

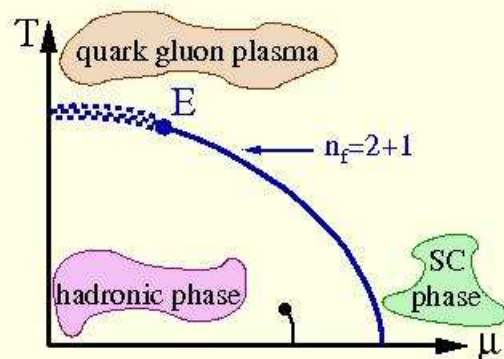
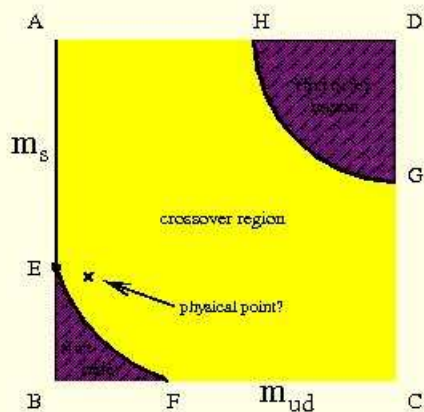
# Lattice QCD thermodynamics at $\mu=0$ and $\mu\neq 0$

Zoltán Fodor

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1. Standard picture of the phase diagram
2. Lattice formulation, fermion doubling, rooting
3. Lattice results at  $L_t=4$  ( $\mu>0$ )
4. Lattice results at  $L_t=4,6$  (equation of state)
5. Lattice results at  $L_t=4,6,8,10$  (nature and  $T_c$ )
6. 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  $\infty$  gives a first order transition

for intermediate quark masses we have an analytic cross over (no  $\chi$ PT)

F. Karsch et al., Nucl. Phys. Proc. 129 (2004) 614; Lattice'07 G. Endrodi, O. Philipsen

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

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

$N_t=4,6,8,10$  lattices correspond to  $a \approx 0.3$  fm, 0.2 fm, 0.15 fm, 0.12 fm

CPU:  $\approx N_t^{12}$  (thermodynamics):  $N_t=10$  needs 50-times more than  $N_t=6$

## Partition function

$$Z = \int dU d\Psi d\bar{\Psi} e^{-S_E}$$

$S_E$  is the Euclidean action

Parameters:

gauge coupling  $g$

quark masses  $m_i$  ( $i = 1..N_f$ )

(Chemical potentials  $\mu_i$ )

Volume ( $V$ ) and temperature ( $T$ )

Finite  $T \leftrightarrow$  finite temporal lattice extension

$$T = \frac{1}{N_t a}$$

Continuum limit:  $a \rightarrow 0$

Renormalization: keep the physical spectrum constant

at finite  $T$ :

continuum limit  $\iff N_t \rightarrow \infty$

CPU grows like  $N_t^{13}$ , thus  $N_t=10$  instead of  $N_t=6$  needs 50-100 $\times$  more CPU







## Overlap improving multi-parameter reweighting

Z. Fodor and S.D. Katz, Phys. Lett. B534 (2002) 87

$$\begin{aligned} Z(m, \mu, \beta) &= \int \mathcal{D}U \exp[-S_g(\beta, U)] \det M(m, \mu, U) = \\ &\int \mathcal{D}U \exp[-S_g(\beta_0, U)] \det M(m_0, \mu = 0, U) \\ &\left\{ \exp[-S_g(\beta, U) + S_g(\beta_0, U)] \frac{\det M(m, \mu, U)}{\det M(m_0, \mu = 0, U)} \right\} \end{aligned}$$

first line = **measure**, field configurations of the Monte-Carlo

curly bracket = **can be measured on each configuration**, weight

simultaneously changing several parameters: better overlap

e.g. transition configurations are mapped to transition ones

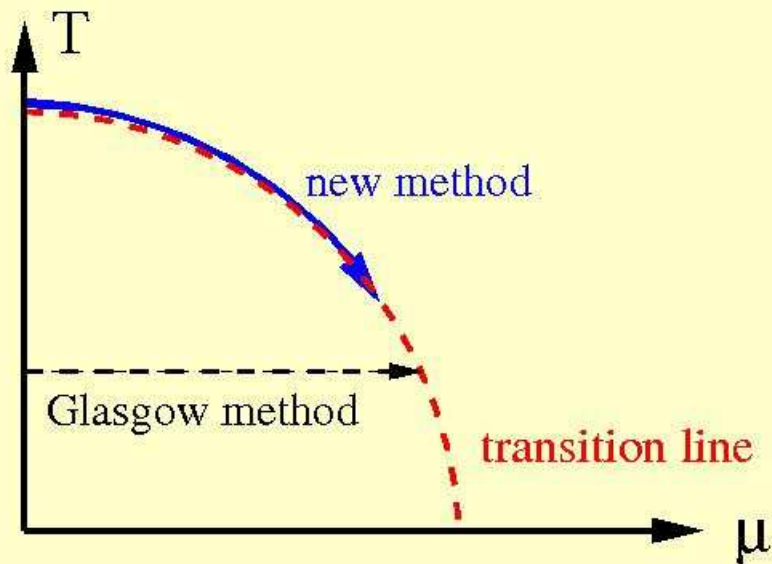
expectation value of an observable  $O$ :

$$\langle O \rangle_{\beta, \mu, m} = \frac{\sum w(\beta, \mu, m) O(\mu, m)}{\sum w(\beta, \mu, m)}$$

observables to get the transition points at  $\mu \neq 0$  (susceptibilities)



## Comparison with the Glasgow method



one parameter reweighting  
single parameter ( $\mu$ )  
purely hadronic  
configurations

New method  
two parameters ( $\mu$  and  $\beta$ )  
transition configurations

## $\mu \neq 0$ multi-parameter reweighting with Taylor expansion

C.R. Allton et al., Phys. Rev. D66 074507,'02, D68 014507,'03

$$Z(m, \mu, \beta) = \int \mathcal{D}U \exp[-S_g(\beta, U)] \det M(m, \mu, U) = \\ \int \mathcal{D}U \exp[-S_g(\beta_0, U)] \det M(m_0, \mu = 0, U) \\ \left\{ \exp[-S_g(\beta, U) + S_g(\beta_0, U)] \frac{\det M(m, \mu, U)}{\det M(m_0, \mu = 0, U)} \right\}$$

instead of evaluating determinants expand them in  $\mu$  or  $\exp(\mu)$ :

$$\ln \left( \frac{\det M(\mu)}{\det M(0)} \right) = \sum_{n=1}^{\infty} \frac{\mu^n}{n!} \frac{\partial^n \ln \det M(0)}{\partial \mu^n} \equiv \sum_{n=1}^{\infty} R_n \mu^n$$

faster than the complete evaluation of the determinants

only valid for somewhat smaller  $\mu$  values than the full technique



## QCD phase diagram from imaginary chemical potential

P.deForcrand, O.Philipsen, Nucl. Phys. B642 290,'02; B673 170, '03

M.D'Elia, M.P.Lombardo, Phys. Rev. D67 014505,'03

fermion determinant: real for imaginary chemical potential ( $\mu_I$ )

$\Rightarrow$  no sign problem, no need for reweighting

directly obtain the  $(\beta_c, \mu_I)$  transition line

analytically continue it to get the physical  $(\beta_c, \mu)$  line

transition line  $(\beta_c, \mu_I)$  is given by the susceptibility-peak

$$\chi = VN_t \langle (\mathcal{O} - \langle \mathcal{O} \rangle)^2 \rangle, \quad \partial \chi / \partial \beta = 0 \quad \partial^2 \chi / \partial \beta^2 < 0$$

on finite V the analytic  $\chi(\mu_I, \beta)$  can be measured

using the implicitly given  $\beta_c(\mu_I)$  one gets

$$\partial \beta_c / \partial \mu = -i \partial \beta_c / \partial \mu_I$$

## Density of states (DOS) method

### Constrained simulations:

Force some observable to have a given value

this way configurations with all values of the observable present  
overlap problem not so serious

For any observable:

$$\langle O \rangle = \int dx \langle O f(U) \rangle_x \rho(x) / \int dx \langle f(U) \rangle_x \rho(x)$$

$\rho$ , the density of states is the constrained partition function  
for some observable  $\phi$

$$\rho(x) \equiv Z_\phi(x) = \int \mathcal{D}U g(U) \delta(\phi - x).$$

### Possible choices for $\phi$ :

$\phi = \text{PI}$  (Bhanot et.al, '87; Karliner et.al,'88; Azooiti et.al,'90; Luo, '01; Takaishi, '04)

$\phi = \Theta$  (complex phase) (Gocksch, '88)

