QCD thermodynamics from shifted boundary conditions

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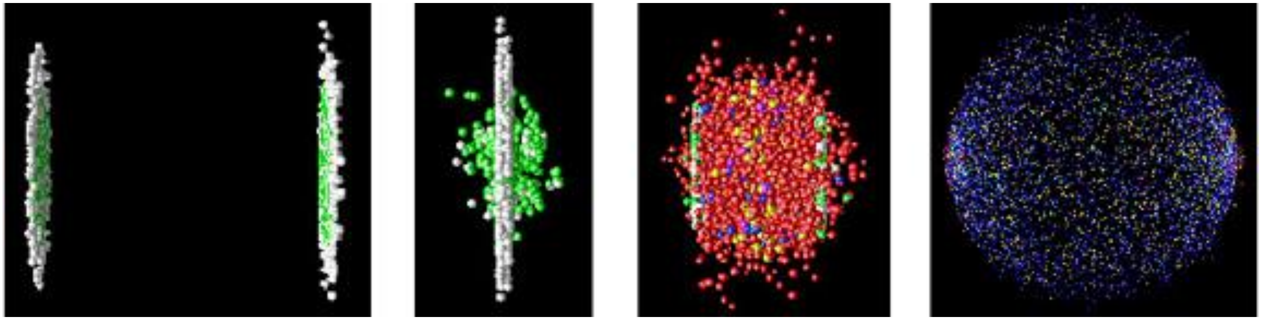
Lattice QCD at finite temperature and density,
KEK, Ibaraki, Japan, 20-22 January 2014

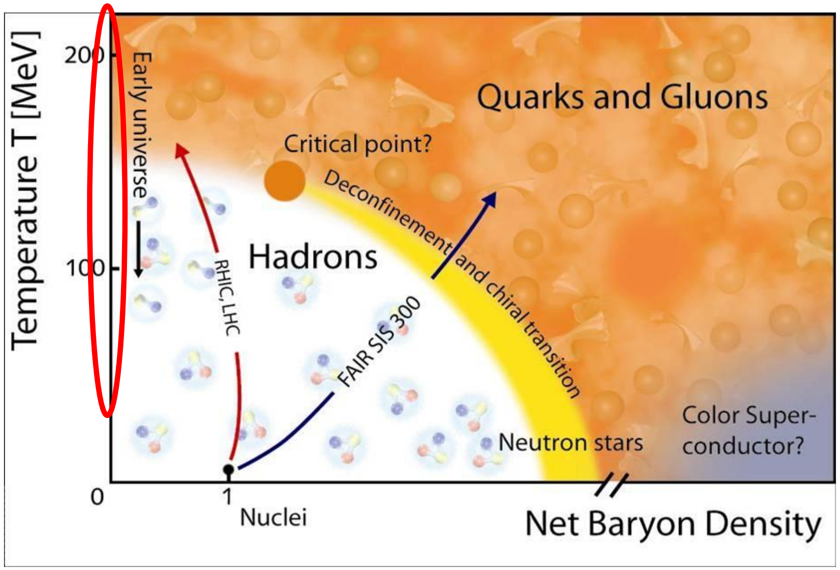
Contents of this talk

- Introduction
  - finite T with Wilson quarks
- Fixed scale approach
  - quenched results
  - Nf=2+1 QCD results
- Shifted boundary conditions
  - EOS
  - Tc
  - Beta-functions (entropy density)
- Summary

Quark Gluon Plasma in Lattice QCD



from the Phenix group web-site



http://www.gsi.de/fair/experiments/

Observables in Lattice QCD

- Phase diagram in (T, μ, m_{ud}, m_s)
- Critical temperature
- Equation of state (ε/T^4, p/T^4,...)
- Hadronic excitations
- Transport coefficients
- Finite chemical potential
- etc...

