QCD thermodynamics on the lattice: Continuum limit with physical quark masses

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results of the Wuppertal-Budapest group:
Nature, 443 '06 675, JHEP 1009 '10 73, 1011 '10 77, 1102.1356

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SFB
TR55

Outline

User's guide to lattice QCD results

- Full lattice results have three main ingredients

1. (tech.) technically correct (users can not really prove)
2. (m_q) physical quark masses: m_s/m_{ud} ≈28 (and m_c/m_s ≈12)
3. (cont.) continuum extrapolated: at least 3 points with $c \cdot a^n$

only a few full results (spectrum, m_q, nature, T_c, EoS, curvature)

ad 1: obvious condition, otherwise forget it
ad 2: difficult (CPU demanding) to reach the physical u/d mass
BUT even with non-physical quark masses: meaningful questions
e.g. in a world with M_π=M_ρ what would be M_N/M_π
these results are universal, do not depend on the action/technique
ad 3: non-continuum results contain lattice artefacts
(they are good for methodological studies, they just "inform" you)

User's guide to lattice QCD results

- troubleshooting

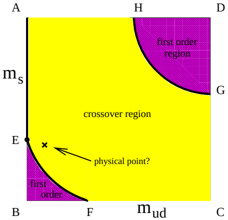
i. clarify if all three conditions were satisfied

ii. if yes: OK with any scale setting (error estimates can be tricky)

iii. if out of the above three ingredients one was missing:
if (1: tech.) was missing: forget it
if (2: m_q) was missing: reliable answer to a well defined case
if (3: cont.) was missing: ask to carry out the continuum limit
show the scaling $c \cdot a^n$ in the scaling regime
n is known from theory c is provided by the simulations
that is why we need at least 3 different lattice spacings

iv. if out of the above three ingredients two were missing: well ...

Phase diagram and its uncertainties



physical quark masses: important for the nature of the transition

n_f=2+1 theory with m_q=0 or ∞ gives a first order transition

intermediate quark masses: we have an analytic cross over (no χPT)

F.Karsch et al., Nucl.Phys.Proc. 129 ('04) 614; G.Endrodi et al. PoS Lat'07 182('07);

de Forcrand, S. Kim, O. Philipsen, Lat'07 178('07)

continuum limit is important for the order of the transition:

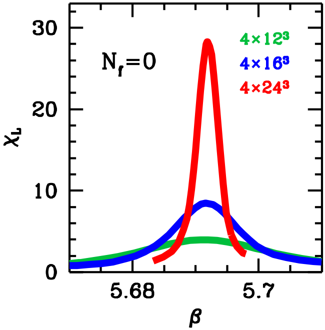
n_f=3 case (standard action, N_t=4): critical $m_{ps}\approx$300 MeV

different discretization error (p4 action, N_t=4): critical $m_{ps}\approx$70 MeV

the physical pseudoscalar mass is just between these two values

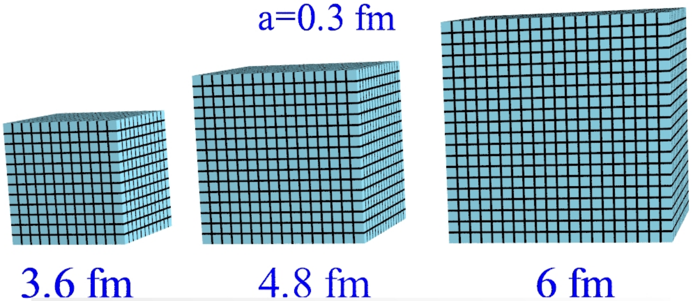
Finite size scaling in the quenched theory

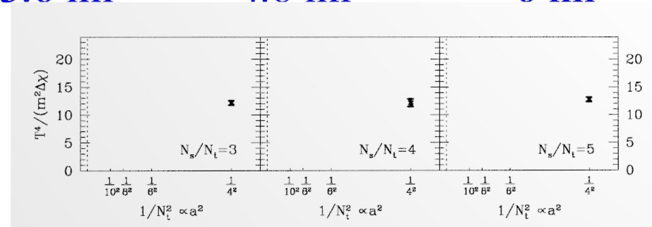
look at the susceptibility of the Polyakov-line
first order transition (Binder) $\Longrightarrow$ peak width $\propto$ 1/V, peak height $\propto$ V



