

# 5. thermodynamic quantities

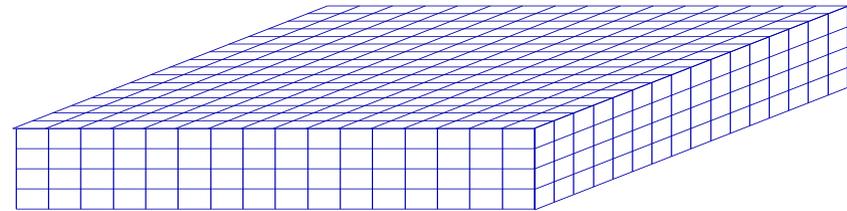
# EOS

$$\epsilon = -\frac{1}{V} \frac{\partial \ln Z}{\partial T^{-1}}, \quad p = T \frac{\partial \ln Z}{\partial V} \quad \text{with} \quad Z = \text{Tr} e^{-H/T} = \int_{b.c.} \mathcal{D}\phi e^{-S}$$

To continuously vary  $T$  and  $V$  independently, we need to (temporarily) introduce anisotropic lattice.

$$a_s \neq a_t$$

$$1/T = N_t a_t, \quad V = (N_s a_s)^3$$



This requires anisotropic beta functions for the variation of  $a_s$  and  $a_t$  independently. They can in principle be estimated by exploring observables in high-dimensional anisotropic coupling parameter space through a systematic study on anisotropic lattices. --- But not easy.

To avoid anisotropic beta functions, the methods discussed in the following subsections are usually adopted.

A crucial point to be noted is that the combination

$$T^{-1} \frac{\partial}{\partial T^{-1}} + 3V \frac{\partial}{\partial V} \propto a_t \frac{\partial}{\partial a_t} + a_s \frac{\partial}{\partial a_s}$$

is nothing but a uniform scale transformation, and thus can be evaluated on just isotropic lattices too.

# EOS (fixed- $N_t$ approach)

$$\epsilon = -\frac{1}{V} \frac{\partial \ln Z}{\partial T^{-1}}, \quad p = T \frac{\partial \ln Z}{\partial V} \quad \text{with} \quad Z = \text{Tr} e^{-H/T} = \int_{b.c.} \mathcal{D}\phi e^{-S}$$

## Trace anomaly

$$\frac{\epsilon - 3p}{T^4} = N_t^4 \left\{ \left\langle a \frac{dS}{da} \right\rangle - \left\langle a \frac{dS}{da} \right\rangle_{T=0} \right\} = \frac{N_t^3}{N_s^3} \sum_i a \frac{db_i}{da} \left\{ \left\langle \frac{\partial S}{\partial b_i} \right\rangle - \left\langle \frac{\partial S}{\partial b_i} \right\rangle_{T=0} \right\}$$

lattice beta functions along LCP

$$b = (\beta, \kappa_{ud}, \kappa_s, \dots) \equiv (b_1, b_2, \dots)$$

measured by the simulation.

$T=0$  subtraction for renormal.

## Integral method for $p$

Differentiate and integrate a thermodyn. relation  $p = (T/V) \ln Z$

$$p = \frac{T}{V} \int_{b_0}^b db \frac{1}{Z} \frac{\partial Z}{\partial b} = -\frac{T}{V} \int_{b_0}^b \sum_i db_i \left\{ \left\langle \frac{\partial S}{\partial b_i} \right\rangle - \left\langle \frac{\partial S}{\partial b_i} \right\rangle_{T=0} \right\}$$

such that  $p(b_0) \approx 0$

numerical integration  
in the coupling param. space

# EOS (fixed- $N_t$ approach)

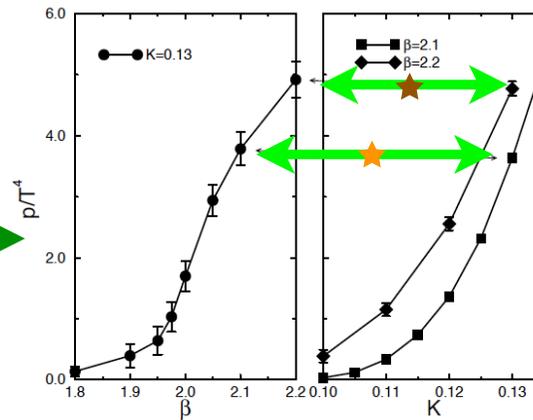
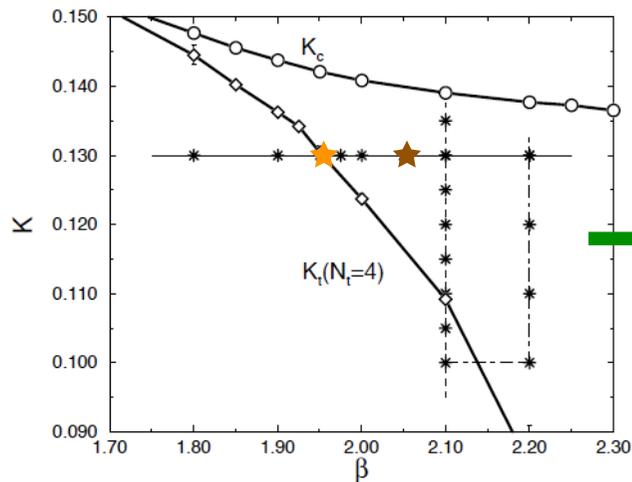
## Integral method for $p$

$$p = \frac{T}{V} \int_{b_0}^b db \frac{1}{Z} \frac{\partial Z}{\partial b} = -\frac{T}{V} \int_{b_0}^b \sum_i db_i \left\{ \left\langle \frac{\partial S}{\partial b_i} \right\rangle - \left\langle \frac{\partial S}{\partial b_i} \right\rangle_{T=0} \right\}$$

such that  $p(b_0) \approx 0$

numerical integration  
in the coupling param. space

The integration path is free to choose as far as  $p(b_0) \approx 0$



[CP-PACS: PRD64, 074510 (2001)]

