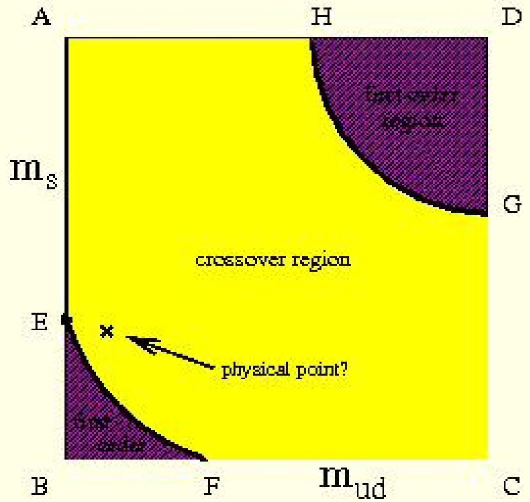
Lattice QCD thermodynamics

Approaching the continuum (limit/calculations)

Z. Fodor

1. Introduction
2. The equation of state at large temperatures
3. The nature of the transition: broad cross-over
4. The transition temperature: T_c
5. Conclusions

Standard picture of the 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

for 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

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

the physical pseudoscalar mass is just between these two values

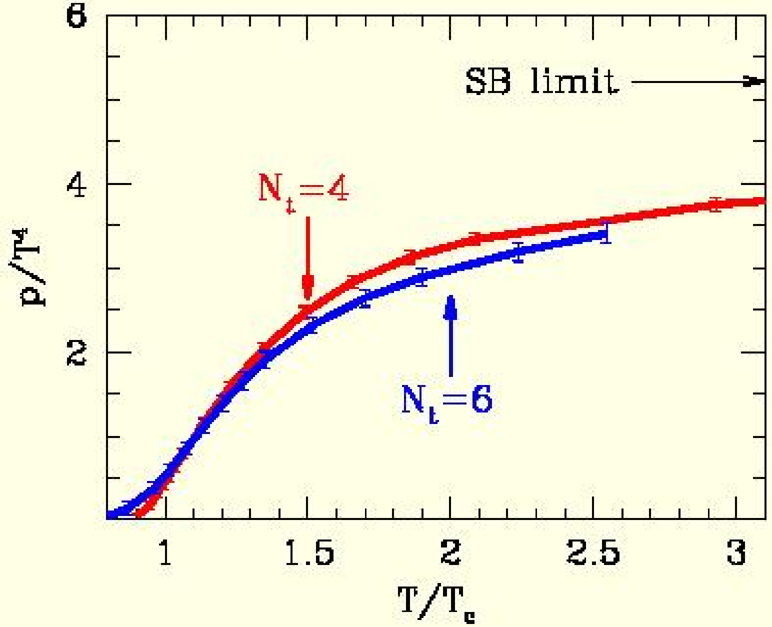
discretization errors change the order of the transition

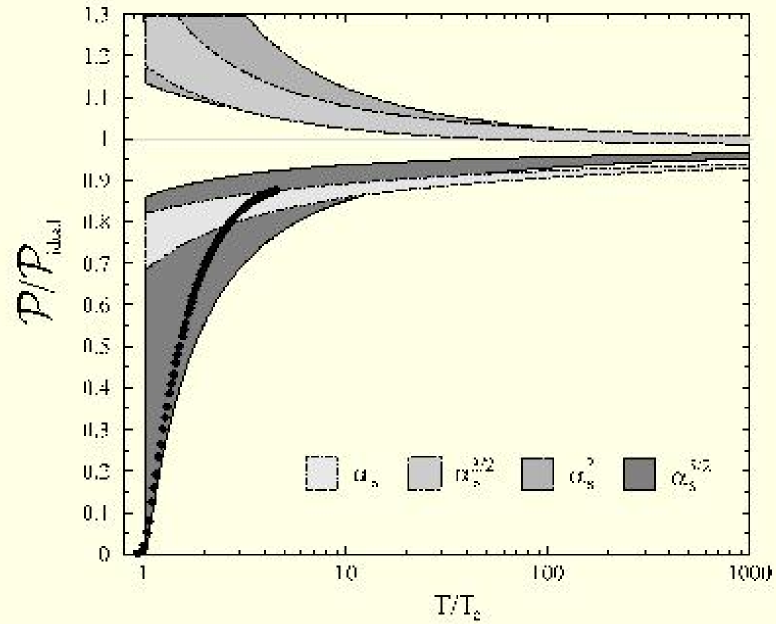
what happens for physical quark masses, in the continuum, at what T_c?

Link to continuum perturbation theory: equation of state at large T

lattice results for the EoS extend upto a few times T_c

perturbative series "converges" only at asymptotically high T





• the standard technique is the integral method:

$\bar{p}$=T/V·log(Z), but Z is difficult ⇒ $\bar{p}$ integral of (∂log(Z)/∂β,∂log(Z)/∂m)

subtract the T=0 term, the pressure is given by: $p(T)$=$\bar{p}(T)$-$\bar{p}(T=0)$

• back of an envelope estimate:

T_c≈150–200 MeV, m_π=135 MeV and try to reach T=20·T_c for N_t=8 (a=0.0075 fm)

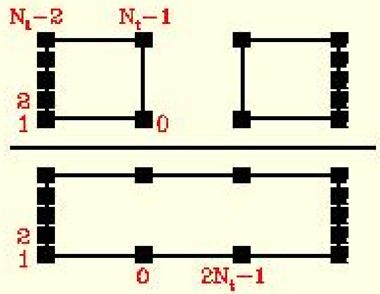
⇒N_s > 4/m_π ≈ 6/T_c = 6·20/T = 6·20·N_t ≈ 1000 ⇒ completely out of reach

a. substract successively: $p(T)=\bar{p}(T)-\bar{p}(T=0)=[\bar{p}(T)-\bar{p}(T/2)]+[\bar{p}(T/2)-\bar{p}(T/4)]+\dots$

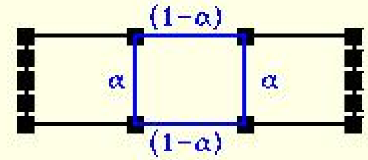
$\Longrightarrow$ for substractions at most twice as large lattices are needed

b. instead of the integral method calculate: $\bar{p}(T)-\bar{p}(T/2)=T/(2V)\cdot\log[Z^2(N_t)/Z(2N_t)]$

$$\frac{Z^2(N_t)}{Z(2N_t)} =$$

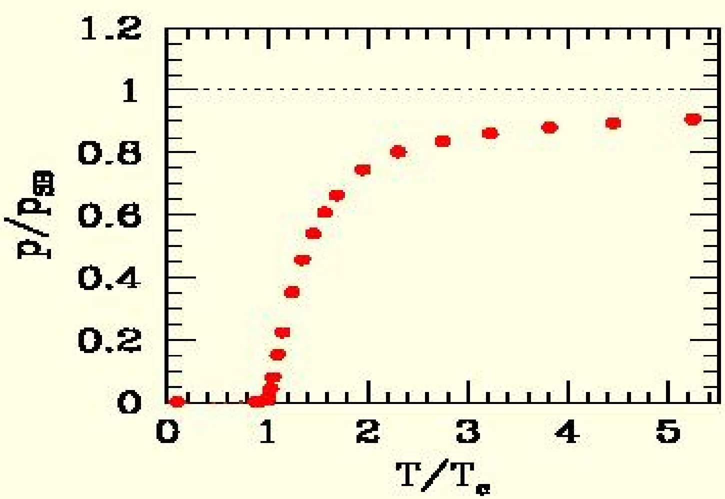


$$\bar{Z}(\alpha) =$$



define $\bar{Z}(\alpha)=\int \mathscr{D}U \exp[-\alpha S_{1b}-(1-\alpha)S_{2b}] \Longrightarrow Z^2(N_t)=\bar{Z}(0)$ and $Z(2N_t)=\bar{Z}(1)$

one gets directly $\bar{p}(T)-\bar{p}(T/2)=T/(2V)\int_0^1 d\log[\bar{Z}(\alpha)]/d\alpha\cdot d\alpha=T/(2V)\int_0^1\langle S_{1b}-S_{2b}\rangle\alpha\cdot d\alpha$



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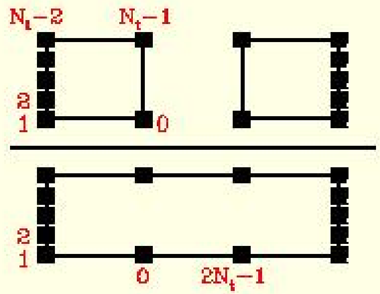

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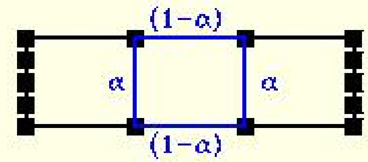

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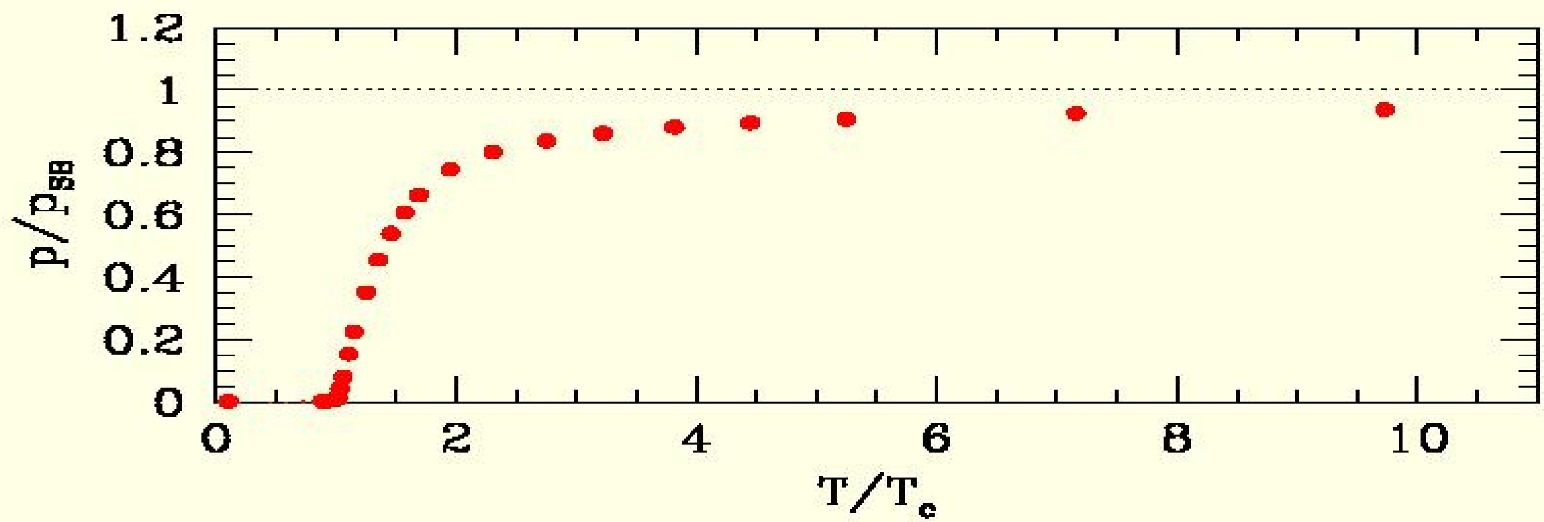

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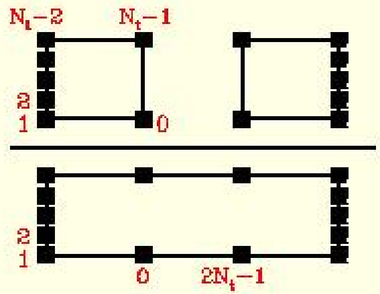

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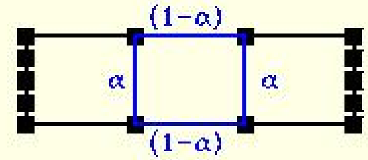

