apeNEXT: Computational Challenges and First Physics Results

Bulk QCD Thermodynamics at small quark masses

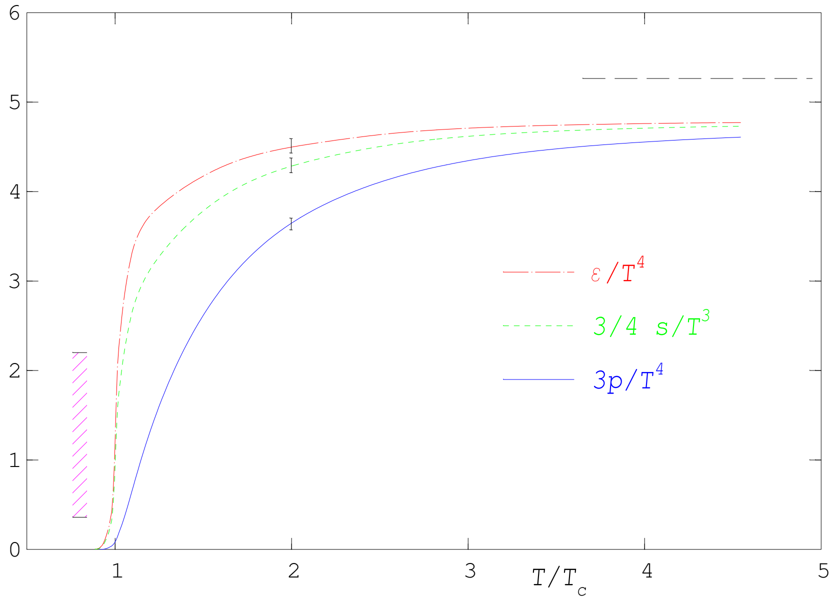
	Introduction
I	**Critical temperature**
II	**Equation of state**

for the
RIKEN –
BNL –
Columbia –
Bielefeld – Collaboration

QCD undergoes a phase transition at large temperature

quenched approximation: bulk thermodynamics solved

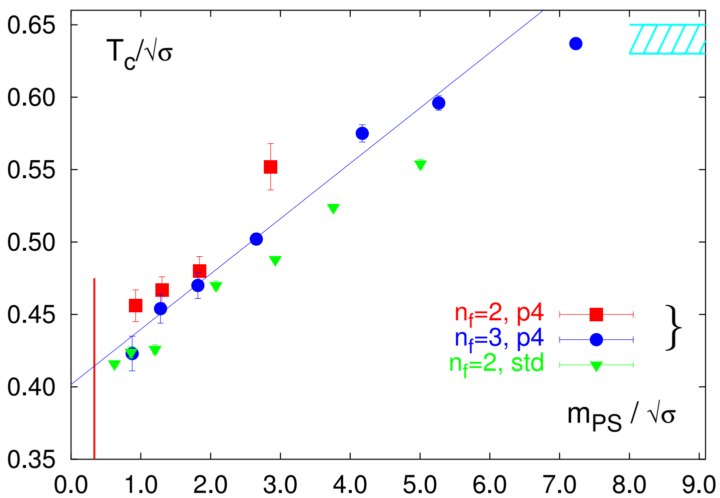
APE100: Equation of state [Boyd et al., 1996]



Questions to be addressed in full QCD (amongst others):

- critical temperature: T_c
- equation of state: $\epsilon(T), p(T), \ldots$

APE1000: full QCD on coarse lattices $a \gtrsim 1/4\text{fm}$ and at quark masses corresp. to $m_\pi \simeq 700\text{MeV}$



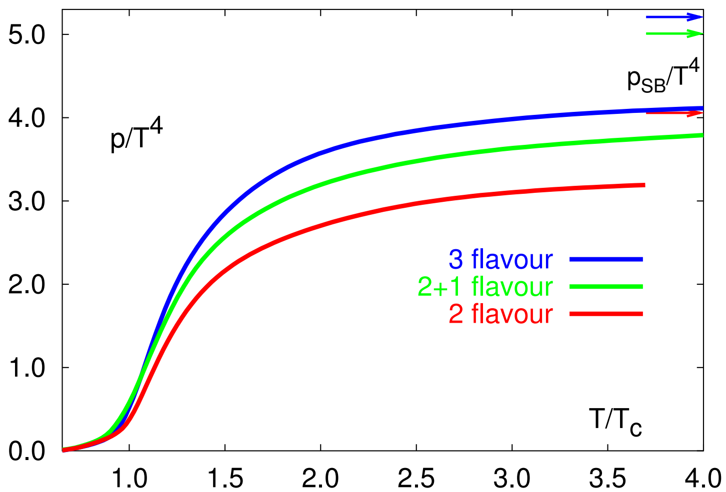
$m \to \infty$

chiral extrapolation $m \to 0$

$$\frac{T_c}{\sqrt{\sigma}} \to \begin{cases} 0.42\,(\pm 0.01)\,(\text{syst.}) & N_F = 2 \text{ Wilson } ^\star \\ 0.42\,(\pm 0.01)\,(\text{syst.}) & N_F = 2 \text{ staggered} \\ 0.40\,(\pm 0.01)\,(\text{syst.}) & N_F = 3 \text{ staggered} \end{cases}$$

improved action

[cp-pacs collaboration, 2001]



strong deviations from ideal gas behavior at $T \lesssim 4T_c$

weak dependence on (large) quark masses

[Karsch, EL, Peikert, 2001]

Quantum Statistics in equilibrium :

$$\text{partition function } Z = \mathrm{tr}\left\{e^{-\hat{H}/T}\right\}$$

→ Feynman path integral

$$Z(T,V) = \int \mathcal{D}\phi(\vec{x},\tau)\,\exp\left\{-\int_0^{1/T} d\tau \int_0^V d^3\vec{x}\,\mathcal{L}_E[\phi(\vec{x},\tau)]\right\}$$

- temporal extent limited by $1/T$
- (anti-) periodic boundary conditions in τ

apply standard thermodynamic relations, e.g.