- ▶ RG-improved gauge +  $N_f=2$  clover-improved Wilson
- ▶  $m_{PS}/m_V = 0.65-0.95$  ( $m_\pi \approx 600-1000$  MeV)
- ▶  $N_t = 4, 6$

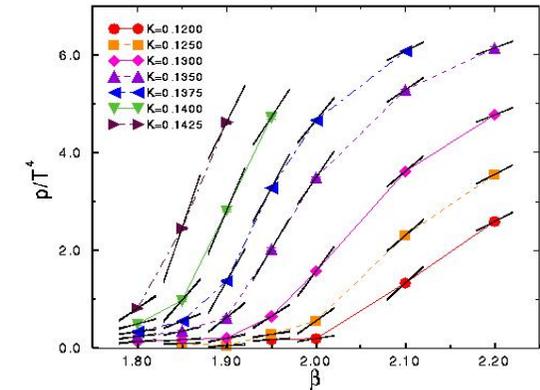
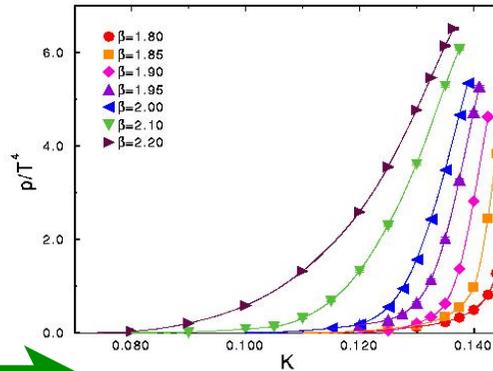
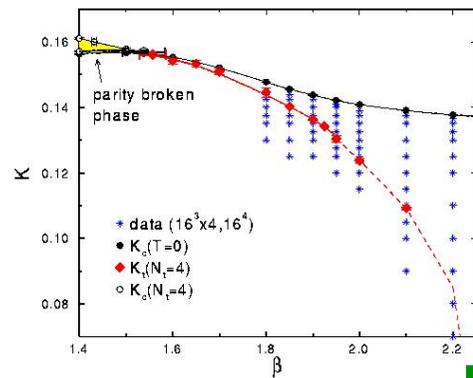
# EOS (fixed- $N_t$ approach)

An alternative test:

From the previous test, we learn that integration in  $K$  leads to smaller errors.

[CP-PACS: PRD64, 074510 (2001)]

- ▶ RG-improved gauge +  $N_f=2$  clover-improved Wilson
- ▶  $m_{PS}/m_V = 0.65-0.95$  ( $m_\pi \approx 600-1000$  MeV)
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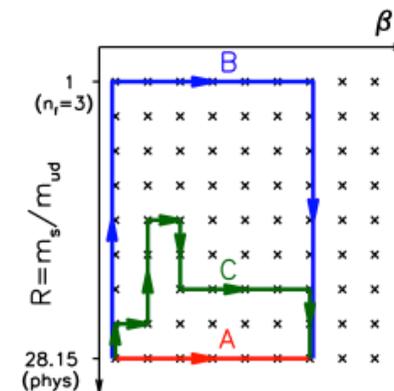
$$\frac{\partial(p/T^4)}{\partial K} = -N_t^4 \left\langle \frac{1}{N_s^3 N_t} \frac{\partial S}{\partial K} \right\rangle_{\text{sub}}$$

Consistent with the slope

measured directly from 
$$\frac{\partial(p/T^4)}{\partial \beta} = -N_t^4 \left\langle \frac{1}{N_s^3 N_t} \frac{\partial S}{\partial \beta} \right\rangle_{\text{sub}}$$

Generalized method taking into account all possible path'

Borsanyi et al. [arXiv:1007.2580].



# beta functions

$$a \frac{db_i}{da} \quad \text{with} \quad b = (\beta, \kappa_{ud}, \kappa_S, \dots) \equiv (b_1, b_2, \dots)$$

In the multi-dimensional parameter space of QCD, we first need to know the line of constant physics (LCP) for the world under investigation.

## LCP

In the scaling region, LCP is defined as the points where the dimension-less ratios of observables are the same at  $T=0$ .

Different LCP's represent different world (different proton mass, different electron mass, etc.).  
On a LCP, different point corresponds to the same world with different lattice spacings.

Off the scaling region, precise location of LCP depends on the definition.

[example] CP-PACS, PR D64('01)074510

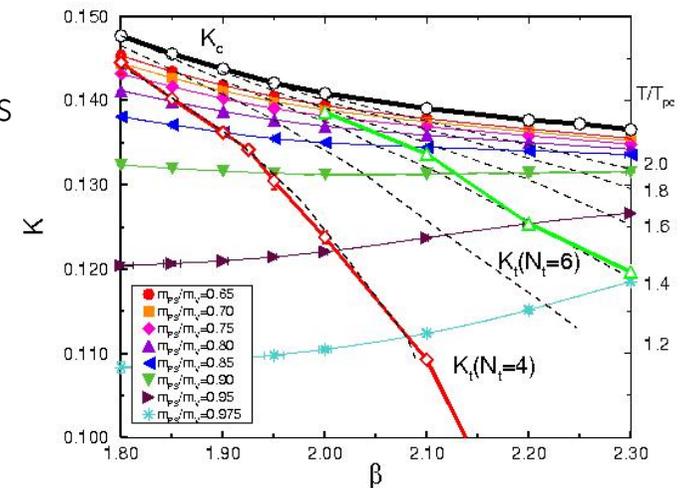
Iwasaki gauge +  $N_F=2$  clover-improved Wilson quarks

