The QCD transition temperature from simulations on BlueGene L supercomputer at LLNL

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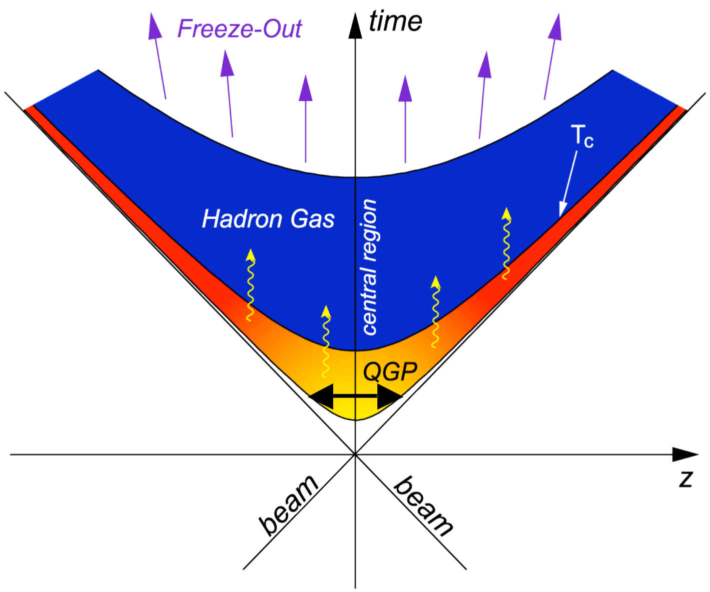
The HotQCD collaboration

(All HotQCD data are preliminary)

RHIC: What we don't know a priori

- The nature (order) of the transition between hadronic matter and QGP
- The transition temperature T_c
- The equation of state (at $< T_c$- 5 T_c)
- The transport properties of the QGP
- Behavior of bound states (onia) in the QGP
- Collective excitations
- The process of hadronization
- The process of thermalization



QCD at finite temperature

HotQCD Collaboration: A unique US wide opportunity for simulating QCD at finite temperature using the BlueGene L Supercomputer at LLNL

- T. Battacharya (LANL)
- M. Cheng (Columbia)
- N. Christ (Columbia)
- C. DeTar (Utah)
- S. Gottlieb (Indiana)
- R. Gupta (LANL)
- U. Heller (APS)
- K. Huebner (BNL)
- C. Jung (BNL)
- F. Karsch (BNL/Bielefeld)
- E. Laermann (Bielefeld)
- L. Levkova (Utah)
- T. Luu (LLNL)
- R. Mawhinney (Columbia)
- P. Petreczky (BNL)
- D. Renfrew (Columbia)
- C. Schmidt (BNL)
- R. Soltz (LLNL)
- W. Soeldner (BNL)
- R. Sugar (UCSB)
- D. Toussaint (Arizona)
- P. Vranas (LLNL)

Timeline

- **Developed collaboration with Ron Soltz and formulated project for *Blue Gene L* at LLNL (Nov-Dec 2005)**
- **Organized US wide meeting to explore doing RHIC phenomenology and Lattice QCD at LLNL (Feb 06)**
- **Developed white paper for calculation of T_c and EOS on the *Blue Gene L* (Feb – May 06)**
- **Got NNSA approval to run on *Blue Gene L* (July 06)**
- **Ported Asqtad and p4fat codes to *Blue Gene L* (Sept 06)**
- **Started N_T=8 lattice QCD simulations (Oct 06)**
- **Continual code Optimization**
- **~10,000 trajectories simulated at 15β for AsqTad & p4**

Restrictive Environment

- **Only T. Luu, R. Soltz and R. Gupta can access the machine or the data**
- **Minimal data can be brought into open**
  - **Print results in ASCI or print figures**
  - **Declassify**
  - **Scan to convert to digital for distribution**

Blue Gene L at LLNL represents a 4-6 Teraflops sustained resource

HotQCD Collaboration: Goals

- **Nature of the transition**
  - **Do deconfinement and χS restoration “coincide”?**
- **Transition temperature Tc**
- **Equation of State (EOS) at (μ=0, $\mu\neq$0)**
- Spectral Functions
- Spatial and temporal correlators versus T
- Transport coefficients of the quark gluon plasma

Order of the transitions and T_c

- Look for discontinuities, singularities, peaks in thermodynamics quantities
  - Polyakov line and its susceptibility
  - Chiral condensate $\langle \bar{\psi}\psi \rangle$ and its susceptibility
  - Quark number $\langle \bar{\psi}\gamma_0\psi \rangle$ and its susceptibility

- Finite size scaling analysis (1^{st} versus 2^{nd})

Previous Staggered simulations →
For 2+1 (ud, s) quark flavors
the transition is a crossover

Observables

Polyakov loop
Quark number susceptibility

} **Deconfinement**

Chiral condensate
Chiral susceptibility

} **χS Restoration**

Issues with previous calculations (in 2005)

- Calculations on coarse lattices: N_T=4,6 and/or small volumes. (a ~ 0.2- 0.13 fermi).
  - Simulate N_T=4,6,8, … and do a→0 extrapolation

- T_c with different actions (different observables) differ by ~ 20 MeV
  - Reduce uncertainty to ~ 5 MeV if transition T is unique

- Need simulations with 2+1 flavors with realistic light (up, down) quark masses holding strange quark mass fixed
  - M_{ud} / m_s = 0.5, 0.2, 0.1 → (physical ~ 0.04)

- Staggered fermions ($\det M^{1/4}$): Creutz/Kronfeld at LAT07

Improving continuum limit results

- Control discretization errors (compare 2 different improved staggered actions)
  - Asqtad Staggered (MILC collaboration)
  - p4 staggered (RBC-Bielefeld collaboration)
  - Explore Domain wall fermions
- New simulations at N_T=8 with 2+1 flavors ($m_{light} \approx 0.1\ m_s$)
- Combine with ongoing/previous N_T = 4,6 simulations to perform $a \rightarrow 0$ extrapolation
- Precise determination of lattice scale

Status report:
HOTQCD data sets

P4 action N_τ=8 simulations: Status 7/21/07

- Lattice Size 8×32×32×32
- Quark mass $m_l/m_s = 0.1$

β	$a\ m_l$	T [MeV]	# trajectories
3.460	0.00313	154	10000
3.490	0.00290	169	10000
3.510	0.00259	179	11280
3.540	0.00240	194	11440
3.570	0.00212	209	12460
3.600	0.00192	225	11790
3.630	0.00170	241	12070
3.660	0.00170	256	11190
3.690	0.00150	271	10760
3.760	0.00139	313	10920
h3.525	0.00240	186	6510
h3.530	0.00240	189	5450
h3.535	0.00240	191	5140
h3.540	0.00240	194	5410
h3.545	0.00240	196	6280
h3.550	0.00240	199	5790
c3.525	0.00240	186	6120
c3.530	0.00240	189	5530
c3.535	0.00240	191	5750
c3.540	0.00240	194	6260
c3.545	0.00240	196	6250
c3.550	0.00240	199	6520

Asqtad action data set as of 7/21/07

Lattice Size 8×32×32×32; Quark mass $m_l/m_s = 0.1$

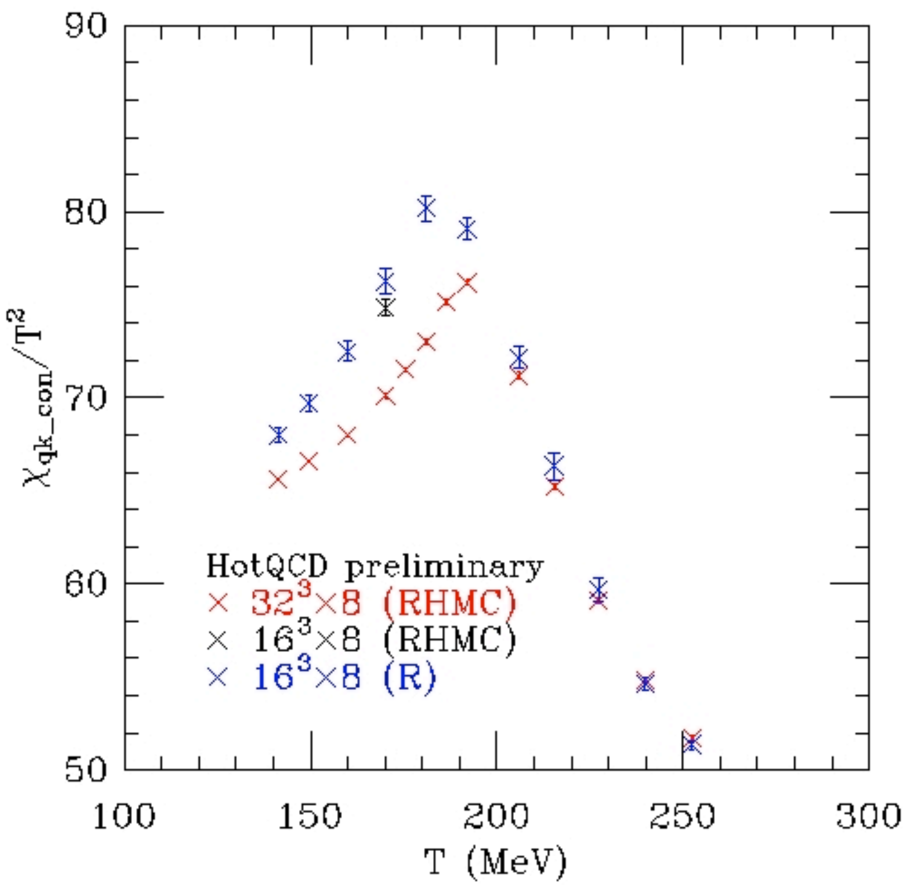
$\beta = 6/g^2$	δt	Acceptance	$\langle \Delta s \exp(-\Delta s/2) \rangle 10^3$		Total # trajectories
6.4580	0.04170	0.66	-4.9 +/-	9.4	12965
6.5000	0.04170	0.72	3.7	7.6	12990
6.5500	0.04170	0.76	-4.5	5.8	12720
6.6000	0.04170	0.78	-1.5	5.9	12405
6.6625	0.04170	0.79	8.1	5.2	12365
6.6500	0.04540	0.76	2.8	6.8	12445
6.6675	0.04540	0.75	3.9	6.1	12660
6.7000	0.04540	0.81	-9.7	5.8	12320
6.7600	0.04540	0.83	2.0	4.2	12530
6.8000	0.04540	0.84	-3.4	4.3	12195
6.8500	0.04540	0.86	2.2	3.3	12405
6.9000	0.04540	0.86	3.4	3.2	12470
6.9500	0.04540	0.86	1.5	3.6	12625
7.0000	0.04540	0.87	-2.9	3.0	12595
7.0800	0.04540	0.86	3.6	3.0	12790

