QCD thermodynamics on QCDOC and APEnext supercomputers

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QCD on Teraflops Computer, Bielefeld, Oct. 11-13, 2006

Motivation & Approach

Quantitative study of QCD thermodynamics
from first principle calculation (Lattice QCD)

T_c, EoS, phase diagram, small μ, etc...

from recent studies, we know
these quantities strongly depend on m_q & N_f

Our aim is QCD thermodynamics with 2+1 flavor
at almost realistic quark masses

e.g. pion mass ≃ 150MeV, kaon mass ≃ 500MeV

- Choice of quark action
  → Improved Staggered quark action
- Continuum limit
  − N_t = 4, 6, (8) → a ≃ 0.24, 0.17, (0.12) fm

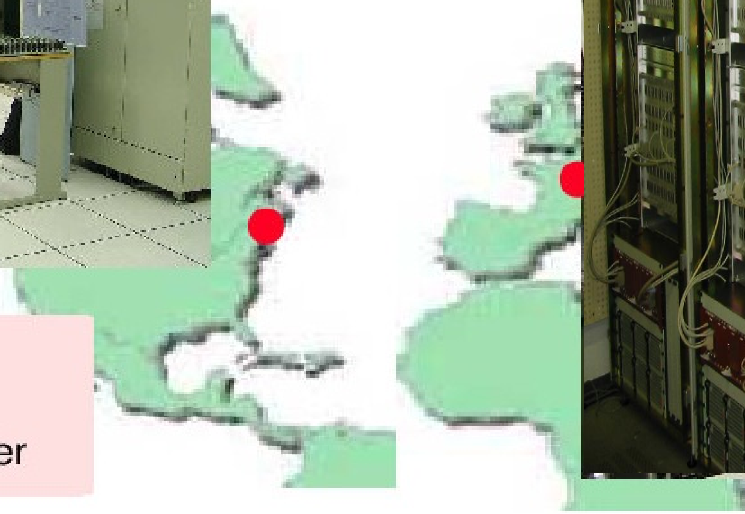
Computers

US/RBRC QCDOC

20.000.000.000.000 ops/sec

BI – apeNEXT

5.000.000.000.000 ops/sec



- critical temperature
- equation of state
- hadron properites in matter

today: 4.0 TFlops

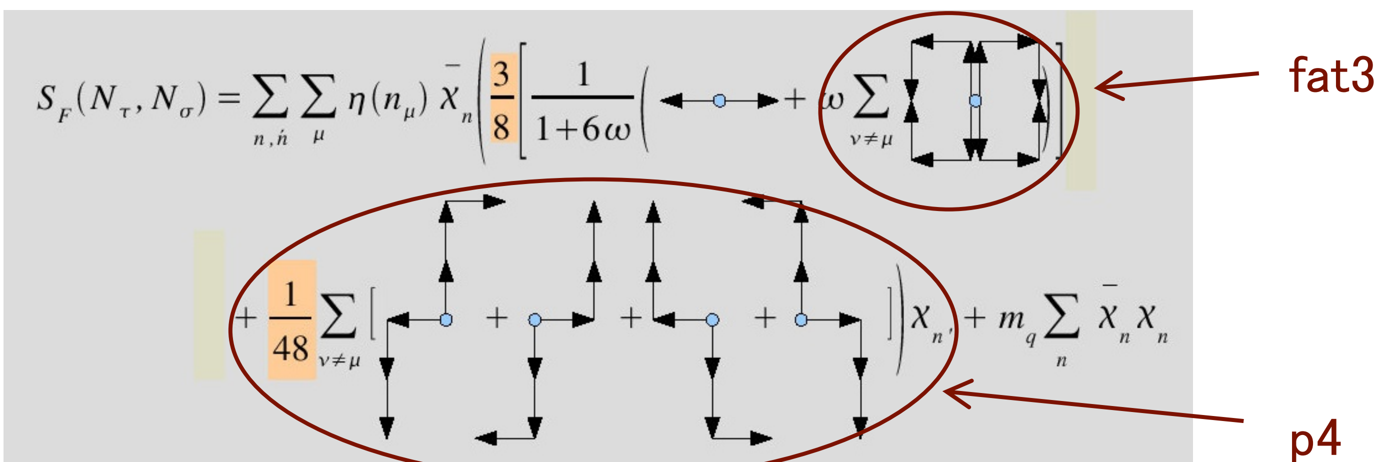
http://quark.phy.bnl.gov/~hotqcd

Choice of Lattice Action

Improved Staggered action : p4fat3 action

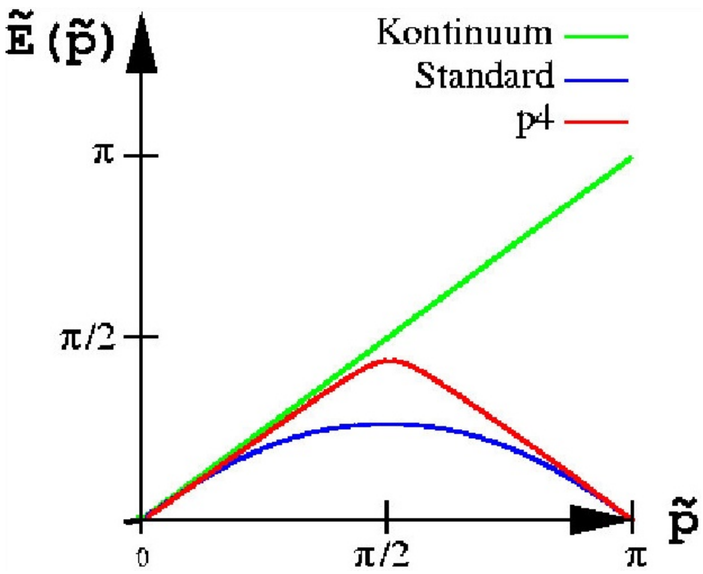
Karsch, Heller, Sturm (1999)

- gluonic part : Symanzik improvement scheme
  - remove cut-off effects of $O(a^2)$
  - tree level improvement $O(g^0)$
- fermion part : improved staggered fermion
  - remove cut-off effects & improve rotational sym.
  - improve flavor symmetry by smeared 1-link term