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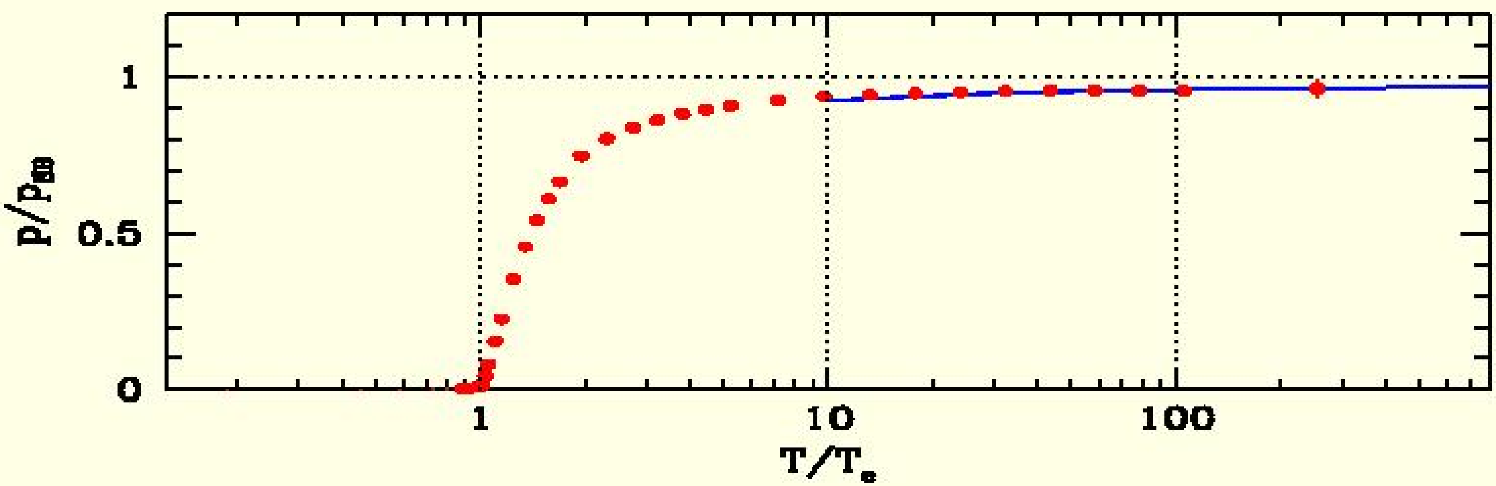

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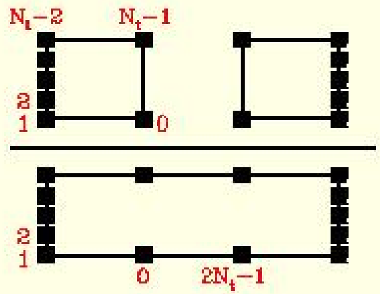

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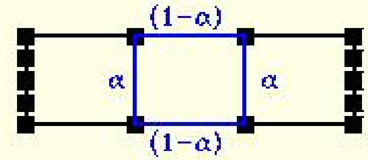

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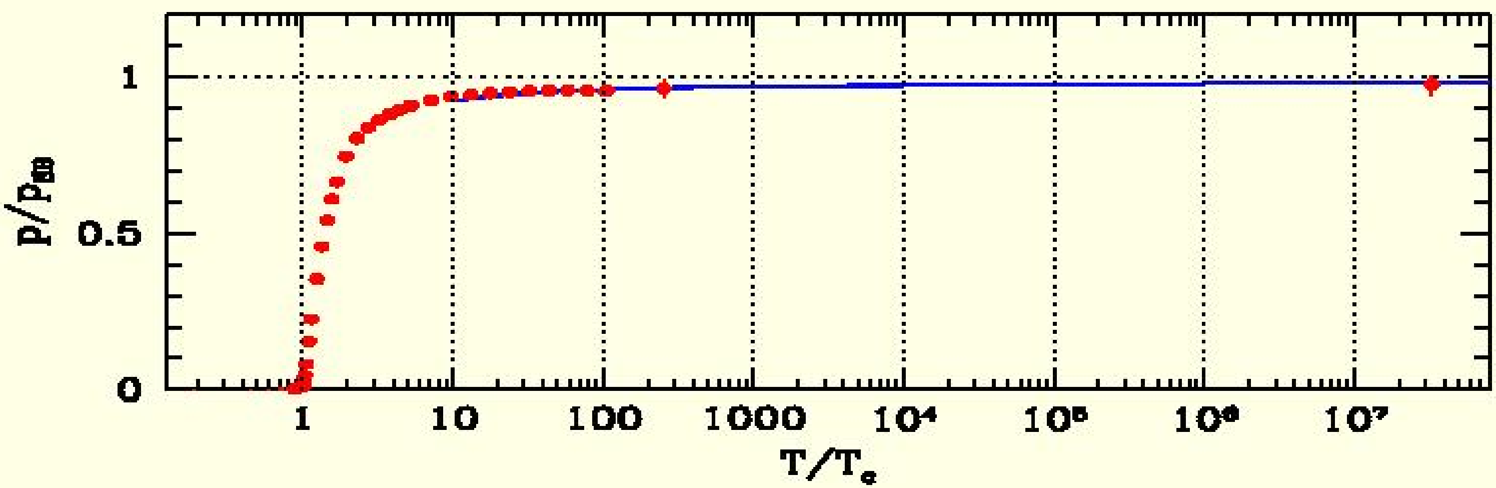

long awaited link between lattice thermodynamics and pert. theory is there

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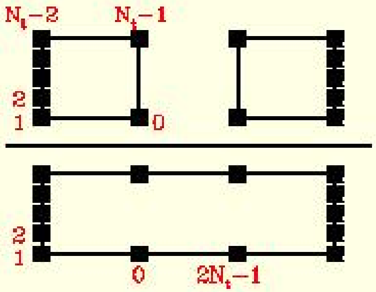

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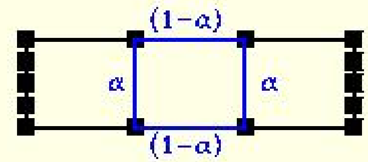

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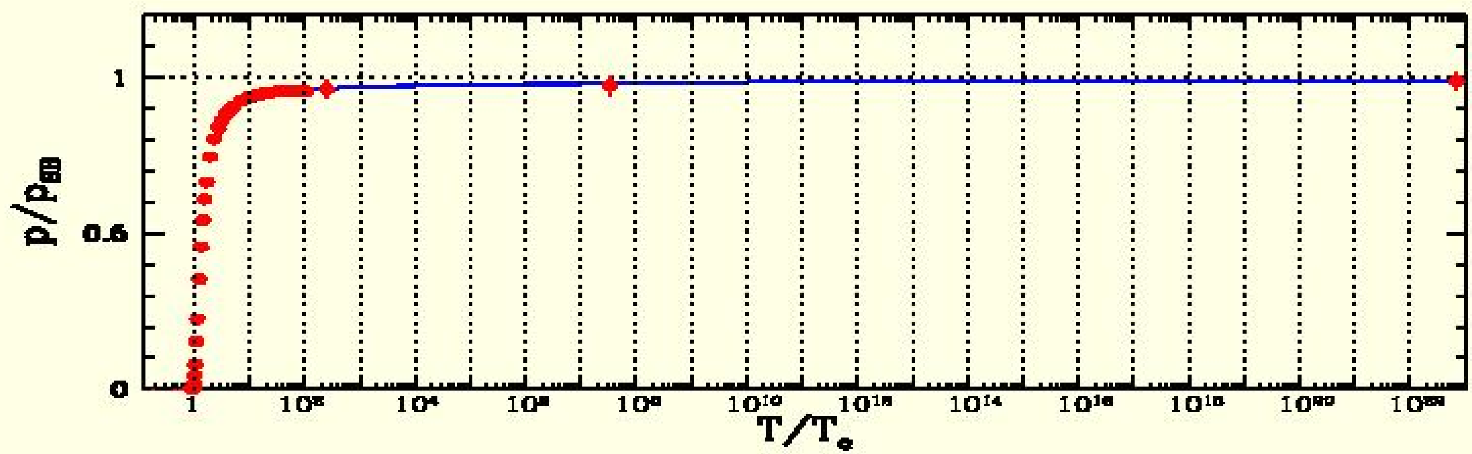


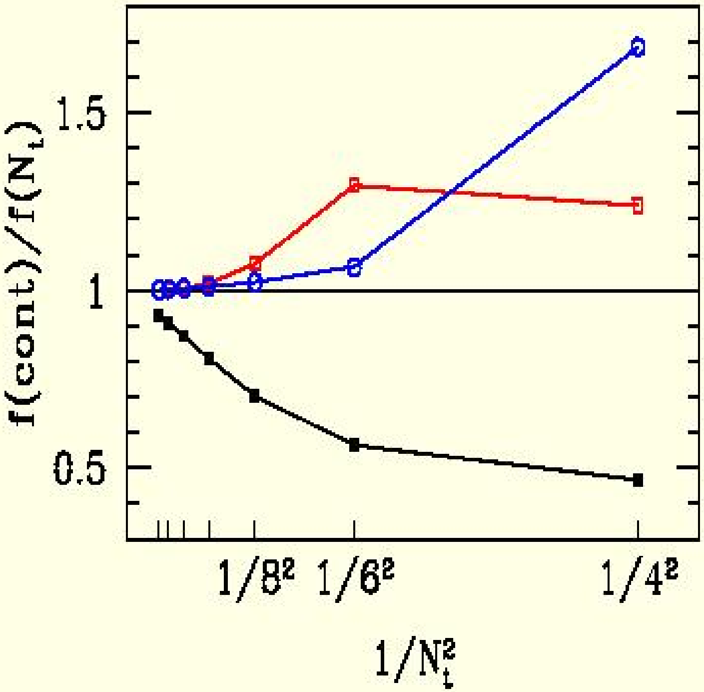
long awaited link between lattice thermodynamics and pert. theory is there

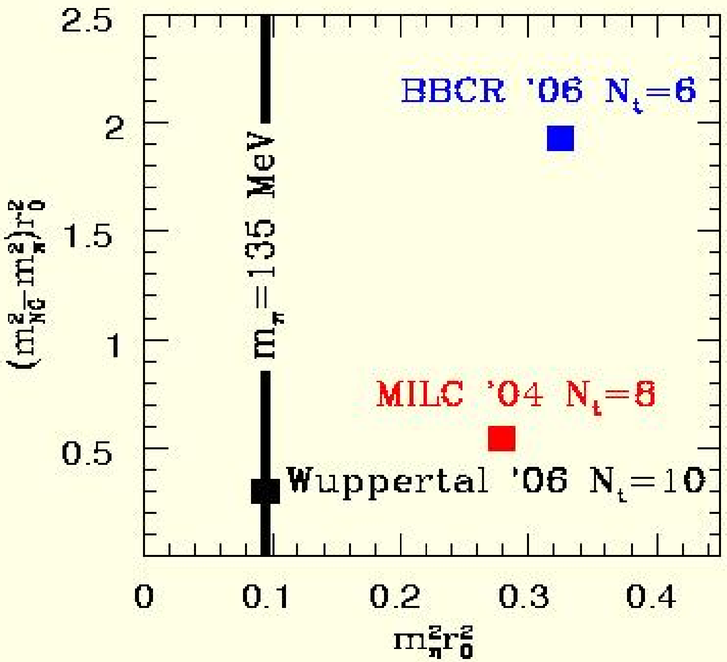
G.Endrodi, Z.Fodor, S.D.Katz, K.K.Szabo, arXiv:0710.4197

The nature of the QCD transition

Y.Aoki, G.Endrodi, Z.Fodor, S.D.Katz, K.K.Szabo, Nature, 443 (2006) 675 [hep-lat/0611014]

Symanzik improved gauge, stout improved n_f=2+1 staggered fermions simulations along the line of constant physics: m_π=135 MeV, m_K=500 MeV