About 70% of target 15000 trajectories (statistics) achieved

AsqTad calculations and deductions

R algorithm and finite size effects

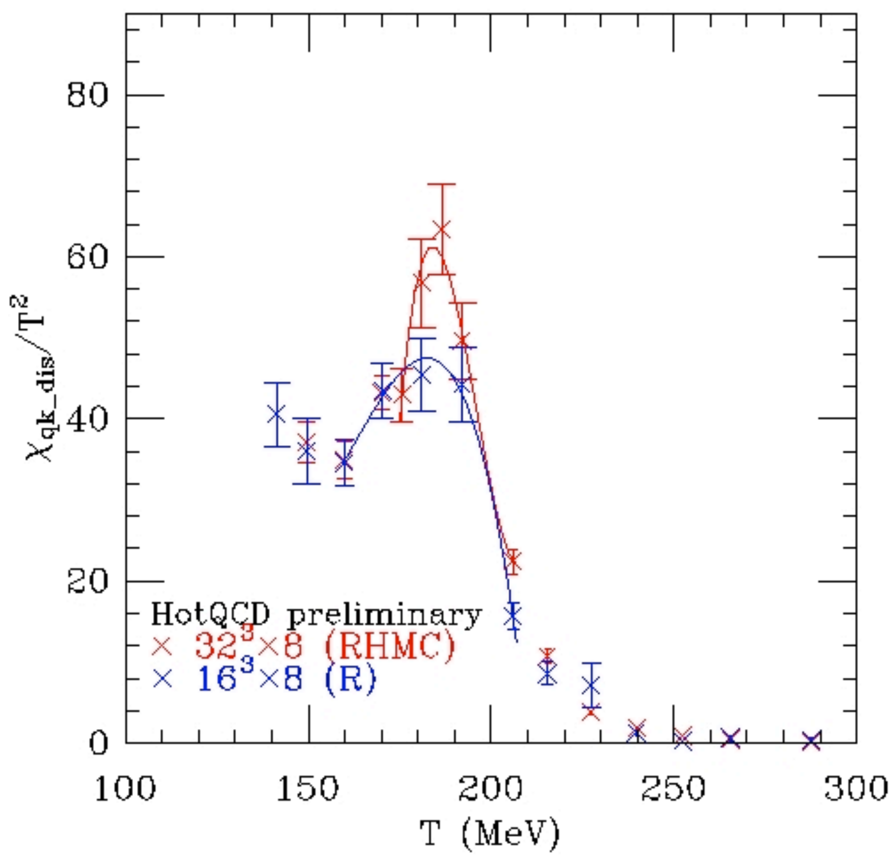
(Connected Chiral Susceptibility)



- Errors in data with R algorithm are small (below resolution)
- Finite size effects are most pronounced at low T

Finite volume correction:

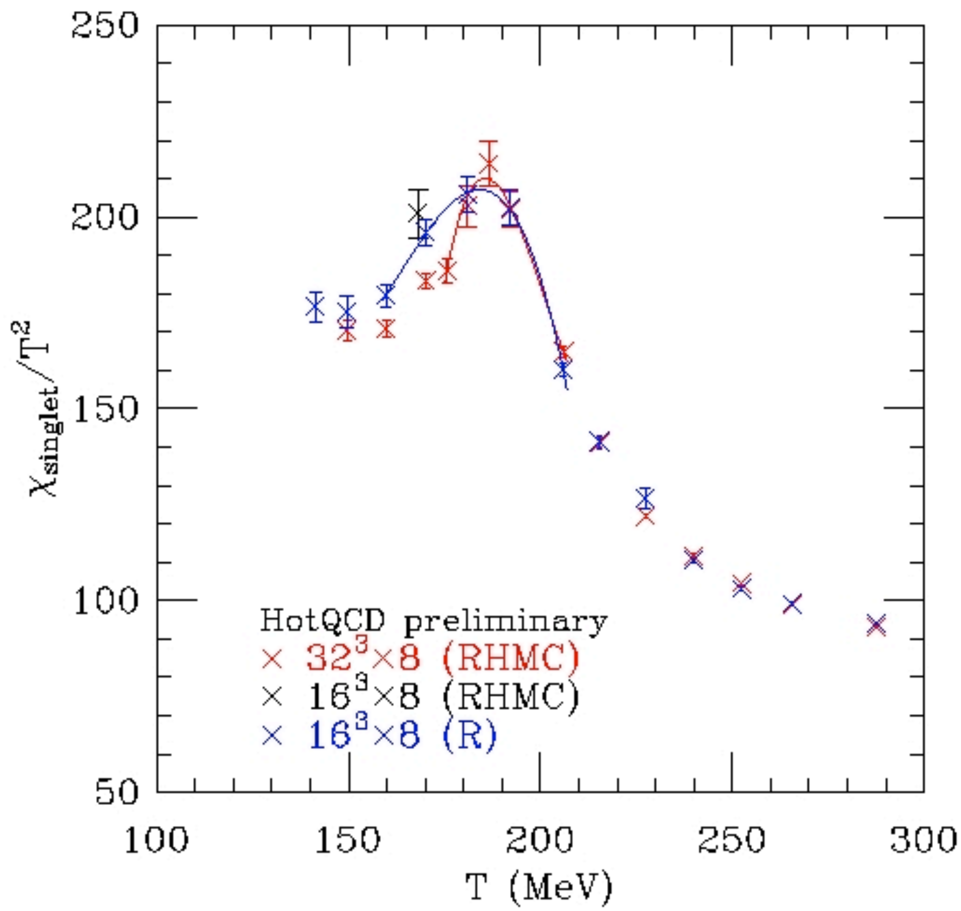
(Disconnected chiral susceptibility)



Large spatial volume is important.

Ns = 4 Nτ ≈ infinite volume

Singlet chiral susceptibility



Finite size effect tends to decrease Tc slightly

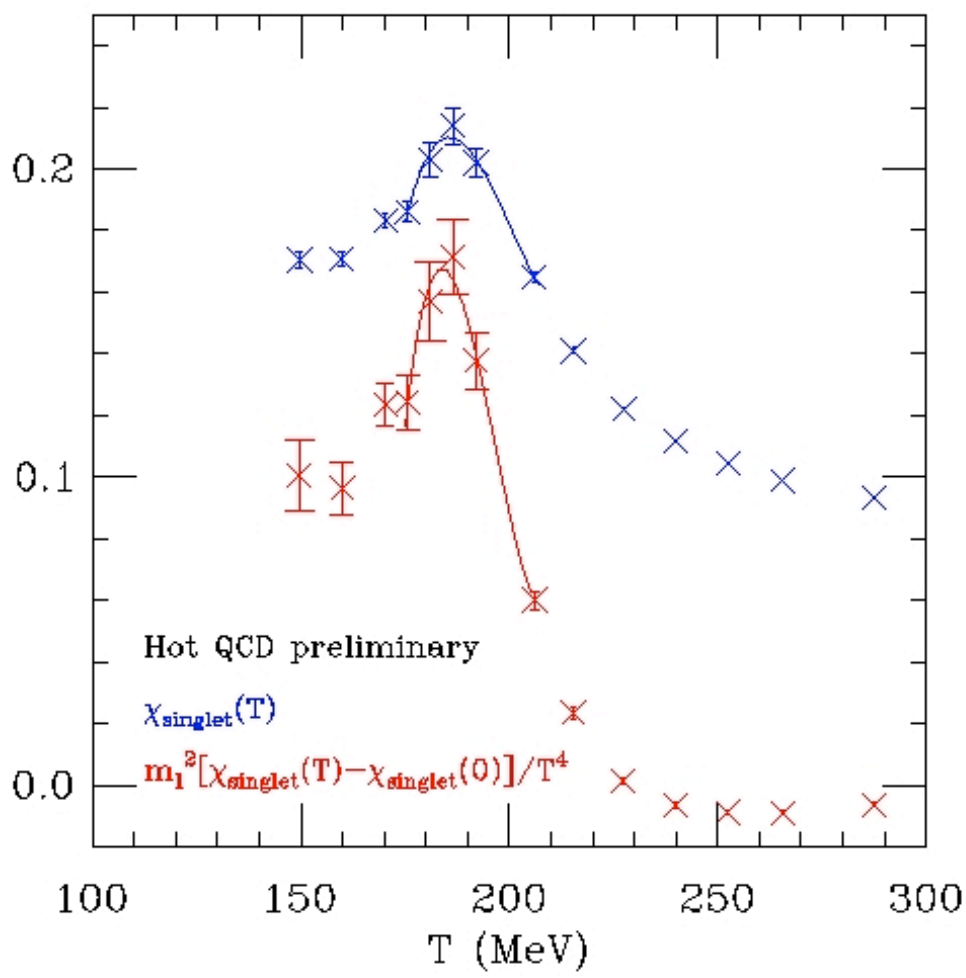
16^3: 184(2)MeV

32^3: 186(2)

Errors shown are only statistical for this fit ansatz!