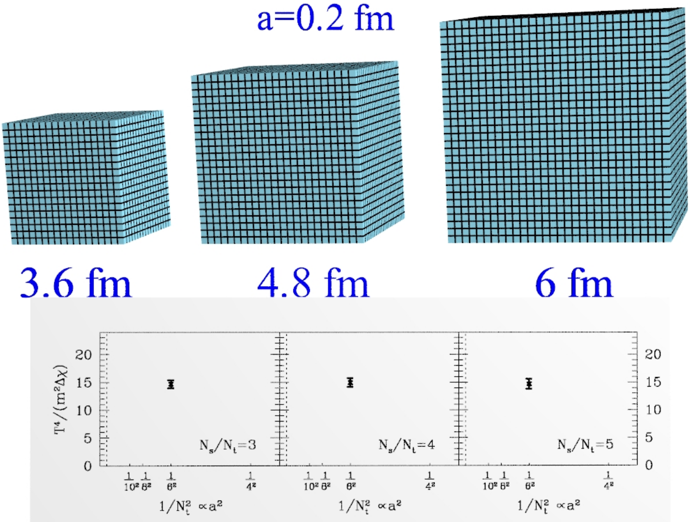
finite size scaling shows: the transition is of first order

Approaching the continuum limuit

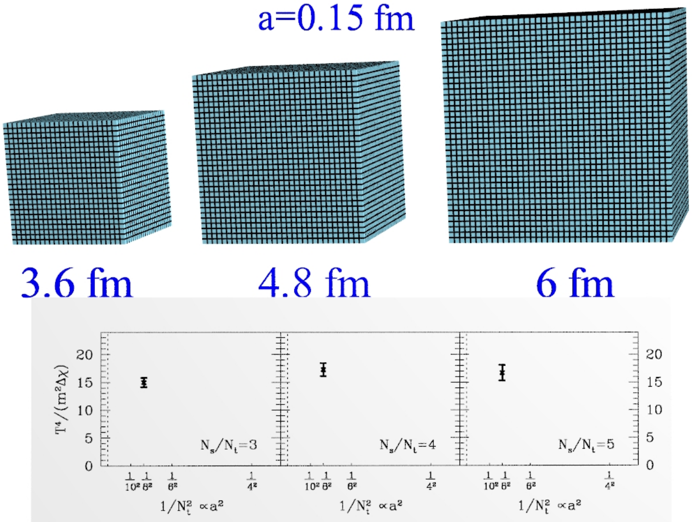




Approaching the continuum limuit

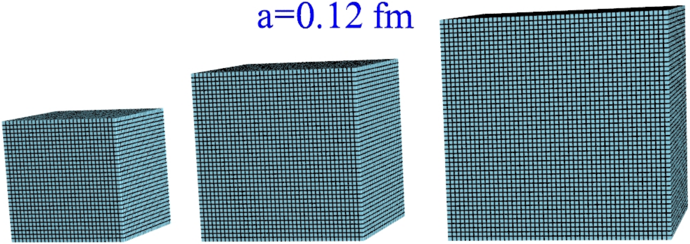


Approaching the continuum limuit

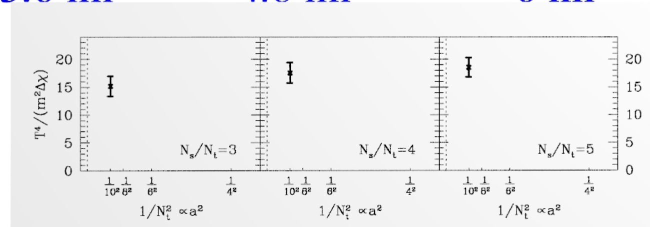


Approaching the continuum limuit

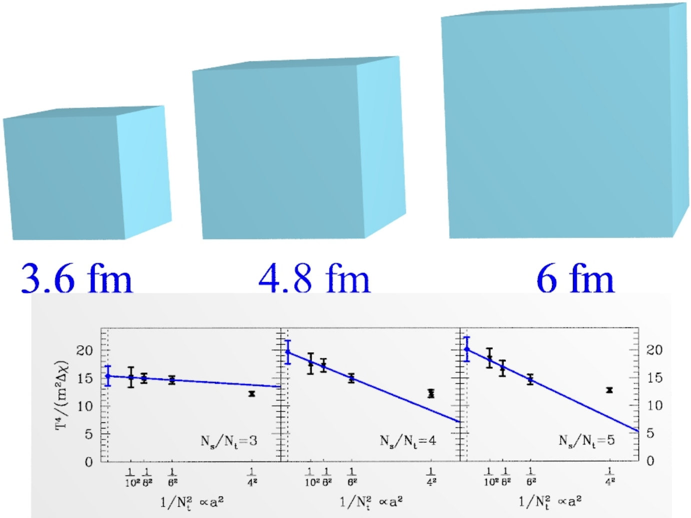
a=0.12 fm



3.6 fm 4.8 fm 6 fm



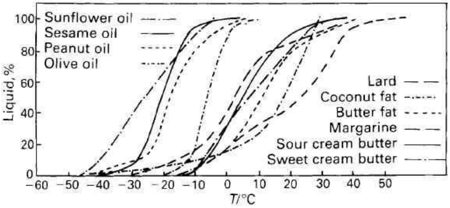
Approaching the continuum limuit

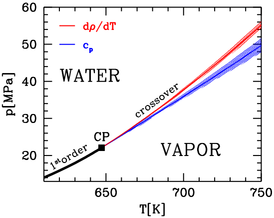


The nature of the QCD transition

Y.Aoki, G.Endrodi, Z.Fodor, S.D.Katz, K.K.Szabo, Nature, 443 (2006) 675

analytic transition (cross-over) $\Rightarrow$ it has no unique T_c:
examples: melting of butter (not ice) & water-steam transition





above the critical point c_p and $d\rho/dT$ give different T_cs.
QCD: chiral & quark number susceptibilities or Polyakov loop
they result in different T_c values $\Rightarrow$ physical difference

Literature: discrepancies between T_c

Bielefeld-Brookhaven-Riken-Columbia Collaboration:

M. Cheng et.al, Phys. Rev. D74 (2006) 054507

T_c from $\chi_{\bar{\psi}\psi}$ and Polyakov loop, from both quantities:

T_c=192(7)(4) MeV

Bielefeld-Brookhaven-Riken-Columbia merged with MILC: 'hotQCD'