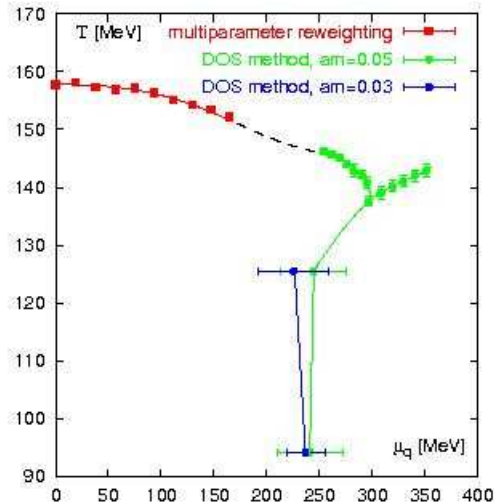
$\Phi = n_q$  (Ambjorn et. al., '02)

Our choice:  $\phi = P$        $g = |\det M| \exp\{-S_G\}$ ,       $f = \exp\{i\theta\}$

## Results for QCD at large $\mu$

Z. Fodor, S.D. Katz, C. Schmidt, JHEP 0703:121,2007 [hep-lat/0701022]

$N_f = 4$  staggered QCD on  $6^4, 8 \cdot 6^3$  lattices



existence of a triple point around  $\mu_q \approx 300$  MeV and  $T \lesssim 135$  MeV

Note,  $L_t=6$  lattices: smallest  $T$  is 73 MeV (if  $m_\rho$  fixes the scale)

Mass dependence checked:

small  $T$  transition point does not depend on pion mass



## Equation of state from lattice simulations

energy density ( $\epsilon$ ) and pressure ( $p$ ) from partition function:

$$\epsilon(T) = \frac{T^2}{V} \frac{\partial(\log Z)}{\partial T} \quad p(T) = T \frac{\partial(\log Z)}{\partial V}.$$

$T, V$  are varied by  $a$ , take derivative with respect of  $a$

$$\frac{\epsilon - 3p}{T^4} = -\frac{L_t^3}{L_s^3} a \frac{d(\log Z)}{da}$$

the pressure ( $p \propto \log[Z]$ ) along the LCP by the integral method:

$$\frac{p}{T^4} = L_t^4 \int d(\beta, m \cdot a) \left( \frac{\partial(\log Z)}{\partial \beta}, \frac{\partial(\log Z)}{\partial(m \cdot a)} \right)$$

## Renormalization of the pressure

We want  $p(T = 0) = 0$  and  $\epsilon(T = 0) = 0 \rightarrow$

Simulations at both

$T > 0$  ( $N_t \ll N_s$ ) and  $T = 0$  ( $N_t \gtrsim N_s$ )

are necessary and then subtraction:

$$\frac{p}{T^4} = \frac{p_T}{T^4} - \frac{p_0}{T^4}, \quad \frac{\epsilon}{T^4} = \frac{\epsilon_T}{T^4} - \frac{\epsilon_0}{T^4}$$

numerical precision needed for the subtraction increases with  $N_t^4$   
 $\rightarrow$  CPU costs grow faster ( $\mathcal{O}(1/\alpha^{13})$ ) than for  $T = 0$  simulations

Today

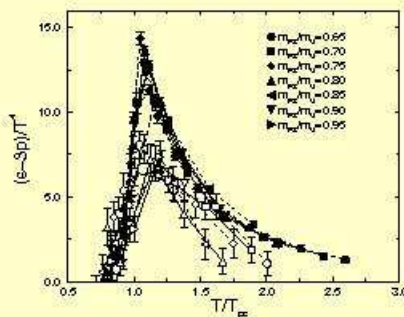
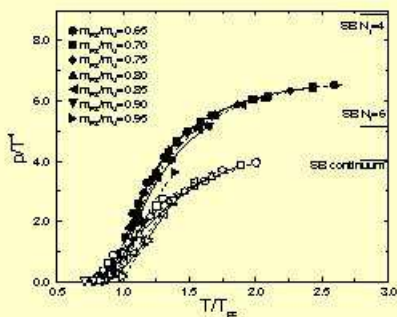
$N_t = 4$  is easy

$N_t = 6$  is difficult

$N_t = 8$  is a challenge

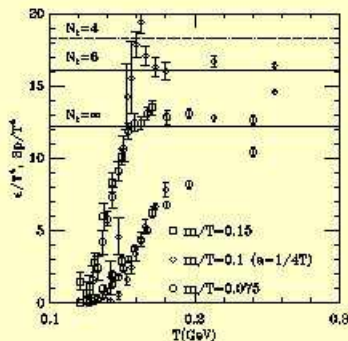
## Previous lattice results

Wilson fermions: slower

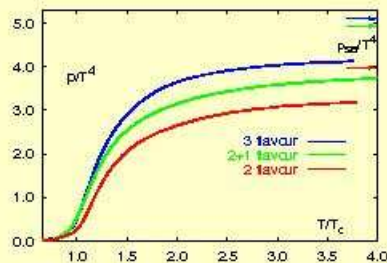


[Ali-Khan et al, '01]

Staggered fermions: faster



[Bernard et al, '96]



[Karsch, Laermann, Peikert, 2000]

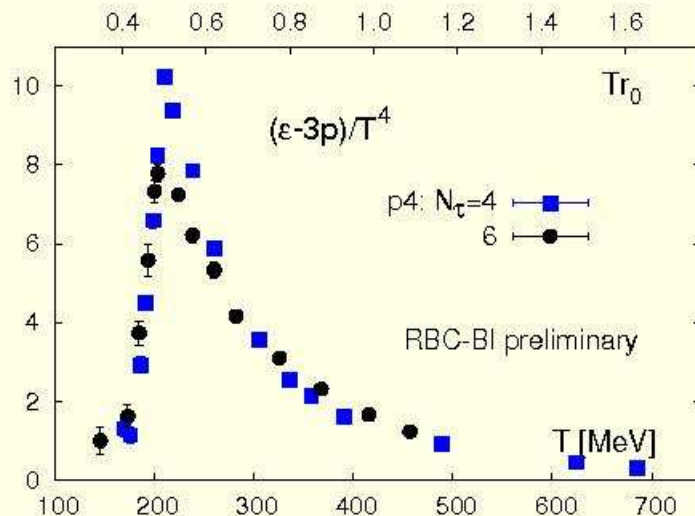
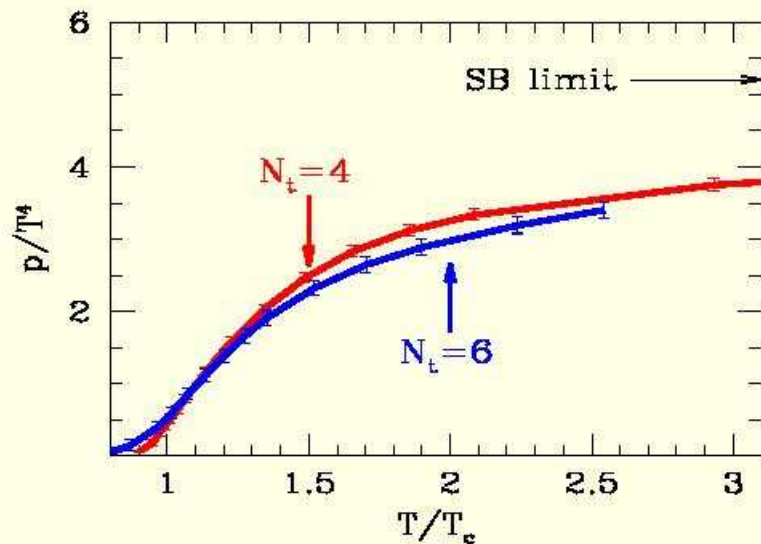
Ongoing project: Bielefeld-Brookhaven-Columbia-Riken



## Equation of state and scaling

Y.Aoki, Z.Fodor, S.D.Katz, K.K.Szabo, JHEP, 0601, 089, 2006.

F.Karsch, hep-ph/0701210

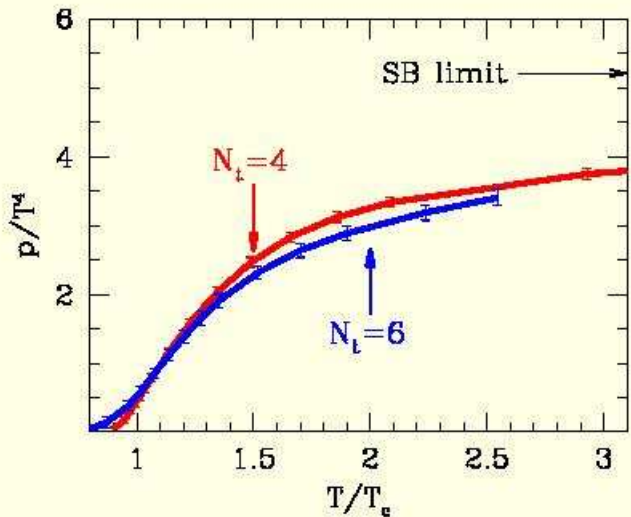


→  $N_t = 8$  is needed for final continuum-extrapolated result

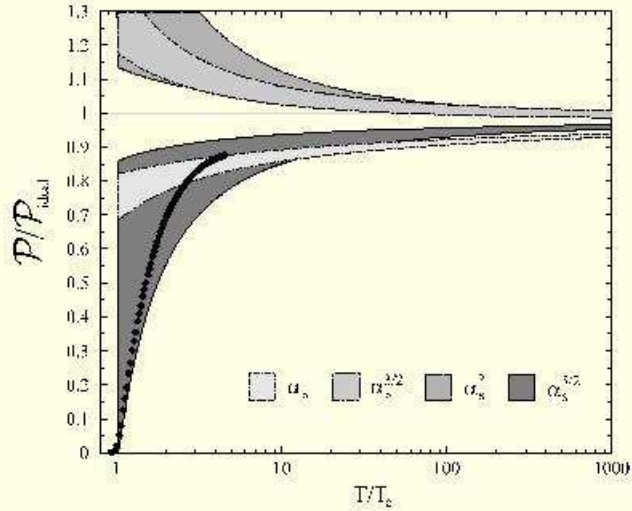
recent  $L_t=4,6$  results also from the MILC collaboration: hep-lat/0611031