LCP:  $m_{PS}/m_V(T=0) = \text{constant}$

Lines of constant  $T/T_{pc}$  for  $N_t=4$

where  $T_{pc}$  determined on the same LCP

**Beta functions are defined as the change of  $b_i$  along LCP.**

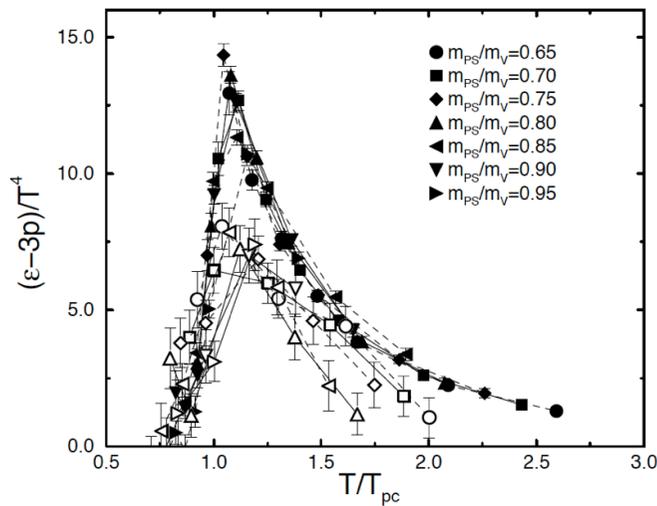


# EOS (fixed- $N_t$ approach)

## Results for $N_F=2$ with clover-improved Wilson quarks

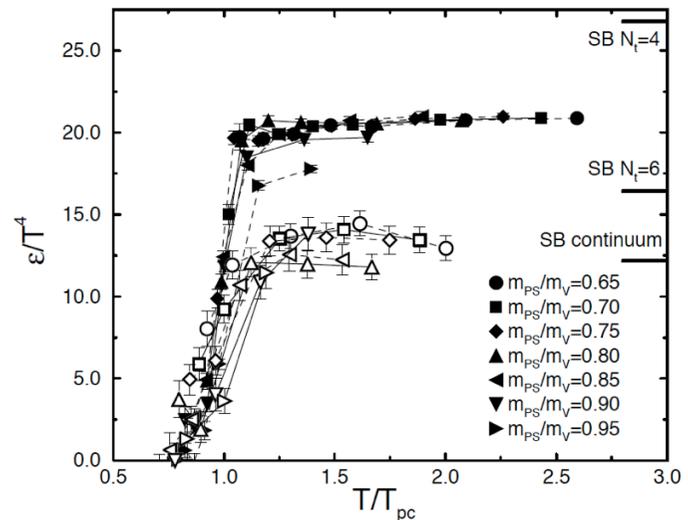
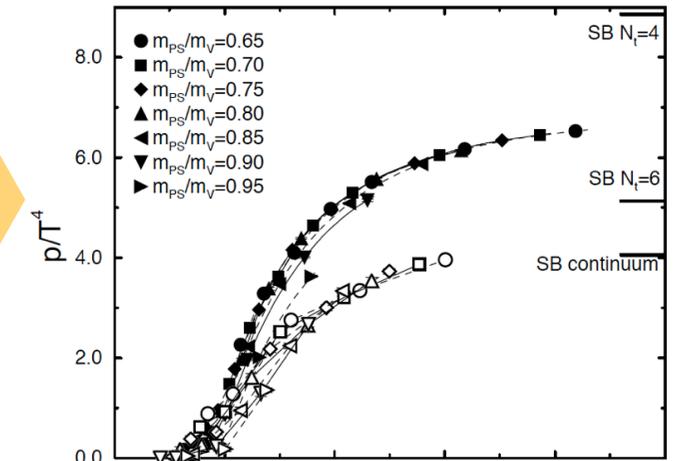
AliKhan et al. (CP-PACS) PRD64('01)

- ▶ RG-improved gauge + clover-improved Wilson
- ▶  $m_{PS}/m_V = 0.65-0.95$  ( $m_\pi \approx 600-1000$  MeV)
- ▶  $N_t = 4, 6$