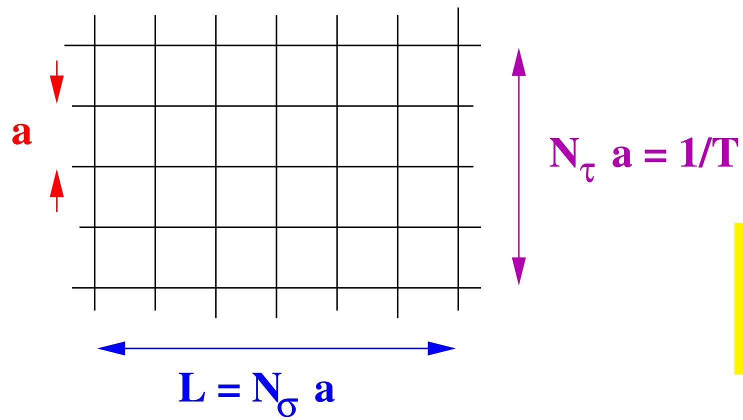
energy density $\qquad \epsilon = \frac{T^2}{V}\frac{\partial \ln Z}{\partial T}\Big|_V$

specific heat $\qquad c_V = \frac{1}{VT^2}\frac{\partial^2 \ln Z}{\partial(1/T)^2}\Big|_V$

thermal field theory can be treated perturbatively at high temperatures – small coupling $g(T)$ but subtle IR problems occur even then numerical treatment of QCD $\Rightarrow$ discretize (Euclidean) space-time

$\Rightarrow$ **lattice**

$N_\sigma^3 \times N_\tau$



$$Z(T,V) = \int \prod_{i=1}^{N_\tau N_\sigma^3} d\phi(x_i) \exp\{-S[\phi(x_i)]\}$$

temperature T introduces a scale $\Rightarrow$

- thermodynamic limit, IR - cut-off effects $\quad LT = \frac{N_\sigma}{N_\tau} \rightarrow \infty \quad$ (finite size scaling)
- continuum limit, UV - cut-off effects $\quad aT = \frac{1}{N_\tau} \rightarrow 0$
- chiral limit $\quad m \rightarrow m_{\rm phys} \simeq 0$

Choice of fermions

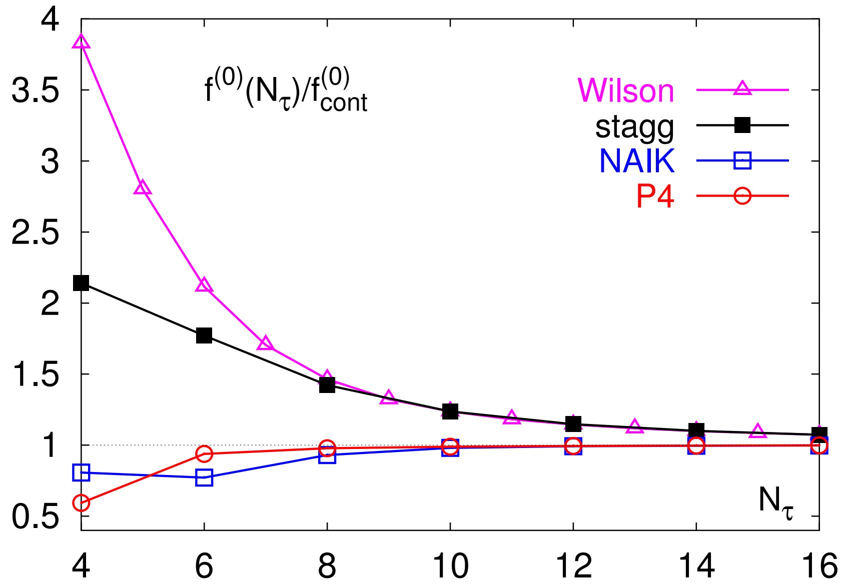
- free energy density, for instance (see later): $f/T^4 \;\sim\; N_\tau^4 \times \text{signal}$

$\Rightarrow$ signal $\sim 1/N_\tau^4$

$\Rightarrow$ keep N_τ small

$\Rightarrow$ coarse lattices $a = 1/N_\tau T$

$\Rightarrow$ improved actions



- Wilson-like fermions have turned out to be notoriously difficult to simulate at small quark masses

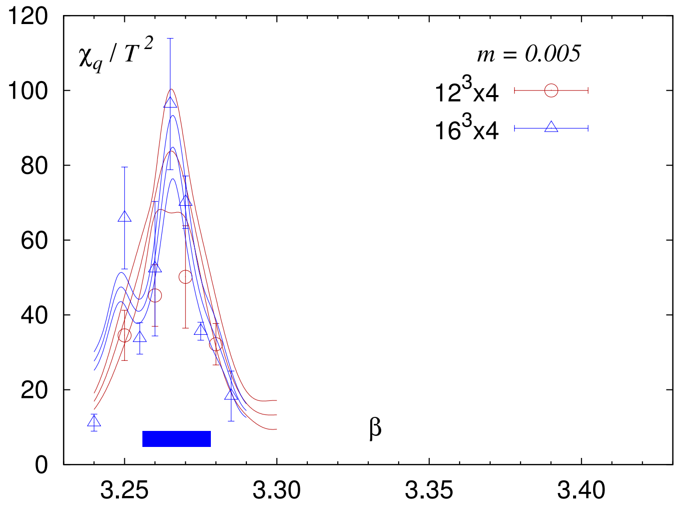
$\star$ in the following: `p4` (to improve thermodynamics) and `fat3` (to improve flavor symmetry)