QCD Thermodynamics with Wilson quarks

Most (T, μ≠0) studies at m_{phys} are done with Staggered-type quarks

4th-root trick to remove unphysical "tastes"

→ non-locality "Validity is not guaranteed"

It is important to cross-check with

theoretically sound lattice quarks like Wilson-type quarks

WHOT-QCD collaboration is investigating
QCD at finite T & μ using Wilson-type quarks

Review on WHOT-QCD studies :

S. Ejiri, K. Kanaya, T. Umeda for WHOT-QCD Collaboration,
Prog. Theor. Exp. Phys. (2012) 01A104 [arXiv: 1205.5347 (hep-lat)]

Recent studies on QCD Thermodynamics

Non-Staggered quark studies at T>0

- Domain-Wall quarks

  hotQCD Collaboration, Phys. Rev. D86 (2012) 094503.

  TWQCD Collaboration, arXiv:1311.6220 (Lat2013).

- Overlap quarks

  S. Borsanyi et al. (Wuppertal), Phys. Lett. B713 (2012) 342.

  JLQCD Collaboration, Phys. Rev. D87 (2013) 114514 .

- twisted mass quarks

  tmfT Collaboration, arXiv:1311.1631(Lat2013).

- Wilson quarks

  S. Borsanyi et al. (Wuppertal), JHEP08 (2012) 126.

  WHOT-QCD Collaboration, Phys. Rev. D85 (2012) 094508.

Fixed scale approach is adopted to study T>0

Fixed scale approach to study QCD thermodynamics

Conventional fixed Nt approach

Temperature $T=1/(N_t a)$ is varied by a at fixed N_t

a : lattice spacing
N_t : lattice size in t-direction

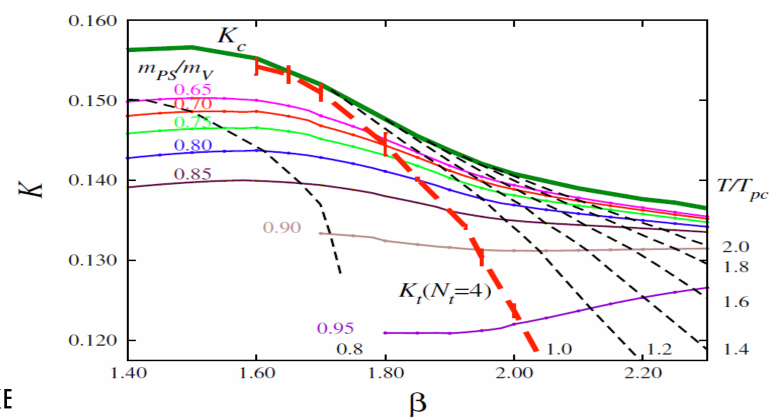
- Coupling constants are different at each T

To study Equation of States

- T=0 subtractions at each T
- beta-functions at each T
- Line of Constant Physics (for full QCD)

} wide range of a

$$\frac{a_{\max}}{a_{\min}} = \frac{T_{\max}}{T_{\min}} > 3$$



These are done in T=0 simulations
- larger space-time volume
- smaller eigenvalue in Dirac op.

→ larger part of the simulation cost

Fixed scale approach to study QCD thermodynamics

Fixed scale approach

Temperature $T=1/(N_t a)$ is varied by N_t at fixed a

a : lattice spacing
N_t : lattice size in t-direction

- Coupling constants are common at each T

To study Equation of States

- T=0 subtractions are common
- beta-functions are common
- Line of Constant Physics is automatically satisfied

