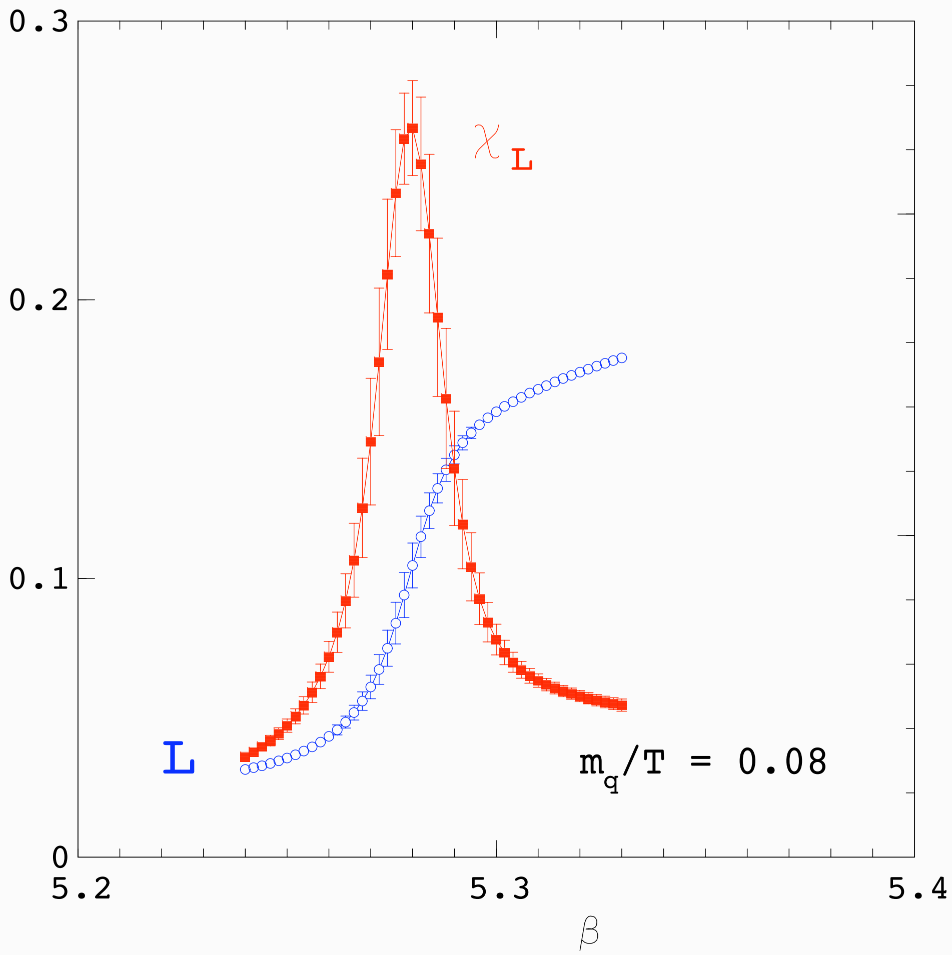
Finding the phase transition: the critical temperature

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

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

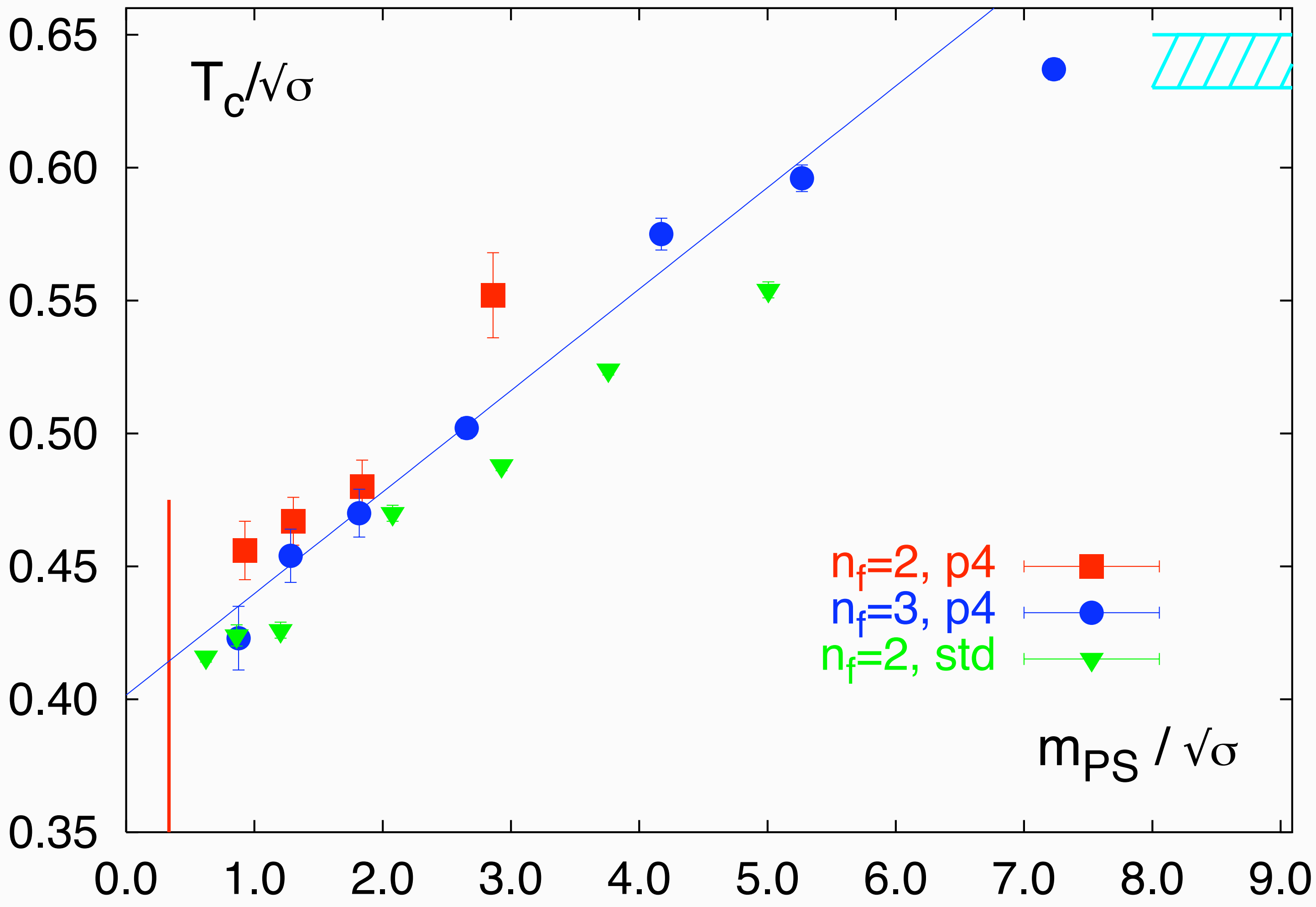
Quark mass dependence of the critical temperature