Wuppertal-Budapest group: WB

Y. Aoki, Z. Fodor, S.D. Katz, K.K. Szabo, Phys. Lett. B. 643 (2006) 46

chiral susceptibility: T_c=151(3)(3) MeV
Polyakov and strange susceptibility: T_c=175(2)(4) MeV

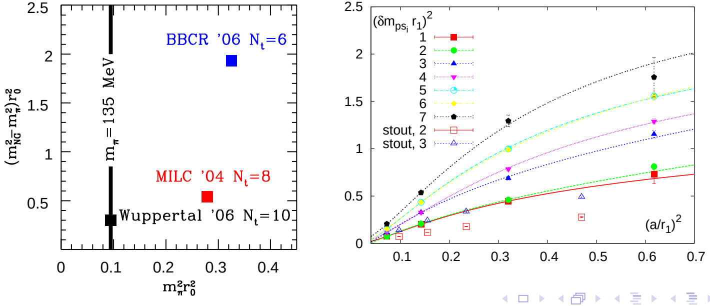
'chiral T_c': ≈40 MeV; 'confinement T_c': ≈15 MeV difference

both groups give continuum extrapolated results with physical m_π

Chiral symmetry breaking and pions

transition temperature for remnant of the chiral transition:
balance between the f's of the chirally broken & symmetric sectors
chiral symmetry breaking: 3 pions are the pseudo-Goldstone bosons

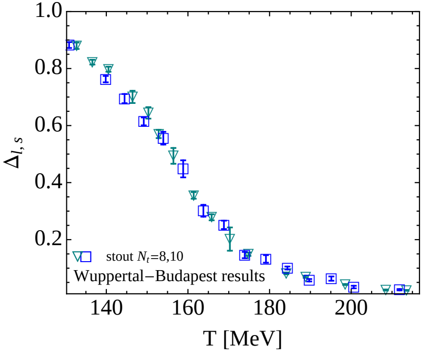
staggered QCD: 1 ($\frac{3}{16}$) pseudo-Goldstone instead of 3 (taste violation)
staggered lattice artefact $\Rightarrow$ disappears in the continuum limit
WB: stout-smeared improvement is designed to reduce this artefact



progress in the transition temperature

Wuppertal-Budapest: physical quark masses (m_s/m_{ud} ≈28)
gauge configs: N_t=8,10 in 2006 ⇒ N_t=12 in 2009 ⇒ N_t=16 in 2010

hotQCD 2009: realistic quark masses (m_s/m_{ud} =10)
hotQCD 2010: preliminary: physical quark masses (m_s/m_{ud} =20)



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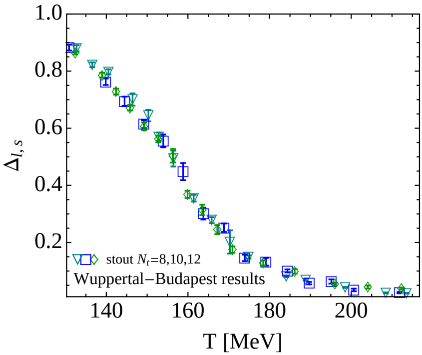