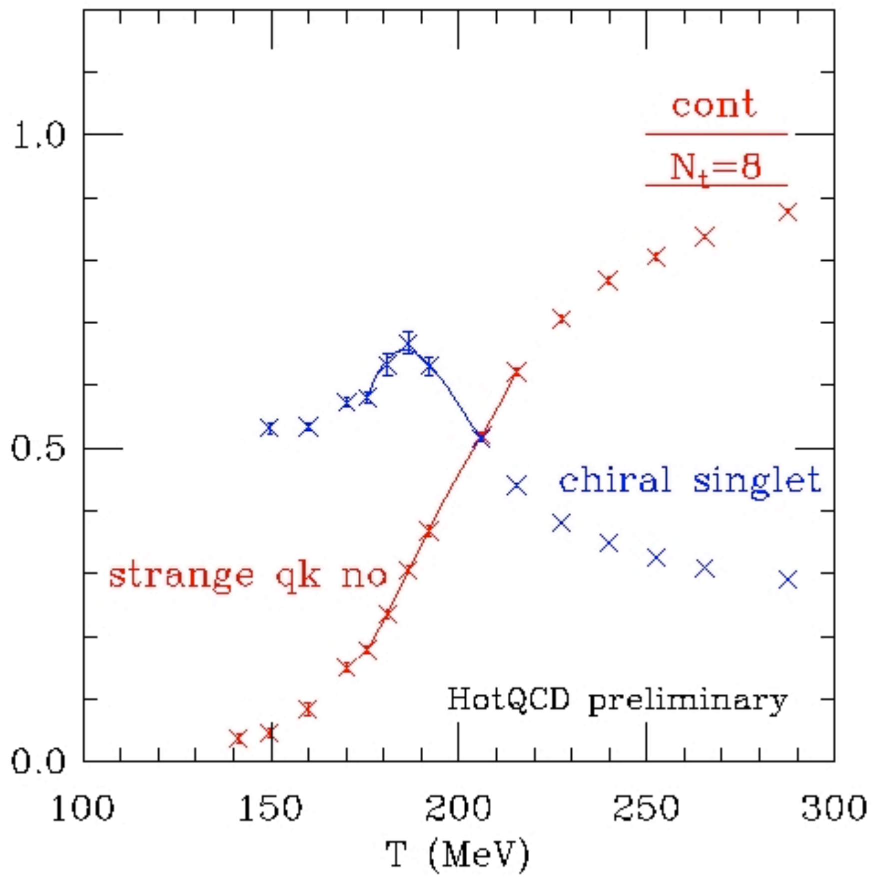
Systematic errors yet to be determined.

Renormalized singlet susceptibility (Raw versus Wuppertal-Budapest method)



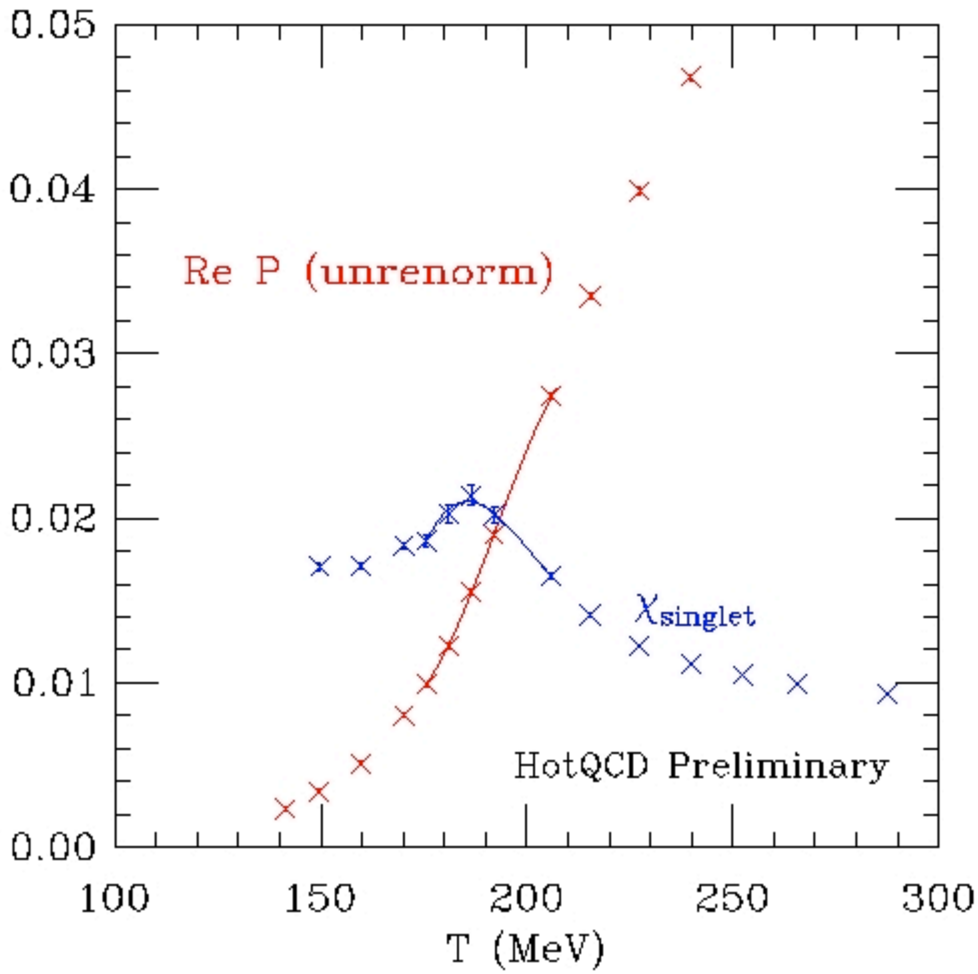
Small (few MeV) difference in peak position

Strange quark number susceptibility



It is more difficult to estimate Tc from fits to determine the inflection point than from a peak.

Polyakov Loop Data



Inflection point in P is difficult to locate accurately

Peak in susceptibility of P hard to distinguish from a plateau/shoulder by N_τ=8.

Data with p4 action

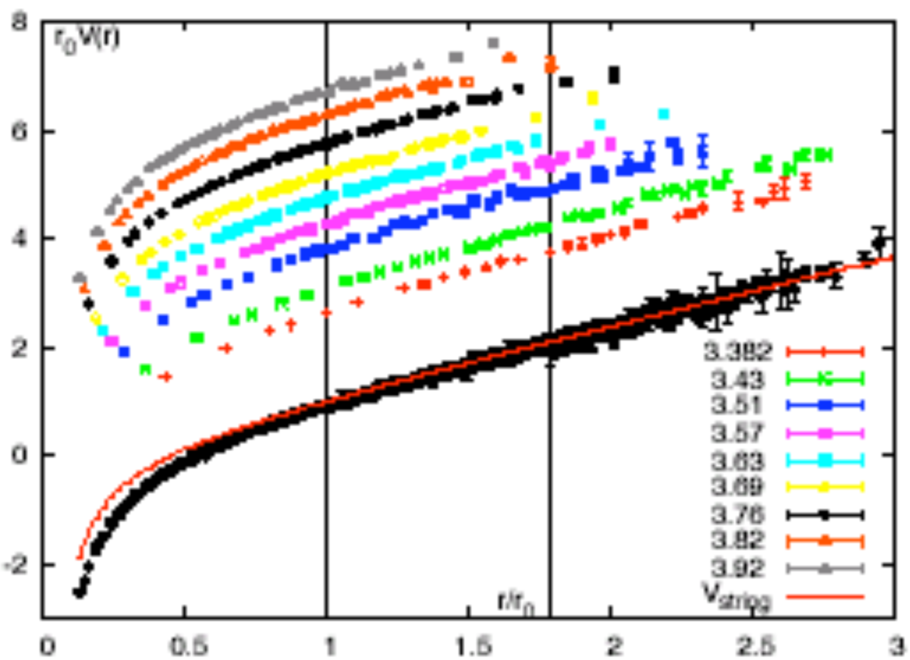
P4: **Line of constant physics (LCP)**

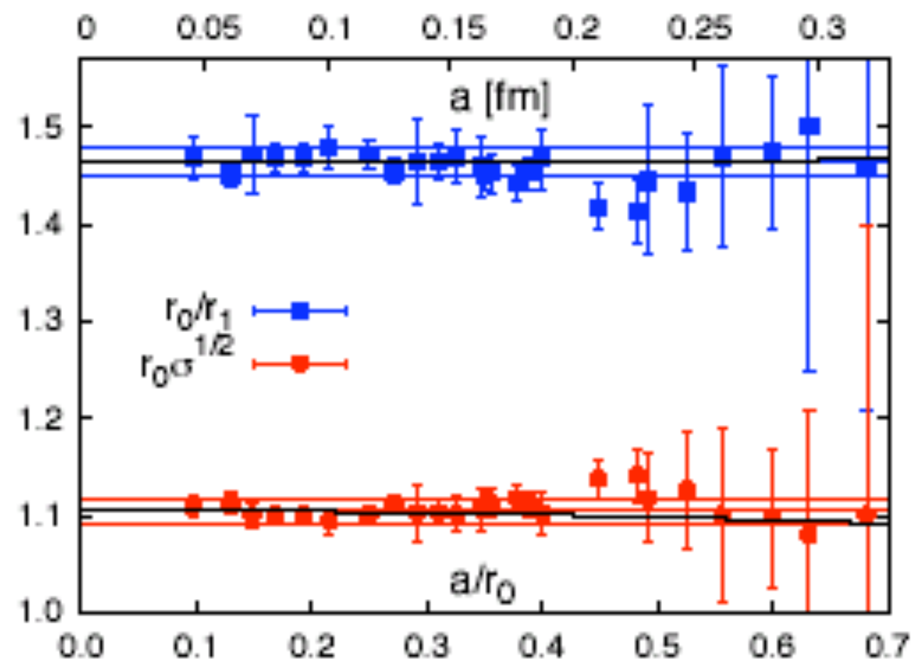
- Use T=0 simulations
- **$M_{ss}\, r_0 = 1.58$ ($M_\pi\, r_0 \approx 0.52 \rightarrow M_\pi \approx 220$ MeV)**
- Quark mass $m_l/m_s = 0.1$ (real world ~0.04)
- Take $a \rightarrow 0$ along this LCP varying just the gauge coupling β

P4: Setting the lattice scale

Jan van der Heide at LAT2007

$$\left(r^2 \frac{dV_{\bar{q}q}(r)}{dr} \right)_{r=r_0} = 1.65 \quad , \quad \left(r^2 \frac{dV_{\bar{q}q}(r)}{dr} \right)_{r=r_1} = 1.0$$



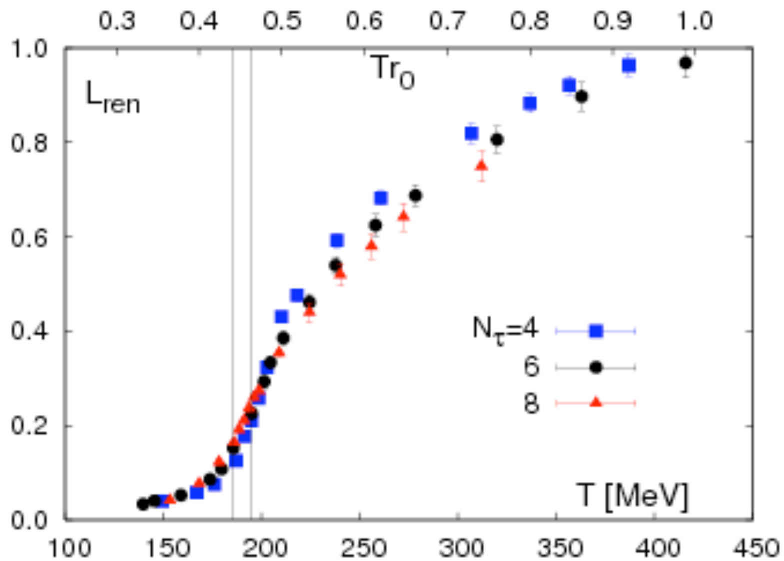


r_0=0.469(7) fm, $r_0\ \sigma^{0.5}$ =1.104(5), r_0/r_1 =1.463(7)