SU(3) pure gauge : $T_c/\sqrt{\sigma} = 0.637 \pm 0.005$

$T_c = (271 \pm 2)\ \mathrm{MeV}$

continuum extrapolated!

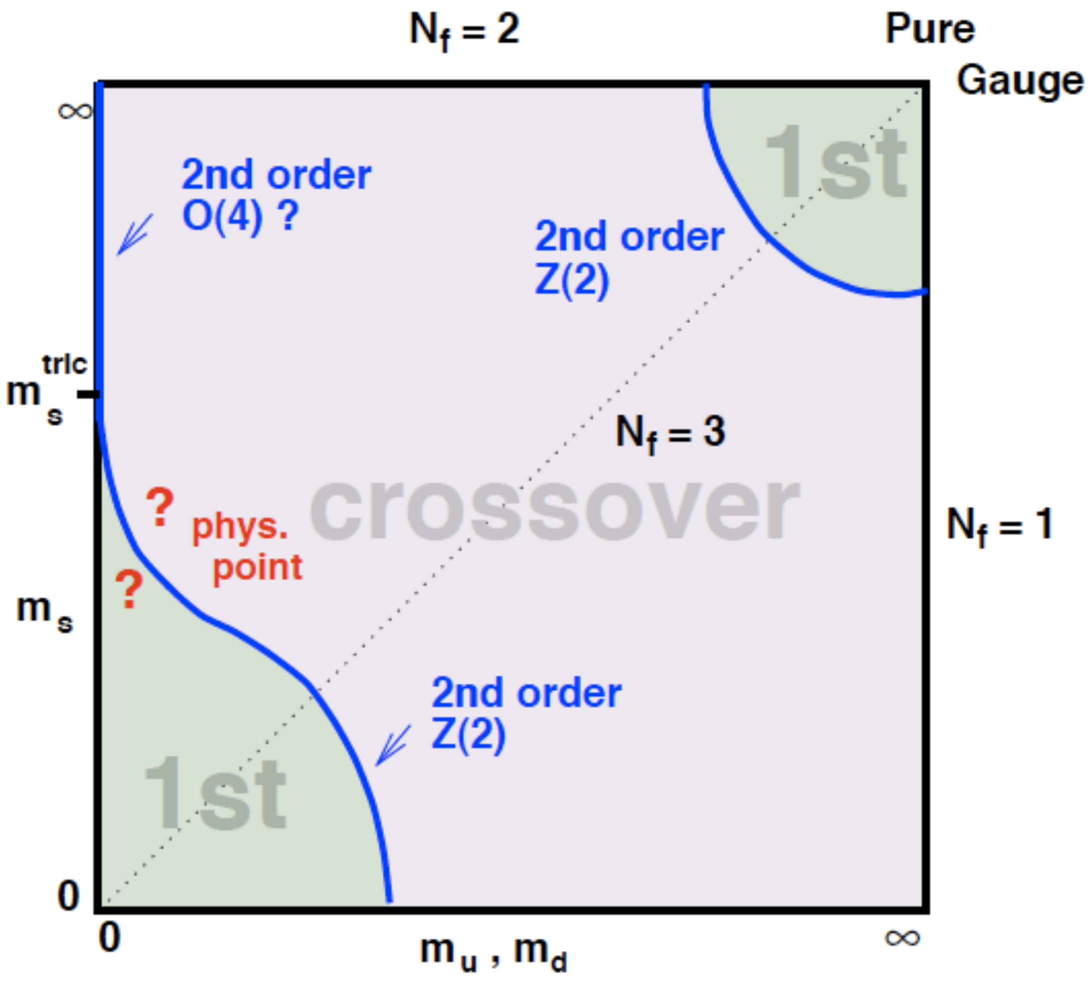
$N_t = 4, a \sim 0.3\mathrm{fm}$



Bielefeld

The order of the p.t., arbitrary quark masses $\mu = 0$