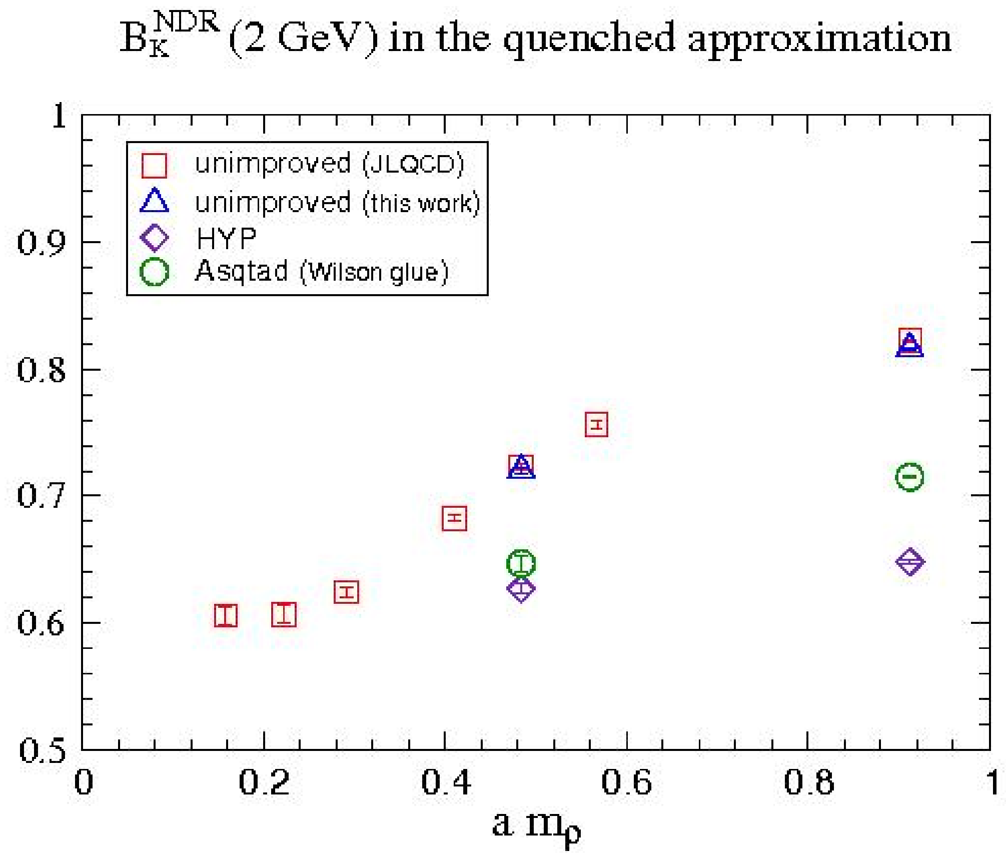


extrapolation from N_t and N_t+2 (standard action) ≈ as good as N_t with p4
N_t=8,10 gives ≈ ±1%, but a<0.15, 0.12 fm needed to set the scale (±1%)
thermodynamic quantities are obtained "more precisely" than the scale
(p4 independent config. is >10× more CPU ⇒ instead balance: a→0)

• Scaling of B_K in Quenched simulations

unimproved action has large scaling violations

HYP smearing: almost perfect scaling

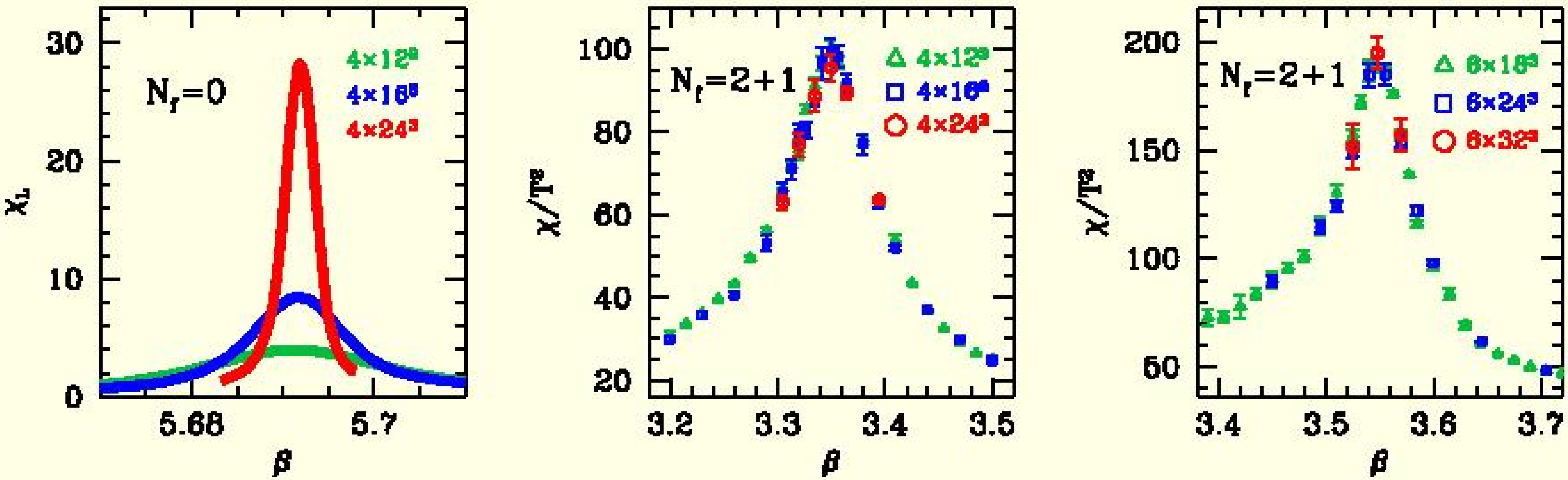


[HPQCD & UKQCD, Phys.Rev.D73 (2006) 114502]

• finite size scaling for the chiral susceptibility: $\chi=(T/V)\partial^2 \log Z/\partial m^2$

first order transition $\Longrightarrow$ peak width $\propto$ 1/V, peak height $\propto$ V

cross-over $\Longrightarrow$ peak width $\approx$ constant, peak height $\approx$ constant



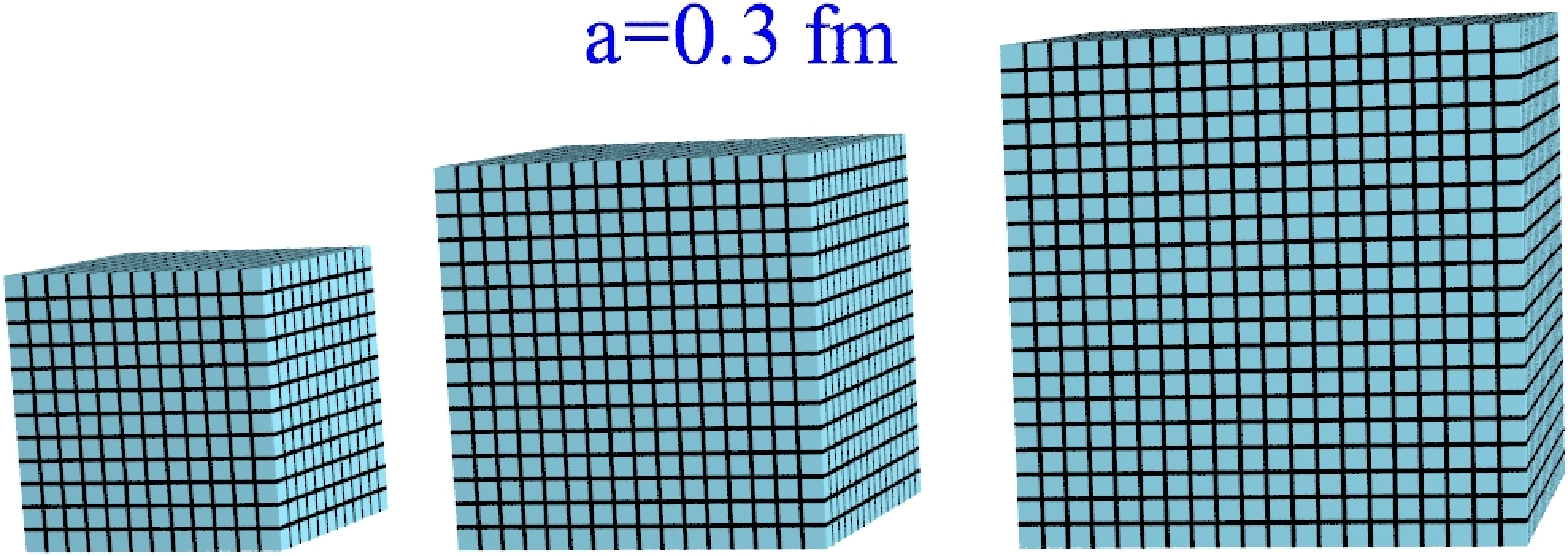
eight times larger volumes: volume independent scaling $\Rightarrow$ cross-over

do we get the same result (cross-over) in the continuum limit?

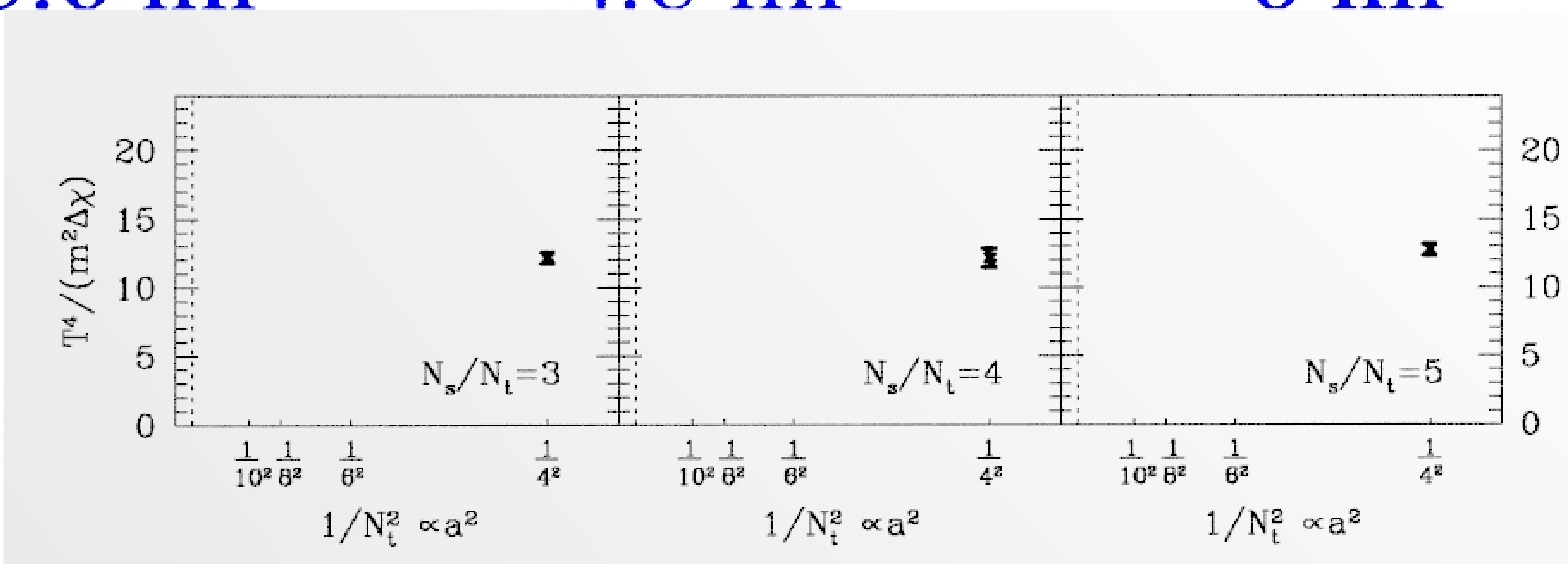
one might have the unlucky case as we had in n_f=3 QCD:

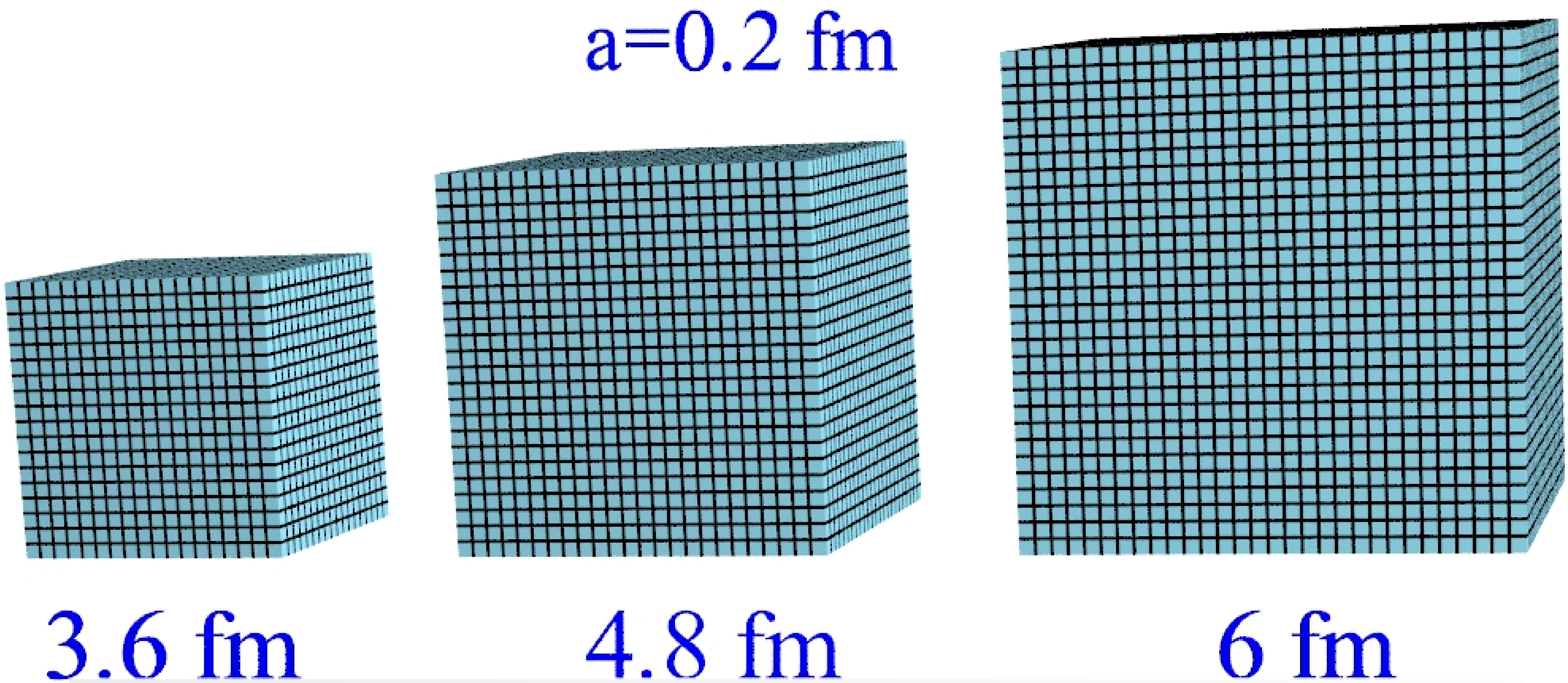
discretization errors changed the nature of the transition for physical m_{ps}