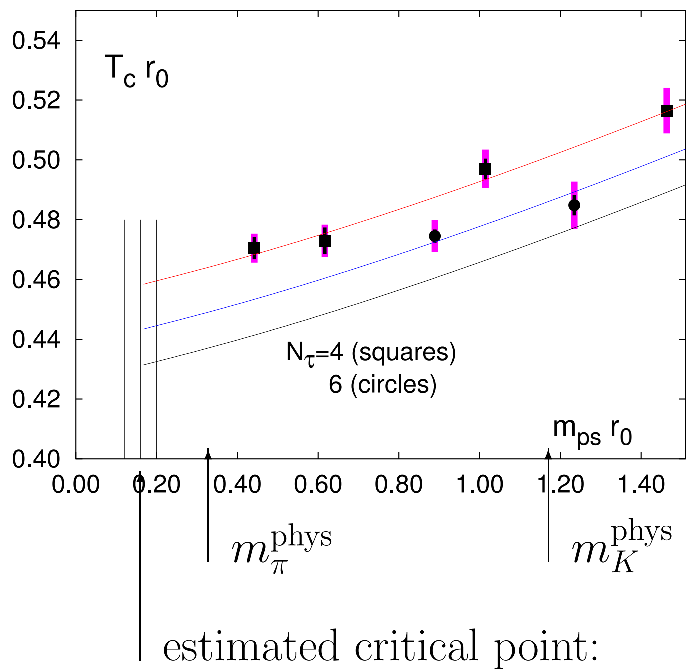
Critical temperature

critical temperature $T_c = 1/N_\tau a(\beta_c)$ signalled by

- chiral condensate $\langle q\bar{q}\rangle \;\sim\; \partial \ln Z/\partial m_q$ rapidly decreasing
- chiral susceptibility $\chi_q \;\sim\; \partial^2 \ln Z/\partial m_q^2$ developing a peak

$N_F = 3$ degenerate light quarks: $N_\tau = 4, 6, \quad N_\sigma = 8, 12, 16$





β_c uncertainty $\leftrightarrow$ $\Delta T_c \simeq 5\text{MeV}$

scale from T = 0 potential

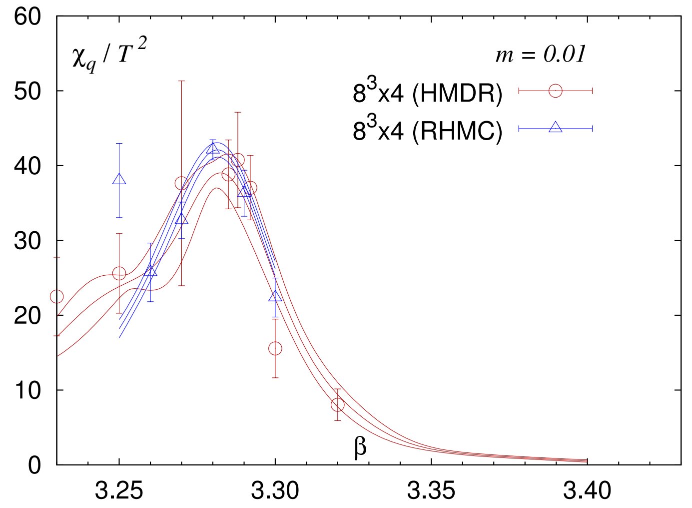
estimated critical point:

$r_0 T_c(m_{PS}^{CP}) = 0.429(8)$

Algorithms:

- from hybrid molecular dynamics (**HMDR**) at $\delta t = am_q/2.5$
- to rational hybrid Monte Carlo (**RHMC**): **exact** Clark, Kennedy

  utilizing multi-shift inversion solvers, Sexton-Weingarten multi-step molecular dynamics



- no systematic difference seen for p4fat3 action
- differences observed for other actions (std. staggered: Forcrand, Philipsen
  p4fat7: RBCBielefeld Coll.)

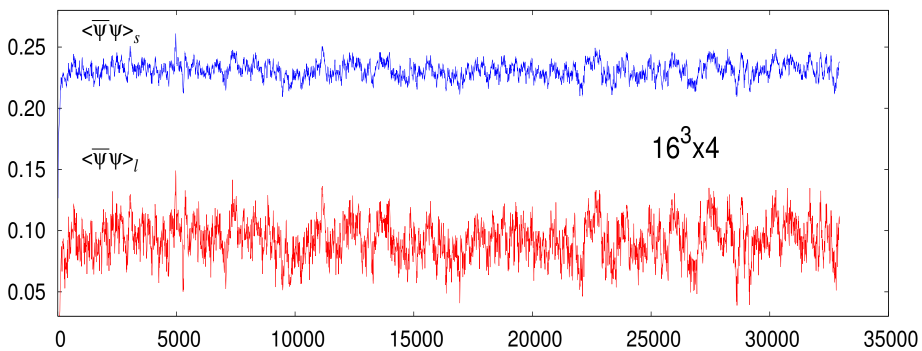
$N_F = 2 + 1$ two light quarks + one strange quark with $m_s \simeq m_s^{\text{phys}}$:

$m_l/m_s \; \epsilon \; [0.05, 0.5]$

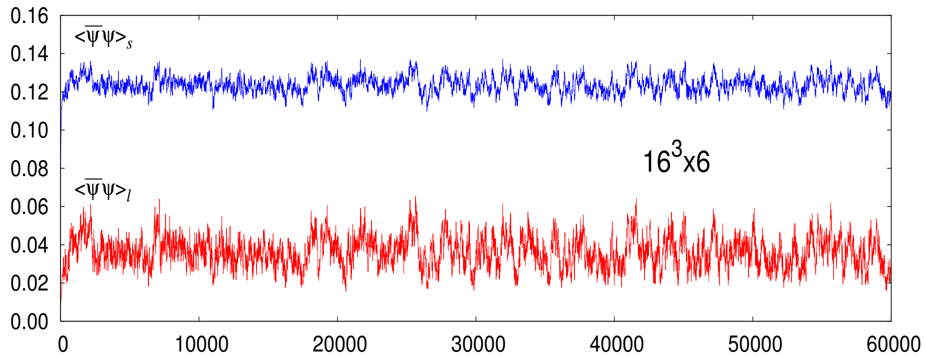
lattice extents: $N_\tau = 4, 6$ $N_\sigma = 8, 16, 24, 32$

statistics between 30,000 and 60,000 traj. at $N_\tau = 4$ $(t = 0.5(\times\sqrt{2}))$ and