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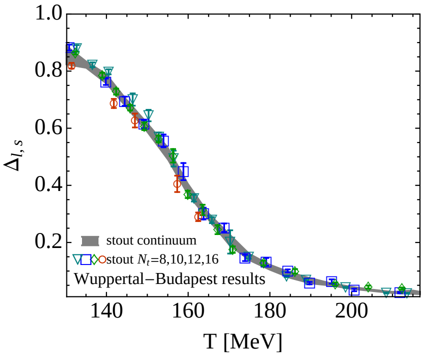

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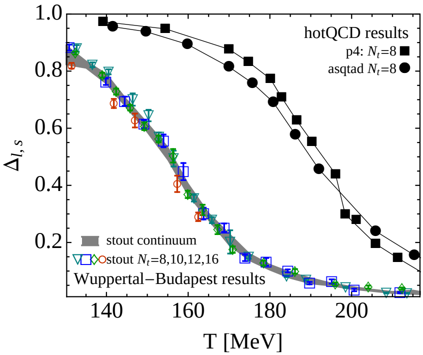

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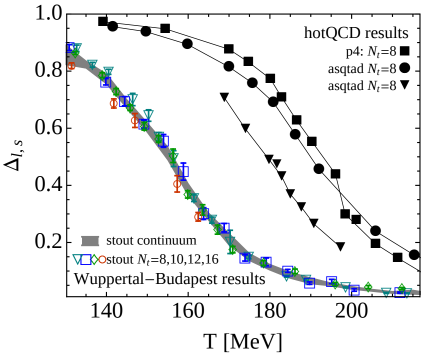

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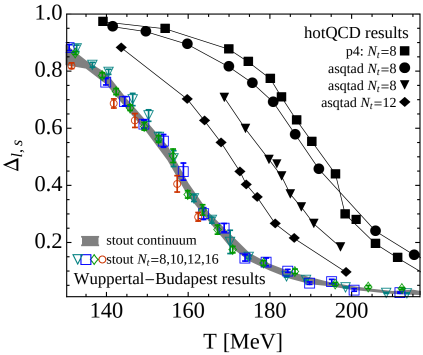

progress in transition temperature

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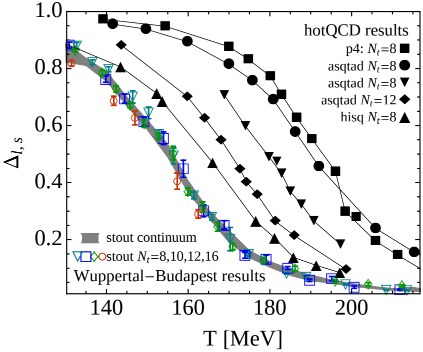
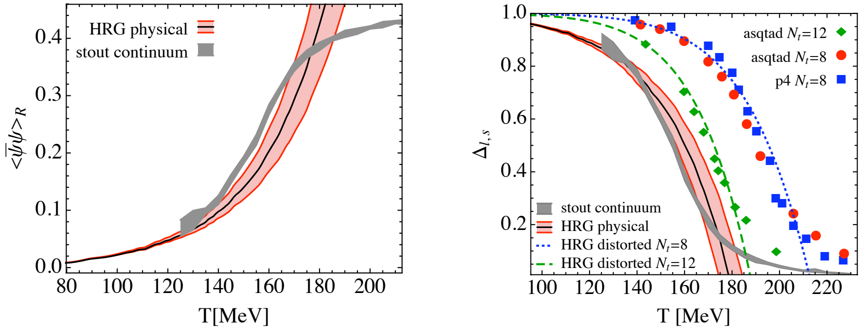


temperature dependence of the chiral condensate



Wuppertal-Budapest: good agreement with the physical HRG

Borsanyi, Fodor, Hoelbling, Katz, Krieg, Ratti, Szabo, JHEP 1009 (2010) 073

hotQCD: agreement only with the distorted spectrum
though their results are gradually getting closer to ours

Equation of state: integral method

J. Engels et al., Phys. Lett. B252 (1990) 625

on the lattice the dimensionless pressure is given by

$$p^{\rm lat}(\beta, m_q) = (N_t N_s^3)^{-1} \log \mathcal{Z}(\beta, m_q)$$

not accessible using conventional algorithms, only its derivatives

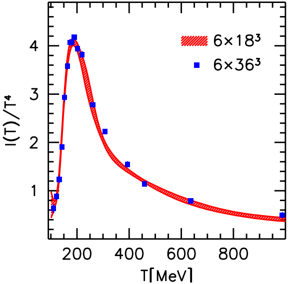
$$p^{\rm lat}(\beta, m_q) - p^{\rm lat}(\beta^0, m_q^0) = (N_t N_s^3)^{-1} \int_{(\beta^0, m_q^0)}^{(\beta, m_q)} \left(d\beta \frac{\partial \log \mathcal{Z}}{\partial \beta} + dm_q \frac{\partial \log \mathcal{Z}}{\partial m_q} \right)$$