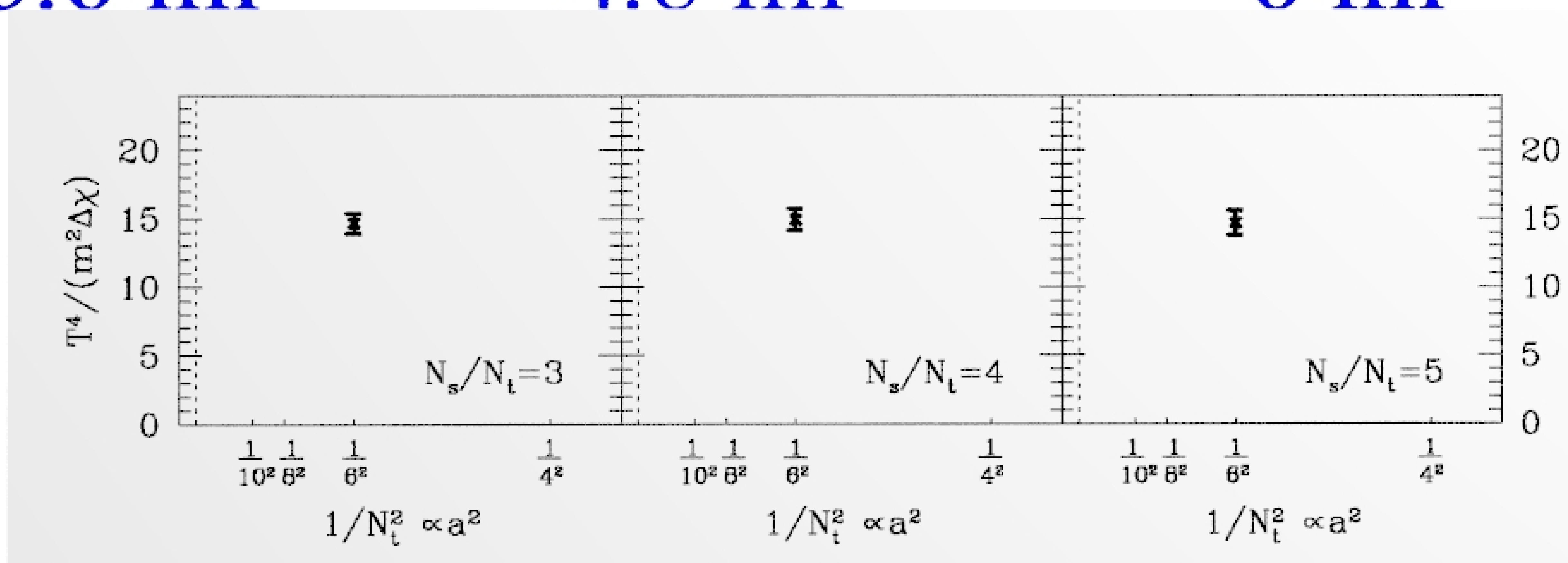
a=0.3 fm

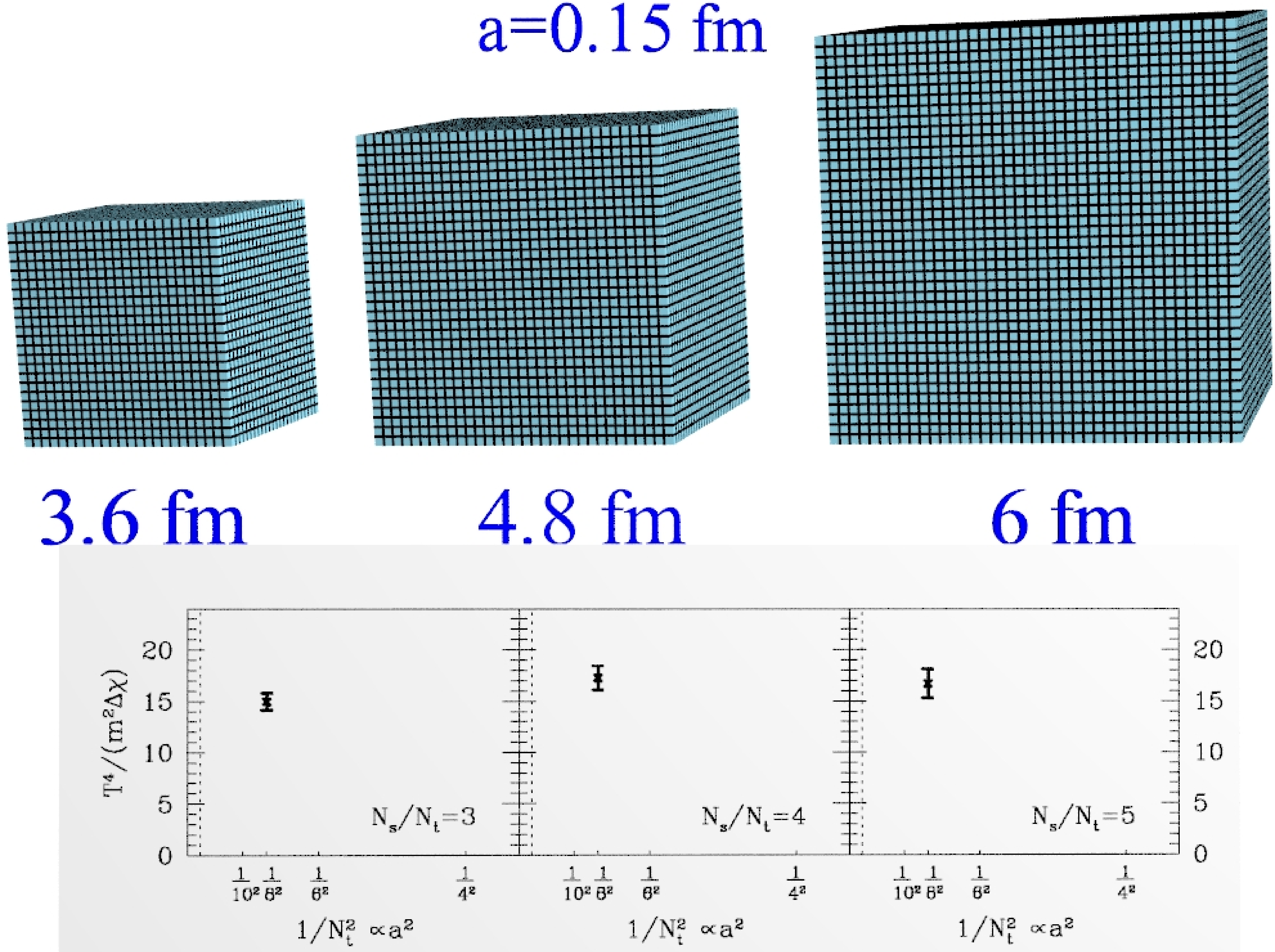


3.6 fm 4.8 fm 6 fm

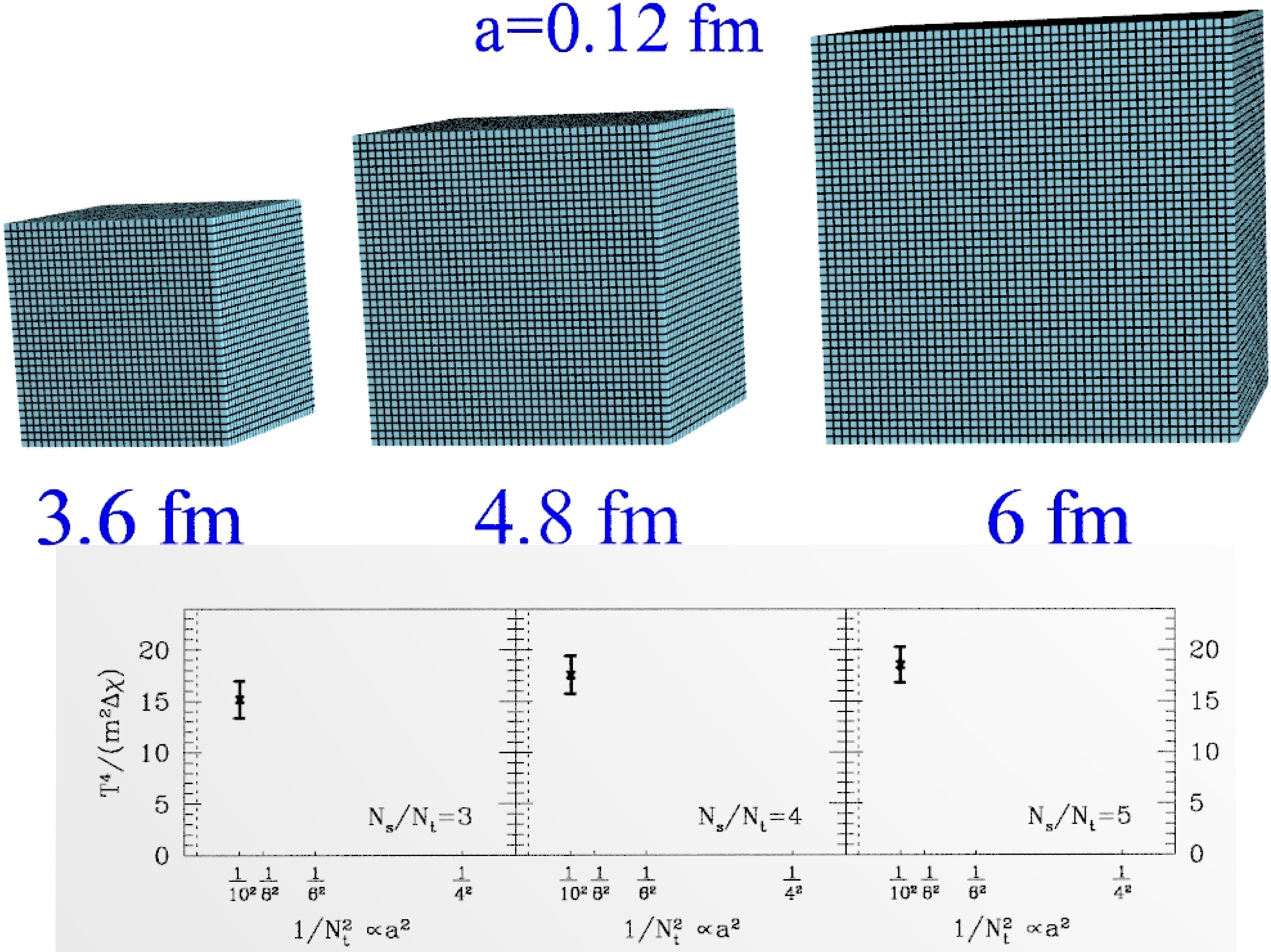



a=0.2 fm
3.6 fm
4.8 fm
6 fm

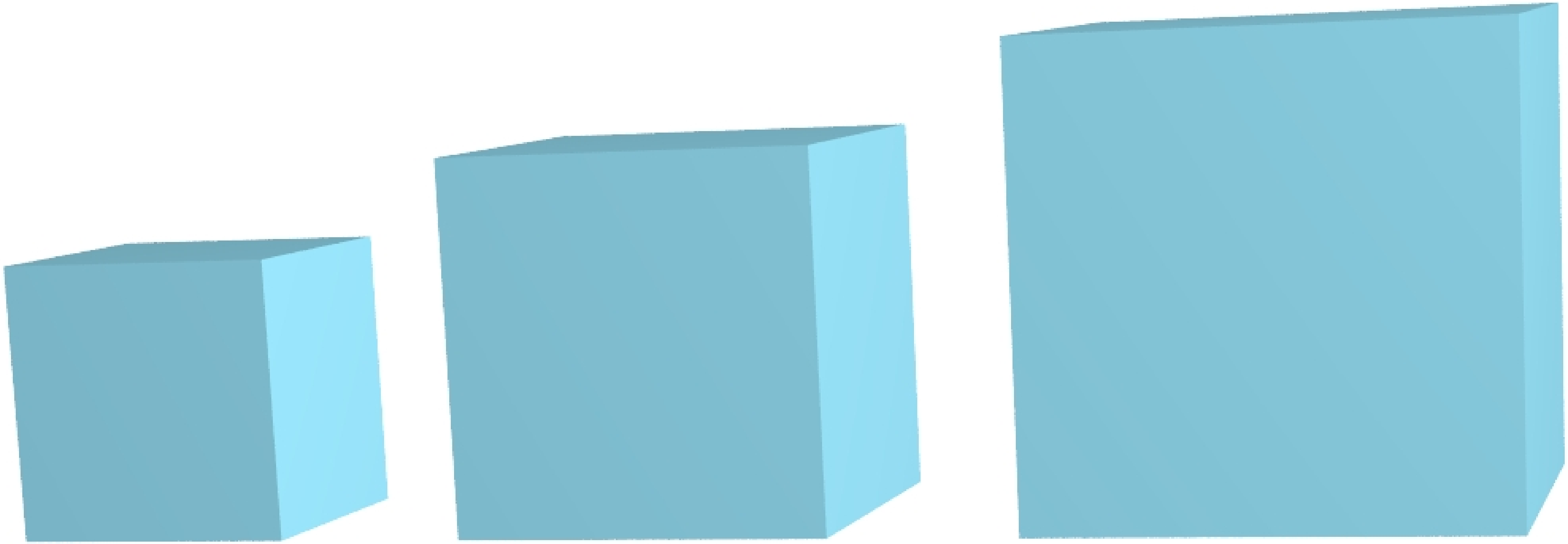

$T^4/(m^2\Delta\chi)$
0
5
10
15
20
$N_s/N_t=3$
$N_s/N_t=4$
$N_s/N_t=5$
$\frac{1}{10^2}$ $\frac{1}{8^2}$ $\frac{1}{6^2}$ $\frac{1}{4^2}$
$1/N_t^2 \propto a^2$



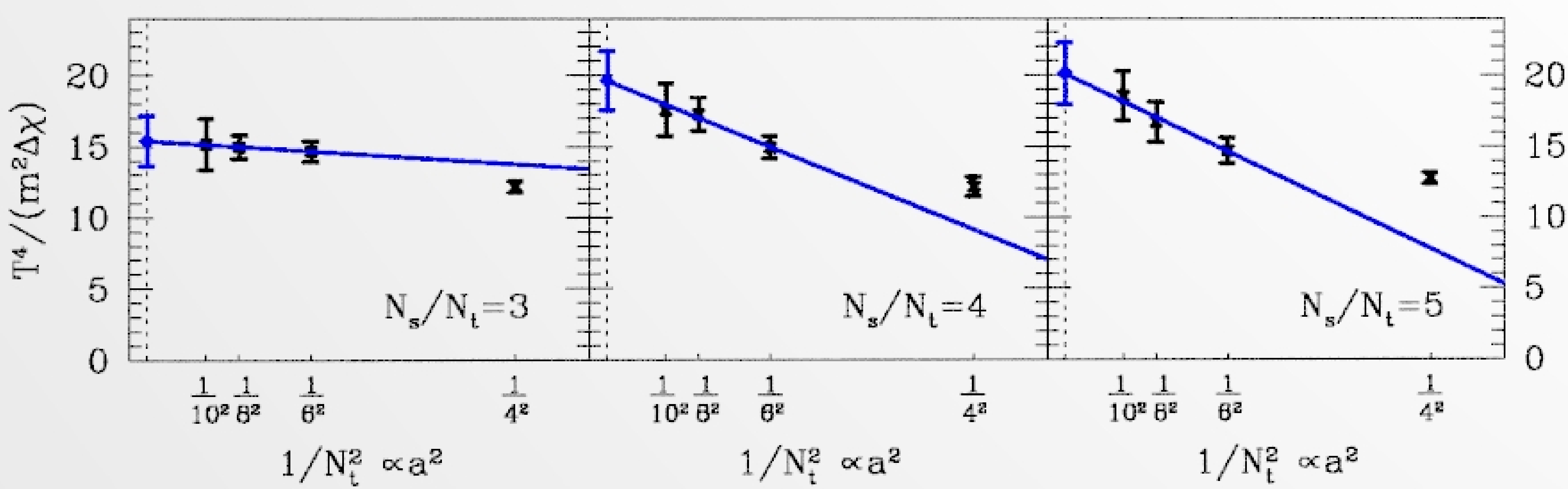
a=0.15 fm
3.6 fm
4.8 fm
6 fm
T⁴/(m²Δχ)
0
5
10
15
20
N_s/N_t=3
N_s/N_t=4
N_s/N_t=5
1/10²
1/8²
1/6²
1/4²
1/N_t² ∝a²



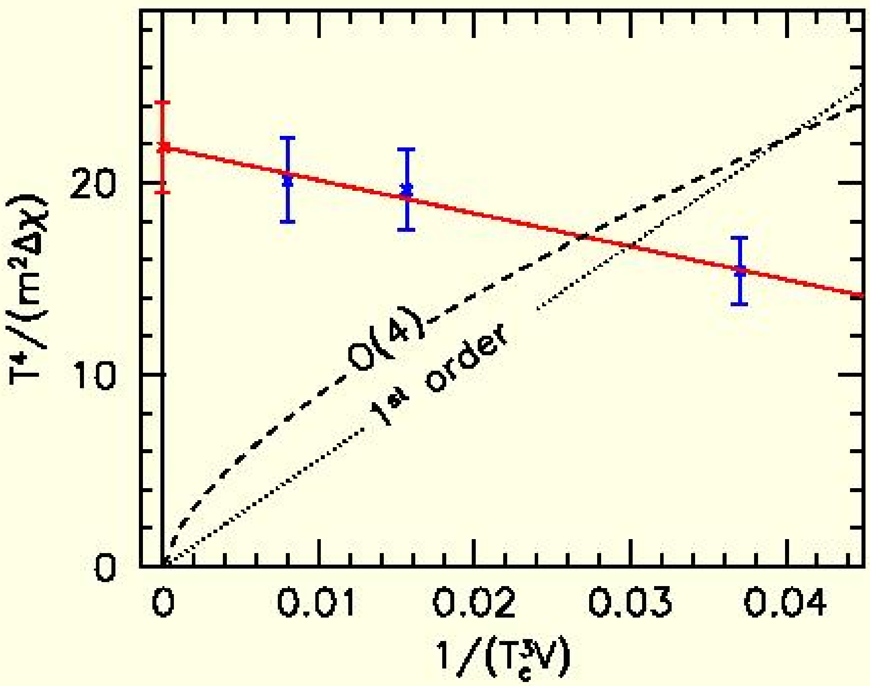
a=0.12 fm
3.6 fm
4.8 fm
6 fm
$T^4/(m^2\Delta\chi)$
$N_s/N_t=3$
$N_s/N_t=4$
$N_s/N_t=5$
$1/N_t^2 \propto a^2$
$1/N_t^2 \propto a^2$
$1/N_t^2 \propto a^2$



3.6 fm 4.8 fm 6 fm



• finite size scaling analysis with continuum extrapolated $m^2\Delta\chi$



the result is consistent with an approximately constant behavior for a factor of 5 difference within the volume range

chance probability for 1/V is 10^{-19} for O(4) is $7 \cdot 10^{-13}$

continuum result with physical quark masses in staggered QCD:

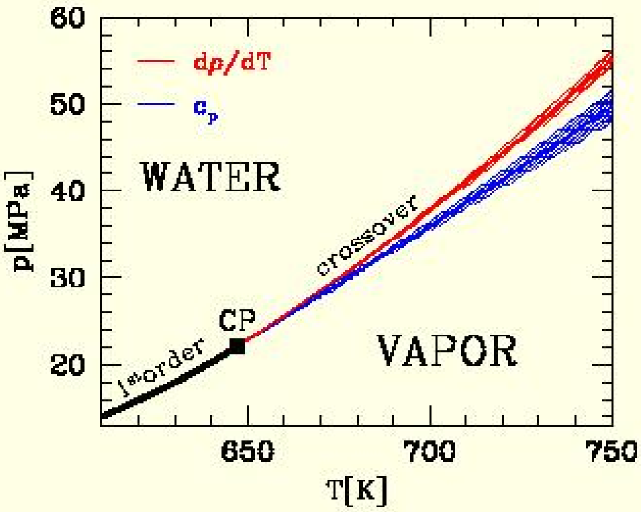
the QCD transition at μ=0 is a cross-over

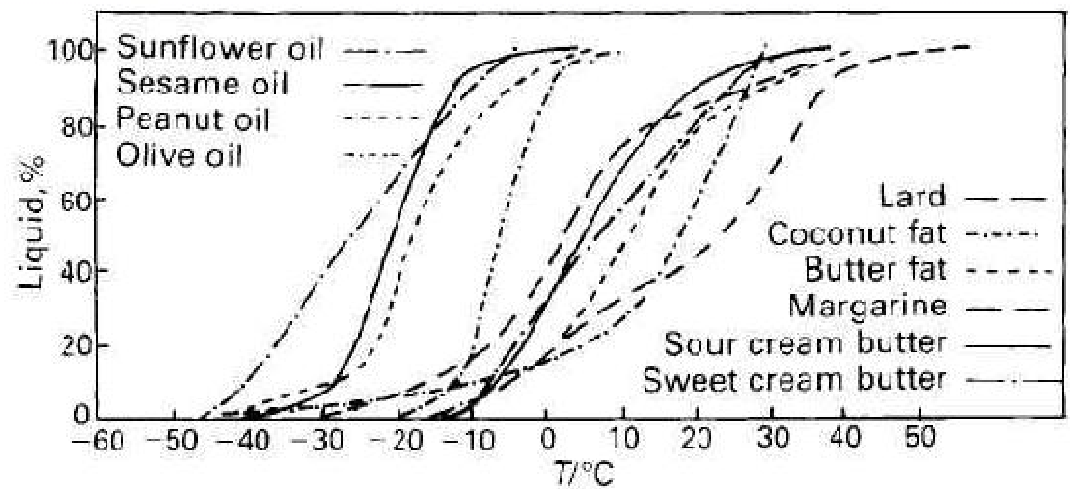
$\Longrightarrow$ Condition for the critical point is fulfilled

The transition temperature (N_t=4,6,8,10)

Y. Aoki, Z. Fodor, S.D. Katz, K.K. Szabo, Phys. Lett. B. 643 (2006) 46 [hep-lat/0609068]

- a cross-over has no unique T_c: example of water-steam transition





above the critical point c_p and $d\rho/dT$ give different T_cs.