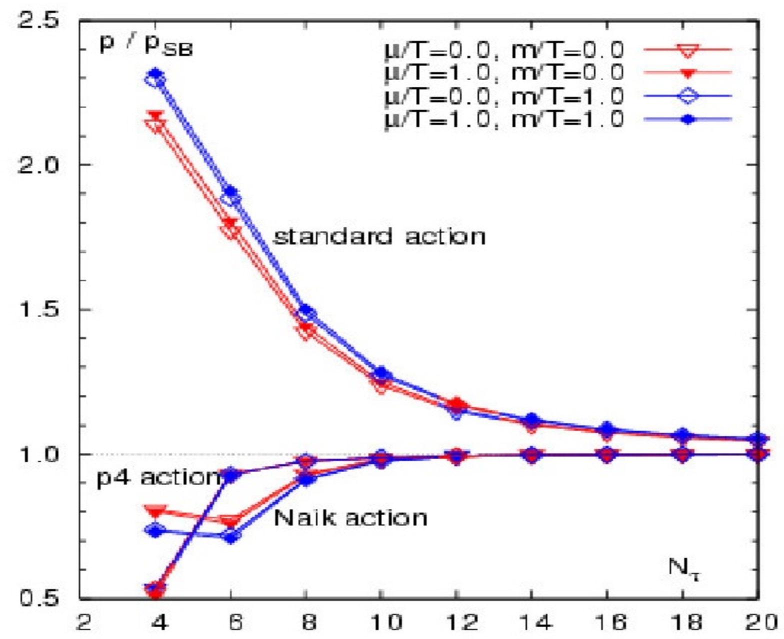
Properties of the p4-action

Dispersion relation



The free quark propagator is rotational invariant up to $O(p^4)$

pressure in high T limit



Bulk thermodynamic quantities show drastically reduced cut-off effects

flavor sym. is also improved by fat link

Contents of this talk

- Motivation and Approach
- Choice of lattice action
- Critical temperature *M.Chen et al. Phys.Rev.D74 054507 (2006)*
    - Simulation parameters
    - Critical β search
    - Scale setting by Static quark potential
    - Critical temperature
- Equation of State
    - Line of Constant Physics
    - Beta–functions
    - Interaction measure & Pressure
- Conclusion

Simulation parameters

- Critical β search at T > 0

N_τ	$\hat{m}_s$	$\hat{m}_l$	V	$\#\beta$ values	max.# conf.
4	0.1	0.5 $\hat{m}_s$	8^3	10	40,000
		0.2 $\hat{m}_s$	8^3	6	12,000
4	0.065	0.4 $\hat{m}_s$	8^3, 16^3	10, 11	30,000, 60,000
		0.2 $\hat{m}_s$	8^3, 16^3	8, 7	30,000, 60,000
		0.1 $\hat{m}_s$	8^3, 16^3	9, 6	34,000, 50,000
		0.05 $\hat{m}_s$	8^3, 16^3	8, 5	30,000, 42,000
6	0.0040	0.4 $\hat{m}_s$	16^3	11	20,000
		0.2 $\hat{m}_s$	16^3	9	60,000
		0.1 $\hat{m}_s$	16^3	7	60,000

(*) conf. = 0.5 MD traj.

to check
m_s dependence for Tc

- T=0 scale setting at $\beta_c(N_t)$ on 16^3x32

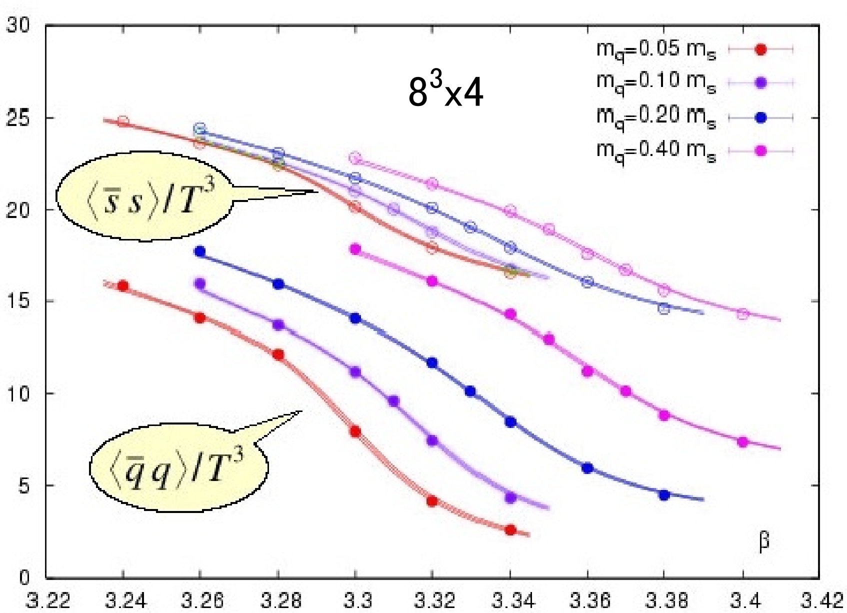
N_τ	$\hat{m}_s$	$\hat{m}_l$	β	# conf.	m_{ps}/m_v	a [fm]
4	0.1	0.5 $\hat{m}_s$	3.409	600	0.520(2)	0.2273(4)
		0.2 $\hat{m}_s$	3.371	238	0.372(5)	0.2336(7)
4	0.065	0.4 $\hat{m}_s$	3.362	500	0.410(2)	0.2312(7)
		0.2 $\hat{m}_s$	3.335	400	0.303(7)	0.2365(6)
		0.1 $\hat{m}_s$	3.310	750	0.212(7)	0.2458(5)
		0.05 $\hat{m}_s$	3.300	400	0.154(5)	0.2475(8)
6	0.0040	0.4 $\hat{m}_s$	3.500	294	0.461(4)	0.1558(7)
		0.2 $\hat{m}_s$	3.470	500	0.343(6)	0.1617(5)
		0.1 $\hat{m}_s$	3.455	410	0.248(4)	0.1670(5)

(*) conf. = 5 MD traj.
after thermalization

Exact RHMC
is used.

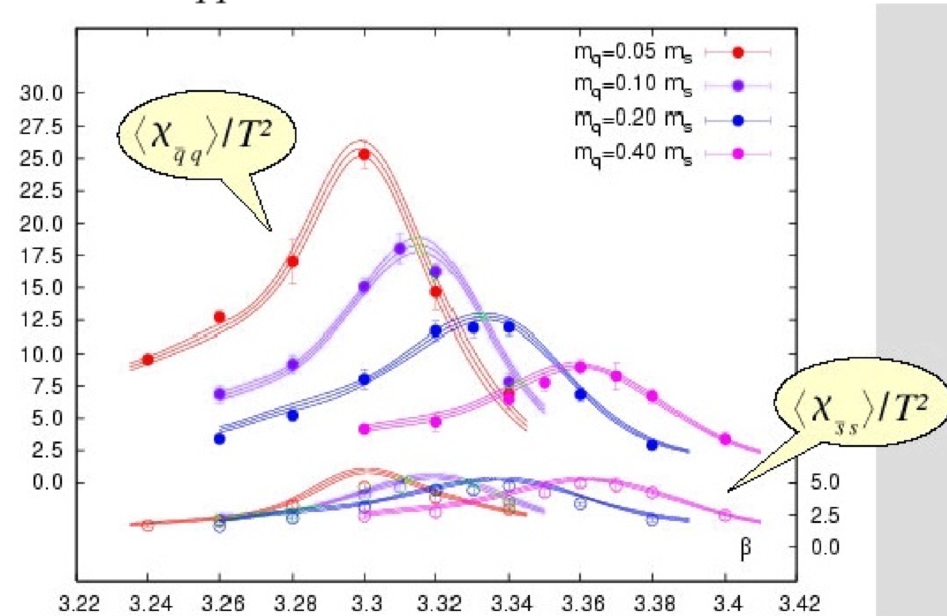
Critical β search

chiral condensate:



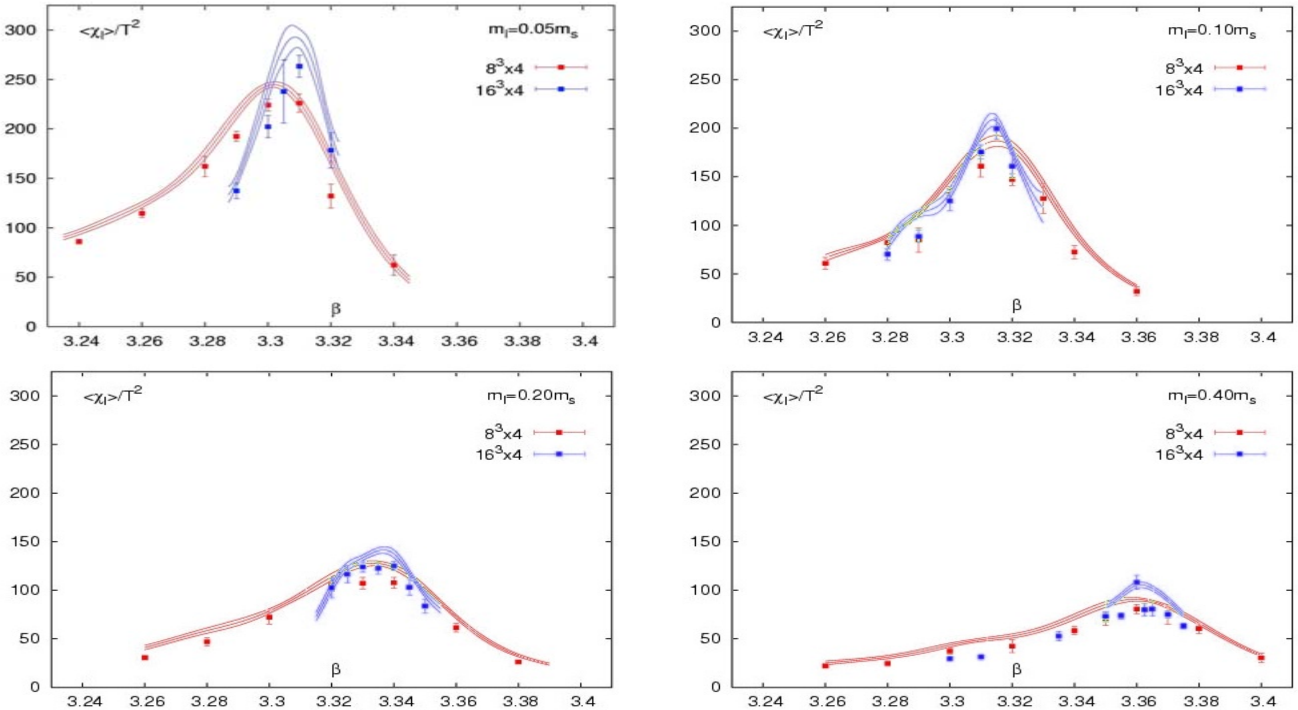
chiral susceptibility:

$$\langle \chi_{\bar q q}\rangle \equiv \langle (\bar q q)^2\rangle - \langle \bar q q\rangle^2$$



- multi-histogram method (Ferrenberg-Swendson) is used
- β_c are determined by peak positions of the susceptibilities
- Transition becomes stronger for smaller light quark masses

Volume dependence of β_c



- No large change in peak height & position

  → consistent with crossover transition rather than true transition

- Reliable calculation of susceptibilities requires large statistics

  at least tens thousands of trajectories are necessary at T>0

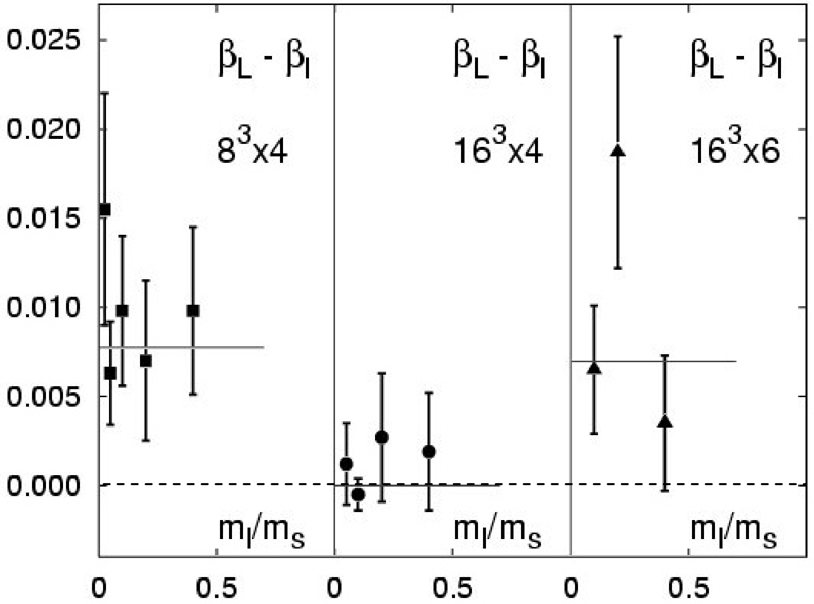
  (we have sometimes 60,000traj.)

Uncertainties in β_c

- Statistical error
  → jackknife analysis for peak-position of susceptibility

- We can find a difference between β_l and β_L
  → small difference but statistically significant
  β_l : peak position of chiral susceptibility.
  β_L : peak position of Polyakov loop susceptibility

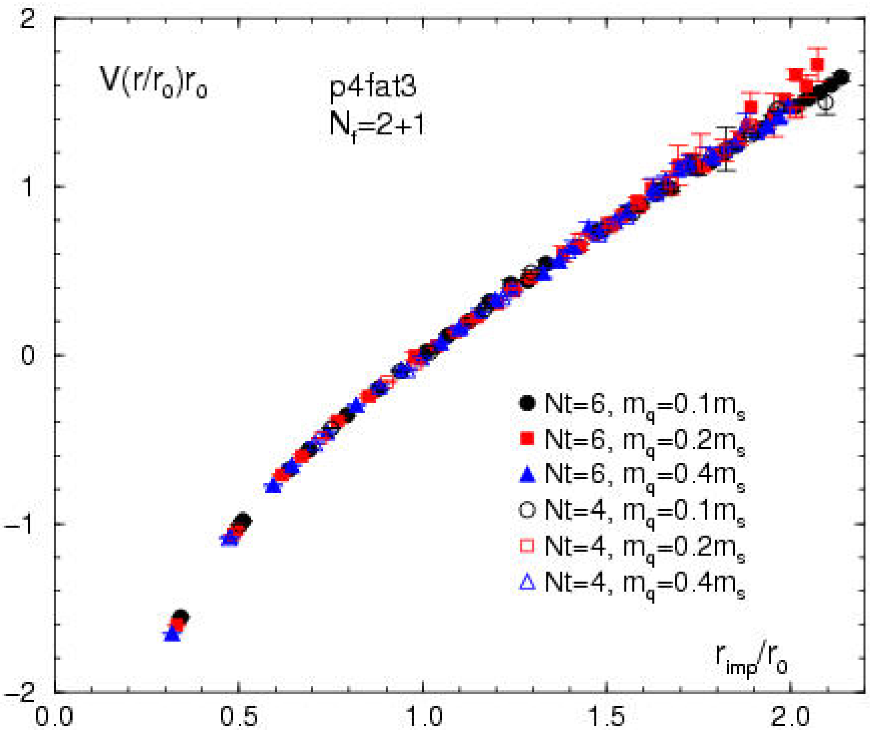
– the difference is negligible at 16^3x4 (N_s/N_t=4)
– no quark mass dependence
– the difference at 16^3x 6 are taken into account as a systematic error in β_c