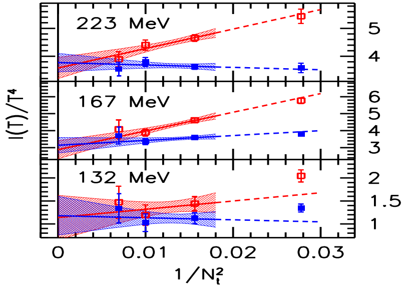
first term: gauge action & second term: chiral condensate

the pressure has to be renormalized: subtraction at T=0 (or T>0)

T≠0 simulations can't go below T≈100 MeV (lattice spacing is large)
physical HRG gives here 5% contribution of SB ⇒
path of M_π=720 MeV ⇒ distorted HRG no contribution at T=100 MeV

Finite volume and discretization effects



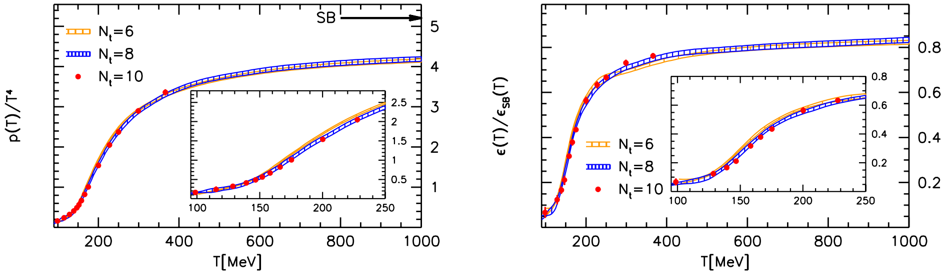


finite V: N_s/N_t=3 and 6 (8 times larger volume): no sizable difference

finite a: improvement program of lattice QCD (action & observables)
tree-level improvement for p (thermodynamic relations fix the others)
trace anomaly for three T-s: high T, transition T, low T
continuum limit N_t=6,8,10,12: same with or without improvement

improvement strongly reduces cutoff effects: slope $\approx$0 (1-2σ level)

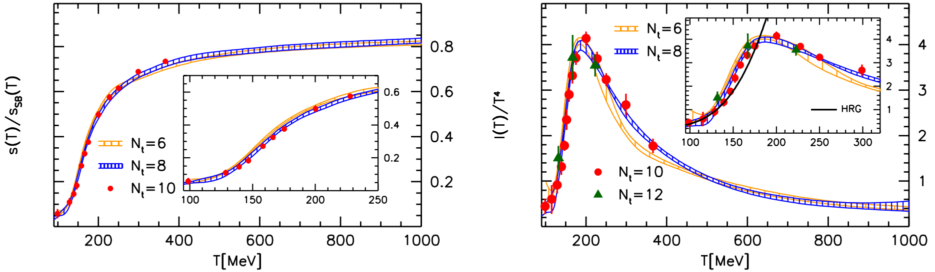
Pressure and energy density



ϵ normalized to the Stefan-Boltzmann limit: $\epsilon(T\to\infty)$=15.7
at 1000 MeV still 20% difference to the Stefan-Boltzmann value

essentially perfect scaling, lines/points are lying on top of each other

Entropy and trace anomaly



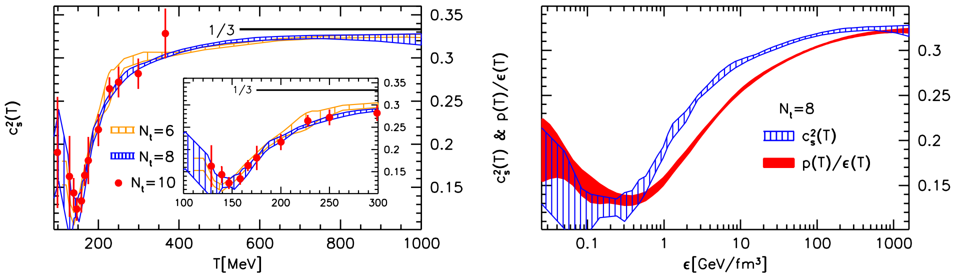
good agreement with the HRG model up to the transition region

T_c can be defined as the inflection point of the trace anomaly

Inflection point of $I(T)/T^4$	154(4) MeV
T at the maximum of $I(T)/T^4$	187(5) MeV
Maximum value of $I(T)/T^4$	4.1(1)

agreement with Aoki, Fodor, Katz, Szabo, JHEP 0601, 089 (2006) [arXiv:hep-lat/0510084]