⇨ Cost for T=0 simulations can be largely reduced

However possible temperatures are restricted by integer N_t

△ critical temperature T_c

○ EOS

T-integration method to calculate the EOS

We propose the T-integration method
to calculate the EOS at fixed scales

T.Umeda et al. (WHOT-QCD), Phys. Rev. D79 (2009) 051501

Our method is based on the trace anomaly (interaction measure),

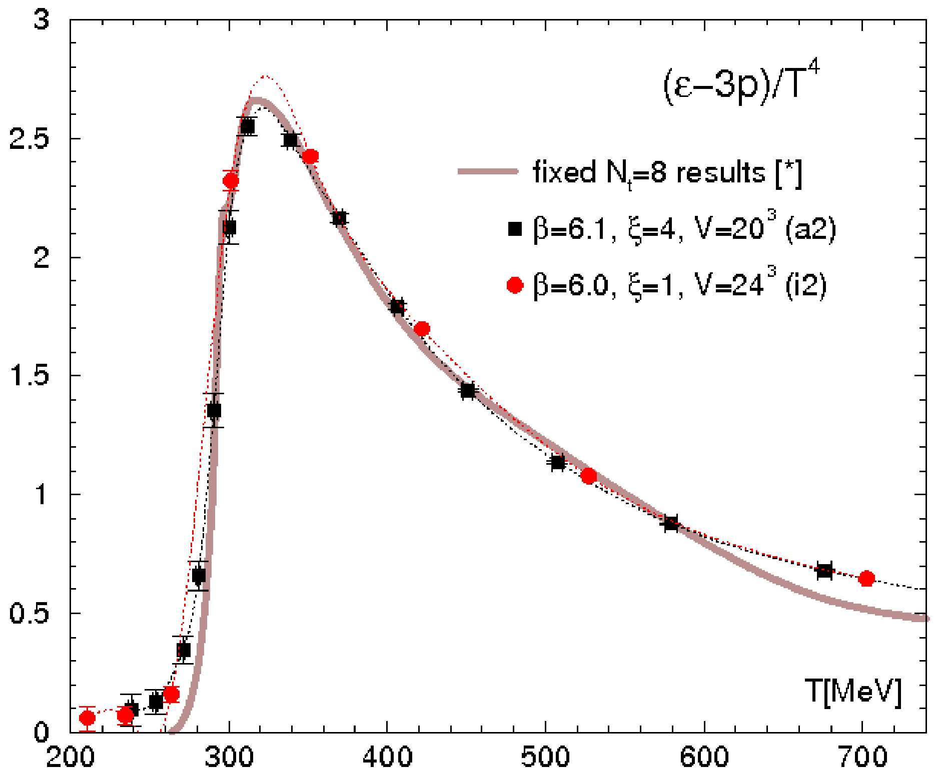
$$\frac{\epsilon - 3p}{T^4} = \left(\frac{N_t^3}{N_s^3}\right) a\frac{d\beta}{da} \left\langle \frac{dS}{d\beta} \right\rangle_{sub}$$

and the thermodynamic relation.

$$\frac{\epsilon - 3p}{T^4} = T\frac{\partial(p/T^4)}{\partial T}$$

$$\Longrightarrow \quad \frac{p}{T^4} = \int_0^T dT' \, \frac{\epsilon - 3p}{T'^5}$$

Test in quenched QCD



[*] G. Boyd et al., NPB469, 419 (1996)

T. Umeda et al. (WHOT-QCD)
Phys. Rev. D79 (2009) 051501.

- Our results are roughly consistent with previous results.
- at higher T
  lattice cutoff effects
  (aT~0.3 or higher)
- at lower T
  finite volume effects
  V > (2fm)^3 is ncessarry T<T_c

Anisotropic lattice is
a reasonable choice

EOS for N_f=2+1 improved Wilson quarks

$$S = S_g + S_q \qquad \begin{aligned} S_g &= -\beta\left\{\sum_{x,\mu>\nu} c_0 W^{1\times1}_{\mu\nu}(x) + \sum_{x,\mu,\nu} c_1 W^{1\times2}_{\mu\nu}(x)\right\} \\ S_q &= \sum_{f=u,d,s}\sum_{x,y}\bar{q}^f_x D_{x,y} q^f_y \end{aligned} \qquad \beta = \frac{6}{g^2}$$

$$D_{x,y} = \delta_{x,y} - \kappa_f \sum_{\mu}\{(1-\gamma_\mu)U_{x,\mu}\delta_{x+\hat{\mu},y} + (1+\gamma_\mu)U^\dagger_{x-\hat{\mu},\mu}\delta_{x-\hat{\mu},y}\} - \delta_{x,y} c_{SW}\kappa_f \sum_{\mu>\nu}\sigma_{\mu\nu}F_{\mu\nu}$$

$$\frac{\epsilon - 3p}{T^4} = \frac{N_t^3}{N_s^3}\left(a\frac{\partial\beta}{\partial a}\left\langle\frac{\partial S}{\partial\beta}\right\rangle_{sub} + a\frac{\partial\kappa_{ud}}{\partial a}\left\langle\frac{\partial S}{\partial\kappa_{ud}}\right\rangle_{sub} + a\frac{\partial\kappa_s}{\partial a}\left\langle\frac{\partial S}{\partial\kappa_s}\right\rangle_{sub}\right)$$