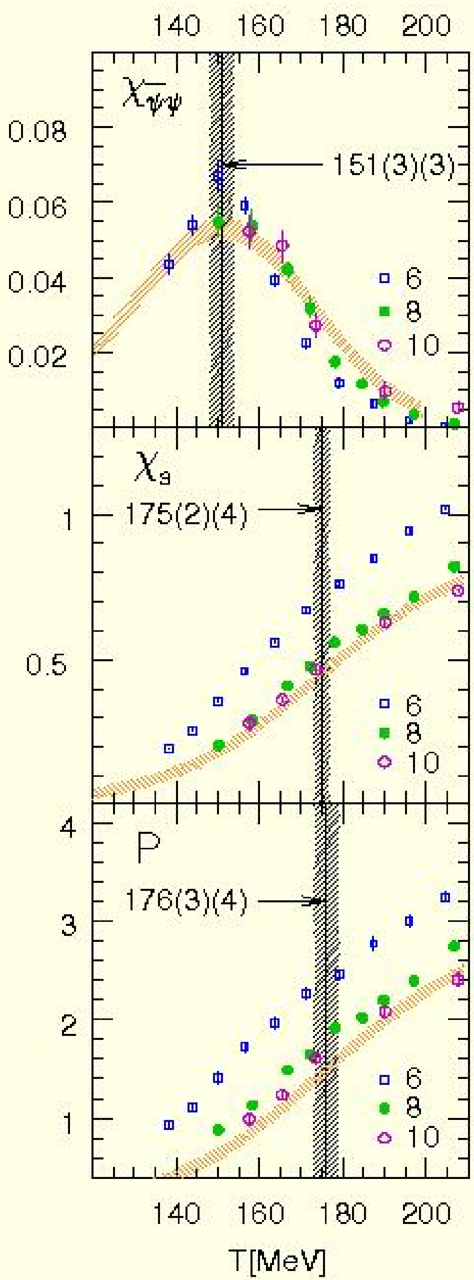
QCD: chiral & quark number susceptibilities or Polyakov loop

they result in different T_c values $\Rightarrow$ physical difference

extrapolations from large a: $\sigma, r_0, m_\rho, m_N, m_{K^*}, m_\Omega, f_\pi, f_K$: different a (in fm)

this lead to different T_c values $\Rightarrow$ non-physical ambiguity

will be removed in the continuum limit (most precise scale is set by f_K)



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

N_t=6,8,10 are in the a^2 scaling regime, N_t=8,10 are practically the same

- $T_c(\chi_{\bar\psi\psi})$ consistent with MILC '2004: $T_c = 169(12)(4)$ MeV

- BBCR collaboration: published result [M. Cheng et.al, Phys. Rev. D74 (2006) 054507]

Transition temperature from $\chi_{\bar\psi\psi}$ and Polyakov loop, from both quantities

T_c=192(7)(4) MeV, $\Longrightarrow$ for $\chi_{\bar\psi\psi}$ contradicts our result ($\approx$40 MeV)

Main differences to our work

normalization changes T_c (multiply a Gaussian by $T^2 \Rightarrow$ peak shifts)

no renormalization, χ/T^2 is used: explains only ≈ 10 MeV difference

only $N_t = 4$ & 6 (cutoff: $a \approx$0.3 fm & 0.2 fm or $a^{-1}\approx$700 MeV & 1 GeV)

scale is set by r_0 instead of f_K (influences only the overall accuracy)

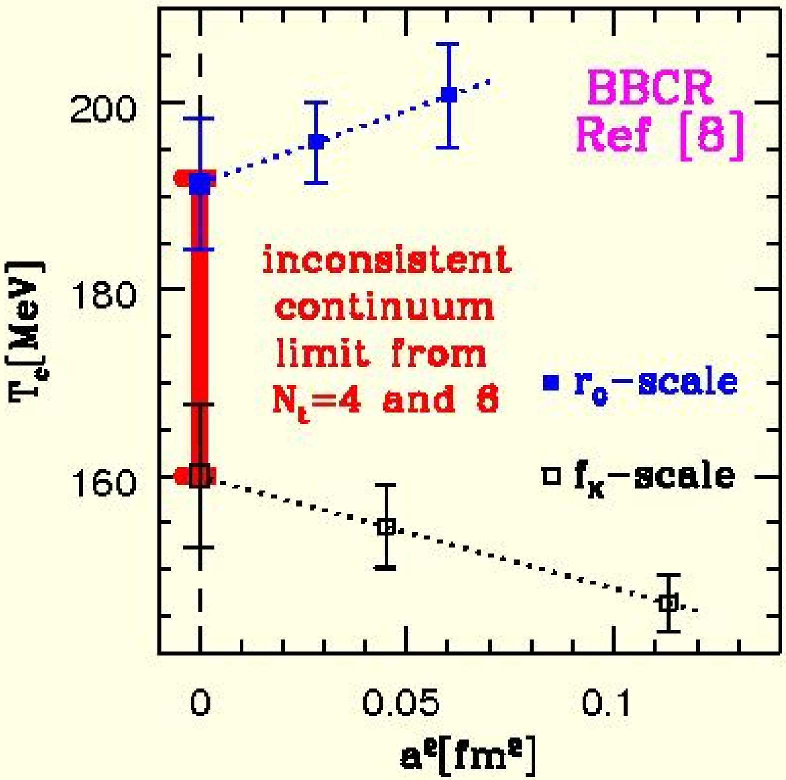
What is the reason for this discrepancy?

Their last concluding remark: it is desirable to

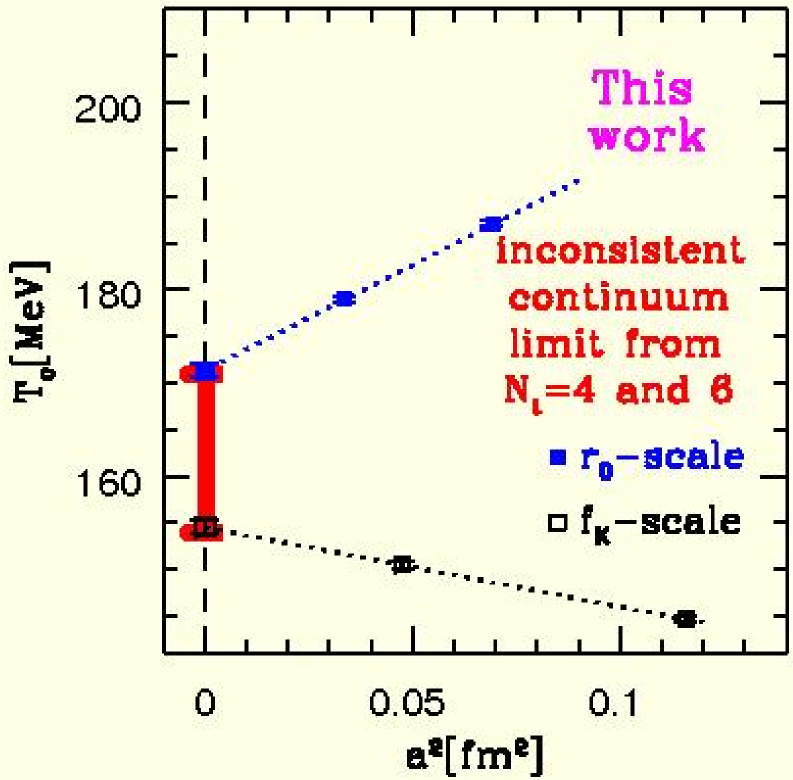
"obtain a reliable independent scale setting for the transition temperature from an observable not related to properties of the static potential".

What if they used f_K to set the scale?

We repeated some of their $T=0$ simulations to determine f_K



Alternatively:
We can use r_0 and only N_t=4,6



Continuum extrapolations from $N_t = 4, 6$ are inconsistent!

not surprising: eg. asqtad at $N_t\approx$10 has $\approx$10% scale difference between r_1 & f_K
Lüscher (Dublin) & DelDebbio et al: a=.06fm $\approx$20% difference between r_0 & m_{K^*}

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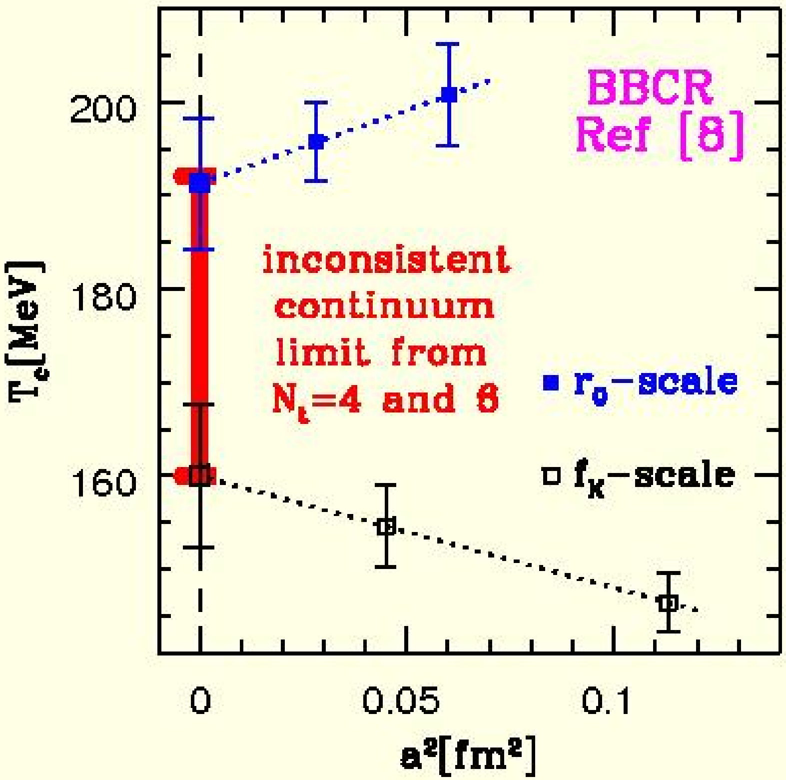

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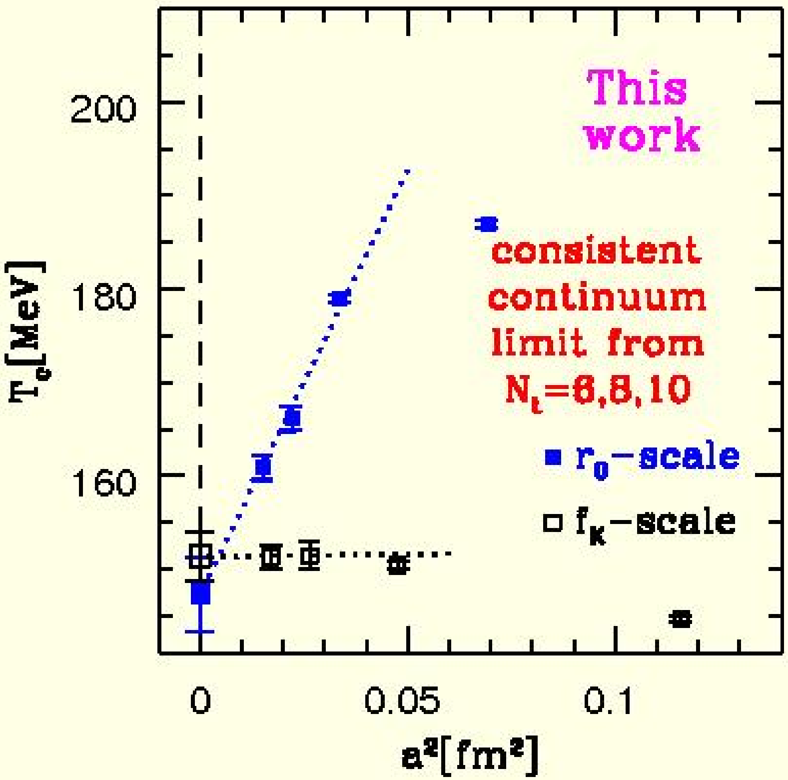


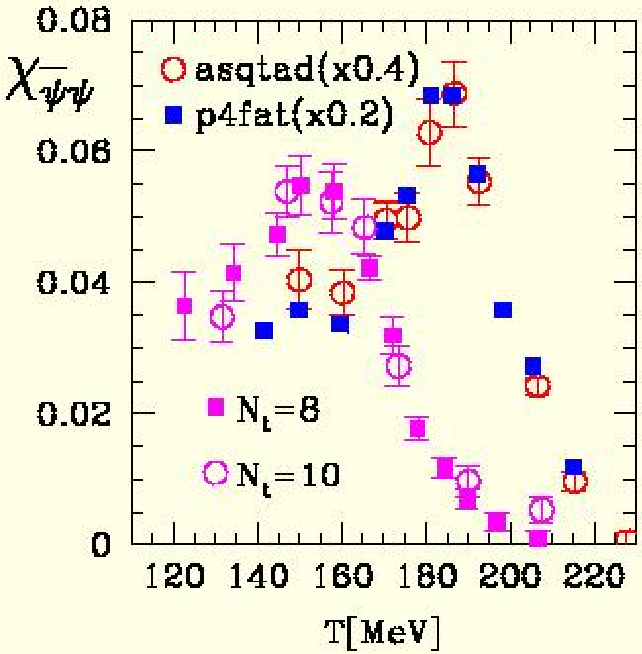
Continuum extrapolations from $N_t = 6, 8, 10$ are consistent!