10,000 and 60,000 traj. at $N_\tau = 6$ per (β, m_l, m_s) set



$\beta \simeq \beta_c$ $m_l = 0.05 m_s$

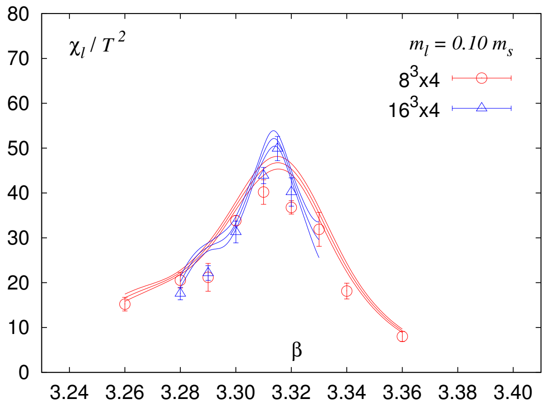


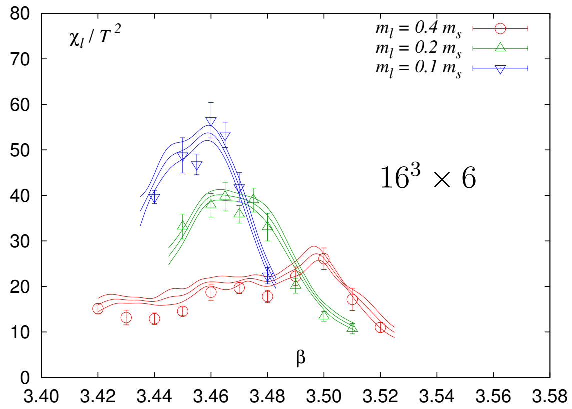
$\beta \simeq \beta_c$ $m_l = 0.1 m_s$

note: quark condensate fluctuations at light quark masses in the vicinity of T_c: $\mathcal{O}(30\%)$

$\Rightarrow$ large statistical samples needed for precision determination of T_c with errors of $\mathcal{O}(\text{few}\%)$

⋆ weak volume dependence, indicating crossover rather than 1st or 2nc order phase transition

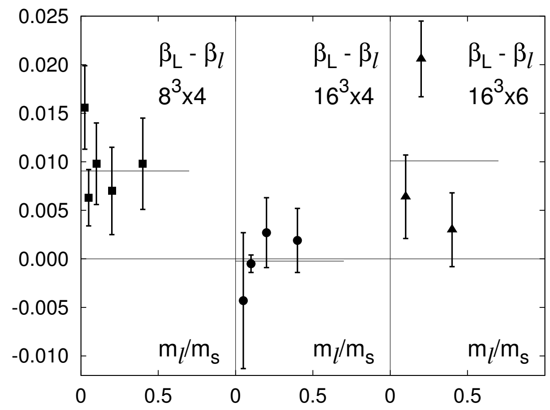




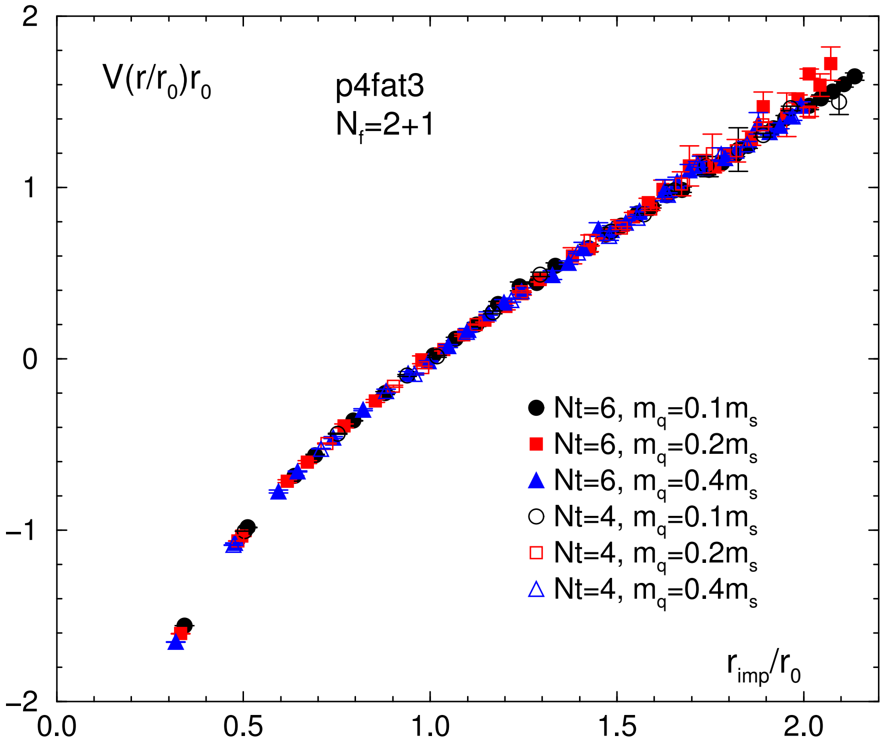
⋆ peak locations from Ferrenberg-Swendsen