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



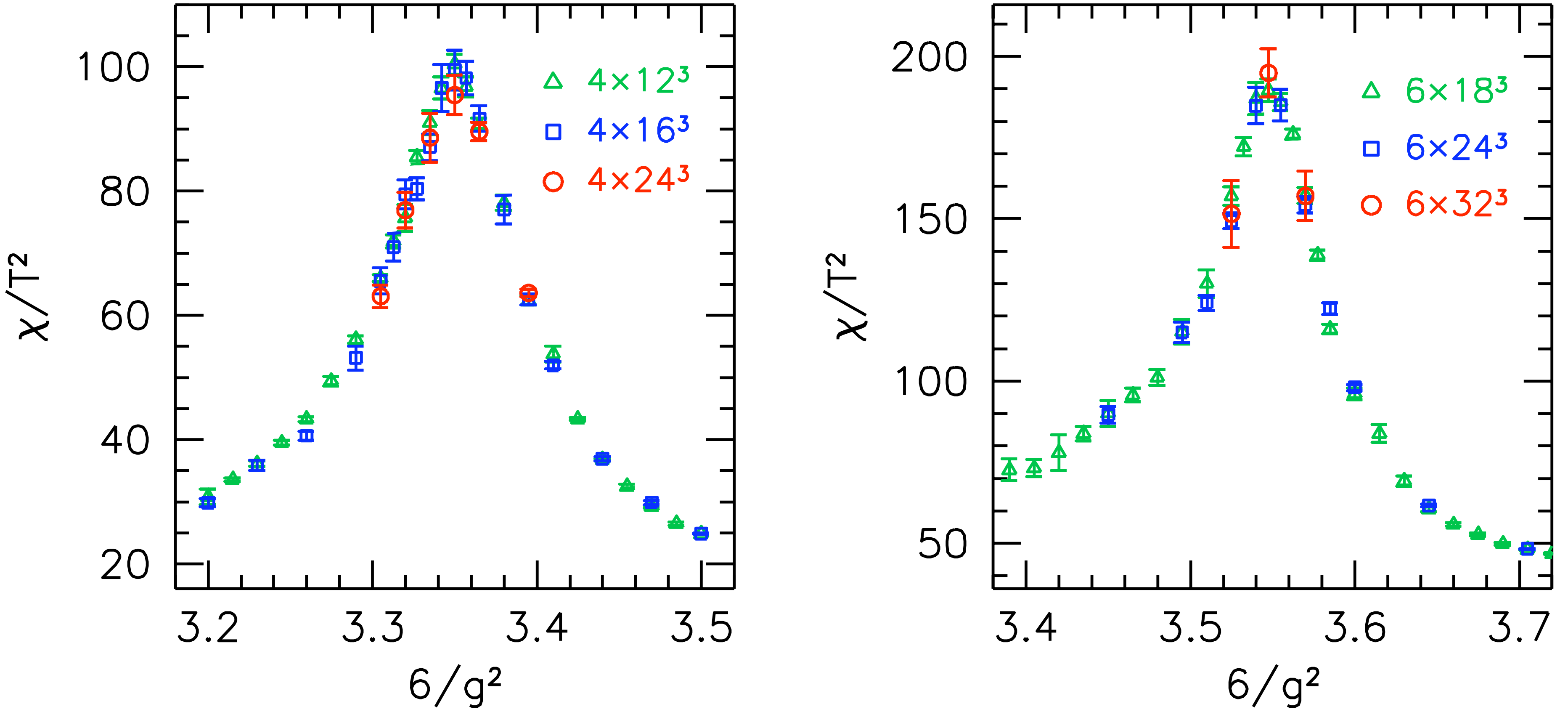
chiral p.t.
restoration of global

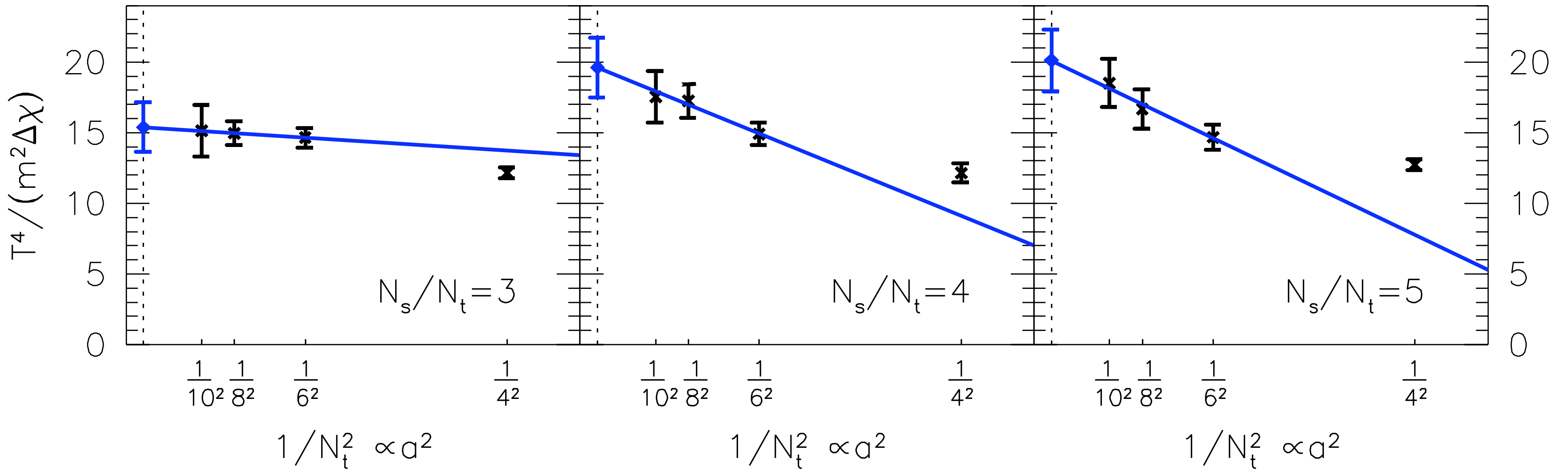
$$SU(2)_L \times SU(2)_R \times \underset{\substack{\uparrow \\ \text{anomalous}}}{U(1)_A}$$