Scale setting at T=0

Lattice scale is determined by a static quark potential V(r)

$$r^2 \frac{dV_{\bar{q}q}(r)}{dr}\Big|_{r=r_0} = 1.65$$



$$V_3(r) = -\frac{\alpha}{r_I} + \sigma r_I + C$$

$$V_4(r) = -\frac{\alpha}{r} + \sigma r - \alpha' \left(\frac{1}{r_I} - \frac{1}{r} \right) + C$$

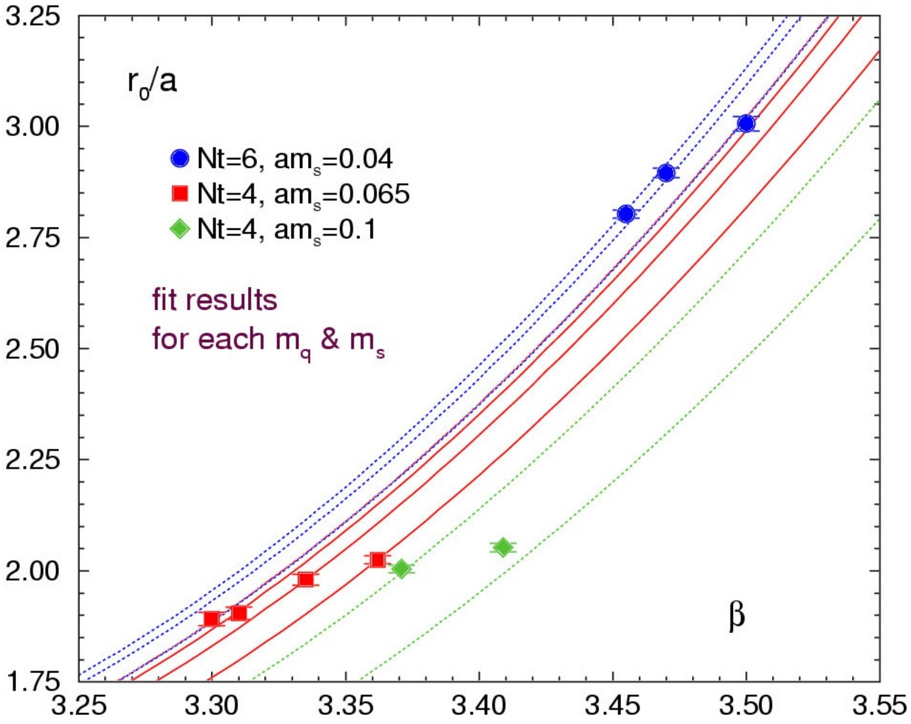
where, r_I is the improve dist.

- statistical error
  → jackknife error
- systematic errors
  → diff. between $V_3(r)$ & $V_4(r)$
  diff. in various fit range
  (r_{min}=0.15−0.3fm, r_{max}=0.7−0.9fm)

β & m_q dependence of r_0

RG inspired ansatz with 2-loop beta-function $R(\beta)$

$$(r_0/a)^{-1} = R(\beta)\left(1 + B\left(\frac{R(\beta)}{R(3.4)}\right)^2 + C\left(\frac{R(\beta)}{R(3.4)}\right)^4\right) e^{A(2\hat{m}_l + \hat{m}_s)+D}$$



$A = -1.45(5),\ \ B = 1.20(17)$

$C = \ 0.21(6),\ \ D = -2.45(5)$

$\chi^2/dof = 0.9$

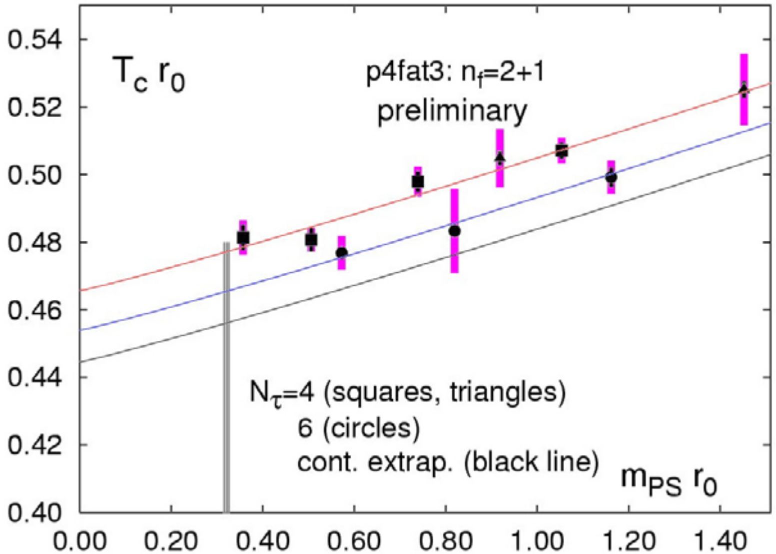
The fit result is used

(1) correction for the diff. between β_c & simulation β at T=0

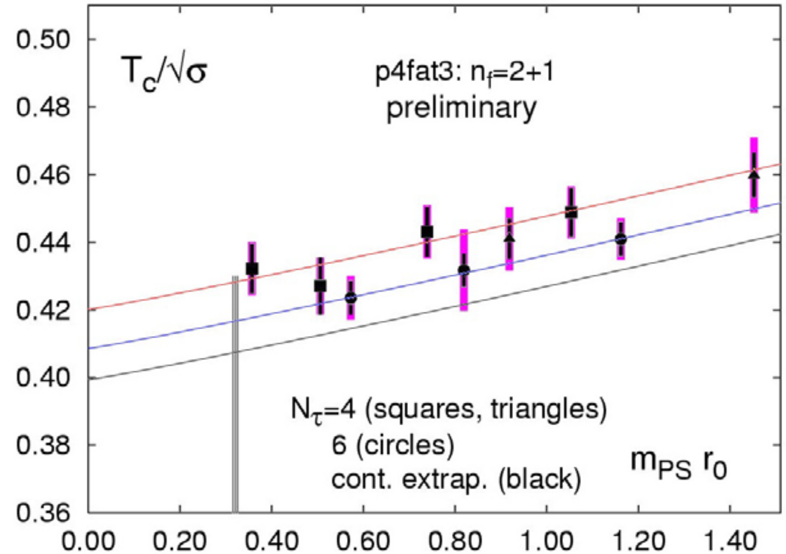
(2) conversion of sys. + stat. error of β_c into error of r_0/a

Critical temperature

ratio to Sommer scale:



ratio to string tension:



$$T_c r_0 = A(m_{ps} r_0)^d + B/N_\tau^2 + C$$ (d=1.08 from O(4) scaling)

$$T_c r_0 = 0.456(7)^{+3}_{-1}, \quad T_c/\sqrt{\sigma} = 0.408(7)^{+3}_{-1}$$ at phys. point,

(fit form dependence → d=1(lower), 2(upper) error)

Finally we obtain T_c=192(7)(4)MeV from r_0=0.469(7)fm

A. Gray et al. Phys. Rev. D72 (2005) 094507

Comment on r_0 scale setting

We use r_0 for scale setting.