Link to perturbation theory: equation of state at large temperatures

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:

$\bar{p} = T/V \cdot \log(Z)$ , but  $Z$  is difficult  $\Rightarrow \bar{p}$  integral of  $(\partial \log(Z)/\partial \beta, \partial \log(Z)/\partial m)$   
 subtract the  $T=0$  term, the pressure is given by:  $p(T) = \bar{p}(T) - \bar{p}(T=0)$

• back of an envelope estimate:

$T_c \approx 150 - 200$  MeV,  $m_\pi = 135$  MeV and try to reach  $T = 20 \cdot T_c$  for  $N_t = 8$  ( $a = 0.0075$  fm)  
 $\Rightarrow N_s > 4/m_\pi \approx 6/T_c = 6 \cdot 20/T = 6 \cdot 20 \cdot N_t \approx 1000 \Rightarrow$  completely out of reach

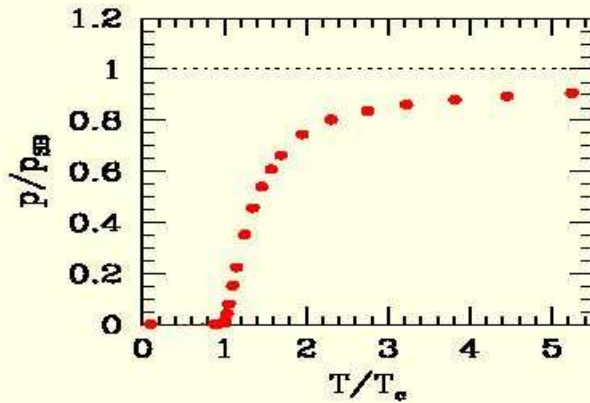
- a. subtract successively:  $p(T) = \bar{p}(T) - \bar{p}(T=0) = [\bar{p}(T) - \bar{p}(T/2)] + [\bar{p}(T/2) - \bar{p}(T/4)] + \dots$   
 $\implies$  for subtractions at most twice as large lattices are needed
- b. instead of the integral method calculate:  $\bar{p}(T) - \bar{p}(T/2) = T/(2V) \cdot \log[Z^2(N_t)/Z(2N_t)]$

$$\frac{Z^2(N_t)}{Z(2N_t)} = \frac{\begin{array}{c} \begin{array}{|c|c|} \hline \text{---} & \text{---} \\ \hline \end{array} \\ \begin{array}{|c|c|} \hline \text{---} & \text{---} \\ \hline \end{array} \\ \hline \begin{array}{|c|c|} \hline \text{---} & \text{---} \\ \hline \end{array} \\ \begin{array}{|c|c|} \hline \text{---} & \text{---} \\ \hline \end{array} \\ \hline \end{array}}{\begin{array}{|c|c|} \hline \text{---} & \text{---} \\ \hline \end{array}} \quad \begin{array}{c} N_t-2 \quad N_t-1 \\ 2 \quad 1 \\ 0 \end{array}$$

$$\bar{Z}(\alpha) = \begin{array}{|c|c|} \hline \text{---} & \text{---} \\ \hline \end{array} \quad \begin{array}{c} (1-\alpha) \\ \alpha \quad \alpha \\ (1-\alpha) \end{array}$$

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

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





- a. subtract successively:  $p(T) = \bar{p}(T) - \bar{p}(T=0) = [\bar{p}(T) - \bar{p}(T/2)] + [\bar{p}(T/2) - \bar{p}(T/4)] + \dots$   
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$$\frac{Z^2(N_t)}{Z(2N_t)} = \frac{\text{Diagram 1}}{\text{Diagram 2}}$$

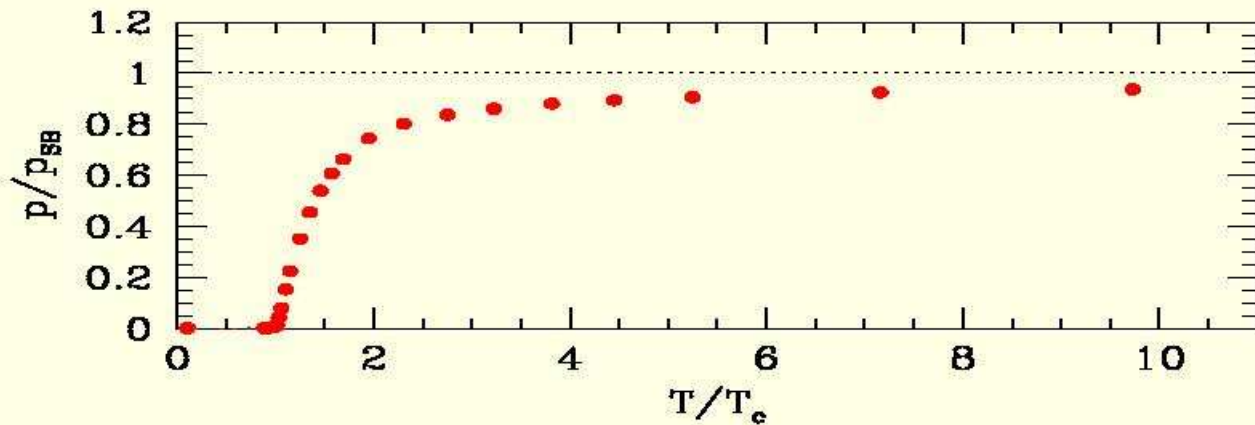
Diagram 1: A diagram representing  $Z^2(N_t)$ . It consists of two separate square lattices of size  $N_t \times N_t$ . The top-left lattice has vertices labeled  $N_t-2$  and  $N_t-1$  at the top, and  $2$  and  $1$  on the left. The bottom-right lattice has vertices labeled  $0$  at the bottom-left and  $2N_t-1$  at the bottom-right. The two lattices are separated by a gap.

Diagram 2: A diagram representing  $Z(2N_t)$ . It is a single large square lattice of size  $2N_t \times 2N_t$ . The vertices are labeled  $2$  and  $1$  on the left,  $0$  at the bottom-left, and  $2N_t-1$  at the bottom-right.

$$\bar{Z}(\alpha) = \text{Diagram 3}$$

Diagram 3: A diagram representing  $\bar{Z}(\alpha)$ . It is a square lattice with vertices labeled  $\alpha$  on the left and right, and  $(1-\alpha)$  at the top and bottom. The lattice is enclosed in a larger square frame with thick black borders on the left and right sides.

define  $\bar{Z}(\alpha) = \int \mathcal{D}U \exp[-\alpha S_{1b} - (1-\alpha)S_{2b}] \implies Z^2(N_t) = \bar{Z}(0)$  and  $Z(2N_t) = \bar{Z}(1)$   
 one gets directly  $\bar{p}(T) - \bar{p}(T/2) = T/(2V) \int_0^1 d\log[\bar{Z}(\alpha)]/d\alpha \cdot d\alpha = T/(2V) \int_0^1 \langle S_{1b} - S_{2b} \rangle \alpha \cdot d\alpha$

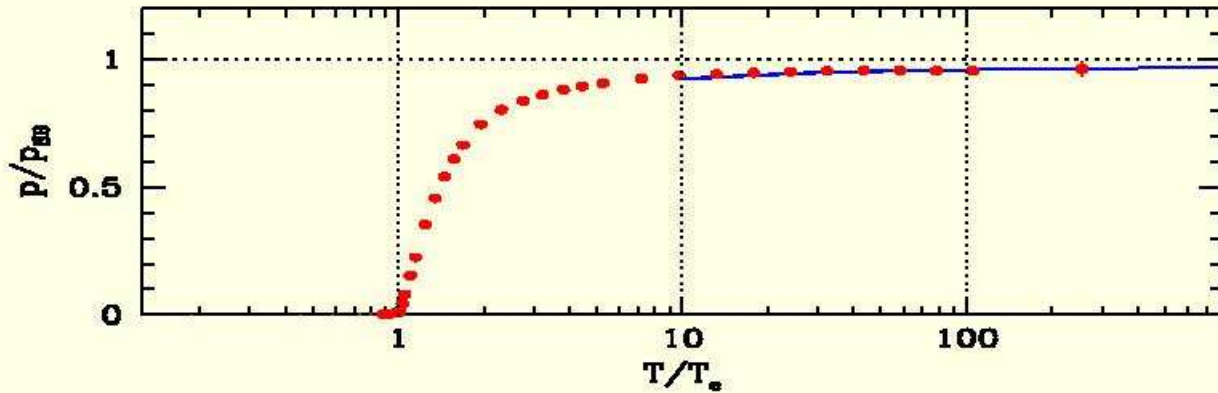


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 $\Rightarrow$  for subtractions at most twice as large lattices are needed
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define  $\bar{Z}(\alpha) = \int \mathcal{D}U \exp[-\alpha S_{1b} - (1-\alpha) S_{2b}] \Rightarrow Z^2(N_t) = \bar{Z}(0)$  and  $Z(2N_t) = \bar{Z}(1)$