Speed of sound & parametrization



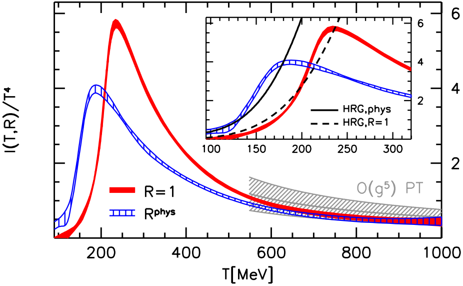
c_s minimum value is about 0.13 at T≈145 MeV

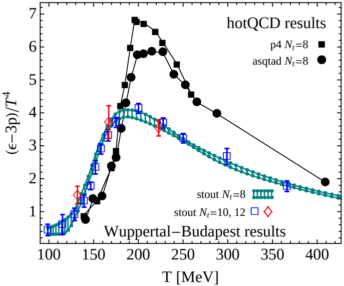
'smaller than error' parametrization T=100...1000 MeV (t=T/200 MeV)

$$\frac{I(T)}{T^4} = \exp(-h_1/t - h_2/t^2) \cdot \left(h_0 + \frac{f_0 \cdot [\tanh(f_1 \cdot t + f_2) + 1]}{1 + g_1 \cdot t + g_2 \cdot t^2} \right)$$

h_0	h_1	h_2	f_0	f_1	f_2	g_1	g_2
0.1396	-0.1800	0.0350	2.76	6.79	-5.29	-0.47	1.04

Equation of state: I(T)=ϵ-3p





two pion masses: $M_\pi \approx$720 MeV (R=1) and M_π=135 MeV (R^{phys})
good agreement with the HRG model up to the transition region
quark mass dependence disappears for high T
good agreement with perturbation theory

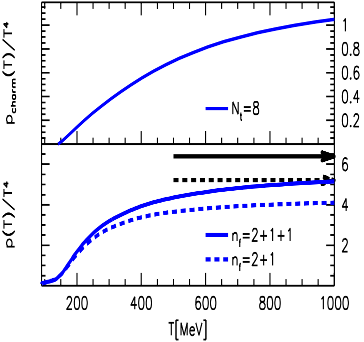
comparison with the published results of the hotQCD collaboration
discrepancy: peak at ≈20 MeV larger T and ≈50% higher

Charm contribution

perturbative indications: important already at $2 \cdot T_c$

M. Laine and Y. Schroder, Phys. Rev. D73 (2006) 085009

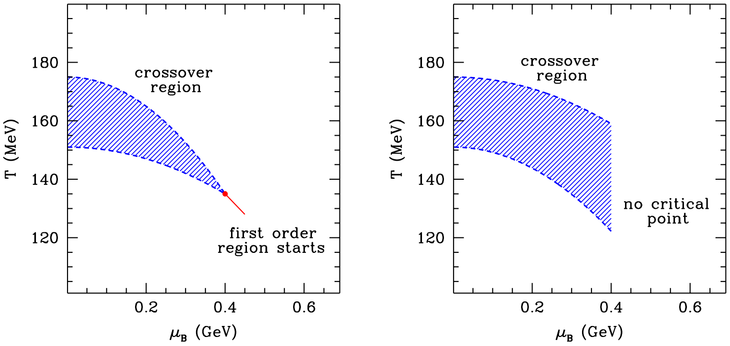
determine it within the partially quenched framwork: m_c/m_s=11.85



charm contribution is indeed non-negligeble from 200 MeV

one has to extend this observation to the dynamical case

Scenarios for $\mu > 0$

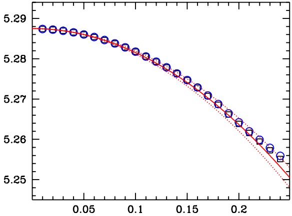


Does the crossover region shrink or expand?
The curvature can affect the existence of the critical endpoint
Estimate: if $\mu_{crit} = 360$ MeV $\rightarrow \Delta\kappa \approx 0.02$

Equivalence of the methods (formal/numerical)

$\Rightarrow$ for moderate μ Taylor and μ_I agree with reweighting

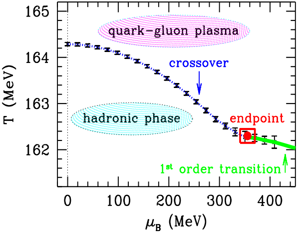
take n_f=2 setting of de Forcrand-Philipsen: $\beta_c(\mu)$ upto 4 digits