$$\left\langle\frac{\partial S}{\partial\beta}\right\rangle = N_s^3 N_t\left(-\left\langle\sum_{x,\mu>\nu} c_0 W^{1\times1}_{\mu\nu}(x) + \sum_{x,\mu,\nu} c_1 W^{1\times2}_{\mu\nu}(x)\right\rangle + N_f\frac{\partial c_{SW}}{\partial\beta}\kappa_f\left\langle\sum_{x,\mu>\nu}\mathrm{Tr}^{(c,s)}\sigma_{\mu\nu}F_{\mu\nu}(D^{-1})_{x,x}\right\rangle\right)$$

$$\left\langle\frac{\partial S}{\partial\kappa_f}\right\rangle = N_f N_s^3 N_t\left(\left\langle\sum_{x,\mu}\mathrm{Tr}^{(c,s)}\{(1-\gamma_\mu)U_{x,\mu}(D^{-1})_{x+\hat{\mu},x} + (1+\gamma_\mu)U^\dagger_{x-\hat{\mu},\mu}(D^{-1})_{x-\hat{\mu},x}\}\right\rangle + c_{SW}\left\langle\sum_{x,\mu>\nu}\mathrm{Tr}^{(c,s)}\sigma_{\mu\nu}F_{\mu\nu}(D^{-1})_{x,x}\right\rangle\right)$$

Noise method (#noise = 1 for each color & spin indices)

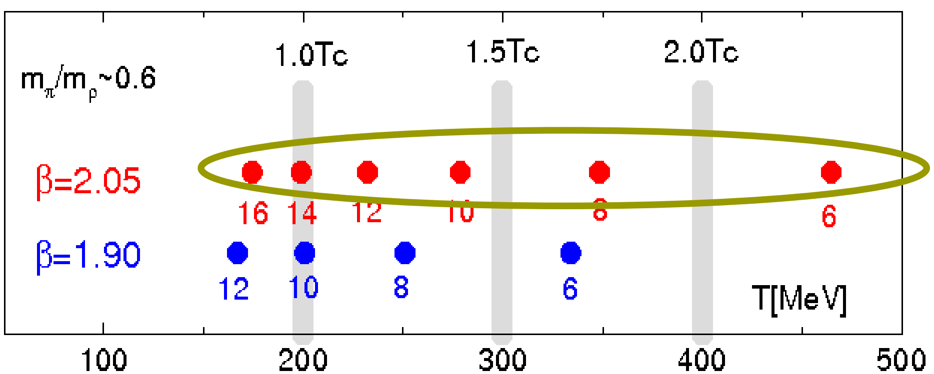
T=0 & T>0 configurations for N_f=2+1 QCD

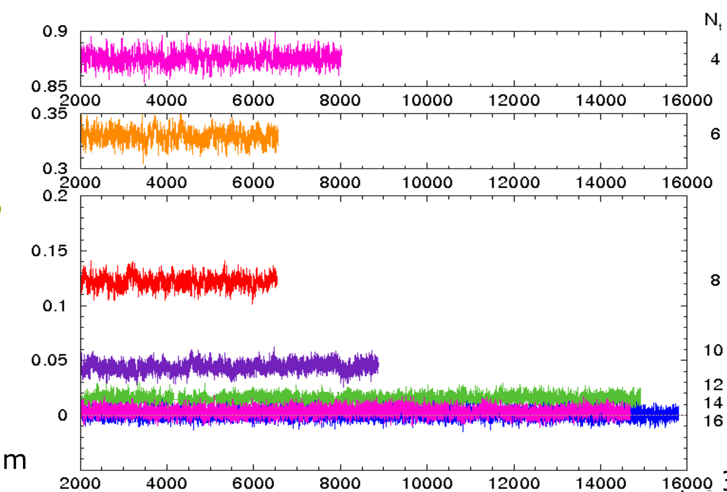
- T=0 simulation: on 28^3 x 56
  - RG-improved glue + NP-improved Wilson quarks
  - V~(2 fm)^3 , a≃0.07 fm, ($m_\pi \sim 634\text{MeV}, \ \frac{m_\pi}{m_\rho} = 0.63, \ \frac{m_{\eta_s s}}{m_\phi} = 0.74$)
  - configurations available on the ILDG/JLDG