Renormalized Polyakov Loop

$$\langle L_R \rangle = Z(\beta)^{N_\tau} \langle L_{Bare} \rangle$$

(Kostya Petrov at LAT07)



- Smooth behavior
- $N\tau$ = 4,6,8 don't show large $O(a^2)$ effects

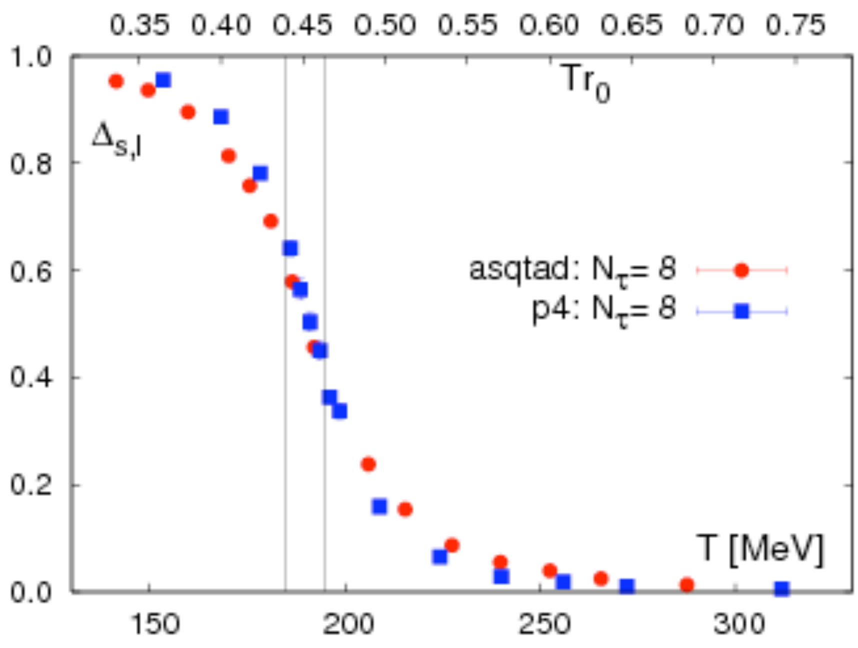
In all figures the band corresponds to the range T=185-195 MeV

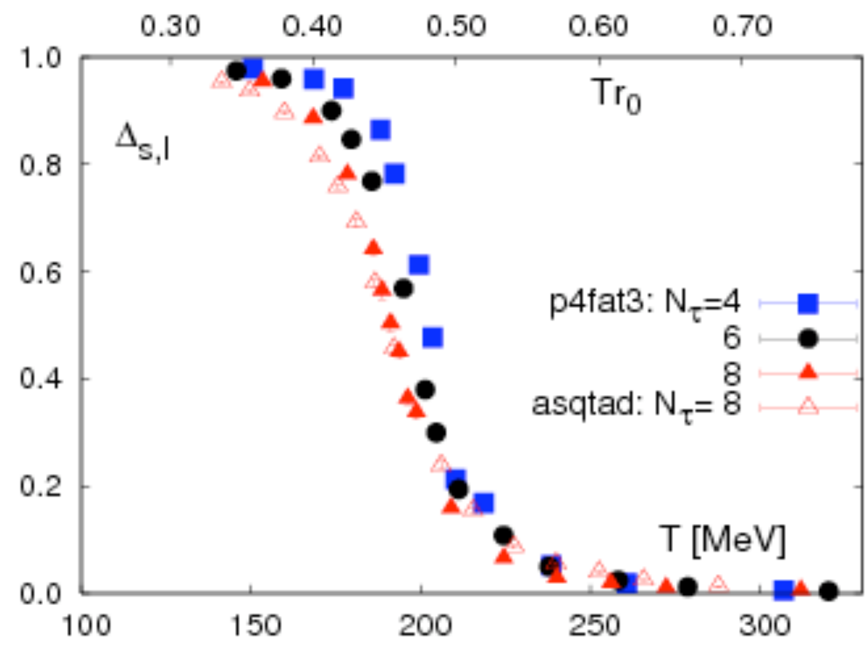
Chiral Condensate: χS restoration

$$\Delta_l = \frac{\langle \bar{l} l \rangle_T - \frac{m_l}{m_s} \langle \bar{s} s \rangle_T}{\langle \bar{l} l \rangle_{T=0} - \frac{m_l}{m_s} \langle \bar{s} s \rangle_{T=0}}$$

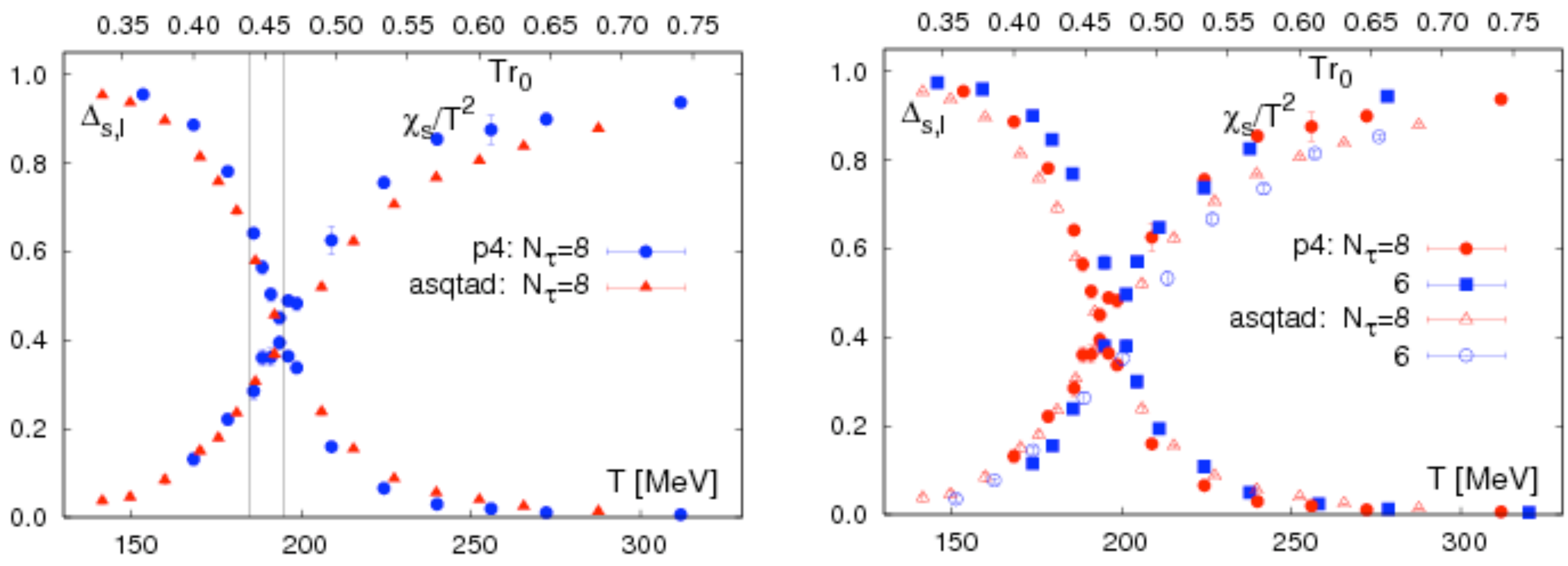
- Subtraction to eliminate additive renormalization
- Sharp decrease in Δ reflects χS restoration

N_τ=8: P4 consistent with AsqTAD





$T_{\chi S\ \text{Restoration}} \approx T_{\text{Deconfinement}}$



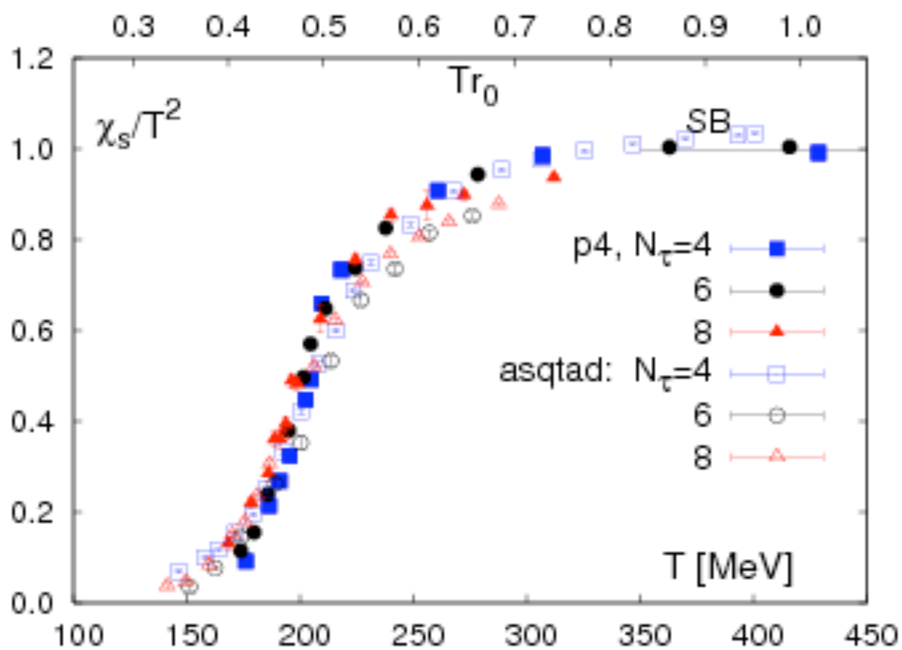
Quark Number Susceptibility

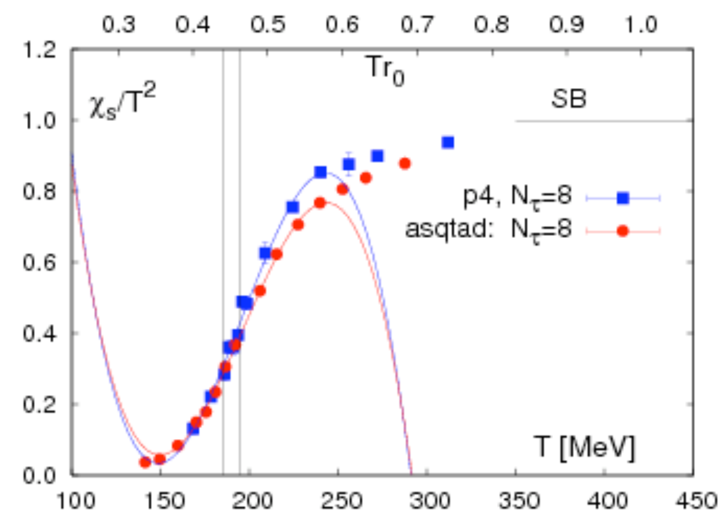
$$\frac{\chi_{l,s}}{T^2} = \frac{1}{TV}\frac{\partial^2 \log Z}{\partial \mu_{l,s}^2}$$

- States carrying such quantum numbers ($\langle\bar{\psi}\gamma_0\psi\rangle$ → **baryon number/strangeness)** are heavy at low T and light at high T. Probe confinement
- Do not require renormalization at $V=\infty$
- Peak in fourth derivative!