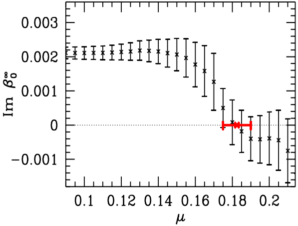


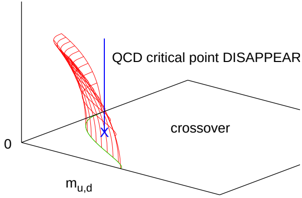
solid/dotted: imaginary μ & error; box: reweighting; circle: Taylor
for larger μ values higher order terms are getting more important

what to choose (depends on the question):
for this particular case imaginary μ has the largest CPU demand;
next one is reweighting; cheapest is Taylor (does not work for large μ)

Critical endpoint discussion (controversy?)







all results are from coarse lattices (a=0.3 fm, read our abstract!)

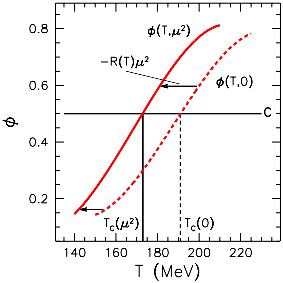
deForcrand-Philipsen: leading order ⇒ not stronger, slightly weaker
same from reweighting: $\mu_I/T\approx$1–3 (μ_{crit}: result of the higher orders)

Taylor & radius of convergence (!) only a lower bound: Lee-Yang

full answer (all the way to the continuum) needs much more CPU

The curvature

we change μ and look at the transition curve
it shifts to the left, we look at its value of a fixed C

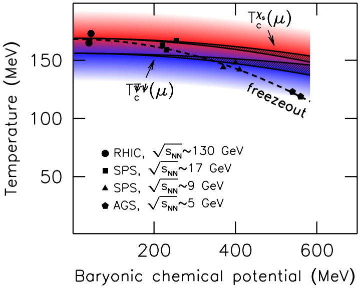


the dimensionless curvature is defined as $\kappa(T) = -T_c(\mu = 0) \cdot R(T)$

$d\kappa/dT$ at T_c tells if the transition is broadening or narrowing
(a point below T_c has a larger or smaller curvature)

Continuum prediction for the curvature: full result

G. Endrodi, Z. Fodor, S.D. Katz, K.K. Szabo, arXiv:1102.1356



lower solid line: T_c from the chiral condensate
upper solid line: T_c from the strange susceptibility

bands (red and blue) indicate the widths of the transition lines
the widths remain in this order approximately the same
in leading order: no critical point (can be anything)

Summary

- old result: QCD transition is an analytic cross-over
- long standing discrepancy in the literature
- overall scale T_c was clarified (Wuppertal-Budapest)
- equation of state (EoS) was determined
- huge discrepancey between WB and hotQCD
- continuum limit of the phase diagram curvature M_π=135 MeV

The nature of the QCD transition

Y.Aoki, G.Endrodi, Z.Fodor, S.D.Katz, K.K.Szabo, Nature, 443 (2006) 675

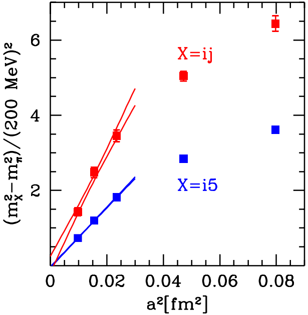
finite size scaling study of the chiral condensate (susceptibility)

$$\chi=(T/V)\partial^2 \log Z/\partial m^2$$

phase transition: finite V analyticity $V \to \infty$ increasingly singular
(e.g. first order phase transition: height $\propto$ V, width $\propto$ 1/V)
for an analytic cross-over χ does not grow with V

two steps (three volumes, four lattice spacings):
a. fix V and determine χ in the continuum limit: a=0.3,0.2,0.15,0.1fm
b. using the continuum extrapolated χ_{max}: finite size scaling

Scaling for the pion splitting



scaling regime is reached if a^2 scaling is observed

asymptotic scaling starts only for $N_t \gtrsim 8$ (a$\lesssim$0.15 fm): two messages

a. N_t=8,10 extrapolation gives 'p' on the $\approx$1% level: good balance

b. stout-smeared improvement is designed to reduce this artefact

most other actions need even smaller 'a' to reach scaling

Overlap improving multi-parameter reweighting

one wants to calculate the following path integral

$$Z(\alpha) = \int [dU] \exp[-S_{bos}(\alpha, U)] \det M(U, \alpha)$$

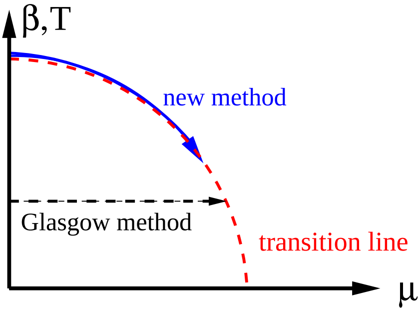
α: parameter set (gauge coupling, mass, chemical potential)
for some parameters α_0 importance sampling can be done