The nature of the transition for phys. masses

Aoki et al. 06

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





The 'sign problem' is a phase problem

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

importance sampling requires
positive weights

Dirac operator: $\not{D}(\mu)^\dagger = \gamma_5 \not{D}(-\mu^*)\gamma_5$

$\Rightarrow \det(M)$ complex for SU(3), $\mu \neq 0$

$\Rightarrow$real positive for SU(2), $\mu = i\mu_i$

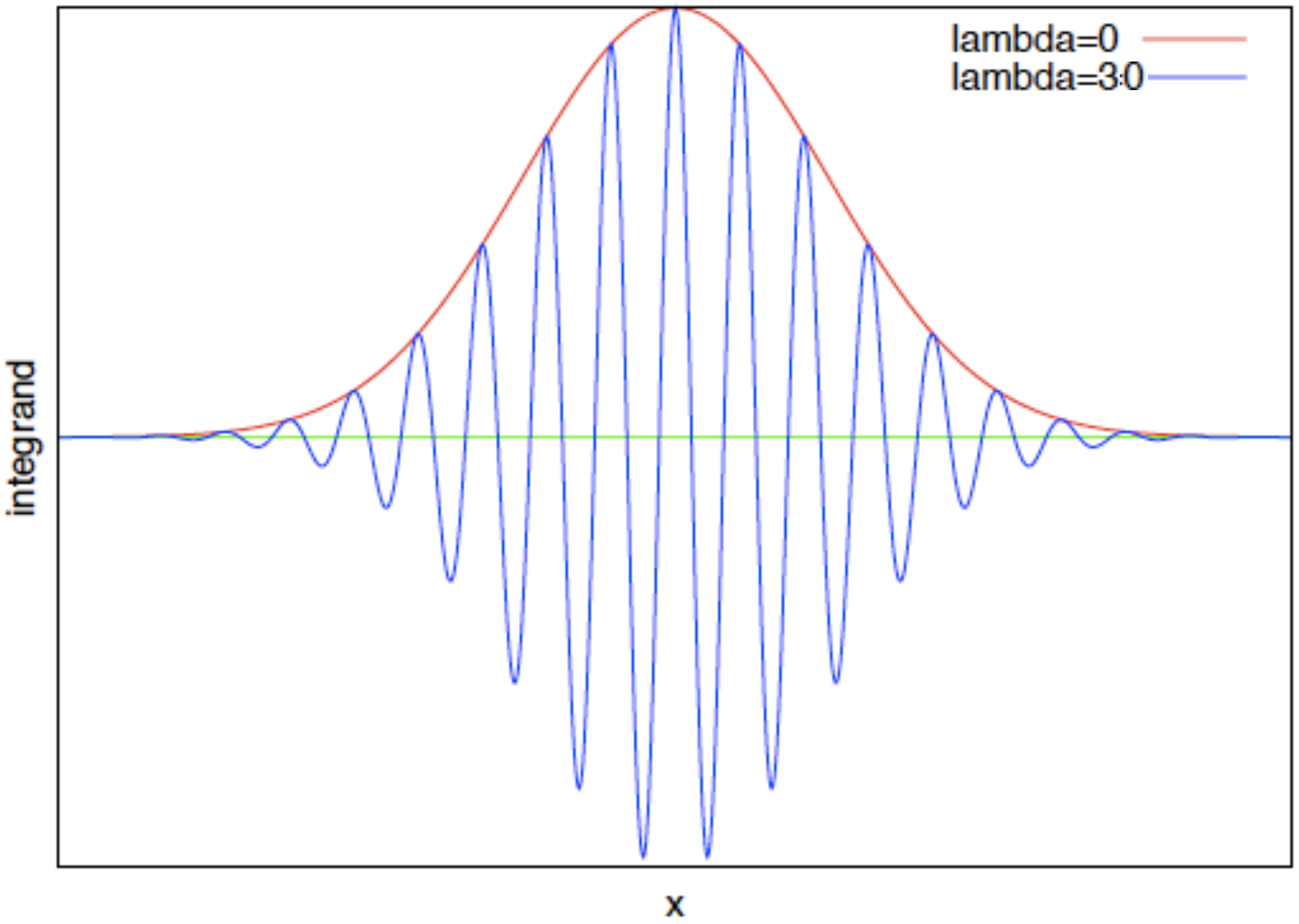
$\Rightarrow$real positive for $\mu_u = -\mu_d$

N.B.: all expectation values real, imaginary parts cancel,
but importance sampling config. by config. impossible!

Same problem in many condensed matter systems!

1 dim. illustration

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

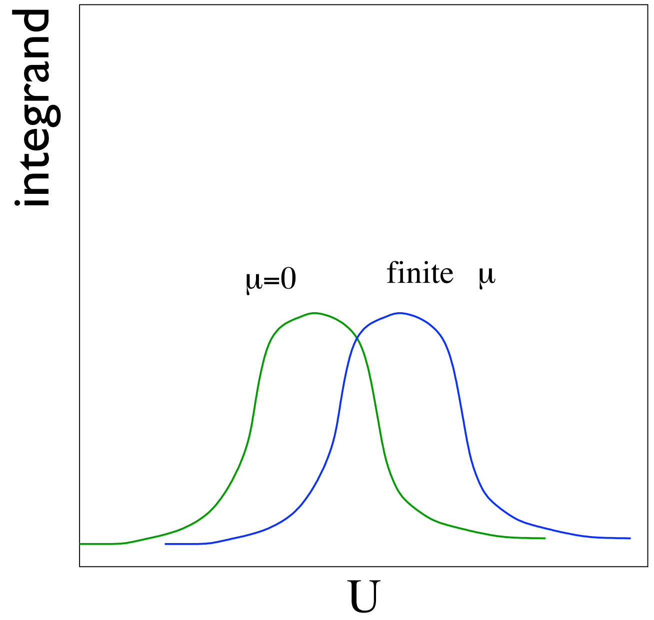


- $Z(\lambda)/Z(0) = \exp(-\lambda^2/4)$: exponential cancellations

$\rightarrow$ truncating deep in the tail at $x \sim \lambda$ gives $\mathcal{O}(100\%)$ error   Splittorff

"Every x is important" $\leftrightarrow$ How to sample?

Finite density: methods to evade the sign problem



- **Reweighting:** $$Z = \int DU \; \det M(0) \frac{\det M(\mu)}{\det M(0)} \, e^{-S_g}$$

  ~exp(V) statistics needed,
  overlap problem

  $\uparrow$ use for MC $\quad$ $\uparrow$ calculate

- **Taylor expansion:**

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

  coeffs. one by one,
  convergence?