Quark Number Susceptibility

P4 data consistent with AsqTAD



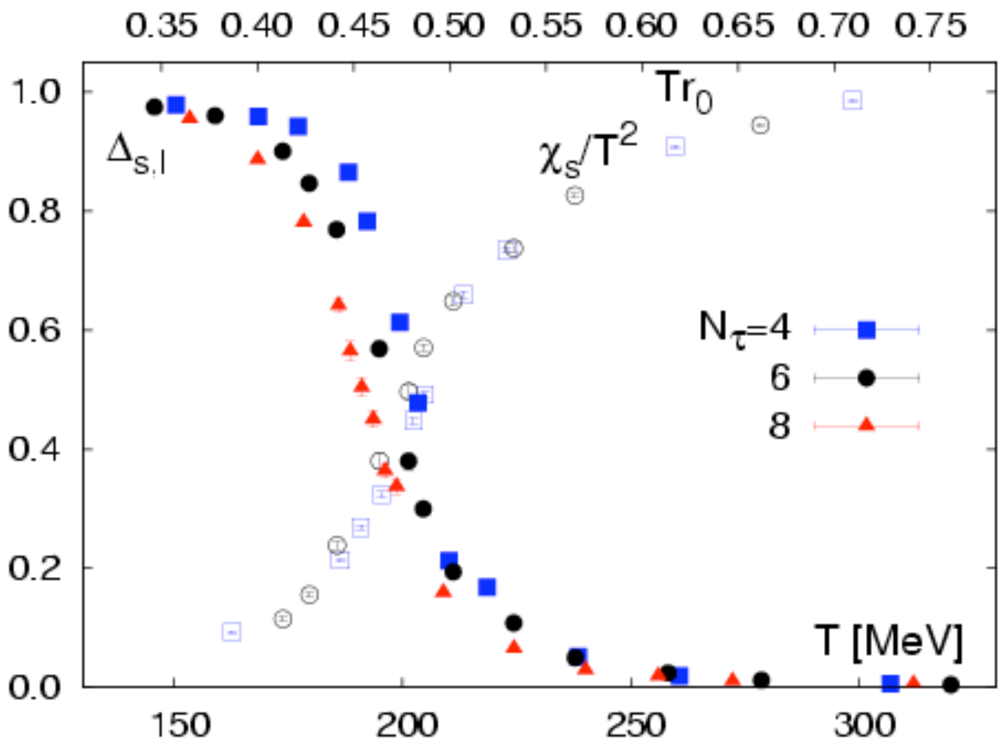


Determination of Tc from inflection point sensitive to

- Range of data points included in the fit (8 points)
- Fit function

$\Delta_{s,l}$ and χ_s/T^2

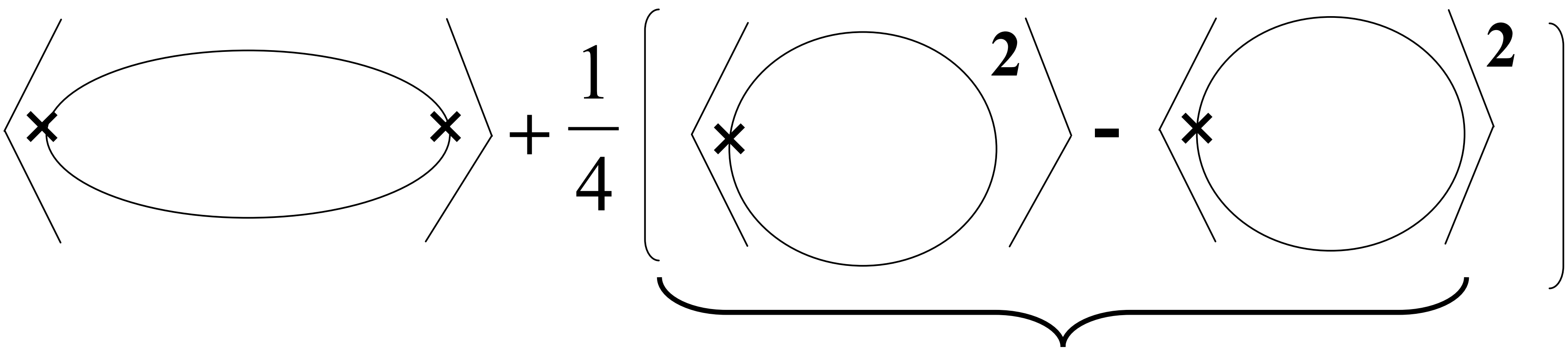
- Smooth behaviour
- $N\tau$ = 4,6,8 don't show large $O(a^2)$ effects
- Crossover at roughly the same T



Chiral Susceptibility: $N_\tau = 4, 6, 8$

One flavor susceptibility for light (l = u,d) and strange (s) quarks:

$$\frac{\chi_{l,s}}{T^2} = \frac{T}{V}\frac{\partial^2 \log Z}{\partial^2 m_{l,s}^2} = \left\langle Tr(M_{l,s}^{-2})\right\rangle + \frac{1}{4}\left(\left\langle (TrM_{l,s}^{-1})^2\right\rangle - \left\langle TrM_{l,s}^{-1}\right\rangle^2\right)$$

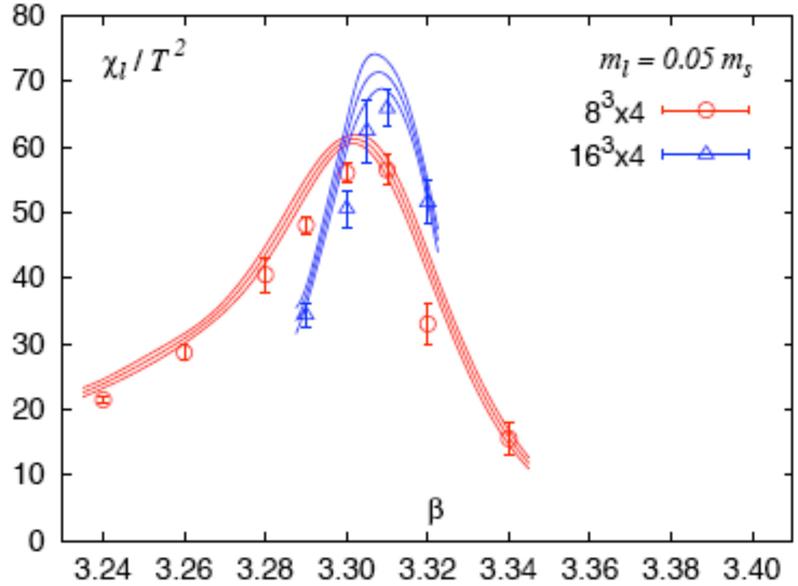


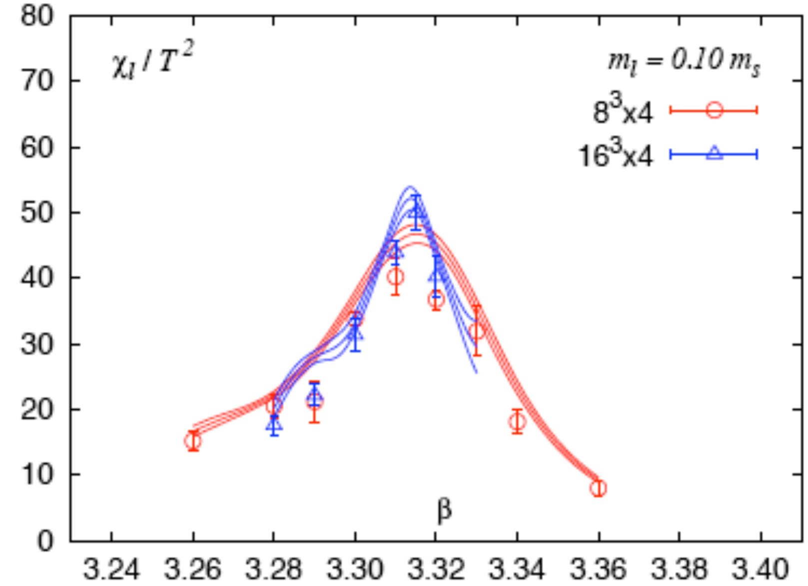
Connected **Disconnected**

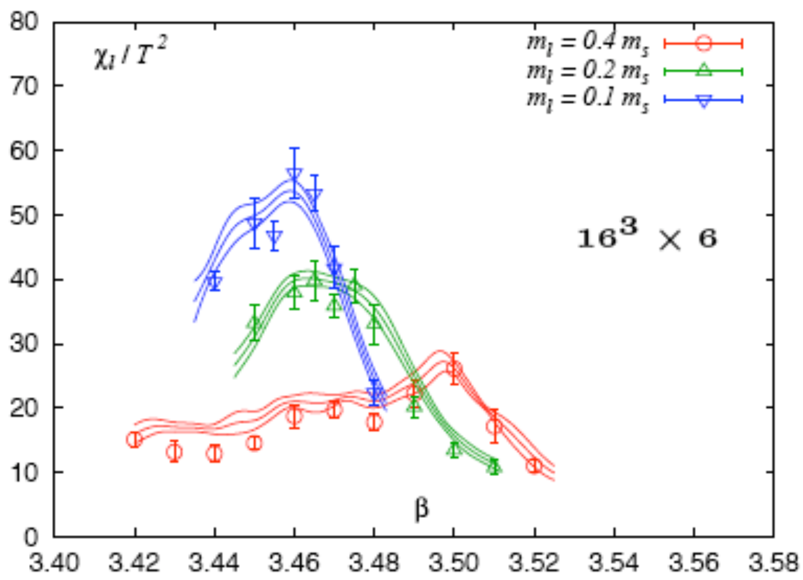
Note: Isosinglet $\chi = \chi_{\text{disconnected}} + 2\chi_{\text{connected}}$