⋆ slight ambiguities in peak locations

⋆ taken into account as systematic error of order 2 to 4 %



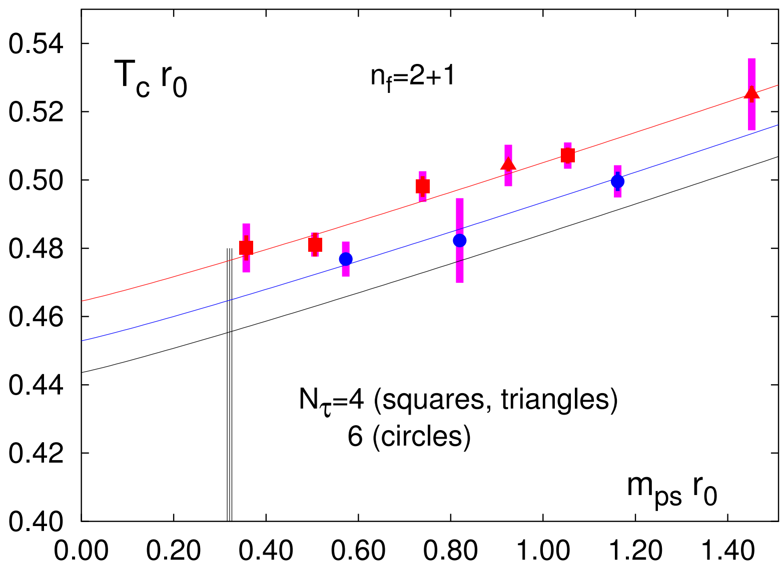
⋆ T = 0 scale taken from heavy quark potential $V(r)$

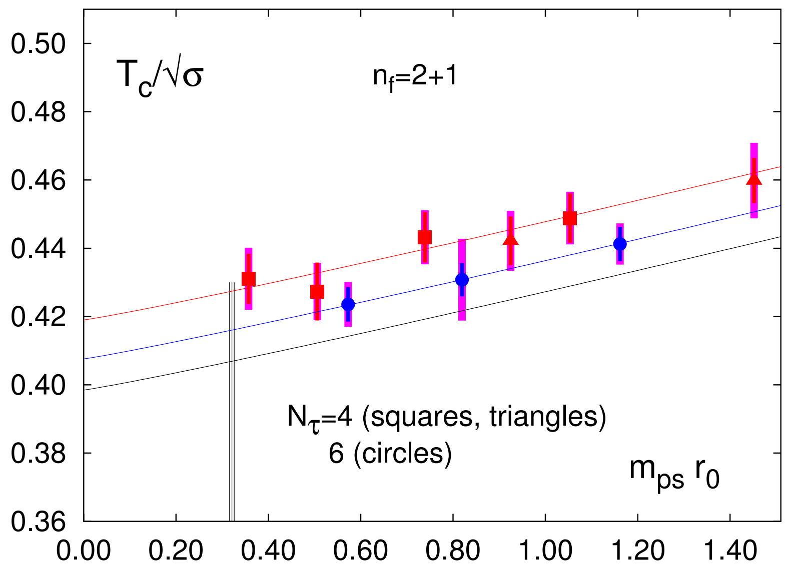


potential well decribed by

$$V(r) = c_0 - \frac{\alpha}{r_{imp}} + \sigma r_{imp} \qquad \text{with} \qquad \frac{a}{r_{imp}} = 4\pi \int_{-\pi}^{\pi} \frac{d^3k}{(2\pi)^3}\, e^{i\vec{k}\vec{r}} \left[4 \sum_i^3 \sin^2(ak_i/2) + \frac{1}{3}\sin^4(ak_i/2)\right]^{-1}$$

ar_0 from $\left. r^2 \frac{dV(r)}{dr} \right|_{r=r_0} = 1.65$ together with $r_0 = 0.469(7)$ fm [A. Gray et al.] $\Rightarrow$ $a(\beta)$





thin error bars: error on r_0/a or $a^2\sigma$; wide error bars: β_c uncertainty

combined continuum/chiral extrapolation ($d = 1.08$ for $O(4)$, $d = 2$ for first order)

$$(T_c\, r_0)_{m_l,N_\tau} = (T_c\, r_0)_{0,\infty} + A(m_{PS}\, r_0)^d + B/N_\tau^2$$

chiral limit $T_c r_0 = 0.444(6)^{+12}_{-3}$ $T_c/\sqrt{\sigma} = 0.398(6)^{+10}_{-1}$ $\begin{smallmatrix} d=2 \\ d=1 \end{smallmatrix}$

phys. point $T_c r_0 = 0.457(7)^{+8}_{-2}$ $T_c/\sqrt{\sigma} = 0.408(8)^{+3}_{-1}$

with new $T = 0$ (lattice) result for $r_0 = 0.469(7)$fm obtain: $T_c = 192\,(7)\,(4)$ MeV at phys. point

stat. on β_c, r_0, σ; syst. on N_τ extrapolation

Equation of State

start from energy-momentum tensor $\frac{\Theta^\mu_\mu(T)}{T^4} = \frac{\epsilon - 3p}{T^4} = T\frac{d}{dT}(p/T^4)$

where $p = \frac{T}{V}\ln Z(T,V) - \lim_{T\to 0}\frac{T}{V}\ln Z(T,V)$ subtracting T = 0 normalization

thus $$\frac{p(T)}{T^4} - \frac{p(T_0)}{T_0^4} = \int_{T_0}^{T} dT' \frac{1}{T'^5}\Theta^\mu_\mu(T')$$

now $Z(T,V;g,m_l,m_s) = Z(N_\tau,N_\sigma,a;\beta,\hat{m}_l,\hat{m}_s) \to Z(N_\tau,N_\sigma,a;\beta,m_\pi,m_K)$

and tune bare lattice parameters $\hat{m}_l, \hat{m}_s$ with β such that $m_{\pi,K} = \text{const} \Rightarrow \hat{m}_{l,s}(\beta), a(\beta)$