- **Imaginary** $\mu = i\mu_i$ **:** no sign problem, fit by polynomial, then analytically continue

  $$\langle O \rangle(\mu_i) = \sum_{k=0}^{N} c_k \left(\frac{\mu_i}{\pi T}\right)^{2k}, \qquad \mu_i \rightarrow -i\mu$$

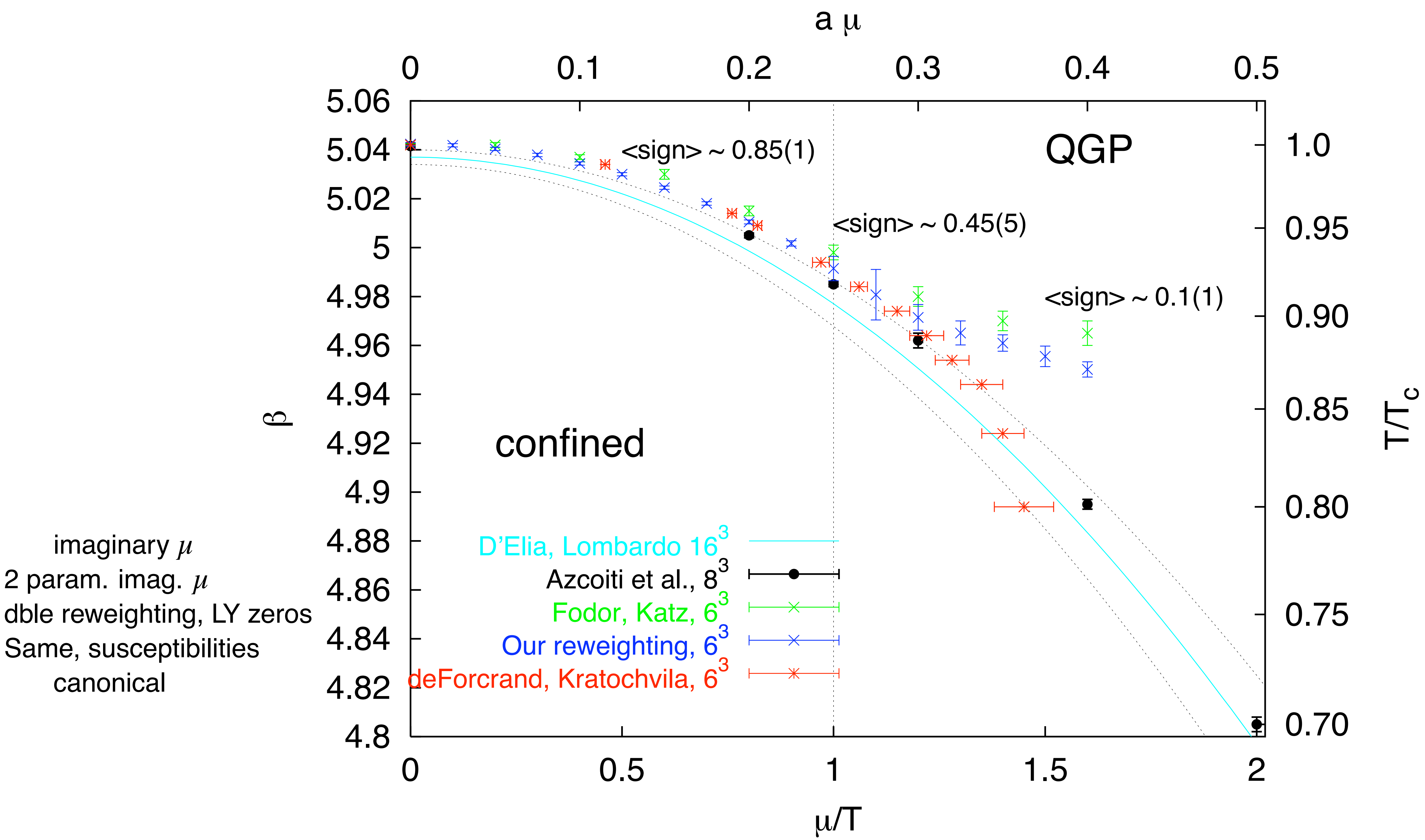
  requires convergence
  for anal. continuation

All require $\mu/T < 1$!