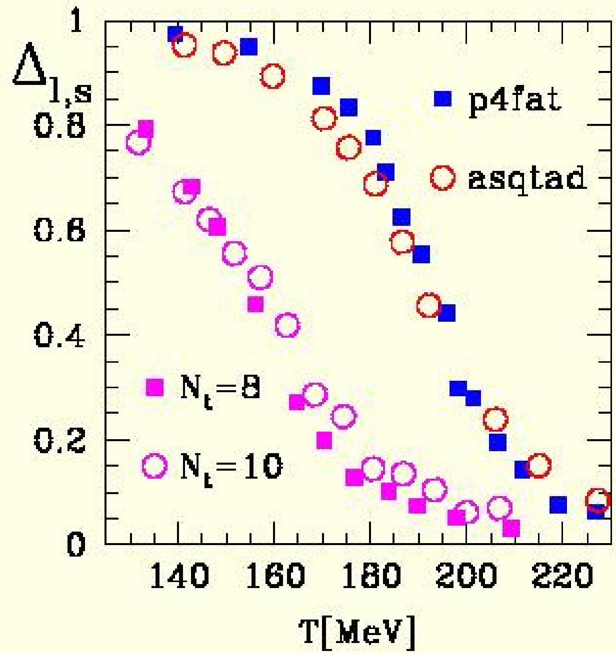
Conclusion: continuum limit from N_t=4,6 isn't safe (a≈0.3, 0.2 fm or 0.7, 1GeV)

hotQCD collaboration: new results ⇒ differences/problems remained (1)

hotQCD: [0710.1655, 0711.0661, 0804.4148, RBRC workshop 04.08]

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





chiral susceptibility, rescaled (quark masses are different)

$$\chi_{\bar\psi\psi} = m_l^2 \frac{\partial^2}{\partial m_l^2}(f(T) - f(T=0))$$

chiral condensate

$$\Delta_{l,s} = \left(\langle \bar{l}l \rangle - m_l/m_s \langle \bar{s}s \rangle\right) / \left(\langle \bar{l}l \rangle_{T=0} - m_l/m_s \langle \bar{s}s \rangle_{T=0}\right)$$

Another difference/problem is related to the width (2)

there is no phase transition, only an analytic cross-over
$\Longrightarrow$ different definitions lead to different temperature scales

our claim:
Polyakov-loop, strange number susceptibility inflection points give quite higher T_c (175 MeV) than the chiral susceptibility peak (151 MeV)

hotQCD claim:
"no large differences in the transition temperature from observables related to deconfinement and chiral symmetry restoration, both lie in the range T=(185-195) MeV" 0711.0661

due to crossover 'Problem 2.' is less severe as 'Problem 1.',
even in our case it is possible to define chiral/deconfinement operators with same transition temperatures e.g. by multiplying by some powers of T
e.g. instead of the dimensionless $m^2\chi_{\bar{\psi}\psi}/T^4$ definition one might use $\chi_{\bar{\psi}\psi}$
(can be less precisely measured on the lattice) $\Rightarrow$
peak of the chiral susceptibility (this definition) is between 170 and 175 MeV

Possible resolutions

Y. Aoki, Z. Fodor, S.D. Katz, K.K. Szabo, Phys. Lett. B. 643 (2006) 46 [hep-lat/0609068]

$N_t = 4, 6$ of 'p4fat3' are too coarse, no controlled continuum limit

present status: fine $N_t = 8$ somewhat better but still large discrepancy

our simulations:

- scale set by f_K, non-Goldstone pions distort chiral extrapolation or continuum limit
- naive staggered dispersion relation has large artefacts

hotQCD:

- nonphysical quark masses $\to \sim$ 5 MeV Soeldner's talk at Lattice'08
- scale set by $r_0^{\mathrm{HPQCD,UKQCD}}$=0.469(7) fm

r_0^{ETM}=0.444(4) fm, r_0^{QCDSF}=0.467(6) fm, $r_0^{\mathrm{PACS-CS}}$= 0.492(6)(+7) fm

both:

- universality problem of staggered discretization
- bug in computer code
- ...

maybe a bit of all

systematic errors are simply underestimated

Improving our previous results

1. improving $T = 0$ simulations

previously: $m_\pi \geq 240$MeV + chiral extrapolations

now: $\boxed{m = m^{\text{phys}}}$, no need for chiral extrapolations

$\Rightarrow$ more precise scale/renormalization

2. improving $T > 0$ simulations

previously: $N_t = 4, 6, 8, 10$ at the physical point

now: $\boxed{N_t = 12}$ at the physical point

$\Rightarrow$ more control over lattice artefacts

Simulation setup: T>0, machine

nVidia GeForce 8800 Ultra
768 MB video memory
103.7 GB/sec bandwidth
two cards per machine

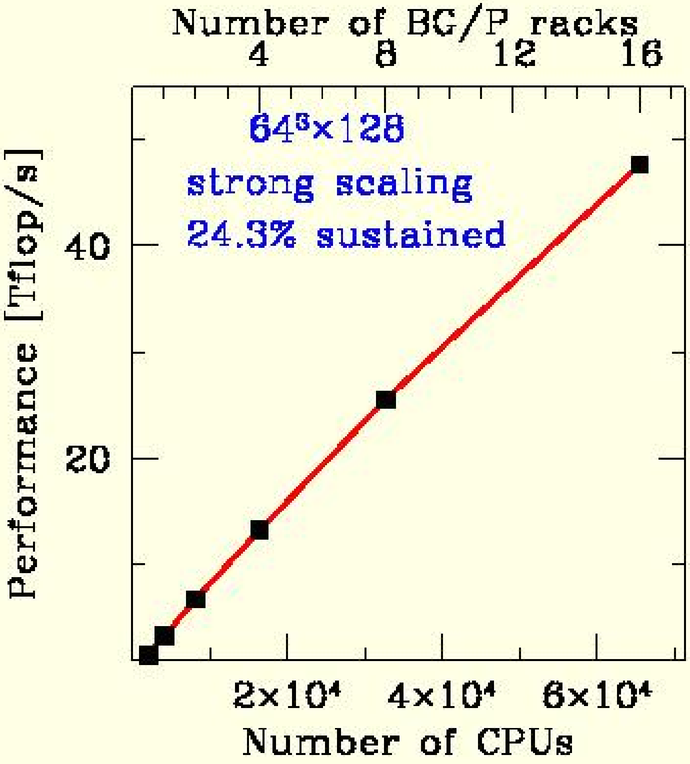
multishift inverter on $12 \cdot 36^3$ fits to the video memory and runs with 32 Gflop
gauge force on the video card: 15 Gflop

only single precision arithmetics, HMC-force is not needed more precisely,
for HMC-energy mixed precision inverters ($\varepsilon = 10^{-8}$)

100 GPU-s in dual PC's in Wuppertal $\rightarrow$ 3 Tflops $\sim$ 1 BGP rack
cluster computing: ideal for finite T with many parameter sets

Simulation setup: T=0, machine

zero T lattices are too large for a single video card
→ BG/P supercomputer in Juelich



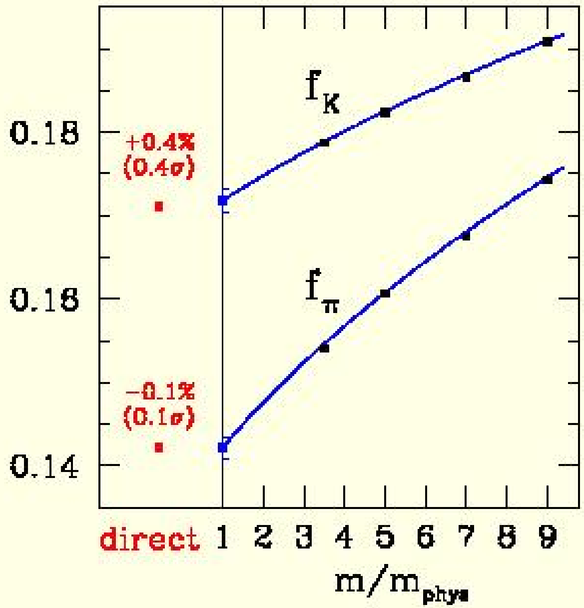
Simulation setup: T=0, volumes and statistics

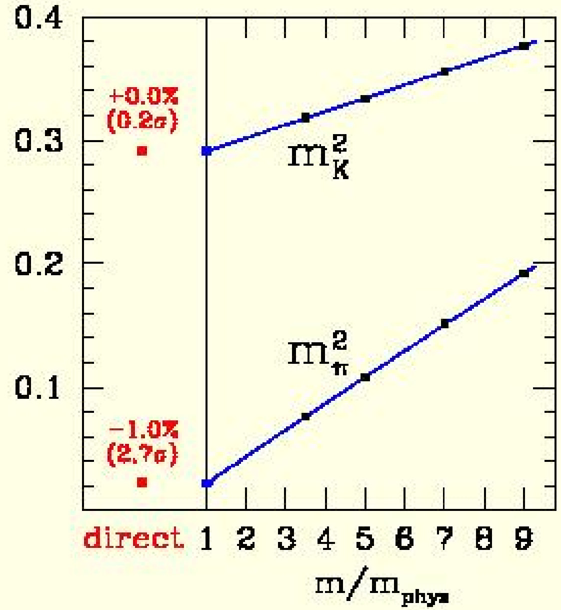
simulations directly at the physical point

choose lattice sizes, so that finite volume corrections are below 0.5% for f_π, m_π, f_K, m_K (cont. formula of Colangelo, Durr, Haefeli '05)

β	$N_t^{\rm crit}$	lattice	#traj
3.45	~ 4	$24^3 \times 32$	1500
3.55	~ 6	$24^3 \times 32$	3000
3.67	~ 8	$32^3 \times 48$	1500
3.75	~ 10	$40^3 \times 48$	1500
3.85	~ 13	$48^3 \times 64$	1500

T=0 results at the physical point, pseudoscalars





chiral extrapolations (not staggered χPT !) work amazingly well

for all analyzed spacings the extrapolation error for f_π, m_π, f_K, m_K is $\leq$ 1%

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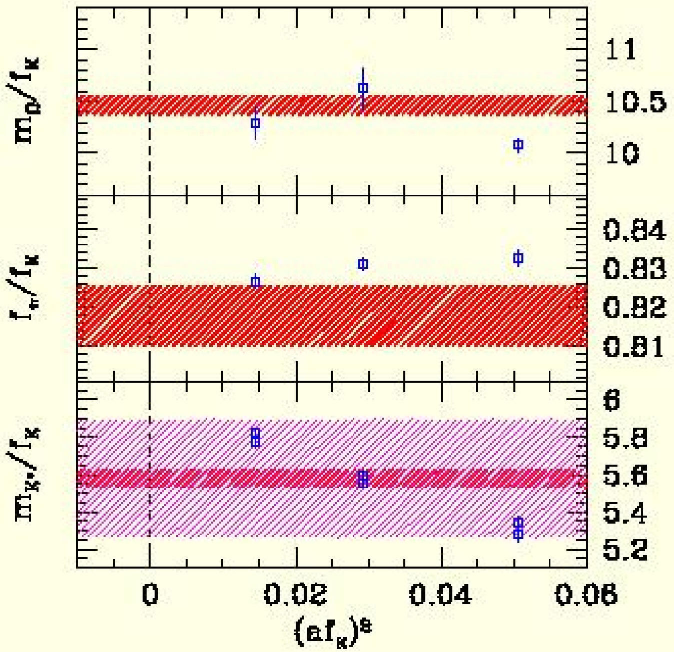
"2% is the accuracy of our LCP."