$\Rightarrow$ $$\frac{\Theta^\mu_\mu(T)}{T^4} = -R_\beta(\beta)N_\tau^4\left(\left\langle\frac{d\bar{S}}{d\beta}\right\rangle_T - \left\langle\frac{d\bar{S}}{d\beta}\right\rangle_{T=0}\right)$$

with $$R_\beta(\beta). = T\frac{d\beta}{dT} = -a\frac{d\beta}{da}$$

furthermore, will need $(\hat{m}_s(\beta) = \hat{m}_l(\beta)\times h(\beta))$

$$R_m(\beta). = \frac{1}{\hat{m}_l(\beta)}\frac{d\hat{m}_l(\beta)}{d\beta} \qquad R_h(\beta). = \frac{1}{h(\beta)}\frac{dh(\beta)}{dh}$$

action $\quad S = \beta\, S_G \,+\, 2\,\hat{m}_l(\beta)\;\bar{\psi}_l\psi_l \,+\, \hat{m}_s(\beta)\;\bar{\psi}_s\psi_s \,+\, \beta$ independent

such that Θ^μ_μ consists of three pieces

$$\frac{\Theta^{\mu\mu}_G(T)}{T^4} = R_\beta\; N_\tau^4\; \Delta\langle \bar{S}_G\rangle$$

where $\Delta\langle\mathcal{O}\rangle = \langle\mathcal{O}\rangle_{T=0} - \langle\mathcal{O}\rangle_T$

$$\frac{\Theta^{\mu\mu}_F(T)}{T^4} = -R_\beta\, R_m\; N_\tau^4\; \{\, 2\,\hat{m}_l\,\Delta\langle\bar{\psi}\psi\rangle_l \,+\, \hat{m}_s\,\Delta\langle\bar{\psi}\psi\rangle_s \,\}$$

$$\frac{\Theta^{\mu\mu}_h(T)}{T^4} = -R_\beta\, R_h\; N_\tau^4\; \hat{m}_s\,\Delta\langle\bar{\psi}\psi\rangle_s$$

need: β functions $R_\beta(\beta), R_m(\beta), R_h(\beta)$

“action differences” $\Delta\bar{S}_G, \Delta\langle\bar{\psi}\psi\rangle_{l,s}$

simulations:

$16^3\times 4,\ 24^3\times 6,\ 16^3\times 32,\ 24^3\times 32$ lattices

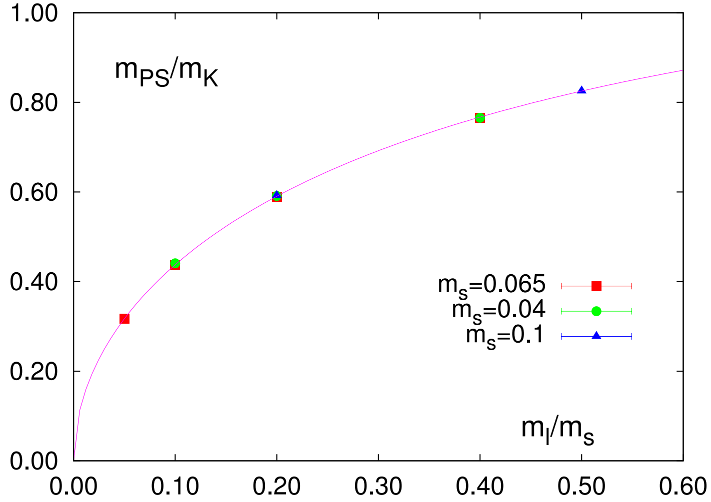
(β, m_l, m_s) on LoCP

$m_{\pi,K} = \text{const}$: Line of Constant Physics (LoCP)

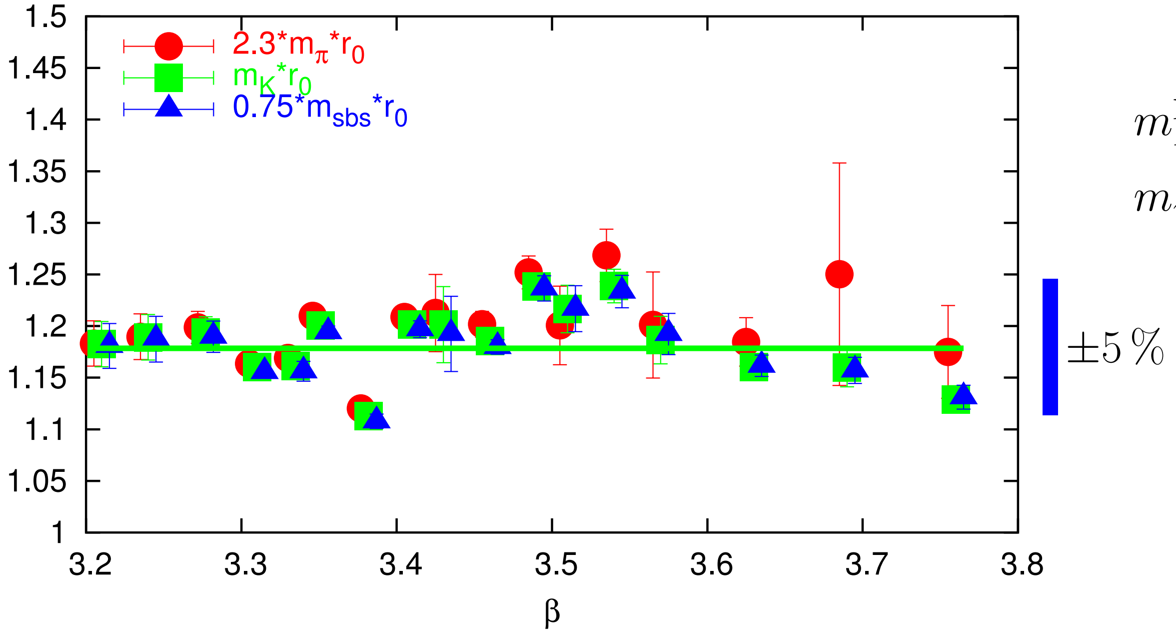
- to sufficient precision,
  m_π/m_K depends on $h = \hat{m}_s/\hat{m}_l$ only