CP-PACS/JLQCD Phys. Rev. D78 (2008) 011502

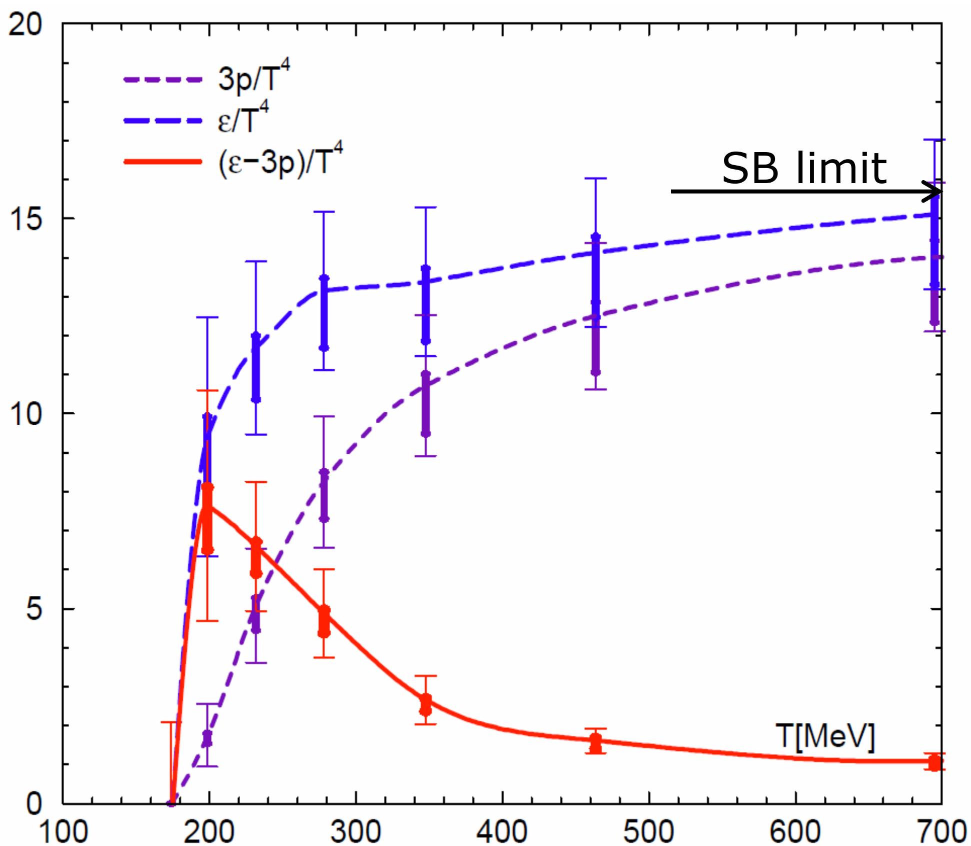
- T>0 simulations: on 32^3 x N_t (N_t=4, 6, ..., 14, 16) lattices

RHMC algorithm, same coupling parameters as T=0 simulation





Equation of State in N_f=2+1 QCD



T. Umeda et al. (WHOT-QCD)
Phys. Rev. D85 (2012) 094508

- T-integration

$$\frac{p}{T^4} = \int_0^T dT' \frac{\epsilon - 3p}{T'^5}$$

is performed by Akima Spline interpolation.

- A systematic error for beta-functions

- numerical error propagates until higher temperatures

Summary on Fixed scale approach

Fixed scale approach for EOS

- EOS (p, e, s, ...) by T-integral method
- Cost for T=0 simulations can be largely reduced
- possible temperatures are restricted by integer N_t
- beta-functions are still a burden

- Some groups adopted the approach
  - tmfT Collaboration, arXiv:1311.1631(Lat2013).
  - S. Borsanyi et al. (Wuppertal), JHEP08 (2012) 126.