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



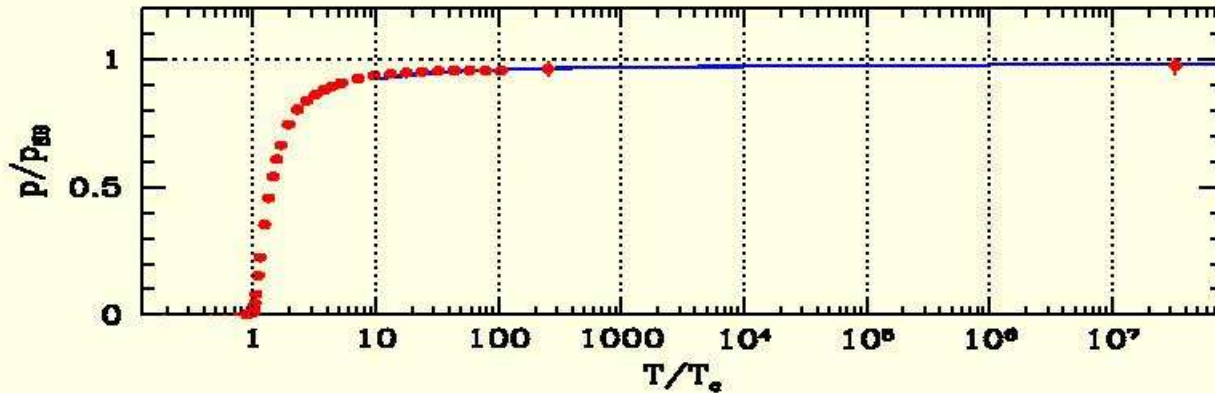
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$$\bar{Z}(\alpha) = \begin{array}{c} (1-\alpha) \\ \begin{array}{|c|c|} \hline \blacksquare \quad \blacksquare \\ \hline \end{array} \\ \alpha \quad \alpha \\ \hline \begin{array}{|c|c|} \hline \blacksquare \quad \blacksquare \\ \hline \end{array} \\ (1-\alpha) \end{array}$$

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



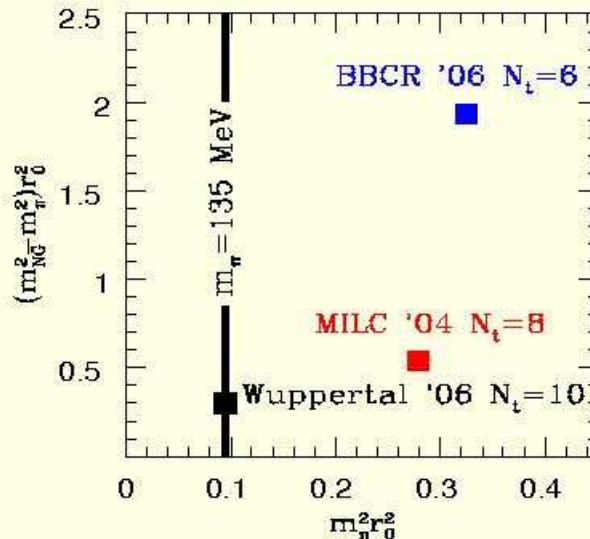
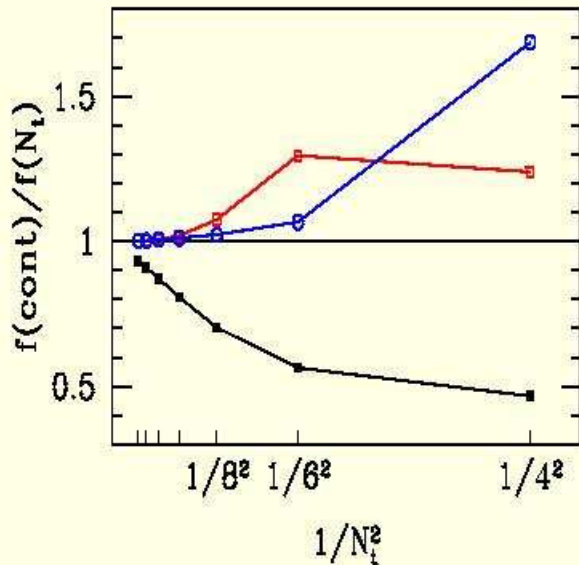




## The nature of the QCD transition

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:  $m_\pi=135$  MeV,  $m_K=500$  MeV

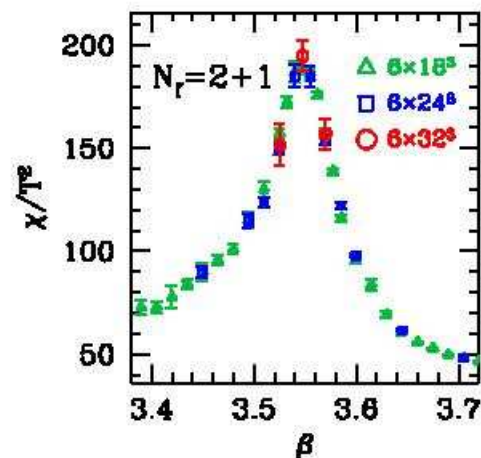
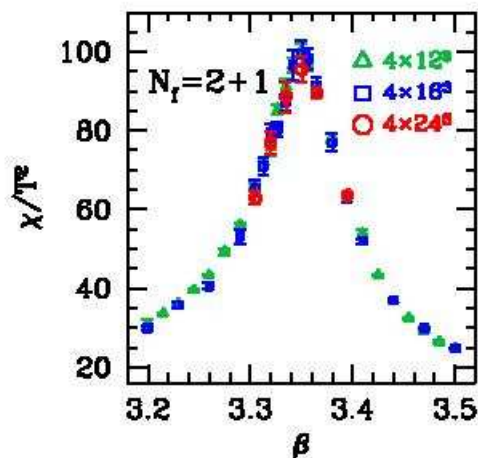
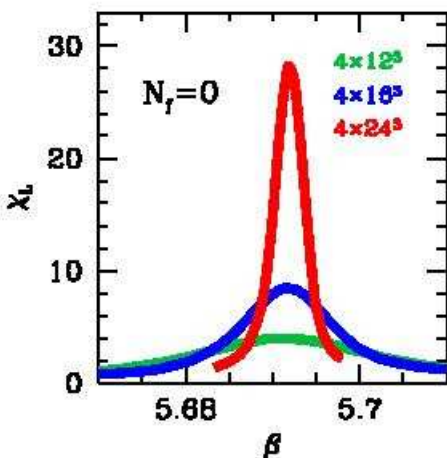


extrapolation from  $N_t$  and  $N_t+2$  (standard action)  $\approx$  as good as  $N_t$  with p4  
 $N_t=8, 10$  gives  $\approx \pm 1\%$ , but  $a < 0.15$ , 0.12 fm needed to set the scale ( $\pm 1\%$ )  
 thermodynamic quantities are obtained "more precisely" than the scale  
 (p4 independent config.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

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

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

cross over  $\implies$  peak width  $\approx$  constant, peak height  $\approx$  constant



for aspect ratios 3–6 (an order of magnitude larger volumes)

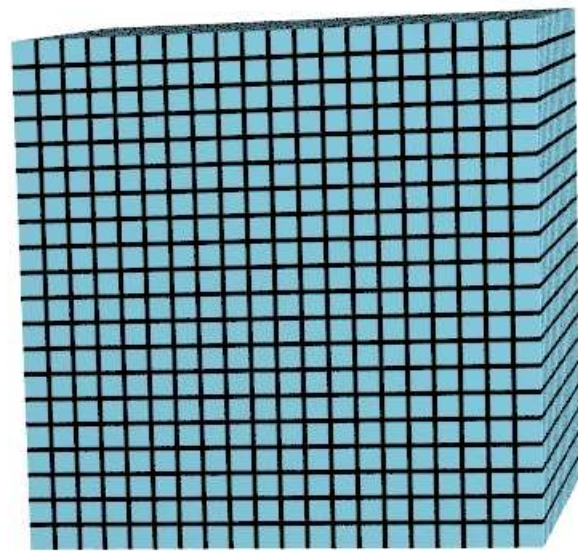
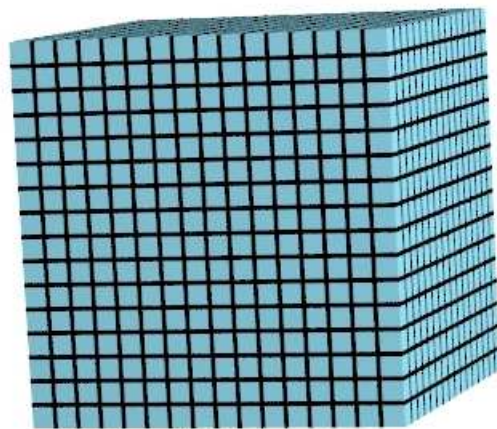
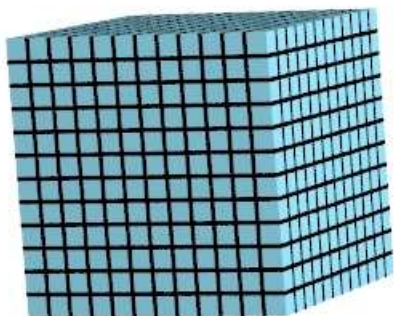
volume independent scaling  $\implies$  cross-over