The good news: comparing $T_c(\mu)$

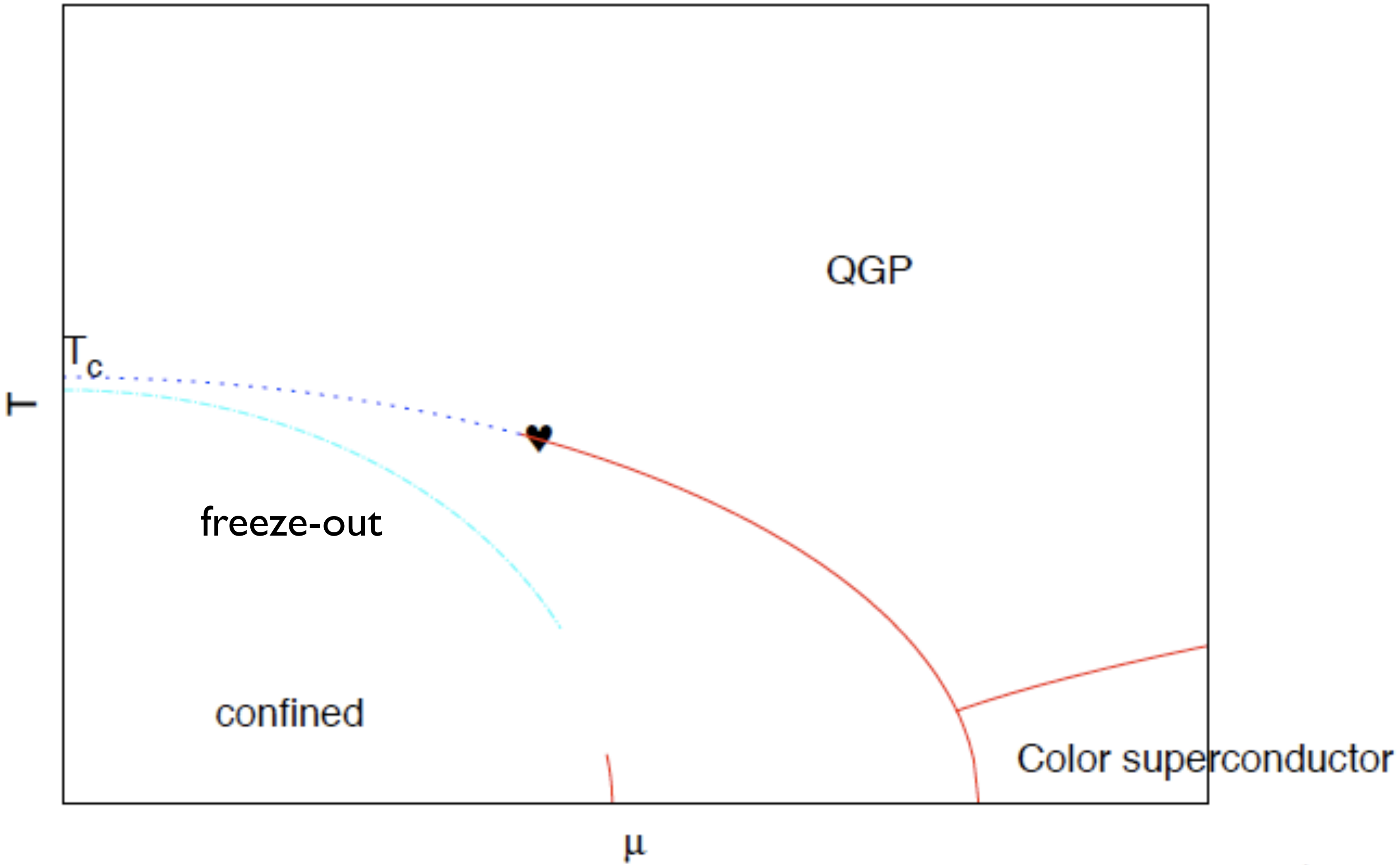
de Forcrand, Kratochvila 05

$N_t = 4, N_f = 4$; same actions (unimproved staggered), same mass



Agreement for $\mu/T \lesssim 1$

Comparison with freeze-out curve



$T_c(\mu)$ considerably flatter than **freeze-out** curve (factor ~ 3 in $\left.\frac{d^2T_c}{d\mu^2}\right|_{\mu=0}$)

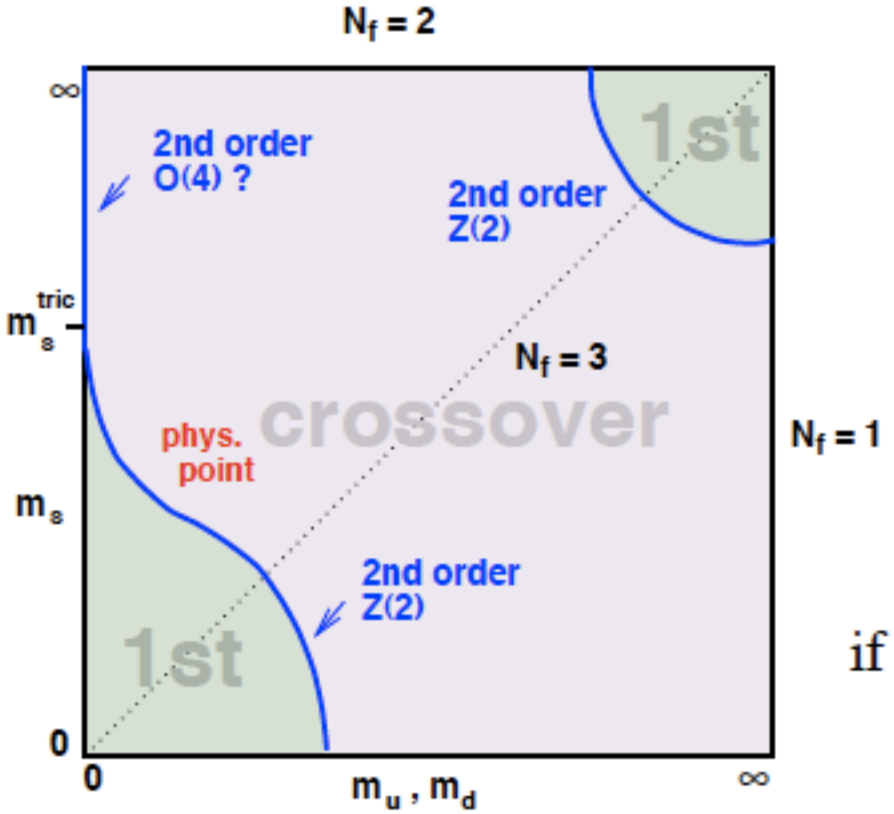
$$\frac{T_c(\mu)}{T_c(0)} = 1 - \kappa(N_f, m_q)\left(\frac{\mu}{T}\right)^2 + \ldots$$