  $\Rightarrow$ fix $h = 10$

  $\Rightarrow$ $R_h(\beta) = 0$

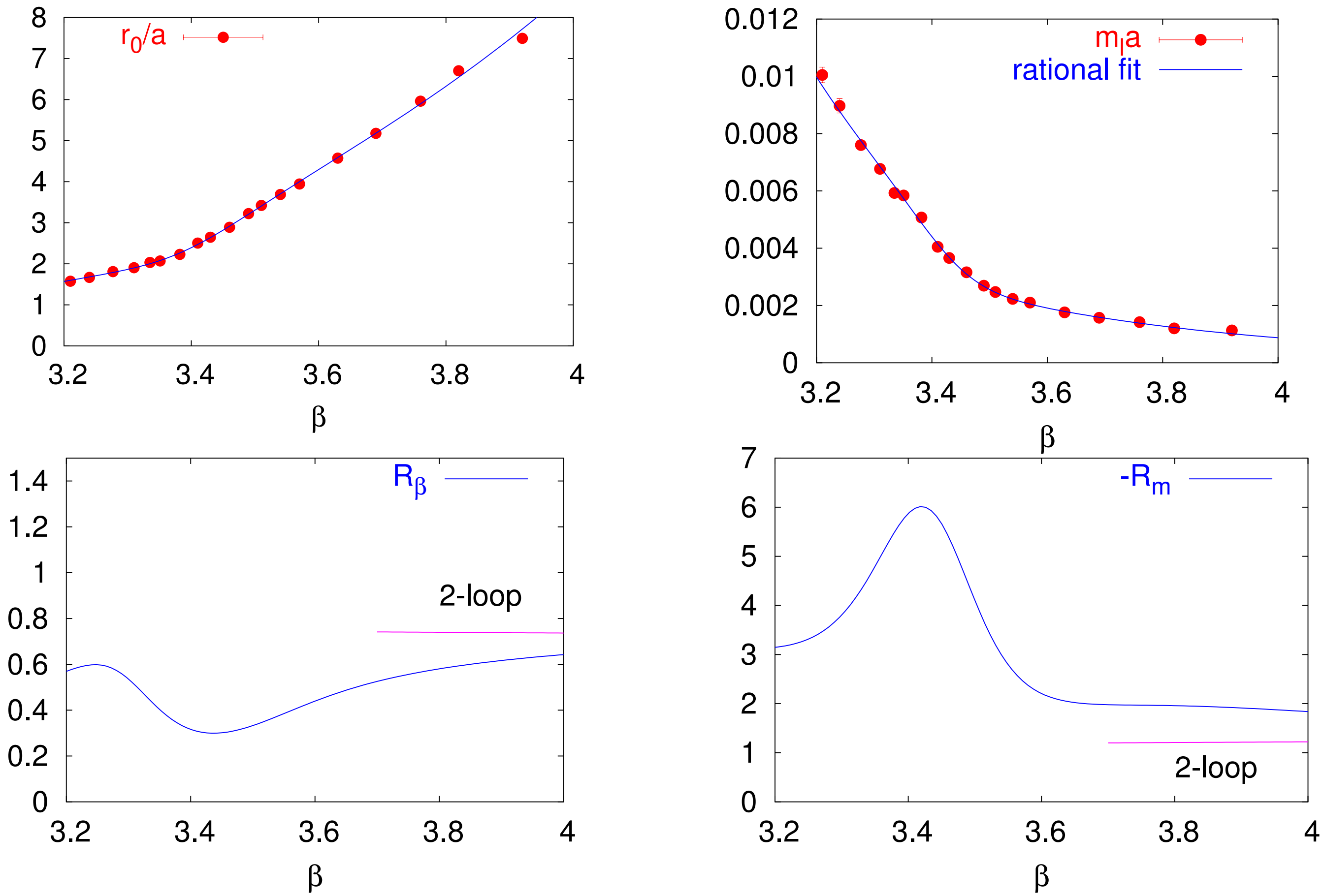


- fine tune $\hat{m}_l(\beta)$



$m_K^{\text{phys}} r_0$ green line

$m_\pi \simeq 215\,\text{MeV}$

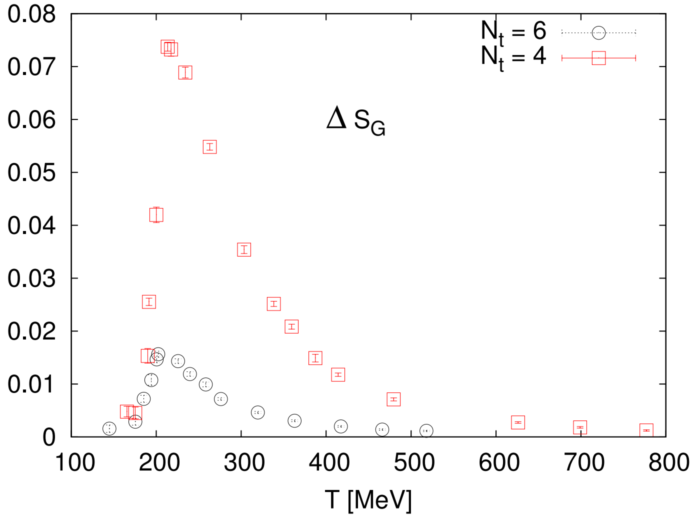


Allton inspired parametrization with rational fct. in $\hat{a}(\beta) = R_\beta^{(2-loop)}(\beta)/R_\beta^{(2-loop)}(\beta = 3.4)$