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:

for physical  $m_\pi$  discretization errors changed the order

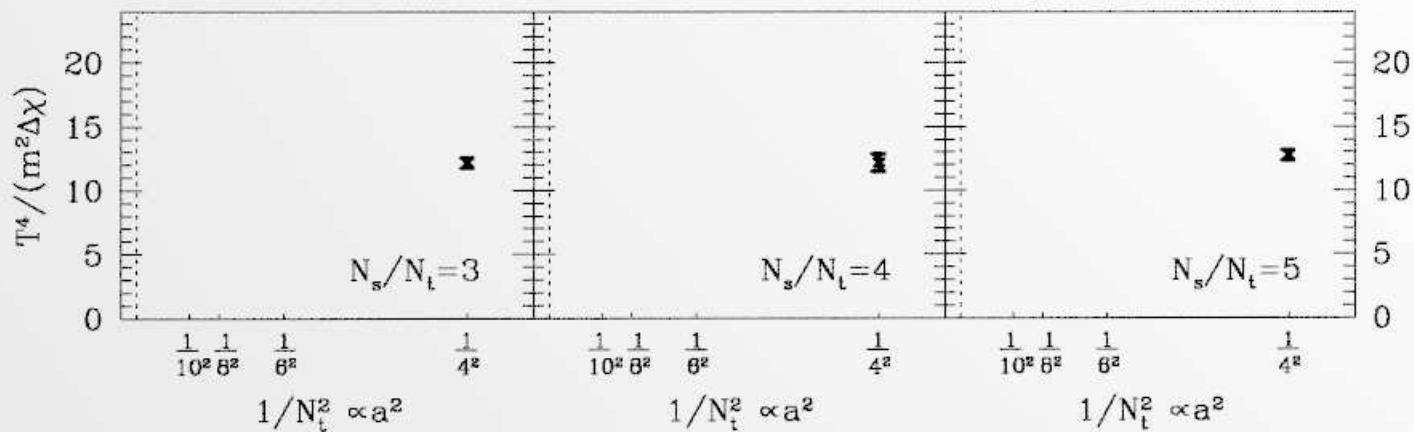
$a=0.3 \text{ fm}$



3.6 fm

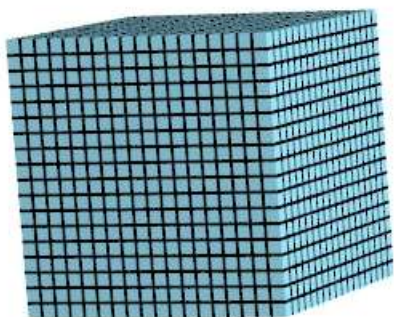
4.8 fm

6 fm

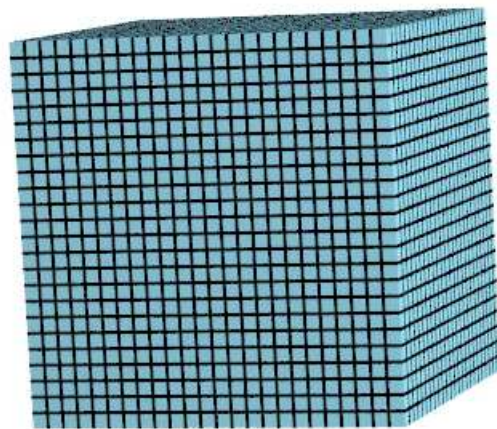




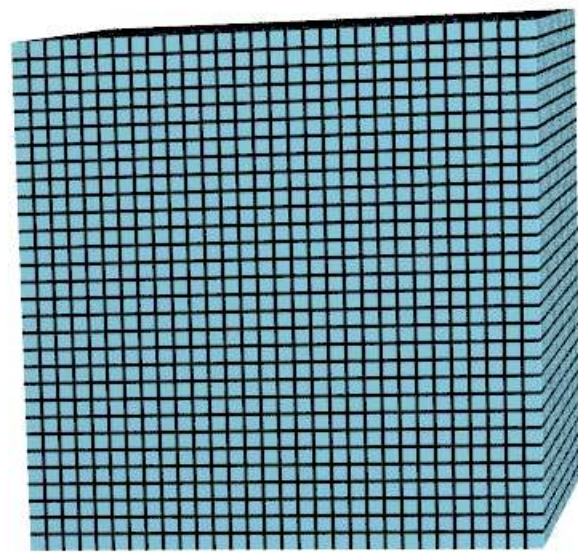
$a=0.2$  fm



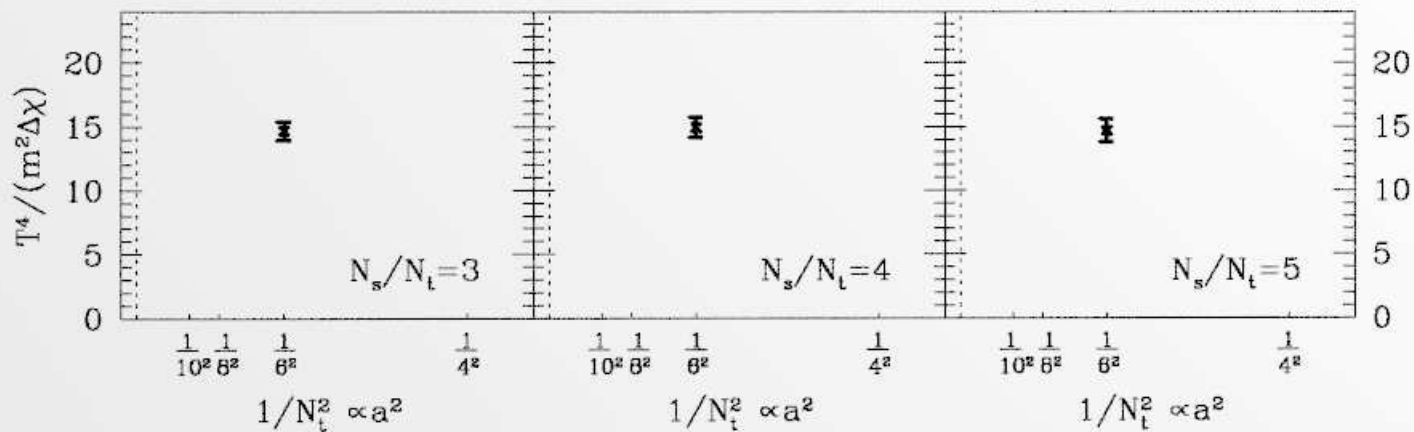
3.6 fm



4.8 fm

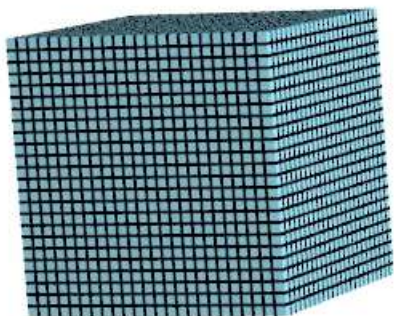


6 fm

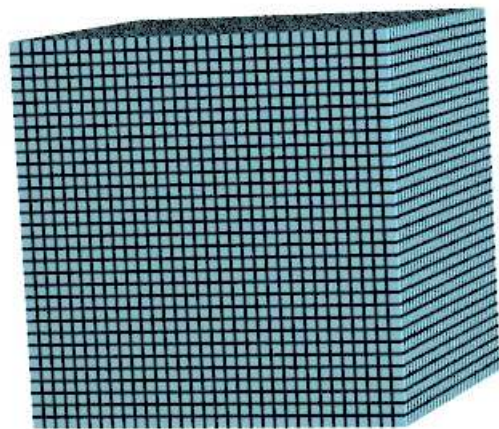




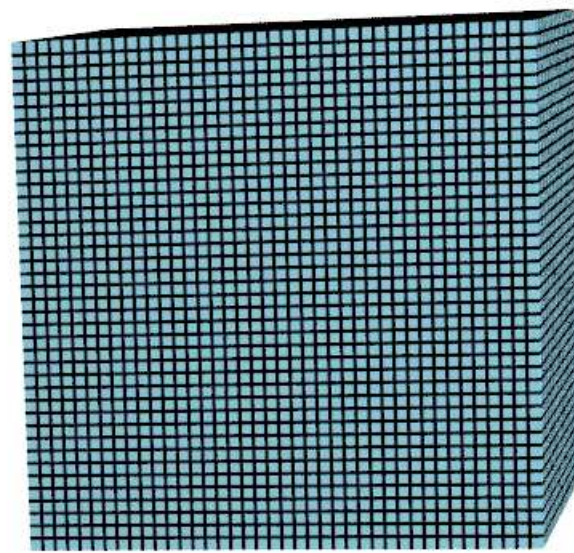
$a=0.15$  fm



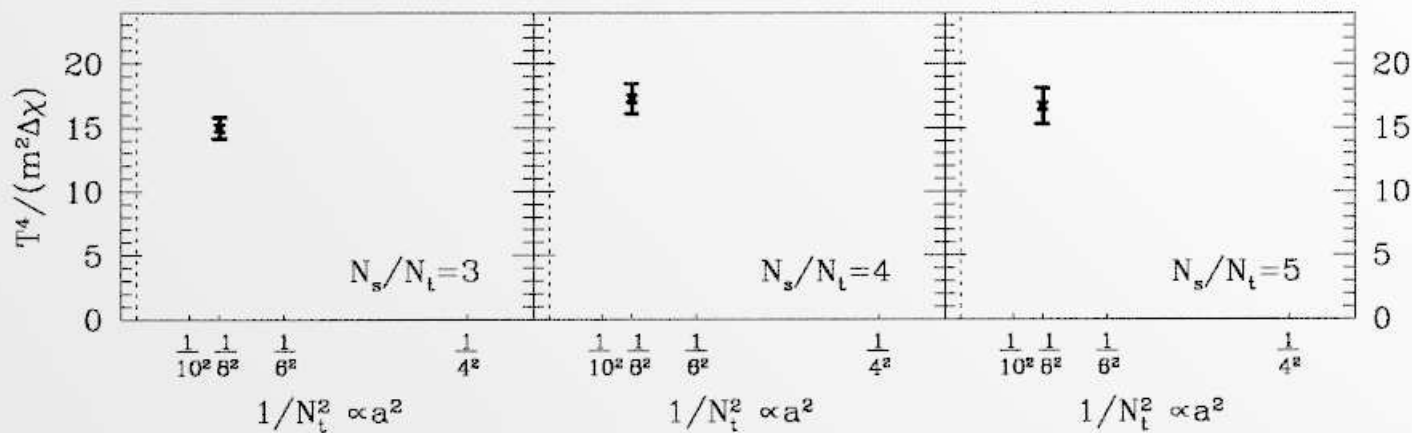
3.6 fm



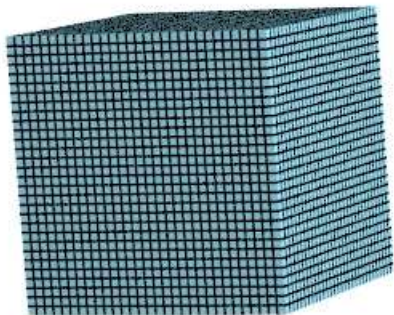
4.8 fm



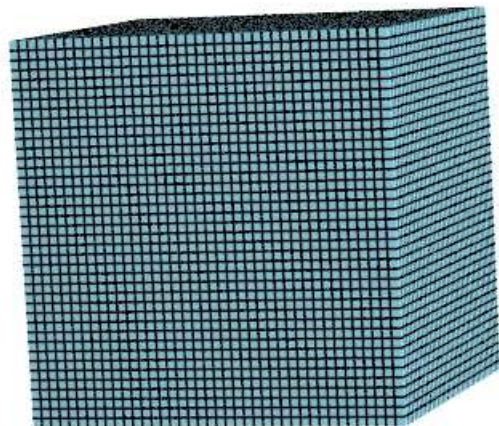
6 fm



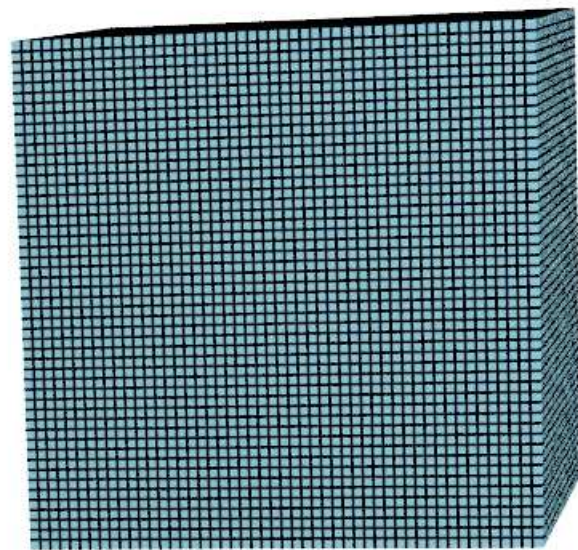
$a=0.12$  fm



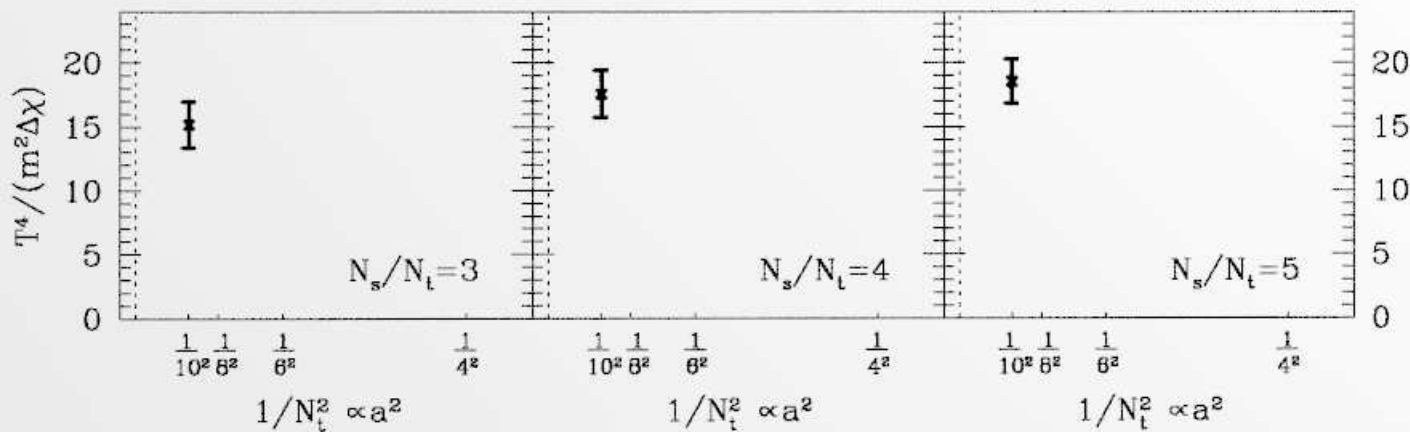
3.6 fm

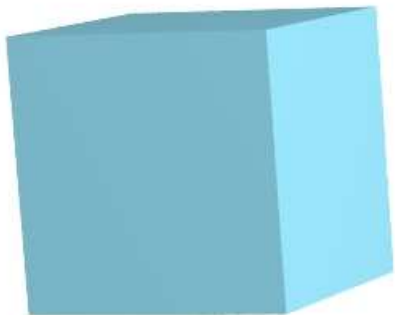


4.8 fm

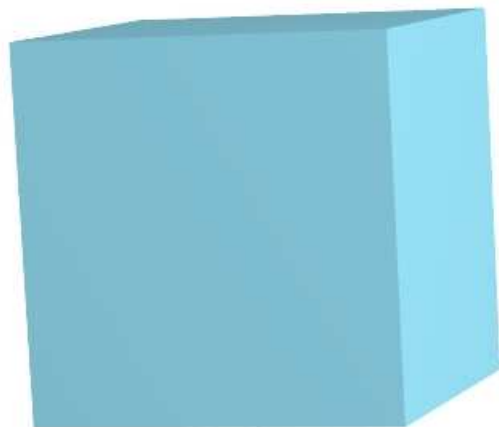