$$p = \frac{T}{V} \int_{b_0}^b db \frac{1}{Z} \frac{\partial Z}{\partial b}$$

integral method

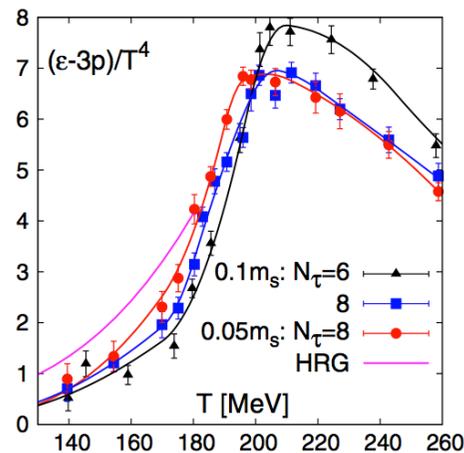


# EOS (fixed- $N_t$ approach)

## Recent results for $N_F=2+1$ with various improved staggered quarks

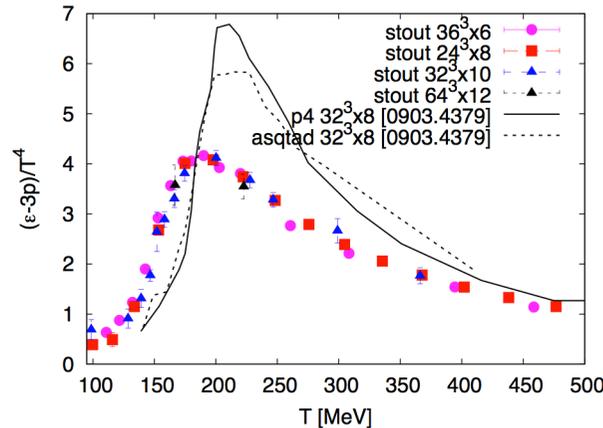
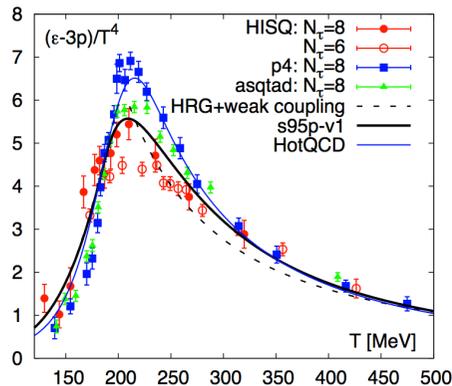
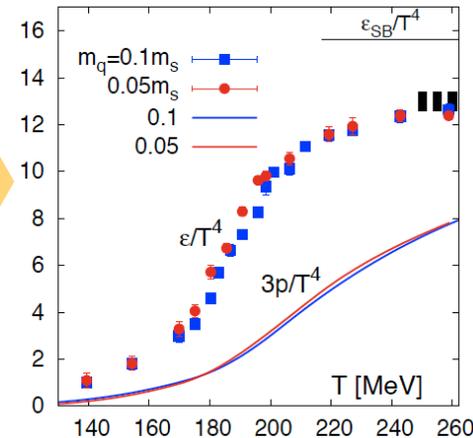
Chen et al. (HotQCD) PRD81('10)

- ▶ tree-level Symanzik gauge + p4-improved stag.
- ▶  $m_s \approx$  "physical",  $m_l/m_s = 0.05$  ( $m_\pi^{\text{pNG}} \approx 154$  MeV)
- ▶  $N_t = 8$



$$p = \frac{T}{V} \int_{b_0}^b db \frac{1}{Z} \frac{\partial Z}{\partial b}$$

integral method



Difference among different stag. quarks = errors due to the remaining taste violation

HotQCD and Wuppertal-Budapest proceedings of Lattice 2010

# EOS (fixed-scale approach)

## (Our) motivations

- Results from staggered-type quarks should be cross-checked by other lattice quarks whose theoretical basis is rigid.
- Conventional EOS calculation requires a large scale systematic simulation, and is still expensive with Wilson-type and chiral lattice quarks.

A large fraction of the cost  $\leq T = 0$  simulations

- ▶ Determination of basic information about the simulation point: (lattice scale, etc.)
- ▶ Determination of LCP, and non-perturbative beta functions at all  $T > 0$  simulation points
- ▶  $T = 0$  subtractions  $\Rightarrow T = 0$  simulations needed at all  $T > 0$  simulation points

With the fixed scale approach, all  $T > 0$  simulations are done at the same point of the coupling parameter space.

- ✓ All the simulations are automatically on the same LCP.
- ✓  $T = 0$  simulations needed only at one point.
- ✓ Scale, non-perturbative beta functions, etc. needed only at this point too.

**We may reduce the cost for  $T = 0$  simulations.**

# EOS (fixed-scale approach)

$$\epsilon = -\frac{1}{V} \frac{\partial \ln Z}{\partial T^{-1}}, \quad p = T \frac{\partial \ln Z}{\partial V} \quad \text{with} \quad Z = \text{Tr} e^{-H/T} = \int_{b.c.} \mathcal{D}\phi e^{-S}$$

## Trace anomaly

$$\frac{\epsilon - 3p}{T^4} = N_t^4 \left\{ \left\langle a \frac{dS}{da} \right\rangle - \left\langle a \frac{dS}{da} \right\rangle_{T=0} \right\} = \frac{N_t^3}{N_s^3} \sum_i a \frac{db_i}{da} \left\{ \left\langle \frac{\partial S}{\partial b_i} \right\rangle - \left\langle \frac{\partial S}{\partial b_i} \right\rangle_{T=0} \right\}$$

lattice beta functions along LCP

$$b = (\beta, \kappa_{ud}, \kappa_s, \dots) \equiv (b_1, b_2, \dots)$$

measured on the lattice  
 $T=0$  subtractions for renorm.

Because all the simulations are done at one point in the coupling parameter space, the conventional integral method in the coupling parameter space is not applicable.

# EOS (fixed-scale approach)

## $T$ -integration method for $p$

Umeda et al., PRD79, 051501 ('09)

Using a thermodyn. relation at  $\mu=0$ :

$$T \frac{\partial}{\partial T} \left( \frac{p}{T^4} \right) = \frac{\epsilon - 3p}{T^4} \quad \Rightarrow \quad \frac{p}{T^4} = \int_{T_0}^T dT \frac{\epsilon - 3p}{T^5}$$