One flavor $\chi = \chi_{\text{disconnected}} + 4\chi_{\text{connected}}$

p4 (RBC-B) analysis

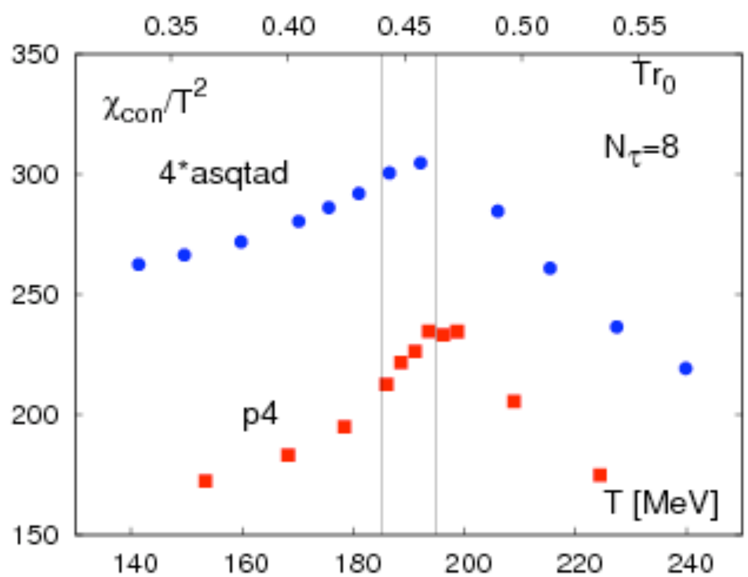




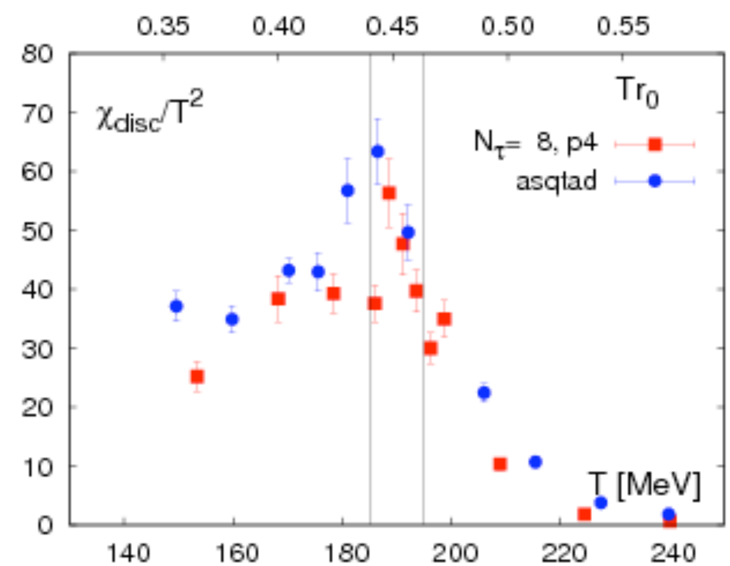


- Very Weak Volume dependence → Crossover
- Peaks become sharper with increasing V and decreasing quark mass
- Peak shift towards smaller β

Chiral Susceptibility: $N_\tau = 8$



Connected

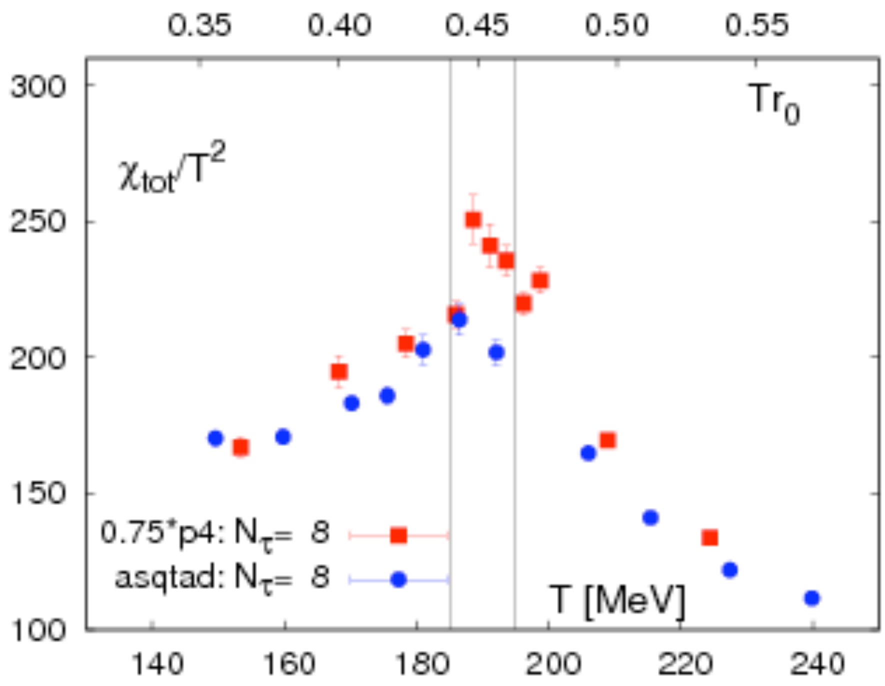


Disconnected

Chiral Susceptibility χ: $N_\tau = 8$

Total Susceptibility for light (l = u,d) quarks:

Unrenormalized ⇒ only examine shape not value



Need more N_t=8 data to quantify [dis]agreement in the region of the peak before combining with N_t=4, 6 to extract T_c(a=0)

HotQCD: Future

- Complete N_τ=8 simulations
- Finish analysis of all the variables
- Combine N_τ=4,6,8 calculations
- Extract transition temperature at which bulk quantities show largest fluctuations
- Resolve Deconfinement versus χS restoration

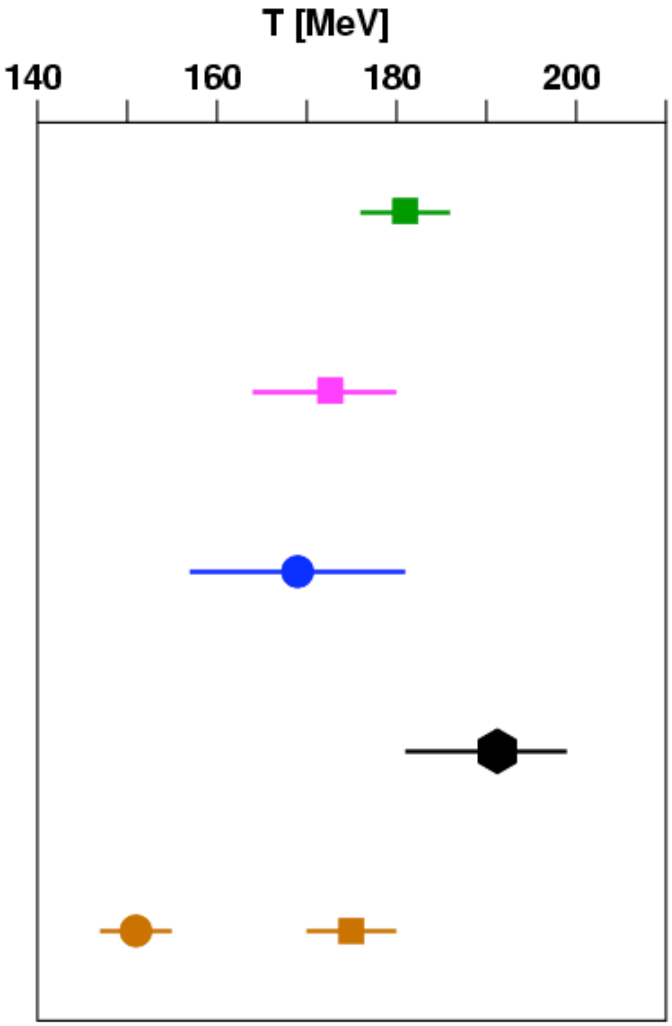
Much progress with staggered 2+1 simulations in last 2 years

- Exact Algorithm -- RHMC
- Finite Volume
  - $N_s \geq 4 N_\tau$
  - Peaks become sharper with larger V
  - Height approx. independent of V (→ crossover)
- Renormalization of observables
- Improvement of action works
  - (N_τ =6,8) P4 and AsqTad ≈ (N_τ=8,10) Stout
- Reaching physical masses
  - P4 and AsqTad (ml = 0.1ms); Stout (ml=0.04ms)
- Setting the scale with T=0 simulations
  - Using r_0, f_K (~10 MeV difference)
- Continuum extrapolations (N_τ=4,6,8,….)