6 fm

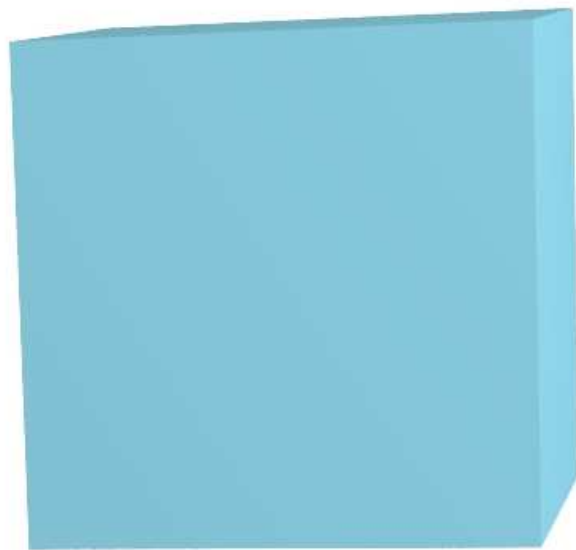




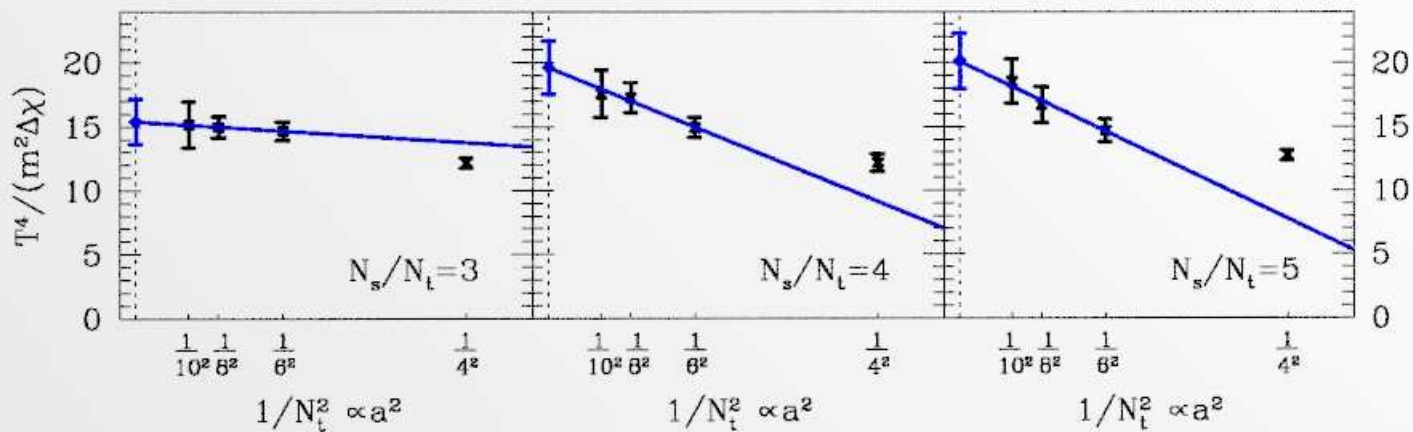
3.6 fm



4.8 fm

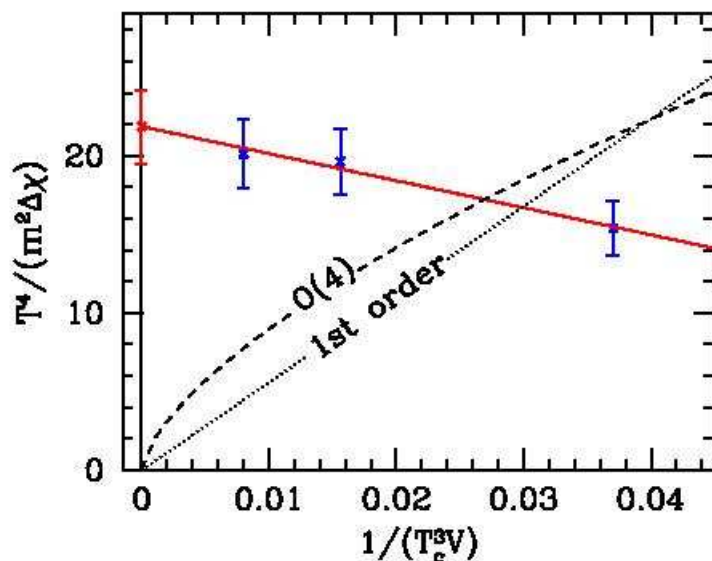


6 fm





- finite size study of continuum extrapolated  $m^2 \Delta \chi$  ( $N_t=4$ : off)



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  $\mu=0$  is a cross-over



## The transition temperature

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

$T = 0$ :

set the physical scale and locate the physical point

Three quantities are needed ( $m_\pi$  and  $m_K$  for the quark masses)

Several possibilities for the third quantity

- string tension (not existing in full QCD)
- static quark potential at intermediate distances ( $r_0^2 \cdot dV/dr=1.65$ )
- directly measurable quantities (e.g.  $f_K$ )

Further quantities are predictions (e.g.  $r_0, f_\pi, m_{K^*}$ )

$T > 0$ :

cross-over  $\rightarrow$  different definitions give different  $T_c$