$$\kappa^{(\chi_s/T^2)} = 0.0089(14)$$

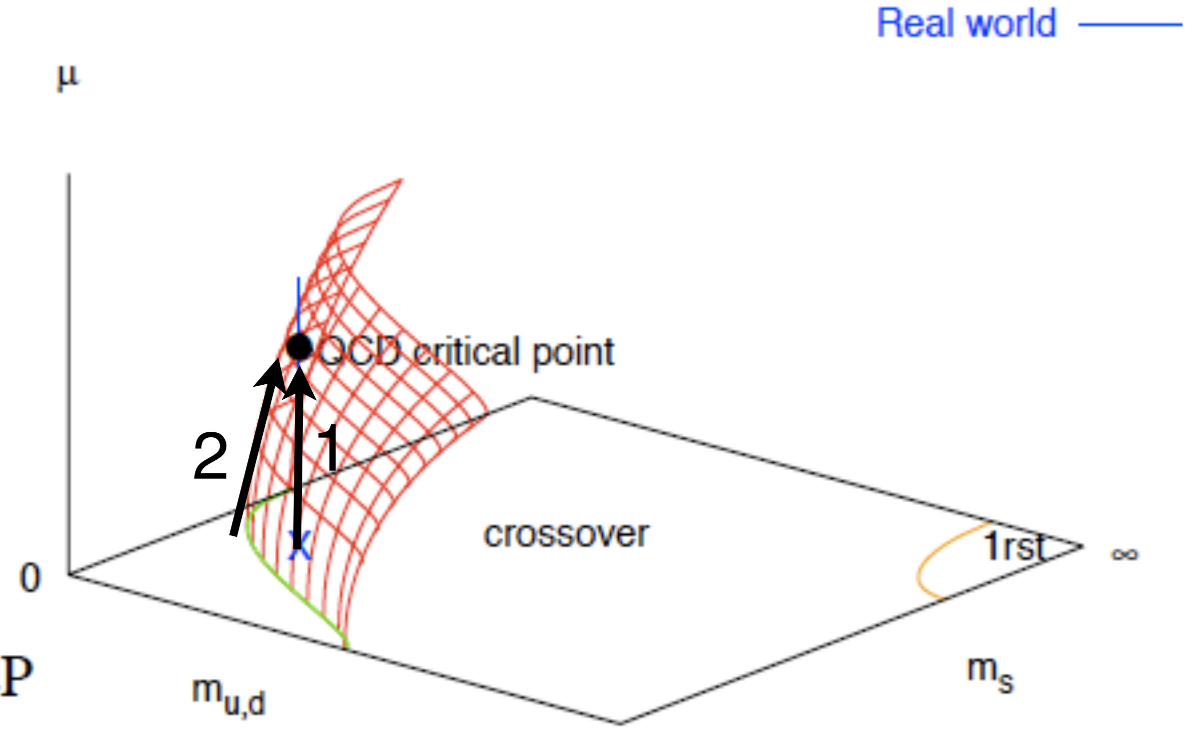
hotQCD 11 Endrödi et al. 11

$$\kappa^{(\bar\psi\psi_r)} = 0.0066(20)$$

Much harder: is there a QCD critical point?



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



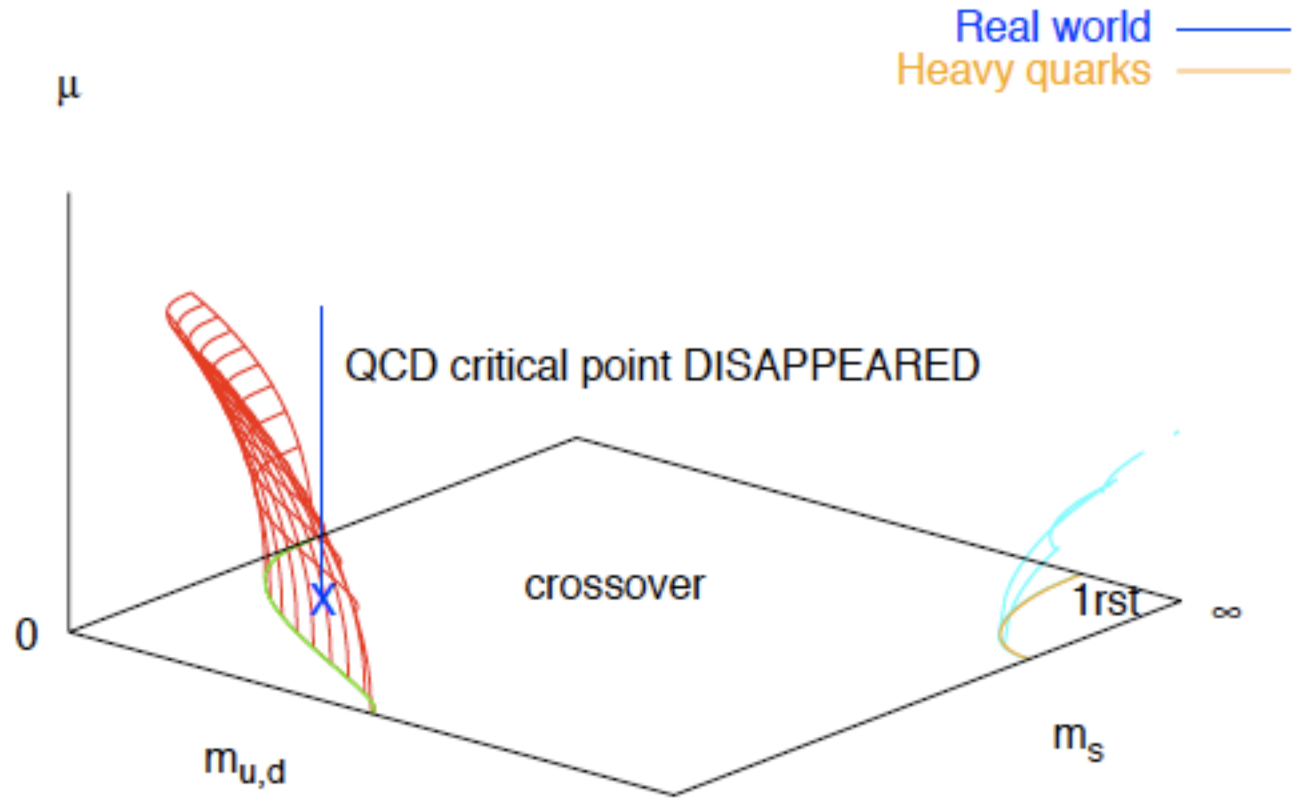
Two strategies:

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

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

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

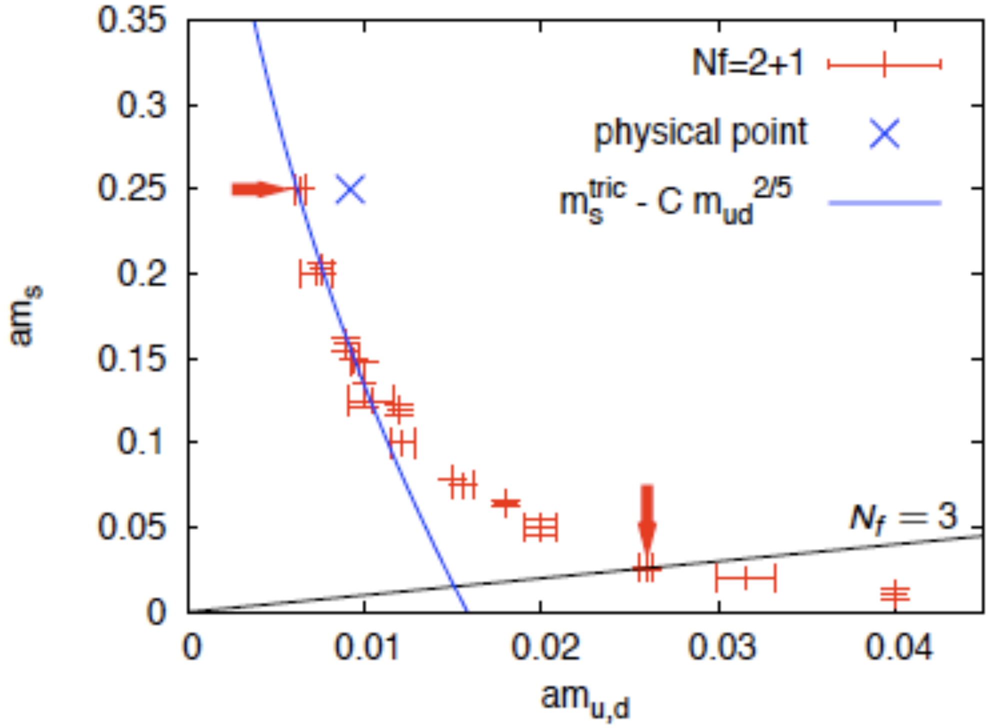
On coarse lattice exotic scenario: no chiral critical point at small density



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

-Heavy quarks	Fromm, Langelage, Lottini, O.P. 11
-Light quarks with finite isospin density	Kogut, Sinclair 07
-Electroweak phase transition with finite lepton density	Gynther 03

Curvature of the chiral critical surface



$N_f = 3$

$N_f = 2+1,\ m_s = m_s^{\rm phys}$

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

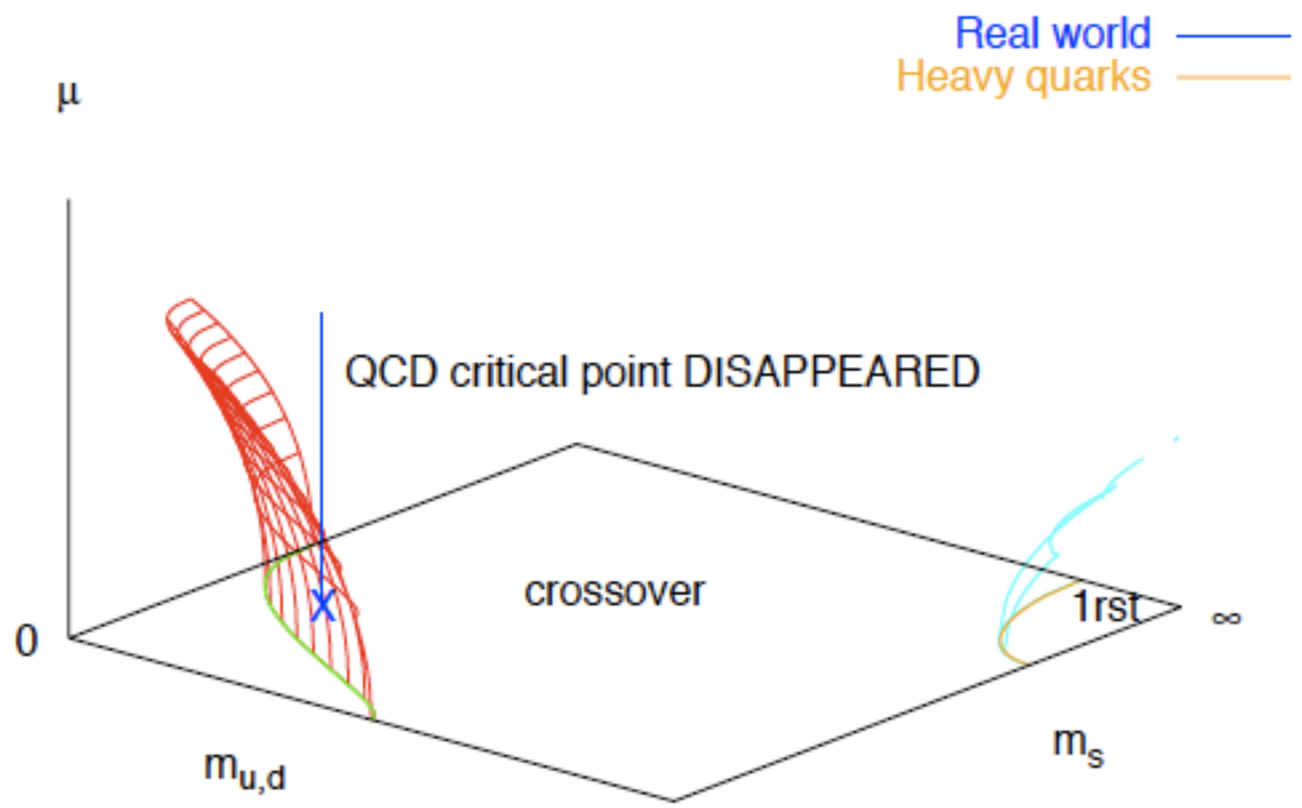
$$\frac{m_c(\mu)}{m_c(0)} = 1 - 3.3(3)\left(\frac{\mu}{\pi T}\right)^2 \underbrace{- 47(20)\left(\frac{\mu}{\pi T}\right)^4}_{\text{8th derivative of P}} - \ldots$$

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

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

de Forcrand, O.P. 08,09

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



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References and Sources

- O.Philipsen, "Introduction to Quantum Field Theory"
- M.Walzl and G.Münster, "Introduction to Lattice Gauge theory"
- I have copied smaller and larger bits and pieces from publicly available lecture slides of:
  D. Gütersloh, F. Krauss, J.Heitger, U.Husemann, H.-J.Pirner and H.-C. Schultz-Coulon, H.Wittig