$\leftarrow p(T_0) \approx 0$

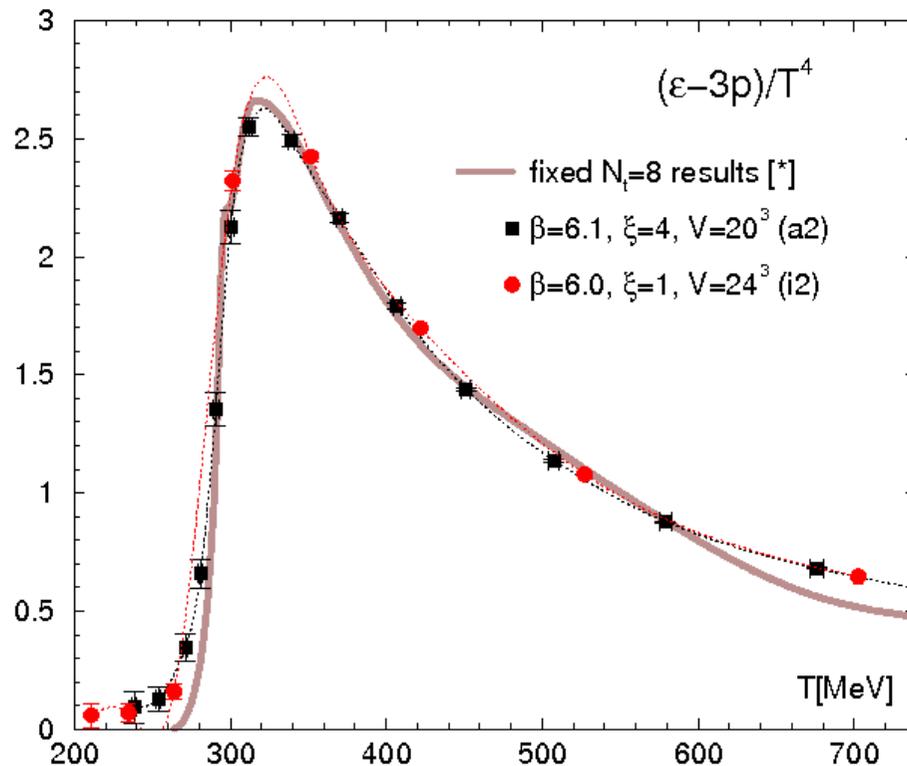
Disadvantages/challenges:

- ▶ The resolution in  $T$  is limited due to the discreteness of  $Nt$ .
  - => interpolation in  $T$
  - <=  $a$  should be sufficiently small / odd  $Nt$  programs /  
combine different  $\beta$  in a scaling region / ...
- ▶ Large statistics required at low  $T$  (large  $Nt$ ) to compete a big cancellation by the  $T=0$  subtraction

# EOS (fixed-scale approach)

## Test in quenched QCD

Umeda et al., PRD79, 051501 ('09)



Results compared for

★ isotropic lattices

( $a_s \sim 0.095$  fm,  $N_t = 3-10 \Rightarrow$   
 $T = 200-700$  MeV,  $L_s \sim 1.5$  fm)

★ anisotropic lattice with  $\xi = 4$

(4-times smaller  $a_t \Rightarrow$  4-times finer  $T$ -  
resolution)

★ result of the fixed  $N_t$  approach

( $N_t = 8$  by Boyd et al. NPB469(96):  
 $N_s = 32 \Rightarrow L_s \sim 2.7$  fm around  $T_c$ )

Note: effects due to small  $L_s$  are physical finite  
volume effects, i.e not a matter of the algorithm.

Besides understandable deviations, results consistent with each other

➡ consistent with the fixed  $N_t$  approach

➡  $T$ -interpolation under control on the isotropic lattice

➡ computation costs much reduced

# fixed scale approach vs. fixed $Nt$ approach

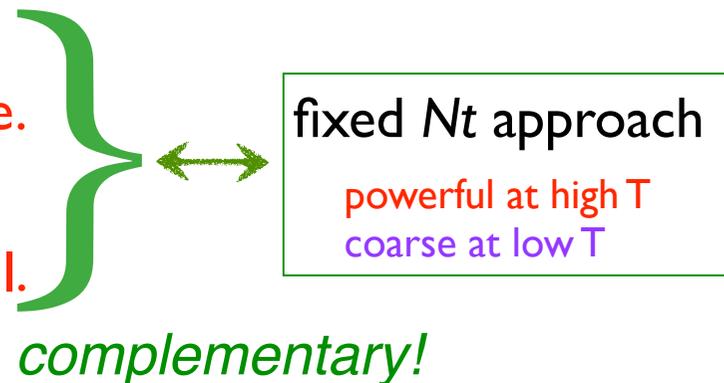
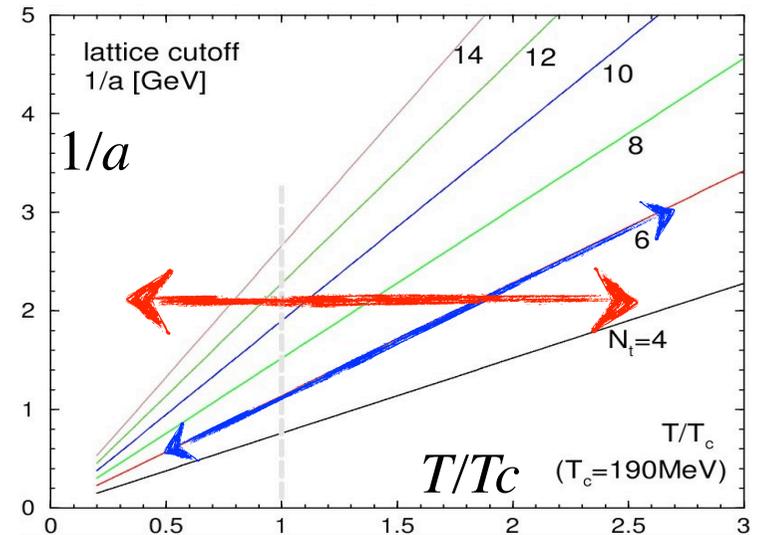
## Pros and cons:

- A common  $T=0$  simulation enough for all  $T=0$  subtractions.
- We can even borrow publicly available high statistic configurations on 
- Automatically on a LCP w/o fine tuning.

→  $T=0$  simulation costs redusable.

- The resolution in  $T$  is limited because  $Nt$  is discrete. => under control for EOS (see Umeda et al., PRD79, 051501 ('09))

- At high  $T$ :  
( $T > 2-3T_c$ )
- $Nt$  too small => another source of errors
  - Keep the lattice volume large.
- Low  $T$  / around  $T_c$  :
- More costs due to larger  $Nt$ .
  - Keep the lattice spacing small.