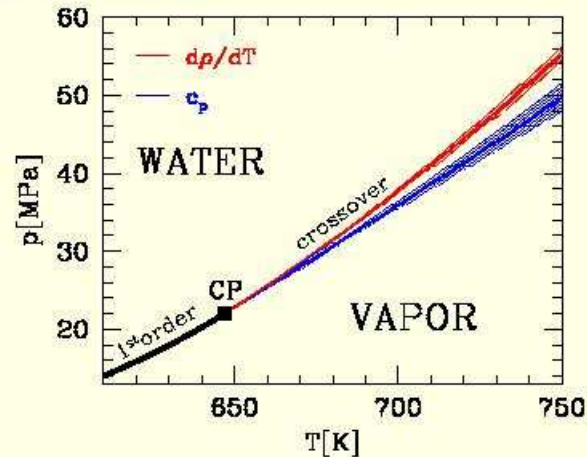
Possible choices:

- Chiral susceptibility
- Quark number susceptibility
- Polyakov-loop

## T>0 Simulations

No well defined  $T_c$

Example of water-steam transition



above the critical point  $c_p$  and  $dp/dT$  give different  $T_c$ s.

Our choices in QCD

$$\frac{m^2 \Delta \chi}{T^4} \rightarrow \text{chiral transition}$$

Quark number susceptibility  $\rightarrow$  de-confinement transition  
Polyakov loop

- an even more often experienced example

melting of ice shows singular behavior: ice  $\rightarrow$  water

melting of butter shows analytic behaviour (broad transition, cross-over)

natural fats are mixed triglycerids of fatty acids from  $C_4$  to  $C_{24}$

these are saturated or unsaturated of even carbon numbers

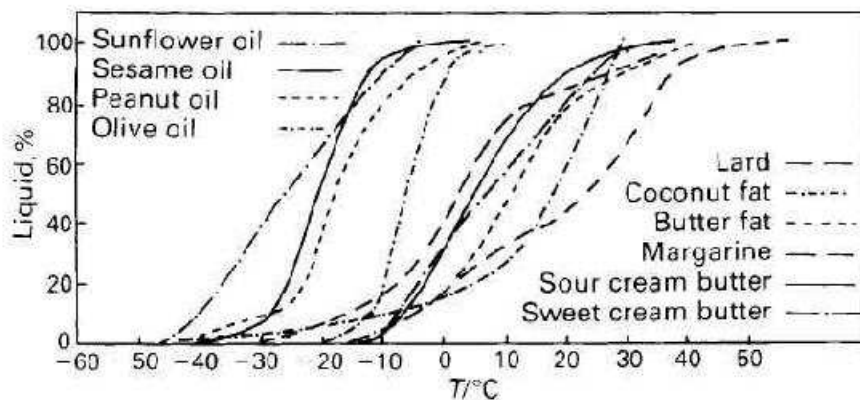
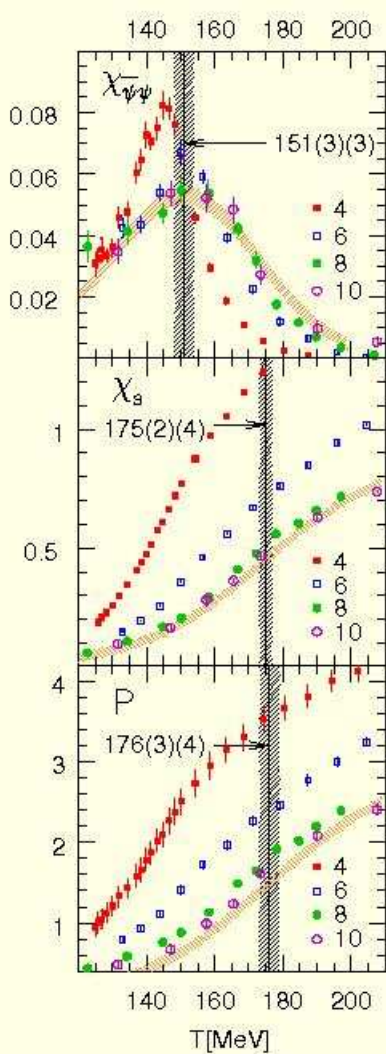