T=0 results at the physical point, scale setting

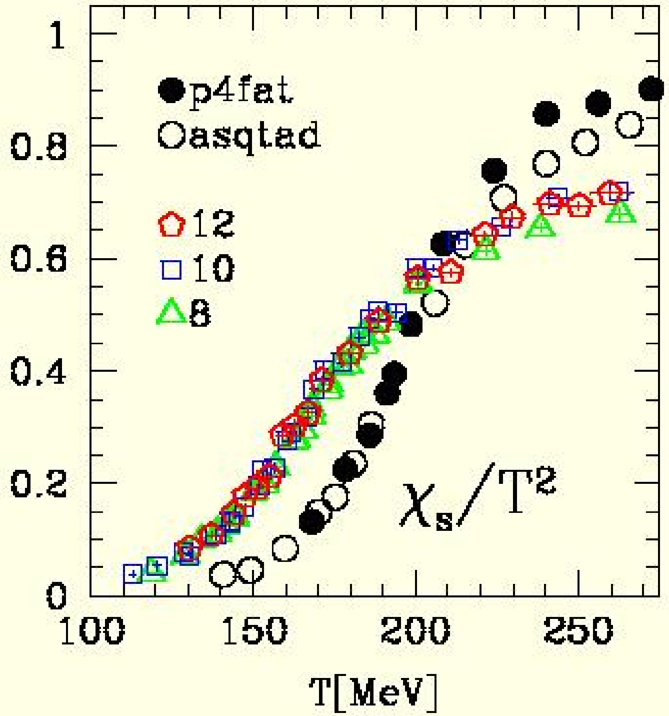
last concluding remark of our competitors: it is desirable to
"obtain a reliable independent scale setting for the transition temperature from an observable not related to properties of the static potential".



extend original f_K scale setting to m_Ω, f_π, m_{K^*} $\Rightarrow$ consistent scales
red bands are the experimental values with uncertainties
K^* decays in the physical point, width is also given (pink)
smaller spacings and r_0 are currently under analysis
V,r_0 "no significant cut-off effects": instead dimensionless combinations

T>0 results

strange quark number susceptibility

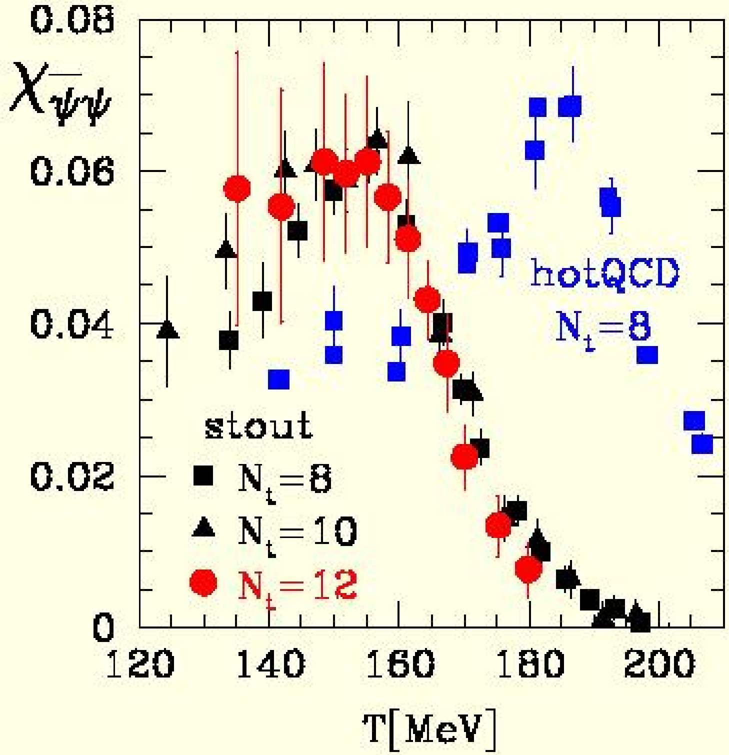


preliminary results, 300-500 trajectories in each point
good agreement with old $N_t = 10$ data

Y. Aoki, Z. Fodor, S.D. Katz, K.K. Szabo, Phys. Lett. B. 643 (2006) 46 [hep-lat/0609068]
"For the transition temperature in the continuum limit one gets: $T_c(\chi_s) = 175(2)(4)$ MeV"

T>0 results

renormalized chiral susceptibility



nice agreement with old $N_t = 8, 10$ data

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"the transition temperature based on the chiral susceptibility reads $T_c(\chi_{\bar{\psi}\psi}) = 151(3)(3)$ MeV"

• universality problem in 2+1 flavour staggered QCD

naively discretizing fermions leads to 16 degenerate fermions
staggered fermions on 2^4 cell leads to 4 degenerate fermions
take the root of the fermion determinant to reach $2+1$ flavours

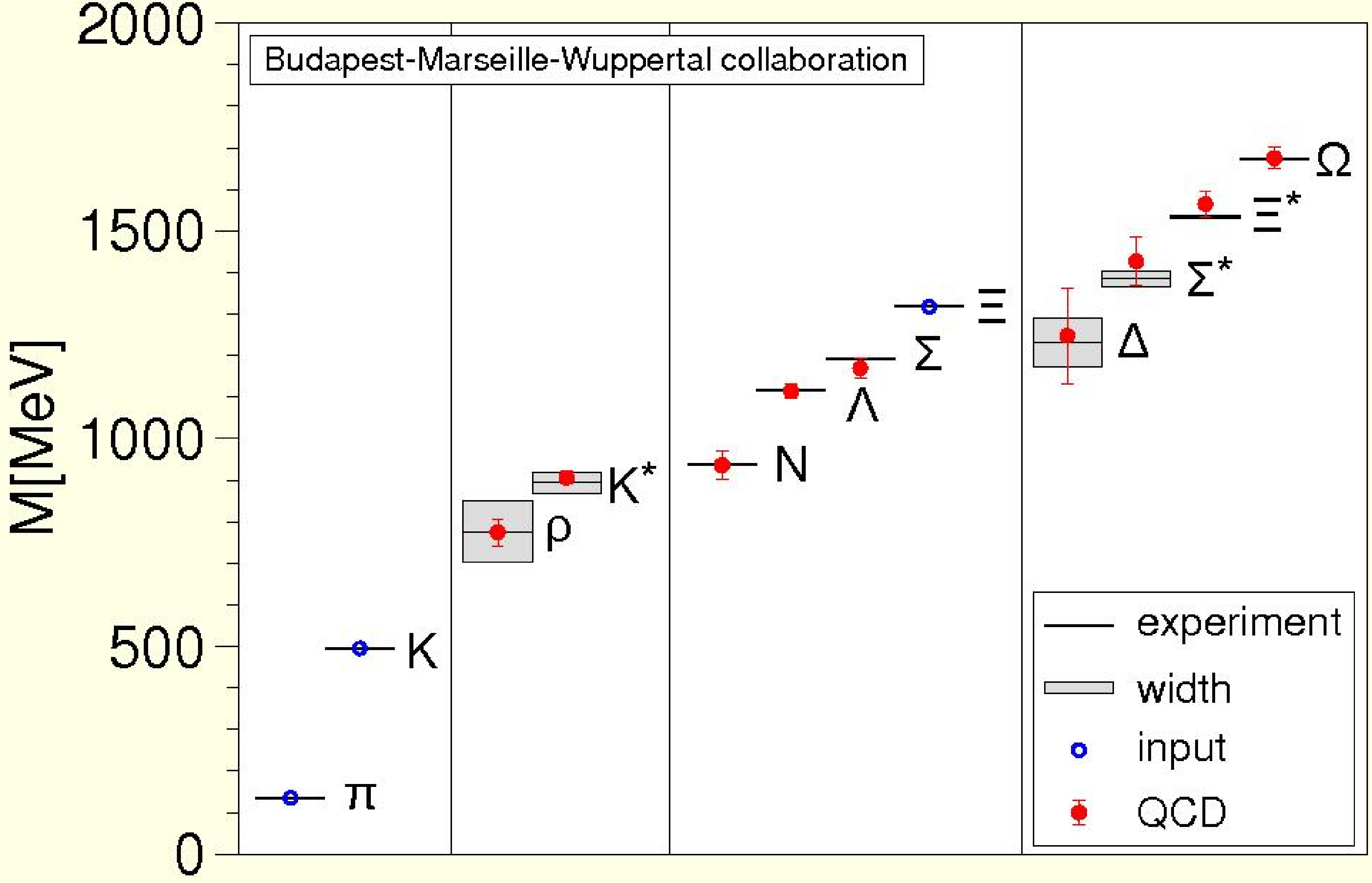
known to be non-local for any non-vanishing lattice spacings

much faster than any other fermion formulation
the largest scale thermodynamics projects are all in staggered QCD

lively discussion: staggered fermions are good, bad or just ugly
M.Cruetz: bad; S.Sharpe: just ugly (Lattice'06 "wouldn't start again")

new algorithms for Wilson fermions (in the universality class of QCD)

one can already control all systematics
lattice spacings, quark masses, finite volume within really n_f=2+1 QCD



⇒ use a formulation, which is known to be in the universality class of QCD

http://www.bmw.uni-wuppertal.de

Summary

- Gap between lattice and perturbative bulk thermodynamics

two new methods to reach (arbitrary) high temperatures

connection to perturbation theory is established

- The nature of the QCD transition was determined

we used physical quark masses and extrapolated to the continuum limit

$\Longrightarrow$ the QCD transition is an analytic cross-over

- The transition temperature is determined (2006)

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

- hotQCD:

they improved their T>0 simulations from N_t=4,6 to N_t=8

- our group:

we improved our T=0 simulations with physical quark masses

we improved our T>0 simulations from N_t=6,8,10 to $N_t = 12$

our chiral extrapolations were correct on the 1% level

consistent scales obtained by f_K, m_Ω, f_π and m_{K^*} (we will give r_0 in fm)

preliminary results for chiral susceptibility and strange susceptibility

$N_t = 12$ are in good agreement with our 2006 results

- discrepancies are not resolved

should we use N_t=16? No, the accumulated data is most probably enough

should hotQCD use other scale settings, too? Probably yes (was their plan)

- n_f=2+1 staggered QCD can be influenced by the universality problem

$\Rightarrow$ use a formulation, which is known to be in the universality class of QCD

recent algorithmic developments allow one to use Wilson fermions

CP violation, K^0–$\bar{K}^0$ mixing and B_K

C: charge conjugation (particle $\leftrightarrow$ antiparticle exchange)
P: space reflection (left $\leftrightarrow$ right exchange)

$|K^0\rangle = |\bar{s}d\rangle$ and $|\bar{K}^0\rangle = |s\bar{d}\rangle$; mass (energy) eigenstates are: $|K_S\rangle$ and $|K_L\rangle$

the universe has a CP preference $\Longrightarrow$ origin of matter (asymmetry)

someone visits us from other end of the universe: matter or antimatter?
$K_L \to e_R^+ \nu_L \pi^-$: 20.2% and $K_L \to e_R^- \bar{\nu}_L \pi^+$: 0% due to maximal C-violation

do we know the absolute definition of left and right?
exchange also left and right $K_L \to e_L^- \bar{\nu}_R \pi^+$: 20.2%

do it more precisely: K_L slightly prefers to decay into $e^+ \nu \pi^-$ than $e^- \bar{\nu} \pi^+$

$$\frac{\Gamma(K_L \to e^+ \nu \pi^-)}{\Gamma(K_L \to e^- \bar{\nu} \pi^+)} = 1.007 = 1 + f(\bar{\eta}, \bar{\rho} \ldots)\langle \bar{K}^0 | \mathscr{H} | K^0 \rangle = 1 + f(\bar{\eta}, \bar{\rho} \ldots)\frac{8}{3} m_K^2 f_K^2 B_K$$

CKMfitter Group, UTfit Collaboration still use quenched B_K from 1997

Chiral susceptibility:

Renormalization: seen before

Quark number susceptibility:

$$\frac{\chi_s}{T^2} = \frac{1}{TV} \frac{\partial^2 \log Z}{\partial \mu_s^2}\bigg|_{\mu_s=0}$$

No renormalization necessary

Polyakov loop:

$$P = \frac{1}{N_s^3} \sum_{\mathbf{x}} \mathrm{tr}[U_4(\mathbf{x},0)U_4(\mathbf{x},1)\ldots U_4(\mathbf{x},N_t-1)]$$

Related to the static quark free energy:

$$|\langle P \rangle|^2 = \exp(-\Delta F_{q\bar{q}}(r \to \infty)/T)$$

Renormalization condition for the potential: $V_R(r_0) = 0$

$$|\langle P_R \rangle| = |\langle P \rangle| \exp(V(r_0)/(2T))$$