Remaining Issues

- Resolving $T_{deconfinement}$ and $T_{\chi SB}$ in $a \rightarrow 0$
- Improve determination of lattice scale

Fodor etal: different observables give different T_c



use T=0 scale: r0=0.469fm

Nf=2:

V.G. Bornyakov et al, POS Lat2005, 157 (2006)
(improved Wilson, Nt=8, 10; input: r0=0.5 fm)
(rescaled to r0)

Y. Maezawa et al., hep–lat/0702005 (QM'2006)
(improved Wilson, Nt=4, 6; input: m–rho)
(no cont. exp. yet)

Nf=2=1:

C. Bernard et al., Phys.Rev. D71, 034504 (2005)
(improved staggered (asqtad), Nt=4,6,8, input r1)
(rescaled to r0)

M. Cheng et al., Phys.Rev D74, 054507 (2006)
(improved staggered (p4), Nt=4,6; input r0)

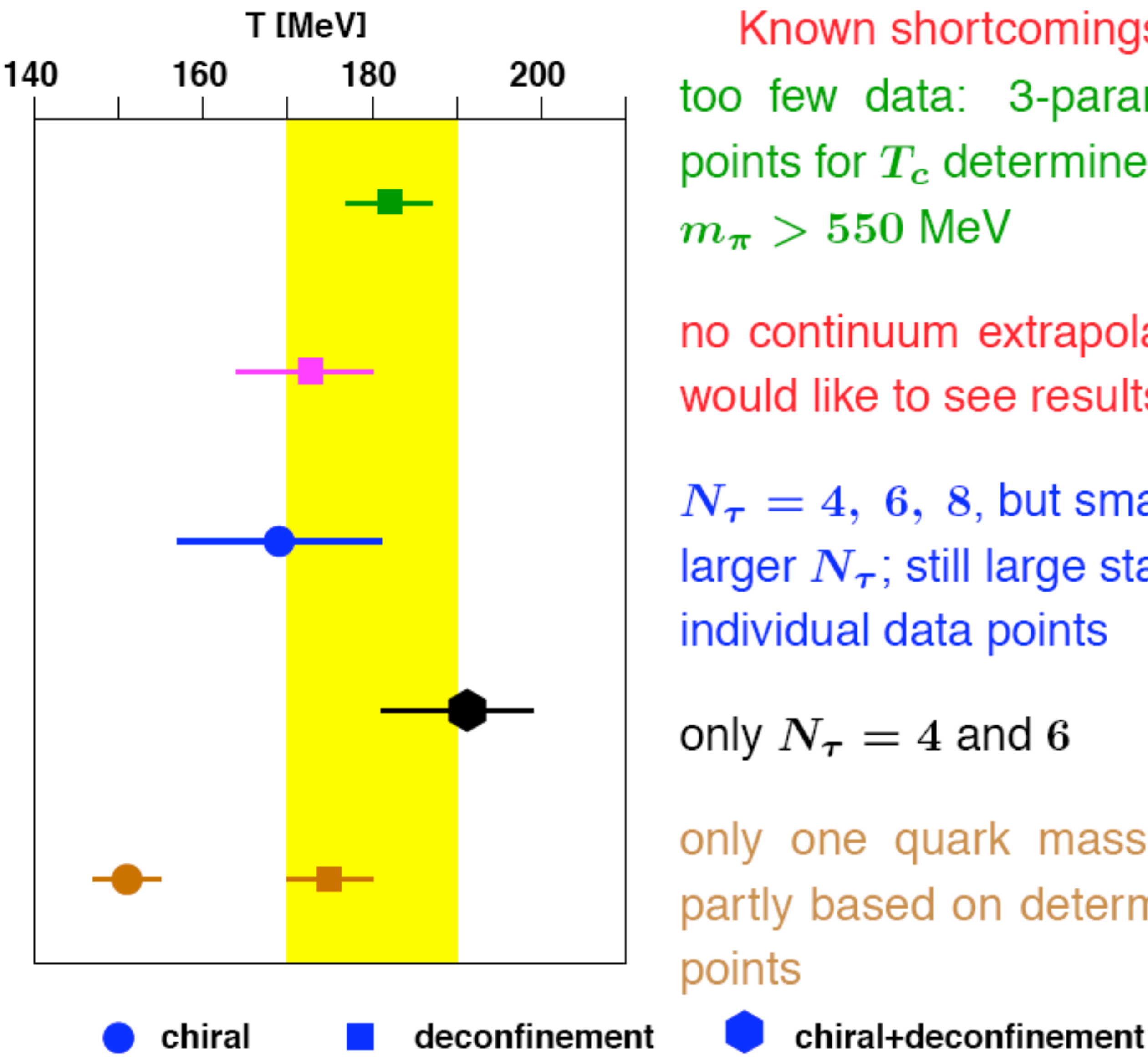
Y. Aoki et al., Phys. Lett. B643, 46 (2006)
(staggered (stout), Nt=4,6,8,10; input fK)
(converted to r0)

● chiral ■ deconfinement ⬢ chiral+deconfinement

Important for RHIC

$\epsilon_c \sim T_c^4$ ⟹ $\epsilon_c = (0.3 - 1.0)\mathrm{GeV/fm}^3$

Issues with "best" calculations



Known shortcomings:

too few data: 3-parameter fit to 4 data points for T_c determined at $m_\pi > 550$ MeV

no continuum extrapolation attempted yet; would like to see results in units of r_0

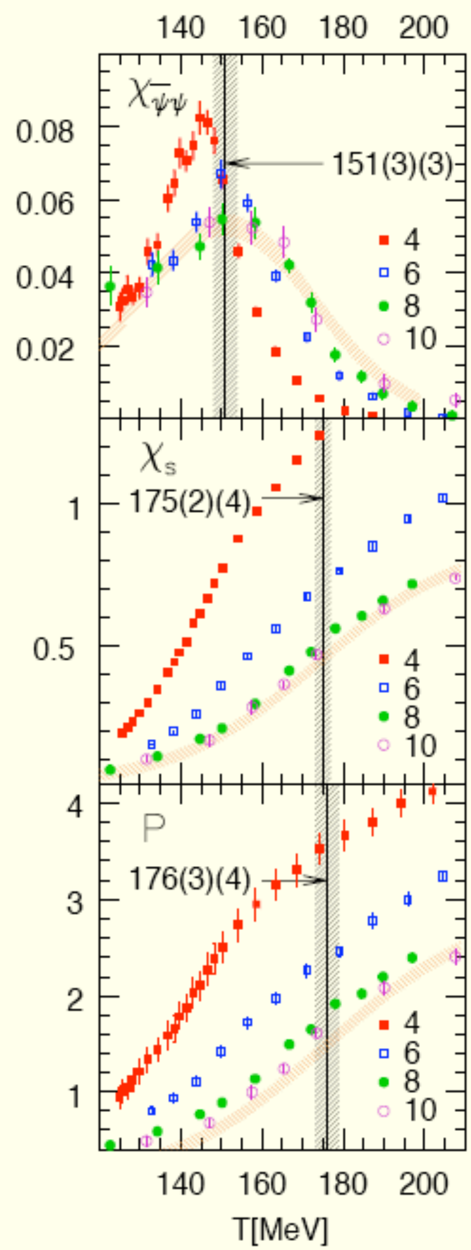
$N_\tau = 4,\ 6,\ 8$, but small spatial volume for larger N_τ; still large statistical errors on individual data points

only $N_\tau = 4$ and 6

only one quark mass; T_c determination partly based on determination of inflection points

Karsch Lat07

Stout Action: Summary (Fodor LAT2007)



Chiral susceptibility

T_c=151(3)(3) MeV

ΔT_c=28(5)(1) MeV

Quark number susceptibility

T_c=175(2)(4) MeV

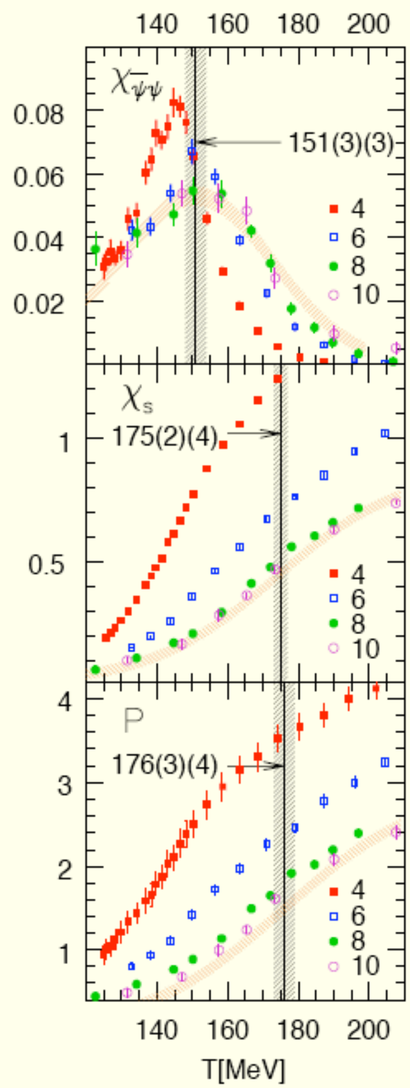
ΔT_c=42(4)(1) MeV

Polyakov loop

T_c=176(2)(4) MeV

ΔT_c=38(5)(1) MeV

Stout Action versus p4/AsqTad



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Polyakov loop

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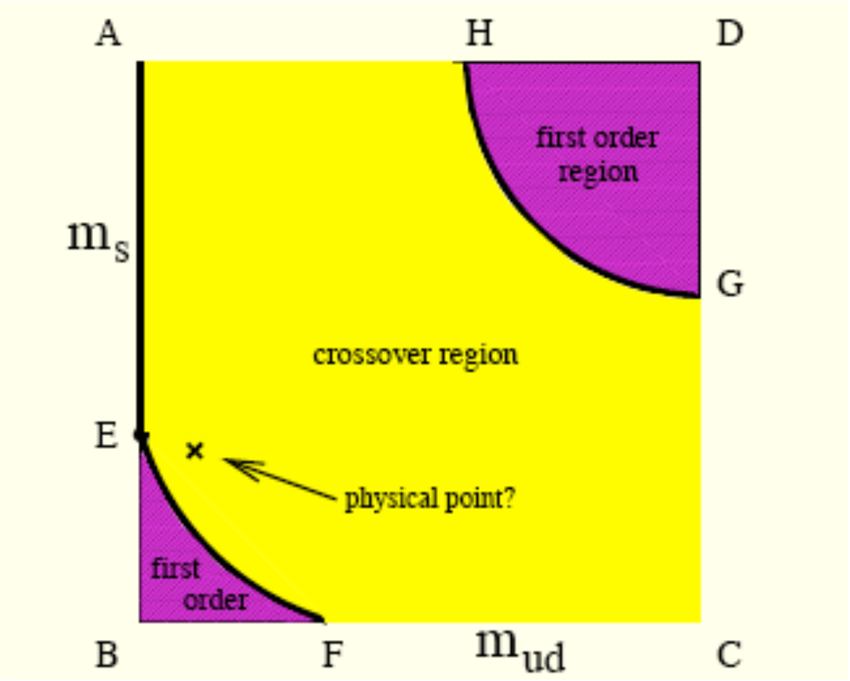
ΔT_c=38(5)(1) MeV