Fig. 4. Liquid proportions of various fats and oils

since in QCD we have an analytic cross-over

we will see very similar temperature dependence for all quantities

e.g. chiral condensate, strange quark susceptibility or Polyakov loop



### Chiral susceptibility

$$T_c = 151(3)(3) \text{ MeV}$$

$$\Delta T_c = 28(5)(1) \text{ MeV}$$

### Quark number susceptibility

$$T_c = 175(2)(4) \text{ MeV}$$

$$\Delta T_c = 42(4)(1) \text{ MeV}$$

### Polyakov loop

$$T_c = 176(3)(4) \text{ MeV}$$

$$\Delta T_c = 38(5)(1) \text{ MeV}$$

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



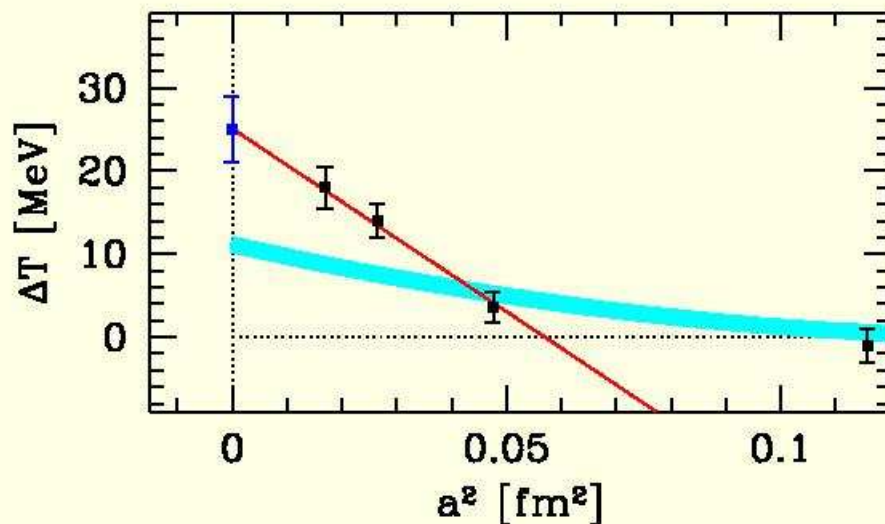
⇒ 25(4) MeV difference between the chiral & the deconfinement transitions

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

continuum: e.g.  $\Delta\chi/T^2$  gives  $\approx 10$  MeV higher  $T_c$  than  $m^2\Delta\chi/T^4$  (blue curve)

the difference can be seen only at small lattice spacings

C. De Tar hotQCD  $N_t=8$  (asqtad):  $T_c$  from  $\chi$  tends to be at smaller values



precise data at  $N_t=8$  and 10 are needed to see the difference

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

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

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

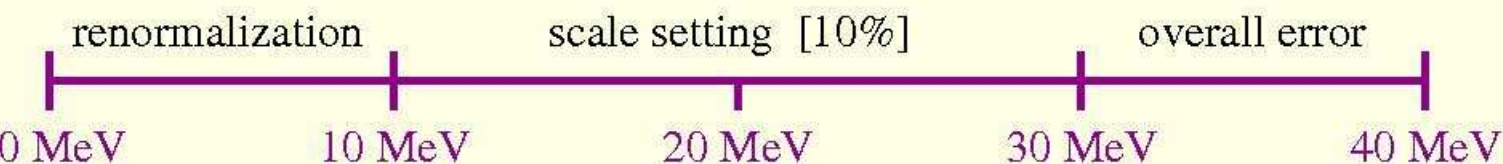
$T_c=192(7)(4)$  MeV,  $\implies$  for  $\chi_{\bar{\psi}\psi}$  contradicts our result ( $\approx 40$  MeV)

### Main differences to our work

no renormalization,  $\chi/T^2$  is used: explains only  $\approx 10$  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)



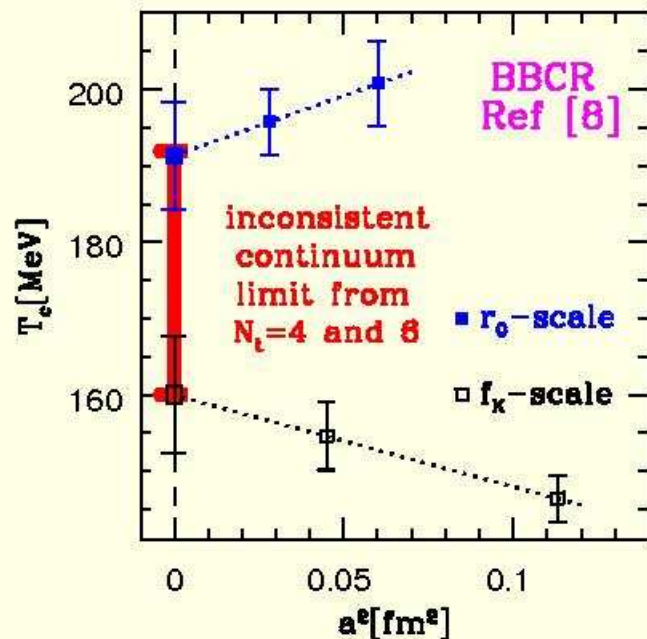
### What is the reason for this discrepancy?

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”.

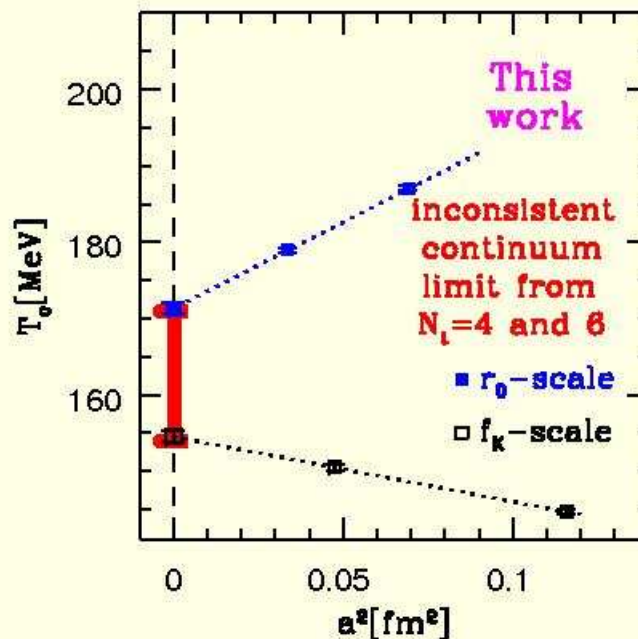
What if they used  $f_K$  to set the scale?

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



Alternatively:

We can use  $r_0$  and only  $N_t=4,6$



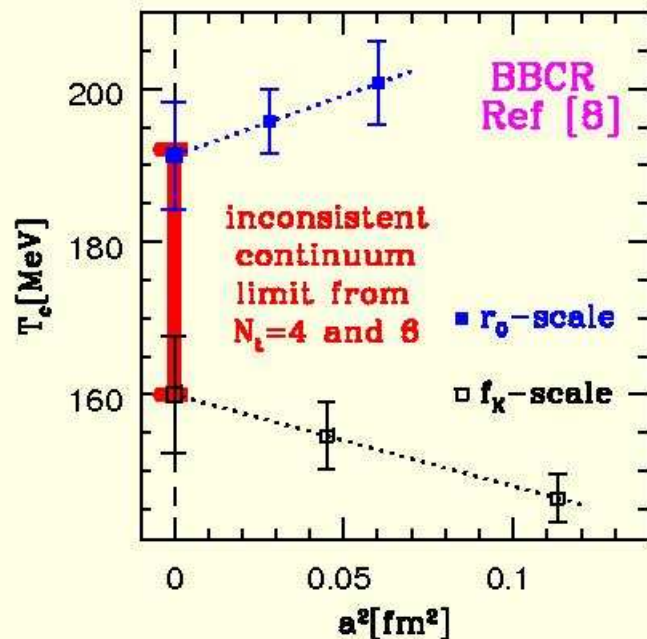
Continuum extrapolations from  $N_t = 4, 6$  are inconsistent!

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



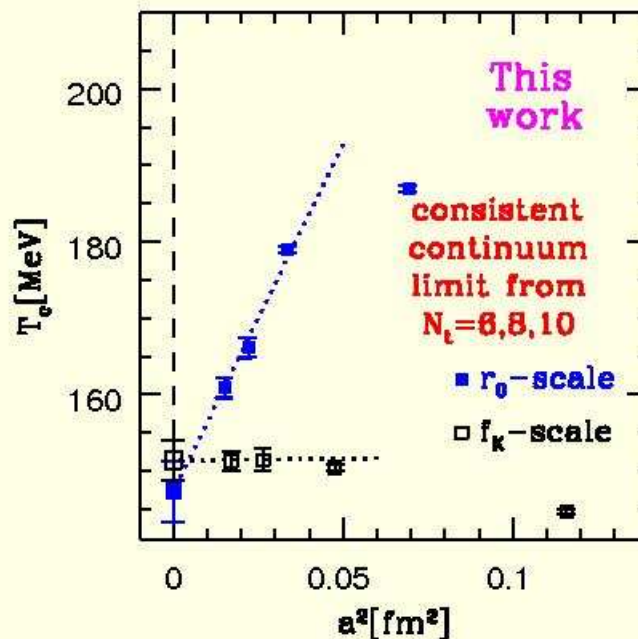
What if they used  $f_K$  to set the scale?

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



Alternatively:

We can use  $r_0$  and only  $N_t=4,6,8,10$



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

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

## Conclusions

lattice thermodynamics: important (already/soon full) results

nature of the transition: analytic transition (cross-over)

$T_c$  discrepancies between groups: resolve it in the continuum

equation of state: still needs a continuum extrapolation

$\mu > 0$  results are quite far from the continuum limit ( $N_t=4$ )

“all” results are within the staggered formalism (non-locality)

$\implies$  closer to the continuum + non-staggered fermions