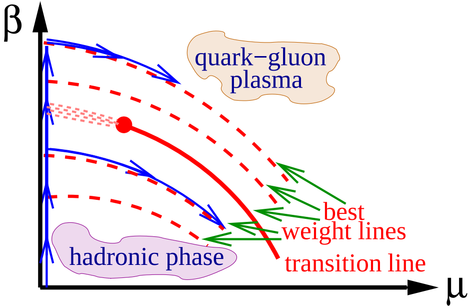
$$Z(\alpha) = \int [dU] \exp[-S_{bos}(\alpha_0, U)] \det M(U, \alpha_0)$$
$$\{\exp[-S_{bos}(\alpha, U) + S_{bos}(\alpha_0, U)] \det M(U, \alpha) / \det M(U, \alpha_0)\}$$

first line: measure; curly bracket: observable (will be measured)
e.g. transition configurations are mapped to transition ones

reweighting factor (ratio of the determinants) can be expressed by the eigenvalues of the (reduced) fermion matrix: closed formula for any μ

Compare with Glasgow (Ferrenberg-Swendsen)



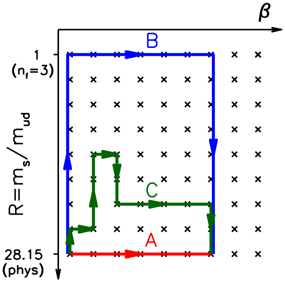


Glasgow method $\Rightarrow$ multiparameter reweighting
single parameter (μ) $\Rightarrow$ two parameters (μ and β)
purely hadronic $\Rightarrow$ transition configurations

map transition configurations to transition ones

All path approach

goal: determine the equation of state for several pion masses
reduce the uncertainty related to the choice of β^0
give the uncertainty related to the integration path



conventional path: A, though B, C or any other paths are possible
generalize: take all paths into account (use derivatives of p)
two-dimensional spline function gives p for any (β,R=m_s/m_{ud})
technically: solution of a large system of linear equations

Finite chemical potential: the sign problem

at μ=0 the fermion matrix is γ_5 hermitian: $M^\dagger = \gamma_5 M \gamma_5$
easy to check $\Longrightarrow$ eigenvalues: either real or conjugate pairs
det(M) is real, which is not true any more for non-vanishing μ

importance sampling (algorithms) for complex det(M) does not work

$$P(U \to U') = \min\left[1, \exp(-\Delta S_g) \det(M[U']) / \det(M[U])\right]$$

sign problem $\Rightarrow$ until 2001: "lattice QCD can not say anything for μ>0"

Fodor-Katz: multiparameter reweighting (hep-lat/0104001, PLB)
Bielefeld-Swansee: det(M) Taylor expanded (hep-lat/0204010, PRD)
de Forcrand-Philipsen: imaginary μ (hep-lat/0205016, Nucl.Phys.B)
D'Elia-Lombardo: imaginary μ (hep-lat/0209146, PRD)

the three methods look different, they are essentially the same

Equivalence of the methods (formal/numerical)

(recent lattice review at μ=0 and μ>0: Fodor-Katz 0908.3341)

det(M) can be given by the eigenvalues of M' (transformed) at μ=0

$$\det M(\mu) = e^{-3V\mu} \prod_{i=1}^{6L_s^3} (e^{L_t\mu} - \lambda_i)$$

observable at μ>0 or μ_I is given by the observable and λ_i at μ=0

$$Pl(\beta,\mu) = \langle Pl \exp[\Delta\beta Pl] e^{-3V\mu} \prod_{i=1}^{6L_s^3} (e^{L_t\mu} - \lambda_i) \rangle$$

det(M) or Pl(β,μ) can be trivially Taylor expanded (Bielefeld-Swansee)
termination of the series & stochastic determination of the coefficients
$\Longrightarrow$ do not expect this method to work for as large μ as the full one

det(M)$>$0 for imaginary μ: impartance sampling still works
determine the phase line $T_c(\mu_I)$ (e.g. use a quadratic/quartic fit)
plug real μ into the same quadratic/quartic function: $c_2\mu^2$+ $c_4\mu^4$
formally: numerical determination of the (μ^2,μ^4) Taylor coefficients