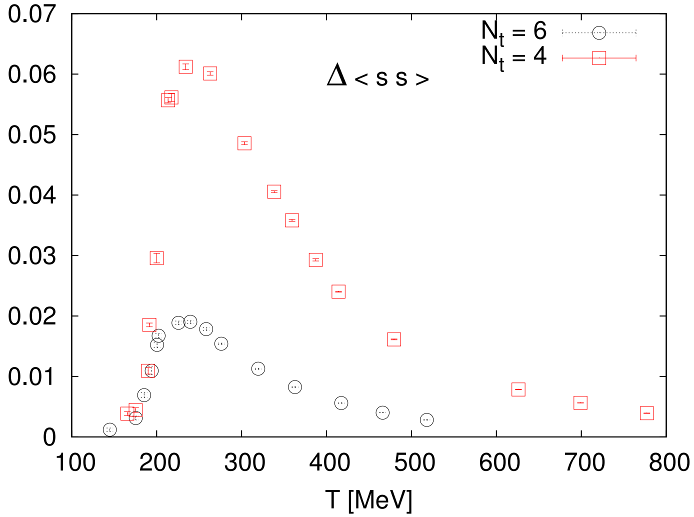
$$\frac{a}{r_0} = a_r R_\beta^{(2-loop)} \frac{1 + b_r\hat{a}^2 + c_r\hat{a}^4 + d_r\hat{a}^6}{1 + e_r\hat{a}^2 + f_r\hat{a}^4} \qquad \Rightarrow \quad R_\beta = \frac{r_0}{a}\left(\frac{dr_0/a}{d\beta}\right)^{-1}$$

$$\hat{m}_l = a_m R_\beta^{(2-loop)} \left(\frac{6b_0}{\beta}\right)^{-4/9} \frac{1 + b_m\hat{a}^2 + c_m\hat{a}^4 + d_m\hat{a}^6}{1 + e_m\hat{a}^2 + f_m\hat{a}^4} \qquad \Rightarrow \quad R_m$$

raw lattice data in lattice units

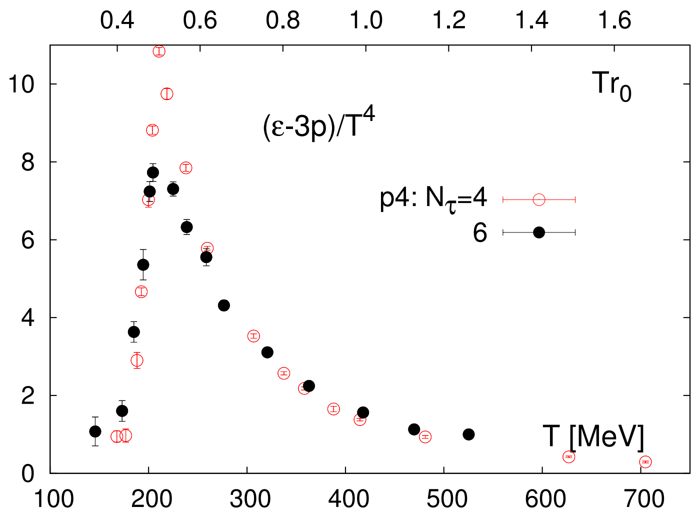


average gauge action difference

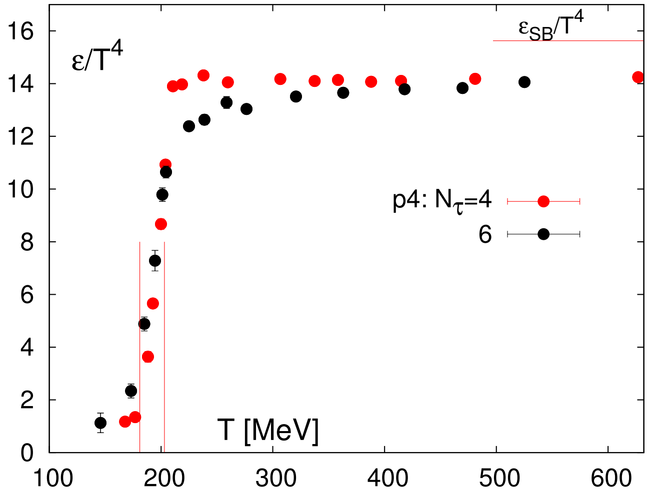


average strange condensate difference

putting everything together ...



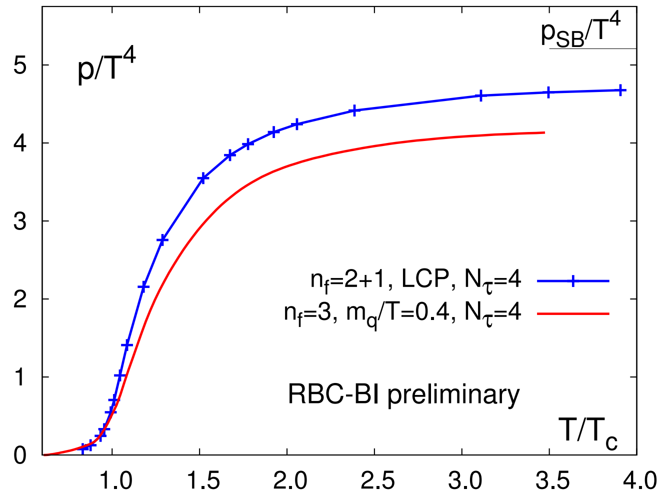
... new energy densities



... compare with old pressure results:

old: m_q/T fixed means m_q rising with T

new: fixed small physical m_q



expected slight rise in p confirmed

at $\gtrsim 2T_c$ almost no discretization effects

at $\gtrsim 2T_c$ 10% deviations from ideal gas

T determination independent of T_c

band indicates $T_c = 192 \pm 11$MeV

Conclusion

- APE computers have had some impact on QCD at finite temperature and density
- apeNEXT opens possibilities for small quark masses and smaller lattice spacings

- so far:
  - ⋆ critical temperature for 2+1 quarks with almost physical masses
  - ⋆ equation of state on LoCP with $m_K^{\rm phys}$ and $m_\pi \simeq 215$MeV

- future: – from near future to future challenges –
  - ⋆ small but phenomenologically relevant non-vanishing baryon densities
  - ⋆ new attempt towards phase diagram
  - ⋆ $N_\tau = 8$
  - ⋆ large baryon densities