■ We can, of course, use other obserbables, e.g. m_ρ

but it is difficult to control

stat. & syst. error of m_ρ on course lattice

■ r0 seems to be the best controlled lattice observable

for scale setting to determine the T_c

The physical value of r_0 have been deduced from

lattice calculations through a comparison with

bottomonium level splitting by MILC Colalb.

Phys. Rev. D70 (2004) 094505

→ also consistent with exp. value in light sector,

e.g. f_π, f_K

Equation of State

Preliminary !!

Equation of State at Nt=4 lattices (Nt=6 is on progress)

by using Integral method
on a Line of Constant Physics (LCP)

T>0 calculations are performed on 16^3x4 lattices

Temp. range is T/Tc = 0.8 – 4.3 (12 data points now)
zero temp. subtraction is calculated on 16^3x32 lattices

Contents of EoS calculation

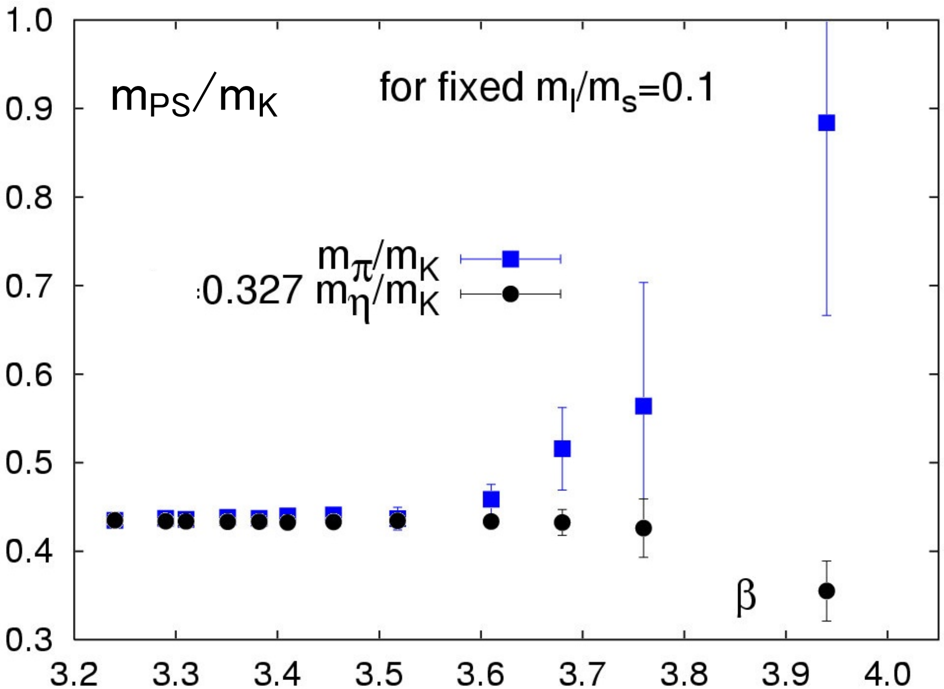
i) Line of Constant Physics
ii) Beta-functions
iii) Interaction measure & Pressure

Line of Constant Physics (LCP)

On a LCP, m_l & m_s are function of β

$\hat{m}_l = \hat{m}_l(\beta),\ \hat{m}_s = \hat{m}_s(\beta)$ ← determined by physical conditions

We define the LCP by (m_{PS}/m_K & $m_{PS}r_0$)



m_{PS}/m_K depends on only Δ

$\Delta = m_l/m_s$

We consider a LCP with (m_l, Δ)

instead of (m_l, m_s)

We assume that

Δ is constant on LCP !!

Line of Constant Physics (LCP)

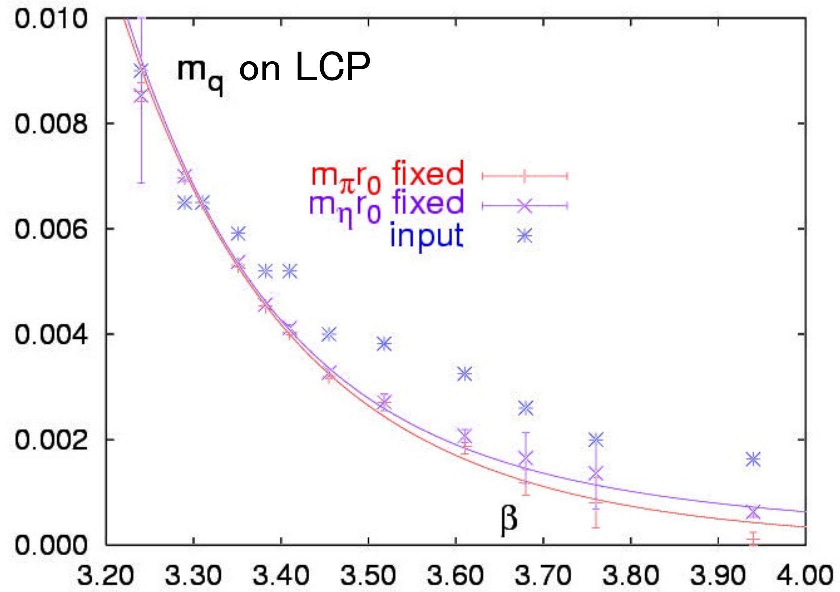
The other parameter to determin the LCP : $\hat{m}_l = \hat{m}_l(\beta)$

$\hat{m}_l$ is determined by the condition for '$m_{PS}r_0$'

We know a good parametrization:

$$m_\pi a = f(\beta)\sqrt{\hat{m}_l}$$
$$r_0/a = h(\beta)\exp\left(-A\hat{m}_l(2+\Delta)\right)$$

$\hat{m}_l$ for fixed $m_{PS}r_0$
at each β (and Δ)



fit with Allton inspired ansatz:

$$\hat{m}_l(\beta) = d_0\left(\frac{6b_0}{\beta}\right)^{-4/9} \times R(\beta)\left(1 + d_2\hat{a}^2(\beta) + d_4\hat{a}^4(\beta)\right)$$

(uncertainty remains
in a choice of fixed $m_{PS}r_0$
→ improved by tuning of input m_l)

Integral method with (m_l, Δ)