- Physical point simulation with Wilson quarks is on going

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Shifted boundary conditions

L. Giusti and H. B. Meyer, Phys. Rev. Lett. 106 (2011) 131601.
Thermal momentum distribution from path integrals
with shifted boundary conditions

New method to calculate thermodynamic potentials
(entropy density, specific heat, etc.)

The method is based on the partition function

$$Z(\vec{z}) = Tr\{e^{-L_0 \hat{H}} e^{i\hat{p}\vec{z}}\}$$

which can be expressed by Path-integral with shifted boundary condition

$$\phi(L_0, \vec{x}) = \pm\phi(0, \vec{x} + \vec{z})$$

- L. Giusti and H. B. Meyer, JHEP 11 (2011) 087
- L. Giusti and H. B. Meyer, JHEP 01 (2013) 140

Shifted boundary conditions

Due to the Lorentz invariance of the theory

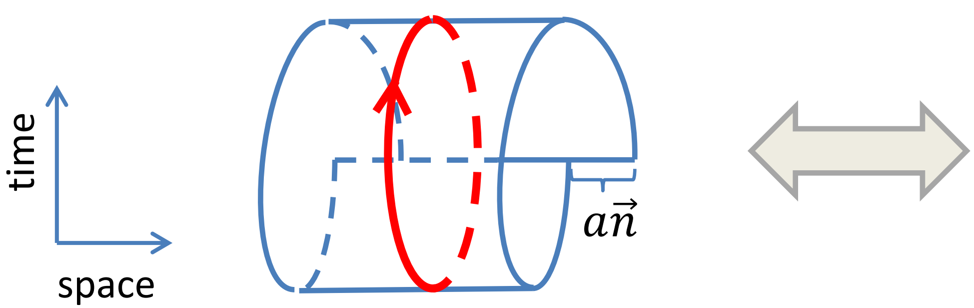
the free-energy depends on L_0 and the boundary shift $\vec{z}$

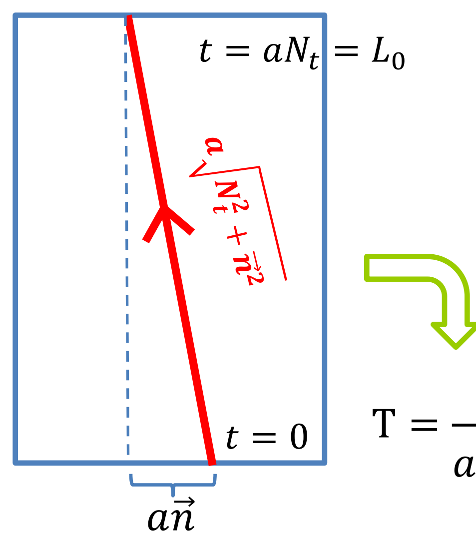
only through the combination $\sqrt{L_0^2 + z^2}$

$$f(L_0, \vec{z}) = f(\sqrt{L_0^2 + z^2}, 0)$$

$$\phi(L_0, \vec{x}) = \pm\phi(0, \vec{x} + \vec{z})$$

$$\vec{z} = a\vec{n}$$



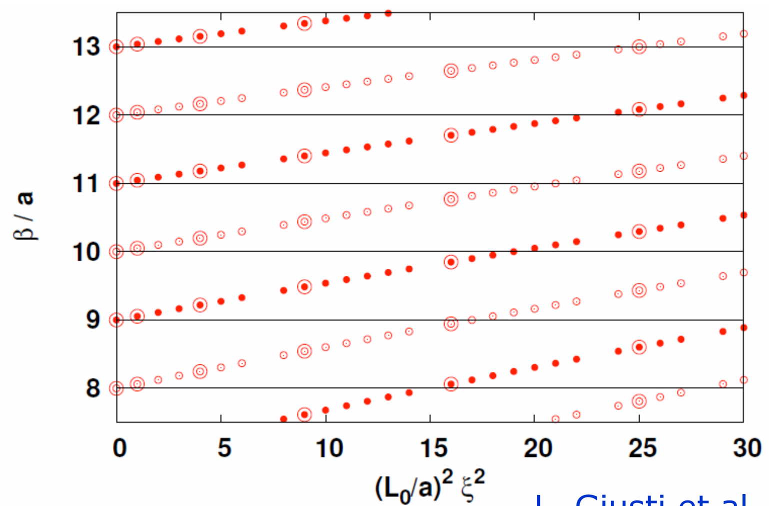


$$T = \frac{1}{a\sqrt{N_t^2 + \vec{n}^2}}$$

Shifted boundary conditions

By using the shifted boundary
various T's are realized with the same lattice spacing