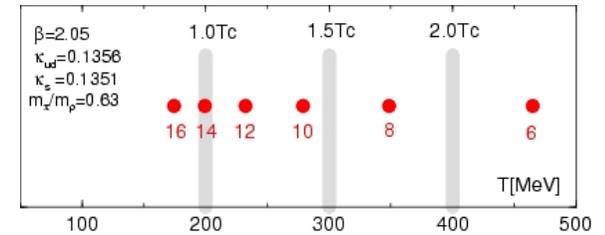


# EOS (fixed-scale approach)

## Trial calculation in $N_F=2+1$ QCD

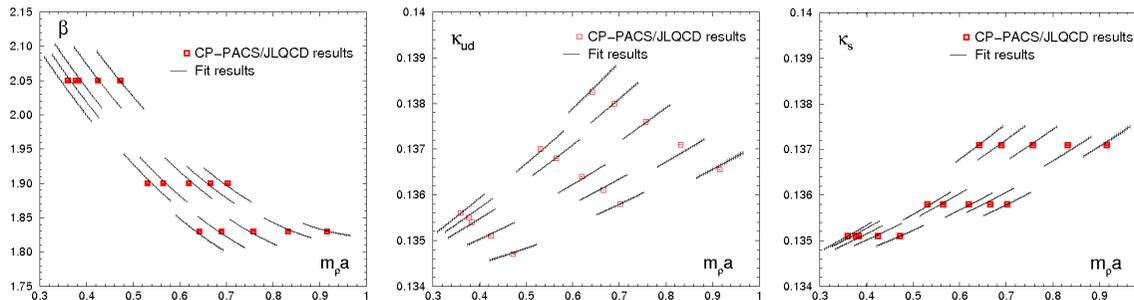
Umeda et al. (WHOT-QCD Collab.)

- $T=0$  simulation: on  $28^3 \times 56$  by CP-PACS/JLQCD Phys. Rev. D78 (2008) 011502
  - RG-improved Iwasaki glue + clover-improved Wilson quarks
  - $\beta=2.05, \kappa_{ud}=0.1356, \kappa_s=0.1351$  ( $m_\pi \sim 634\text{MeV}, \frac{m_\pi}{m_\rho} = 0.63, \frac{m_{\eta_{ss}}}{m_\phi} = 0.74$ )
  - $V \sim (2\text{ fm})^3, a=0.07\text{ fm}$ ,
  - configurations available on the ILDG/JLDG
- $T>0$  simulations: on  $32^3 \times Nt$  ( $Nt=4, 6, \dots, 14, 16$ ) lattices  
RHMC algorithm, same parameters as the  $T=0$  simulation



Beta functions  $\Leftarrow T=0$  meson mass data at 3 ( $\beta$ )  $\times$  5 ( $\kappa_{ud}$ )  $\times$  2 ( $\kappa_s$ ) = 30 data points

fit  $\beta, \kappa_{ud}, \kappa_s$  as functions of  $(am_\rho), \left(\frac{m_\pi}{m_\rho}\right), \left(\frac{m_{\eta_{ss}}}{m_\phi}\right) \Rightarrow a \frac{db}{da} = am_\rho \left. \frac{\partial b}{\partial(am_\rho)} \right|_{LCP}$



with LCP defined by

$$\frac{m_\pi}{m_\rho} = \text{const.}, \quad \frac{m_{\eta_{ss}}}{m_\phi} = \text{const.}$$

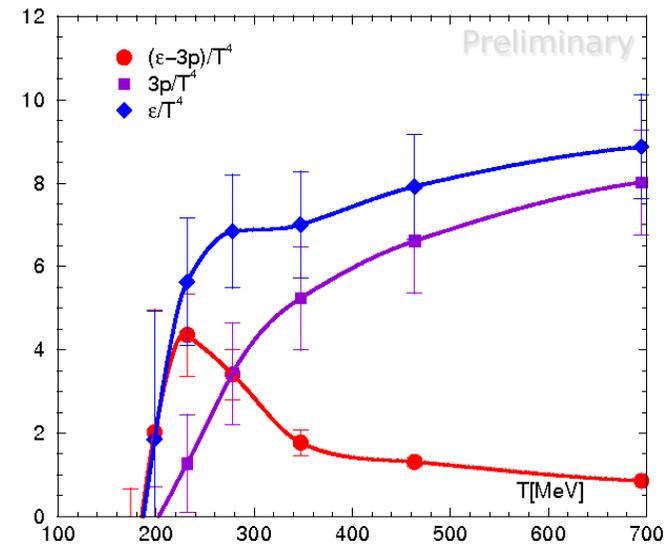
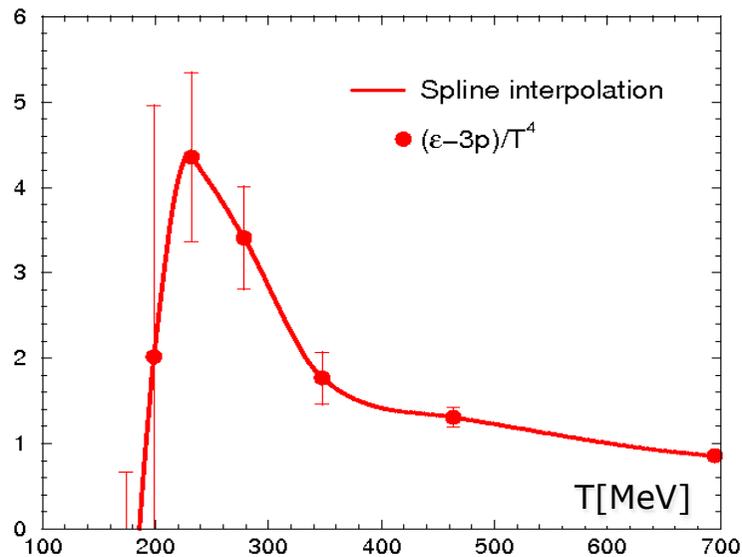
$$\left( a \frac{\partial \beta}{\partial a}, a \frac{\partial \kappa_{ud}}{\partial a}, a \frac{\partial \kappa_s}{\partial a} \right)_{\text{simulation point}} = (-0.334(4), 0.00289(6), 0.00203(5)) \quad (\text{statistical errors only})$$