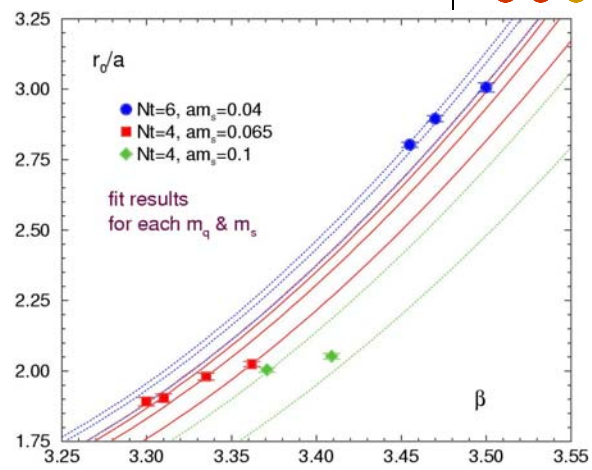
$$\left.\frac{p}{T^4}\right|_{\beta_0}^{\beta} = N_\tau^4 \int_{\beta_0}^{\beta} d\beta' \left[\frac{1}{N_\sigma^3 N_\tau} (\langle S_g \rangle_0 - \langle S_g \rangle_T) \right.$$
$$- (2(\langle\bar\psi\psi\rangle_{l0} - \langle\bar\psi\psi\rangle_{lT}) + \Delta(\langle\bar\psi\psi\rangle_{s0} - \langle\bar\psi\psi\rangle_{sT})) \left(\frac{\partial \hat m_l}{\partial \beta'}\right)_\Delta$$
$$\left. - \hat m_l \left((\langle\bar\psi\psi\rangle_{s0} - \langle\bar\psi\psi\rangle_{sT}) \right) \left(\frac{\partial \Delta}{\partial \beta'}\right)_{\hat m_l} \right]$$

$$\frac{\epsilon - 3p}{T^4} = T\frac{\mathrm{d}}{\mathrm{d}T}\left(\frac{p}{T^4}\right) = a\frac{\mathrm{d}\beta}{\mathrm{d}a}\frac{\partial p/T^4}{\partial \beta}$$
$$= \left(\frac{\epsilon - 3p}{T^4}\right)_g + \left(\frac{\epsilon - 3p}{T^4}\right)_{\hat m_l} + \left(\frac{\epsilon - 3p}{T^4}\right)_\Delta$$

$$\left(\frac{\epsilon - 3p}{T^4}\right)_g = \left(\frac{N_\tau}{N_\sigma}\right)^3 \left(\frac{d\beta}{da}\right) (\langle S_g \rangle_0 - \langle S_g \rangle_T)$$
$$\left(\frac{\epsilon - 3p}{T^4}\right)_{\hat m_l} = N_\tau^4 \left(\frac{d\beta}{da}\right) \left(\frac{\partial \hat m_l}{\partial \beta}\right) \left[2\left(\langle\bar\psi\psi\rangle_{l,0} - \langle\bar\psi\psi\rangle_{l,T}\right) + \Delta\left(\langle\bar\psi\psi\rangle_{s,0} - \langle\bar\psi\psi\rangle_{s,T}\right)\right]$$
$$\left(\frac{\epsilon - 3p}{T^4}\right)_\Delta = N_\tau^4 \left(\frac{d\beta}{da}\right) \left(\frac{\partial \Delta}{\partial \beta}\right) \left(\langle\bar\psi\psi\rangle_{s,0} - \langle\bar\psi\psi\rangle_{s,T}\right)$$

We need beta-functions : $R_\beta = \frac{d\beta}{da},\ R_{\hat m_l} = \left(\frac{\partial \hat m_l}{\partial \beta}\right)_\Delta,\ \left[R_\Delta = \left(\frac{\partial \delta}{\partial \beta}\right)_{\hat m_l} \right]$

Beta-function $-R_\beta-$



$$R_\beta = a\frac{d\beta}{da}\bigg|_{\hat{m}_l,\hat{m}_s} = \frac{a}{r_0}\left(\frac{\partial(a/r_0)}{\partial\beta}\bigg|_{LCP}\right)^{-1}$$

$$\frac{a}{r_0} = e^{A\hat{m}_l(2+\Delta)}R(\beta)\left(1 + B\hat{a}^2(\beta) + C\hat{a}^4(\beta)\right)e^D$$

$$\frac{\partial(a/r_0)}{\partial\beta} = \hat{e}(\beta)\frac{a}{r_0} + R(\beta)\left(2B\hat{e}(\beta)\hat{a}^2(\beta) + 4C\hat{e}(\beta)\hat{a}^4(\beta)\right)e^{D+A\hat{m}_l(2+\Delta)}$$

where $\hat{e}(\beta) = -\frac{1}{12b_0} + \frac{b_1}{2b_0^2\beta}$ and $\hat{a}(\beta) = R(\beta)/R(3.4)$

Finally we obtain

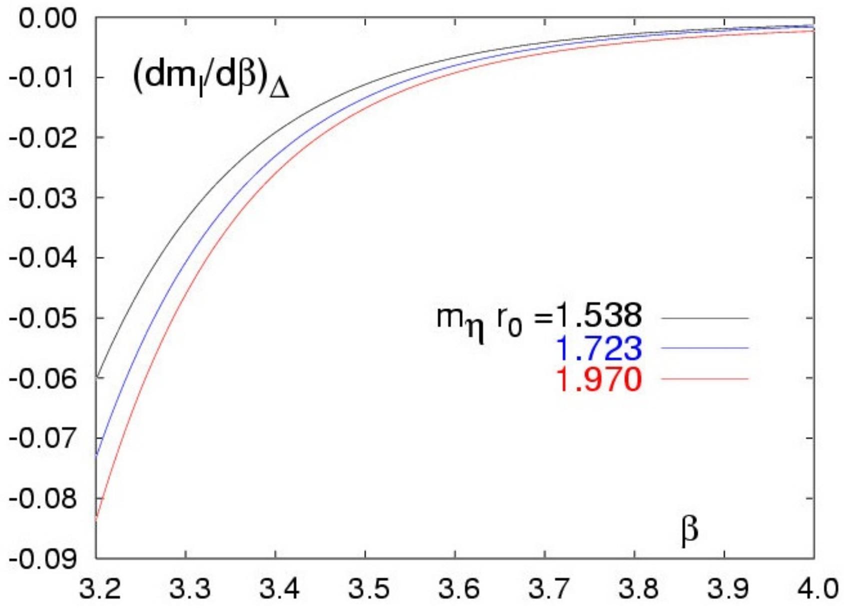
$$R_\beta = \frac{1 + B\hat{a}^2(\beta) + C\hat{a}^4(\beta)}{\hat{e}(\beta)\left(1 + 3B\hat{a}^2(\beta) + 5C\hat{a}^4(\beta)\right)}$$

Beta-function $-R_m-$

fit of m_l on LCP

Allton inspired ansatz

$$\hat{m}_l(\beta) = d_0 \left(\frac{6b_0}{\beta}\right)^{-4/9} R(\beta)\left(1 + d_2\hat{a}^2(\beta) + d_4\hat{a}^4(\beta)\right)$$