Main disagreement with p4 & AsqTad

Tc determined from inflection point

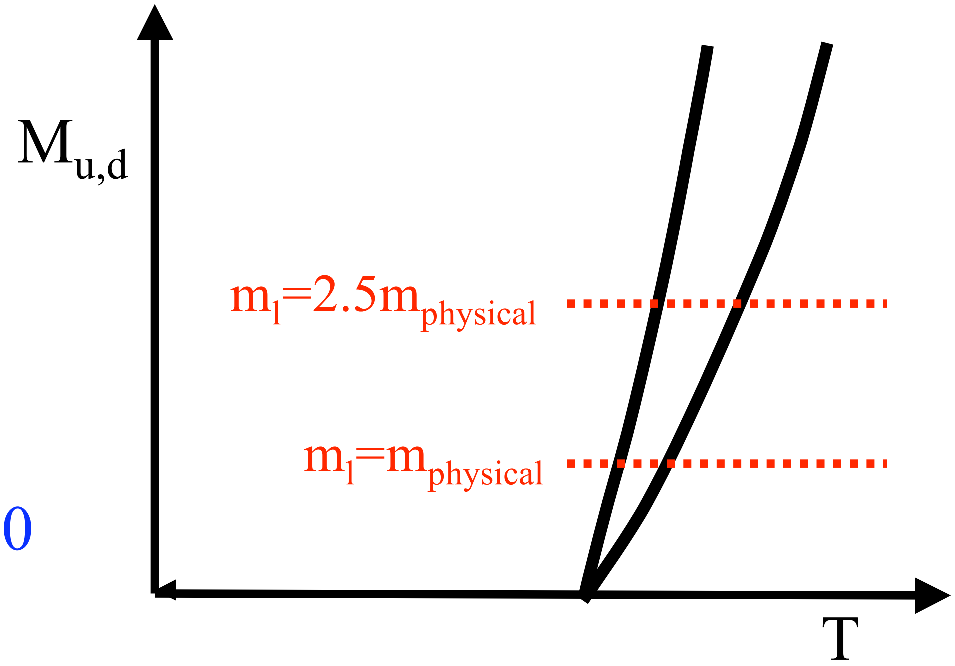
Issues in Crossover phenomena

(emphasized by Y. Aoki etal.)

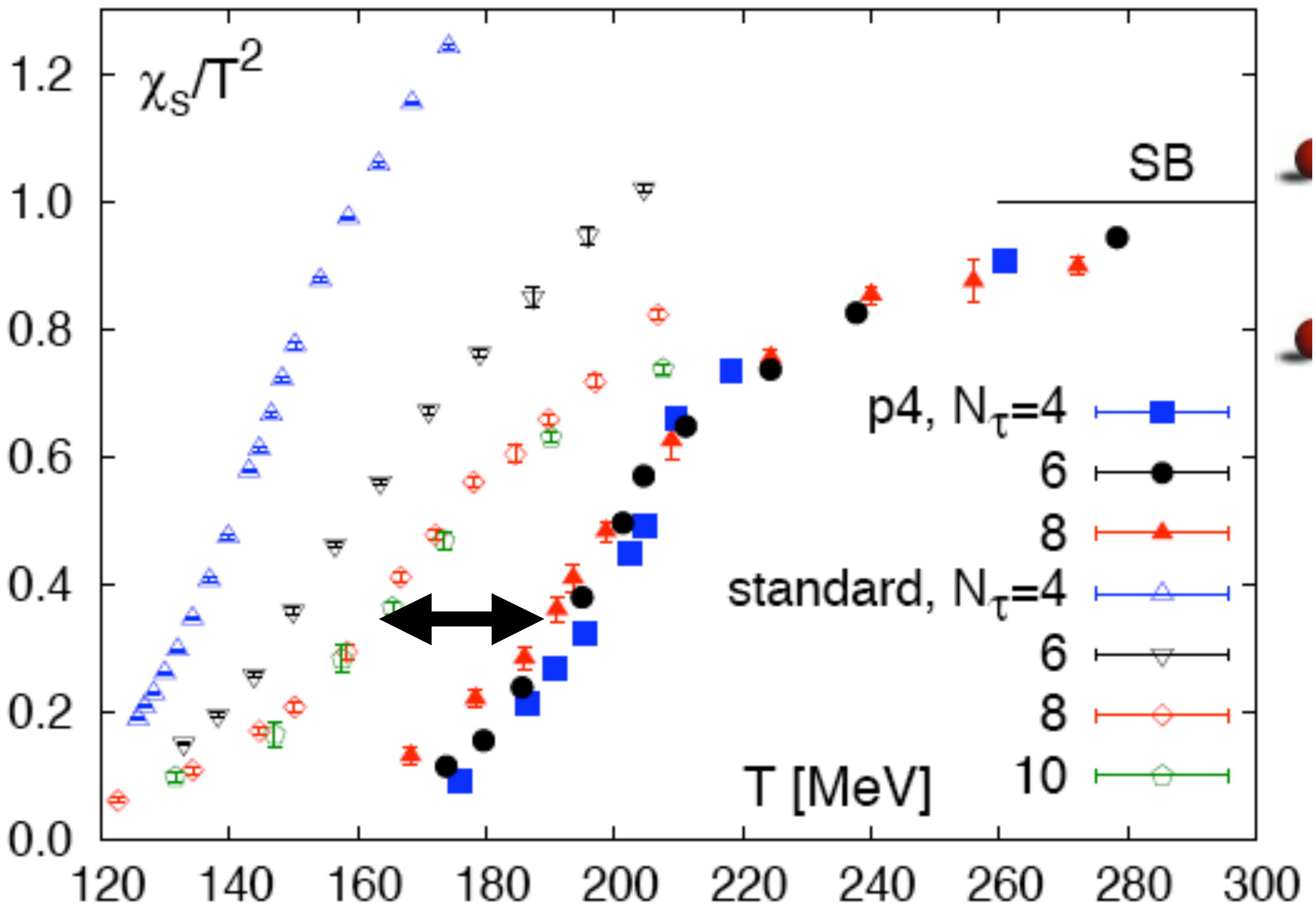


Away from a phase transition, different observables can show largest fluctuations (defining the transition point) at different T

Difference should vanish as $m_l \to 0$



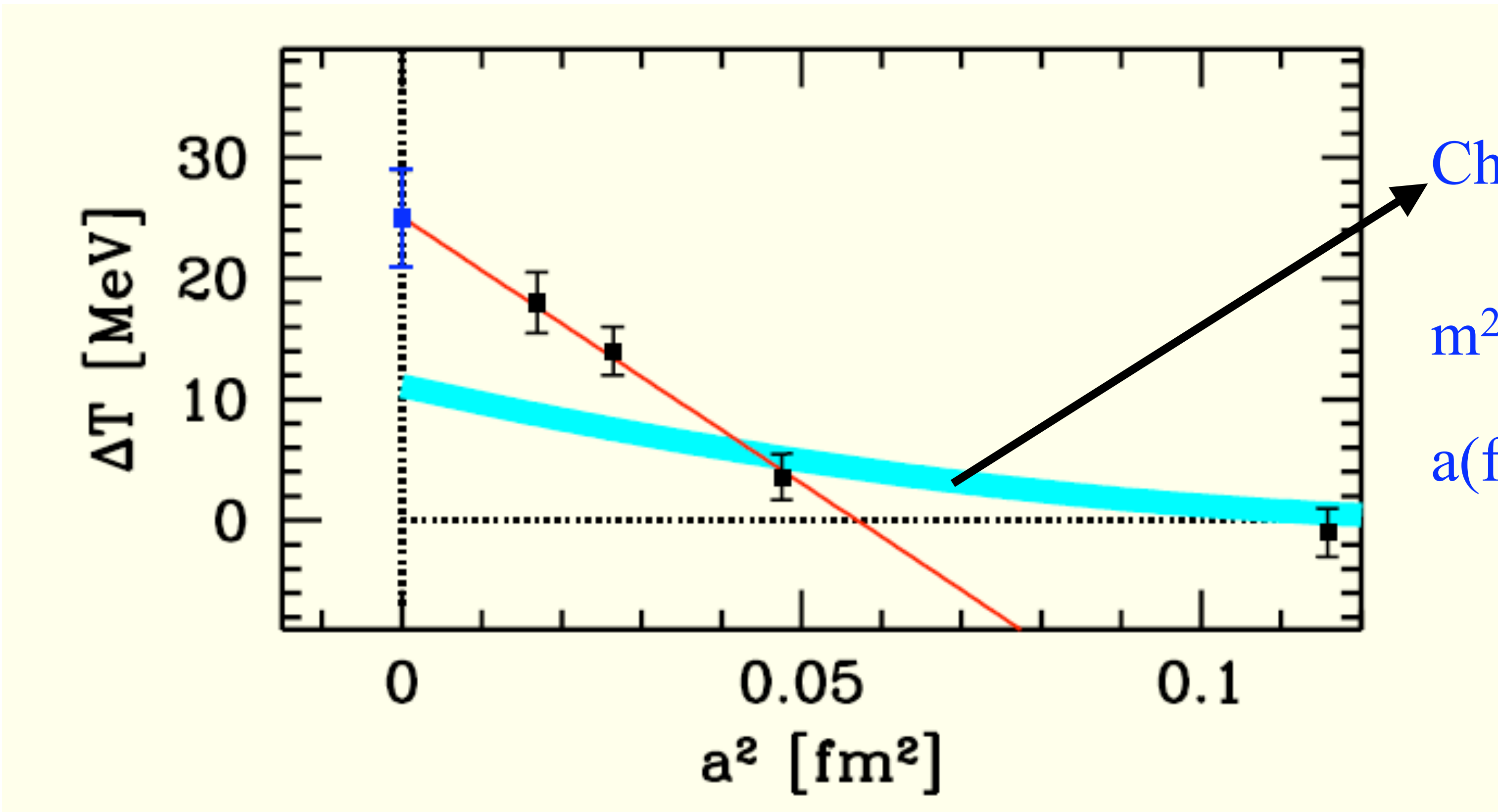
P4 versus stout



Stout: Much Larger O(a^2) errors

T (stout) smaller by ~30 Mev T(p4)

Stout: Can normalization & scale explain the 25 MeV difference between $T_{\chi S\ \mathrm{Restoration}}$ and $T_{\mathrm{deconfinement}}$



Changes made:

$m^2\chi/T^4 \rightarrow \chi/T^2$

$a(f_K) \rightarrow a(r_0)$

Important Role of: Data at N_τ=8, 10

Lattice scale? (Is $a(f_K) \approx a(r_0)$ as $a \rightarrow 0$?)

What next?

- Improve p4 and AsqTad continuum extrapolation (Finalize N_τ=8 HotQCD data)

- Final HotQCD data unlikely to change the current qualitative picture $T_{deconfinement} \approx T_{\chi SB}$ and lying in the band 185-195 MeV

- Resolve difference in $T_{\chi SB}$ between stout and hotQCD results