# EOS (fixed-scale approach)

## Trial calculation in $N_F=2+1$ QCD

EOS (preliminary)

Umeda et al. (WHOT-QCD Collab.) @ Lattice 2010

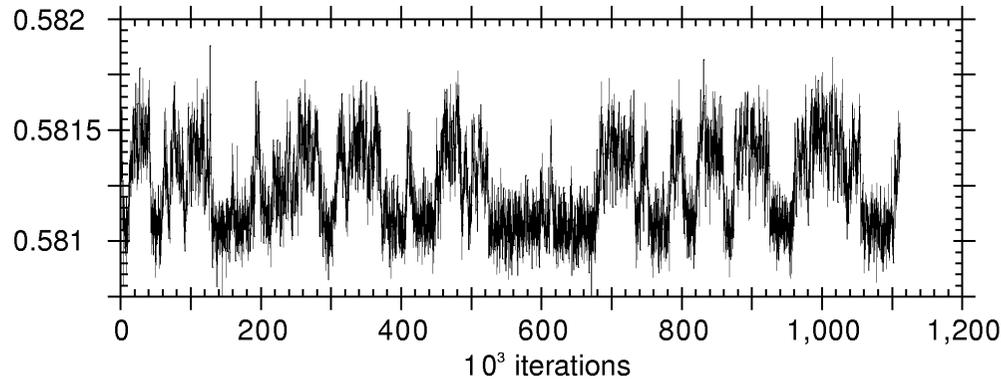


More works needed

- more statistics at low  $T$
- better  $T$ -resolution  $\Rightarrow$  odd  $Nt$ ? / combine with other  $\beta$  on the LCP
- more refined method to evaluate beta functions?  $\Rightarrow$  reweighting?
- just on the physical point (using  $T=0$  configurations generated by the PACS-CS Collab.)

# Latent heat

When the transition is 1st order,



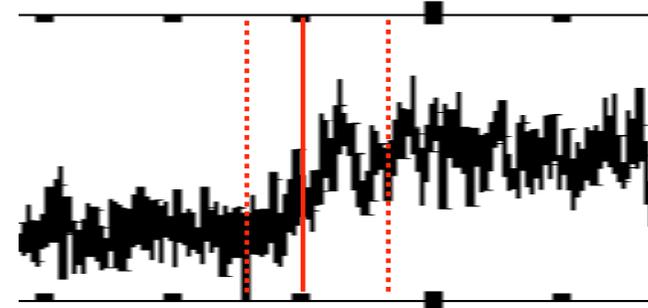
Plaquette history at  $T_c$

Iwasaki et al., PR D46('92)4657

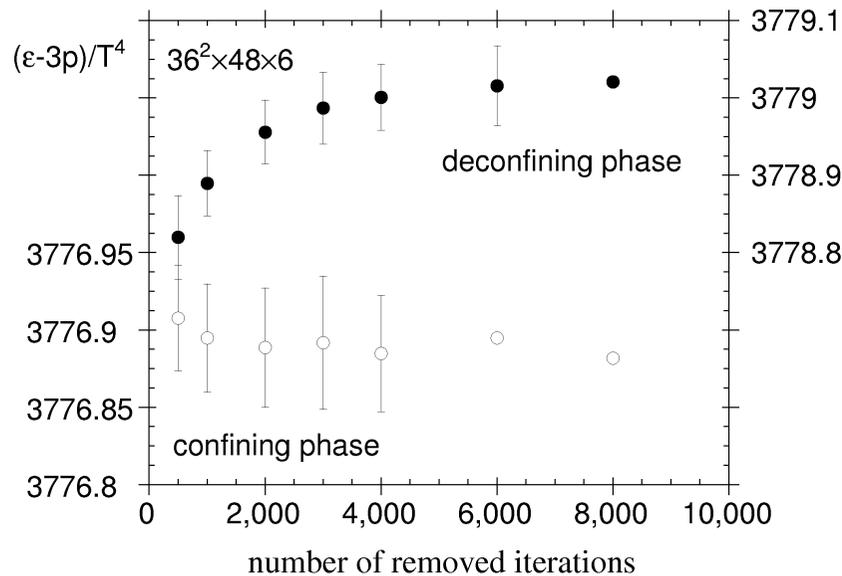
$36^2 \times 48 \times 6$ , 1150,000 iterations

bin=100

Flip-flop among two phases visible.