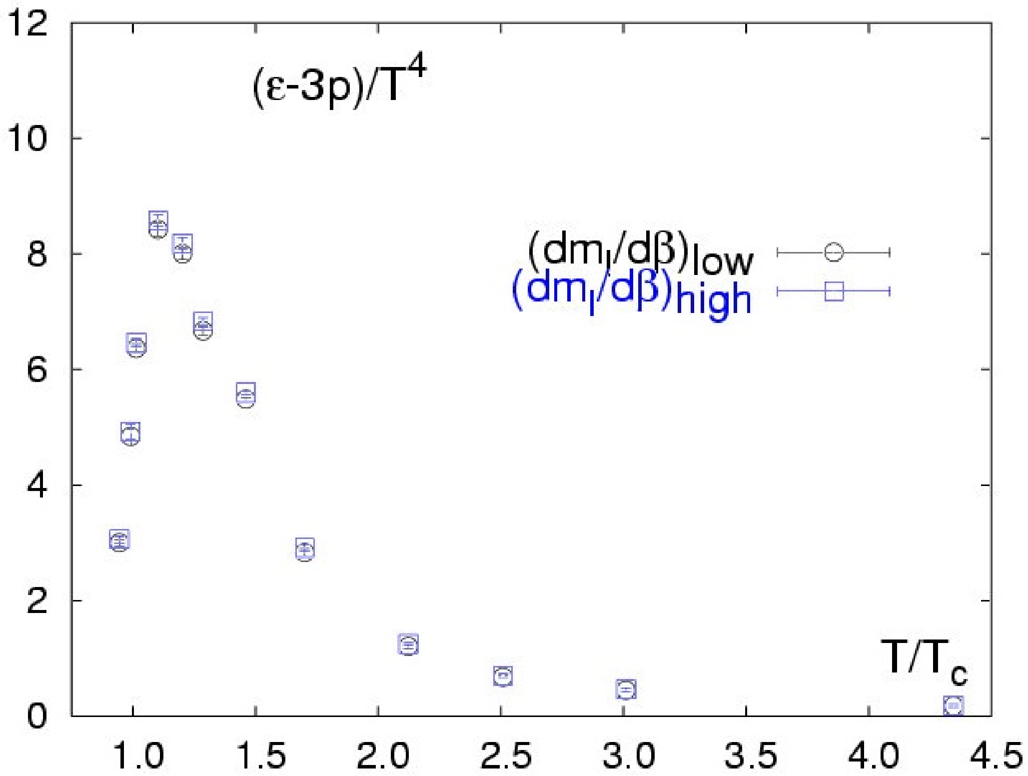


$$\left(\frac{\partial \hat{m}_l}{\partial \beta}\right)_\Delta = \hat{m}_l\left(\hat{e}_m(\beta) + \hat{e}(\beta)\frac{2d_2\hat{a}^2(\beta) + 4d_4\hat{a}^4(\beta)}{1 + d_2\hat{a}^2(\beta) + d_4\hat{a}^4(\beta)}\right)$$

where $\hat{e}_m(\beta) = -\frac{1}{12b_0} + \left(\frac{b_1}{2b_0^2} + \frac{4}{9}\right)\frac{1}{\beta}$

β	m_l	$m_\pi r_0$	$m_\eta r_0$	d_1	d_2	d_4
3.31	0.0065	0.505	1.538	0.0216	1.2087	1.9184
3.455	0.004	0.573	1.723	0.0266	1.0886	1.9267
3.61	0.00325	0.681	1.970	0.0594	0.2294	1.0679

Interaction measure



- small statistical error with current statistics

  T>0 : 10,000–30,000 traj.

  T=0 : 2,000– 9,000 traj.

- uncertainty of beta-func. is well controlled.

β	m_l	$m_\pi r_0$	$m_\eta r_0$	d_1	d_2	d_4
3.31	0.0065	0.505	1.538	0.0216	1.2087	1.9184
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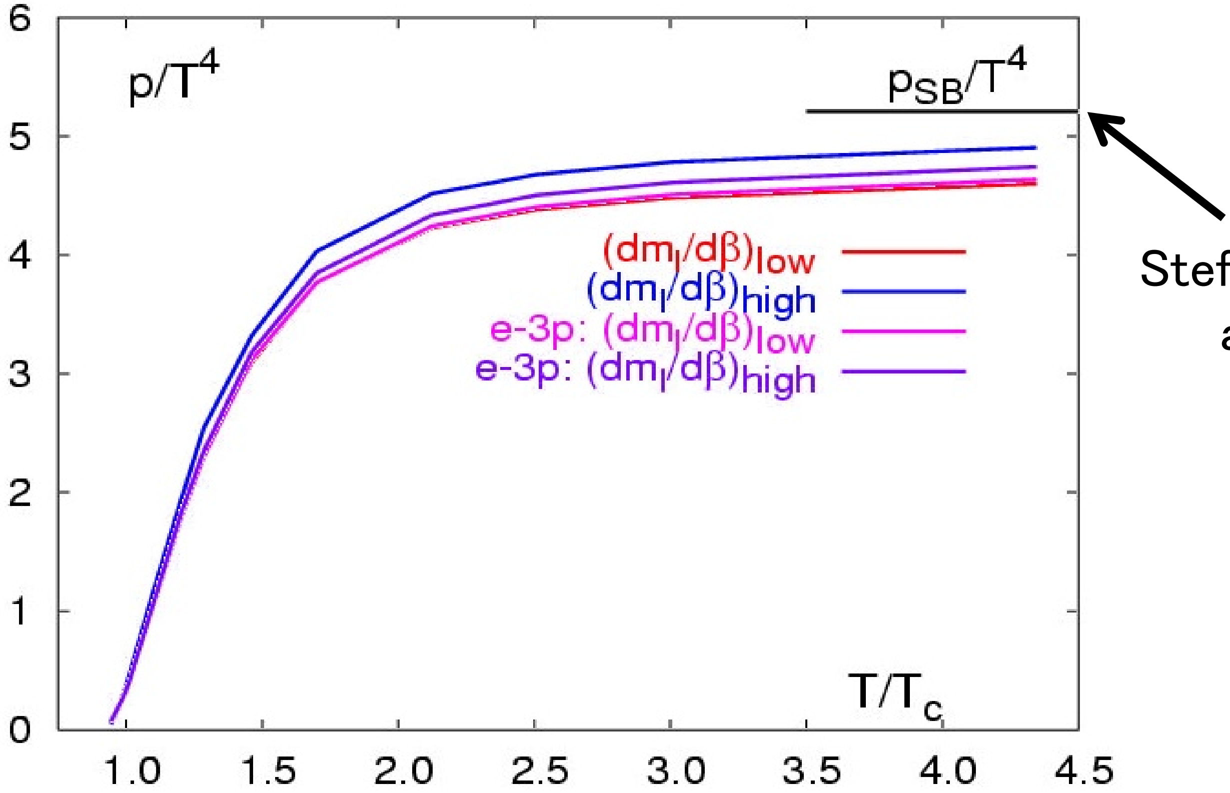
3.61	0.00325	0.681	1.970	0.0594	0.2294	1.0679

← "low" (β = 3.31)

← "high" (β = 3.61)

Pressure



Stefan Boltzmann limit at continuum

$(dm_l/d\beta)$: $\left.\frac{p}{T^4}\right|_{\beta_0}^{\beta} = \frac{1}{VT^3}\int_{\beta_0}^{\beta} d\beta' \left[\frac{\partial \ln Z}{\partial \beta'} + \frac{\partial \ln Z}{\partial \hat{m}_l}\frac{\partial \hat{m}_l'}{\partial \beta'}\right]$

e−3p: $(dm_l/d\beta)$: $\left.\frac{p}{T^4}\right|_{T_0}^{T} = \int_{T_0}^{T} dT' \left(\frac{\epsilon - 3p}{T'^3}\right) = \int_{T_0}^{T} dT' \frac{d}{dT'}\left(\frac{p}{T'^4}\right)$

Conclusion

N_f=2+1 simulation with almost realistic quark masses at N_t=4, 6

- critical temperature

  $T_c r_0$=0.456(7), (T_c=192(7)(4)MeV from r_0=0.469(7)fm)

  – $T_c r_0$ is consistent with previous p4 result
    difference in T_c mainly comes from physical value of r_0
  – however, our value is about 10% larger than MILC result
    and about 30% larger than Fodor et al. result
  – most systematic uncertainties are taken into account
    remaining uncertainty is in continuum extrapolation

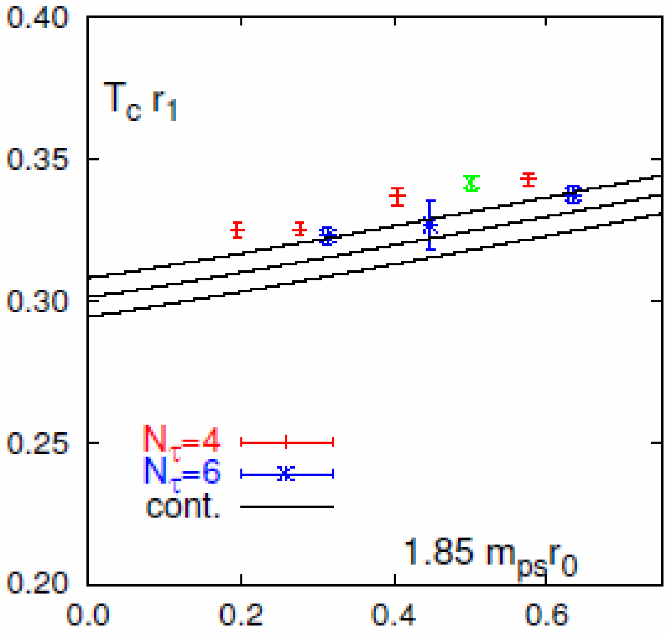
- Equation of state
  – We calculate EoS on a Line of Constant Physics at Nt=4
  – using $\Delta = m_l/m_s$
  – Nt=6 is on progress

appendix

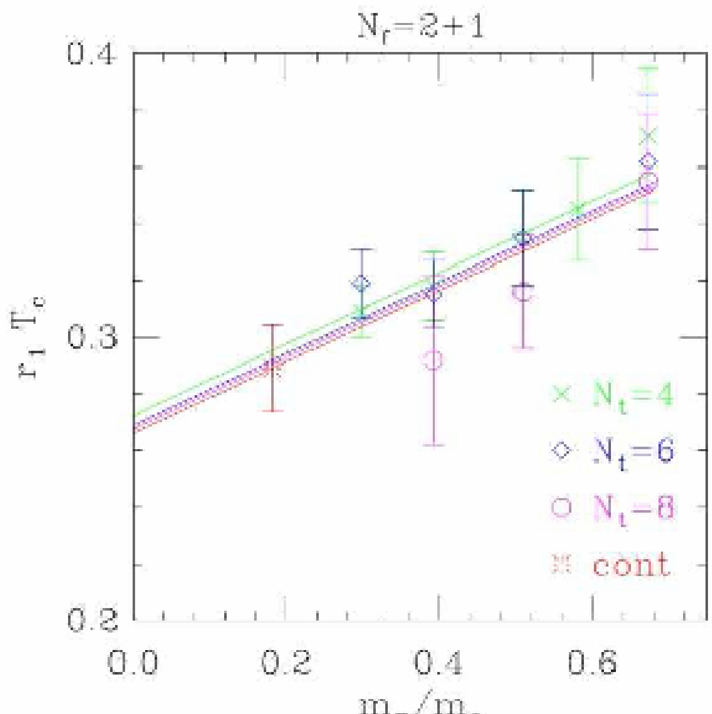
A new determination of the transition temperature in QCD

- calculation of transition temperature with almost physical quark masses and different lattice cut-off values

  $\Rightarrow$ extrapolation to physical limit ($m_\pi = 135$ MeV) and continuum limit ($a \rightarrow 0$)



RIKEN-BNL-Columbia-Bielefeld



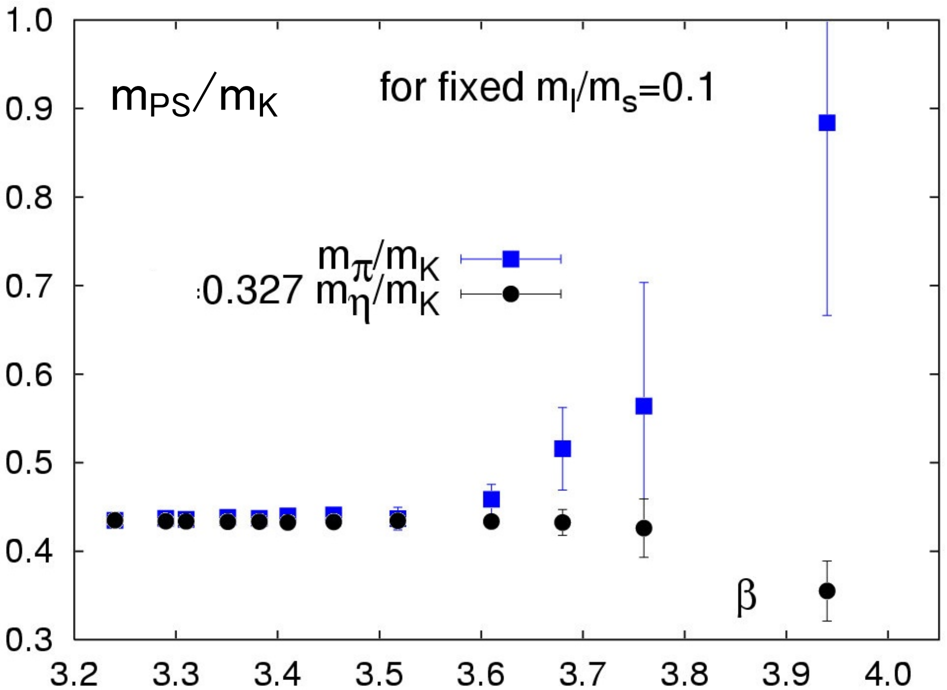
MILC, PRD71 (2005) 034504 (figure unpublished)

Line of Constant Physics (LCP)

On a LCP, m_l & m_s are function of β

$\hat{m}_l = \hat{m}_l(\beta), \ \hat{m}_s = \hat{m}_s(\beta)$ ← determined by physical conditions

We define the LCP by (m_{PS}/m_K & $m_{PS}r_0$)



m_{PS}/m_K depends on only Δ

$\Delta = m_l/m_s$

We consider a LCP with (m_l, Δ) instead of (m_l, m_s)

We assume that Δ is constant on LCP !!