remove transition states



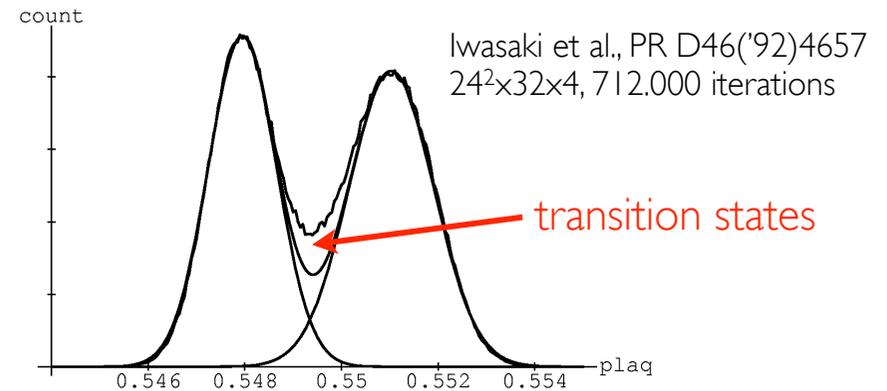
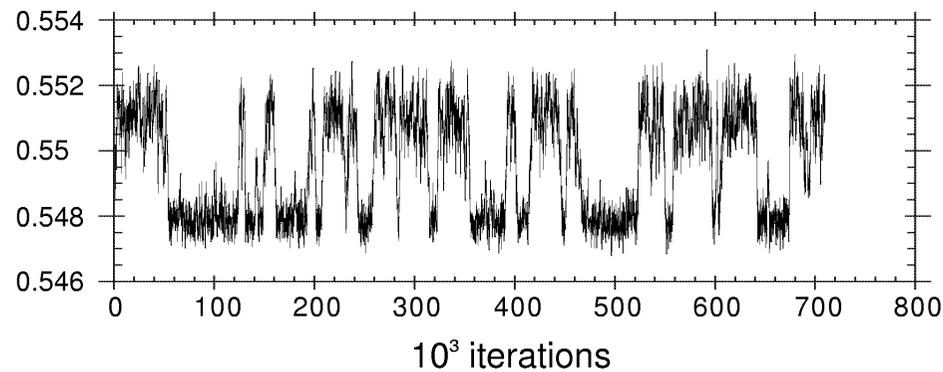
$p$  is continuous at  $T_c \Rightarrow \Delta\varepsilon$

results for SU(3) YM theory:

	$Nt$	$\Delta\varepsilon/T_c^4$
Standard	4	2.27(5)
	6	1.53(4)
Symanzik	4	1.40--1.57 (9--12)

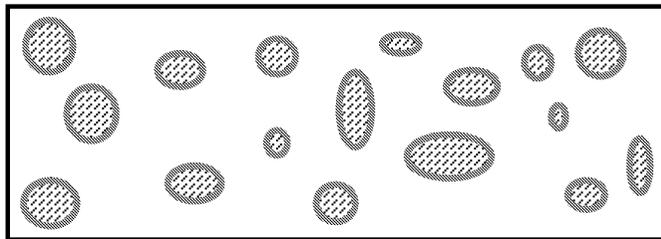
# Interface tension

When the transition is 1st order,

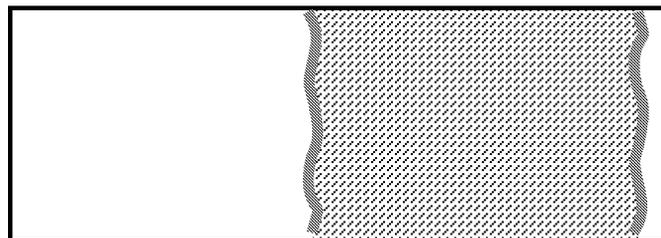


We now extract information from the transition states.

When two phases coexists with a non-zero interface tension:

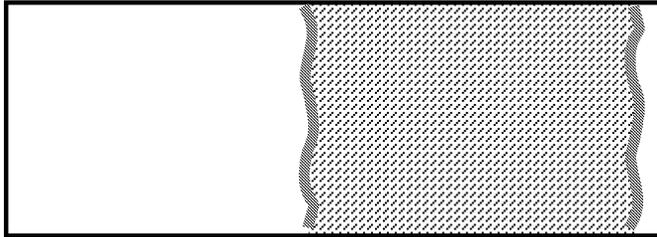


Large interface area  
=> less probable



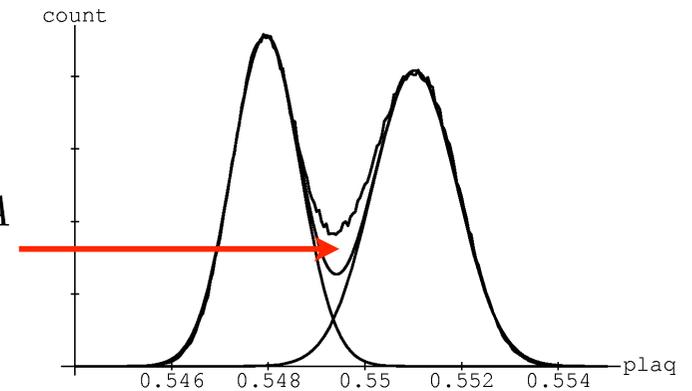
Minimum interface area with p.b.c  
=> dominant contribution

# Interface tension



Interface area approximately known.

=> The probability to have such transition state  $\propto e^{-\sigma_I A}$



In actual calculation, we take into account the effects of

- \* lattice geometry
- \* parallel transports
- \* capillary wave collections on the interface

See Iwasaki et al., PR D49('94)3540 for details.

For the case of SU(3) YM,  $\sigma_I/T_C^3 \approx 0.15 - 0.16$

# Many other interesting quantities

entropy density / sound velocity / ...

transport coefficients / ...

heavy quark potential / screening masses / effective couplings / ...

spectral functions / ...

## **to investigate**

dissociation of charmonia / effective masses and decay rates of them at  $T > 0$  / ...

*Young powers and many new ideas are starved for!!*

thank you

# What will happen at $\mu \neq 0$ ?

Similar to the high  $T$  case,

- restoration of the chiral symmetry

*when the thermal energy  $>$  potential barrier between the sectors.*

$$\mu \sim M_N / 3$$

- breakdown of confinement

*high density  $\Rightarrow$  short average distances between quarks*

*asymptotic freedom:  $g(\mu) \rightarrow 0$  as  $\mu \rightarrow \infty$ .*

$$\mu \sim \Lambda_{\text{QCD}} \sim \mathcal{O}(100) \text{ MeV}$$

$\Rightarrow$  visit the lectures by Atsushi Nakamura