T resolution is largely improved
while keeping advantages of the fixed scale approach



L. Giusti et al. (2013)

Figure 3: Inverse temperature values that become accessible with the use of shifted boundary conditions at a fixed lattice spacing a and for different values of L_0/a. The inverse temperatures accessible with a shift in a single direction, $\boldsymbol{\xi} = (\xi_1, 0, 0)$, are marked by a double circle.

$$\left(\beta = \frac{1}{T},\ \vec{z} = L_0\vec{\xi}\right)$$

Test in quenched QCD

Simulation setup

- quenched QCD
- β=6.0
  a ~ 0.1fm
- 32^3 x N_t lattices, N_t = 3, 4, 5, 6, 7, 8, 9 and 32 (T=0)
  $T_c(N_f=0)$ ~ 2 x $T_c(N_f=2+1, m_{phys})$
- boundary condition
  - spatial : periodic boundary condition
  - temporal: shifted boundary condition

$$U_\mu(L_0, \vec{x}) = U_\mu(0, \vec{x} + \vec{z})$$

- heat-bath algorithm (code for SX-8R)
  only "even-shift" to keep even-odd structure
  e.g. $\vec{z}/a = (0,0,0), (1,1,0), (2,0,0), (2,1,1), (2,2,0), (3,1,0), \ldots$

Test in quenched QCD

Choice of boundary shifts

$$U_\mu(L_0, \vec{x}) = U_\mu(0, \vec{x} + \vec{z}) \qquad \vec{z} = a\vec{n}$$

					Nt							
n^2	n_1	n_2	n_3	e/o	10	9	8	7	6	5	4	3
0	0	0	0	0	10.00	9.00	8.00	7.00	6.00	5.00	4.00	3.00
2	1	1	0	0	10.10	9.11	8.12	7.14	6.16	5.20	4.24	3.32
4	2	0	0	0	10.20	9.22	8.25	7.28	6.32	5.39	4.47	3.61
6	2	1	1	0	10.30	9.33	8.37	7.42	6.48	5.57	4.69	3.87
8	2	2	0	0	10.39	9.43	8.49	7.55	6.63	5.74	4.90	4.12
10	3	1	0	0	10.49	9.54	8.60	7.68	6.78	5.92	5.10	4.36
12	2	2	2	0	10.58	9.64	8.72	7.81	6.93	6.08	5.29	4.58
14	3	2	1	0	10.68	9.75	8.83	7.94	7.07	6.24	5.48	4.80
16	4	0	0	0	10.77	9.85	8.94	8.06	7.21	6.40	5.66	5.00
18	3	3	0	0	10.86	9.95	9.06	8.19	7.35	6.56	5.83	5.20
18	4	1	1	0	10.86	9.95	9.06	8.19	7.35	6.56	5.83	5.20
20	4	2	0	0	10.95	10.05	9.17	8.31	7.48	6.71	6.00	5.39
22	3	3	2	0	11.05	10.15	9.27	8.43	7.62	6.86	6.16	5.57
24	4	2	2	0	11.14	10.25	9.38	8.54	7.75	7.00	6.32	5.74
26	4	3	1	0	11.22	10.34	9.49	8.66	7.87	7.14	6.48	5.92
26	5	1	0	0	11.22	10.34	9.49	8.66	7.87	7.14	6.48	5.92
30	5	2	1	0	11.40	10.54	9.70	8.89	8.12	7.42	6.78	6.24
32	4	4	0	0	11.49	10.63	9.80	9.00	8.25	7.55	6.93	6.40
34	4	3	3	0	11.58	10.72	9.90	9.11	8.37	7.68	7.07	6.56

Trace anomaly (e-3p)/T^4

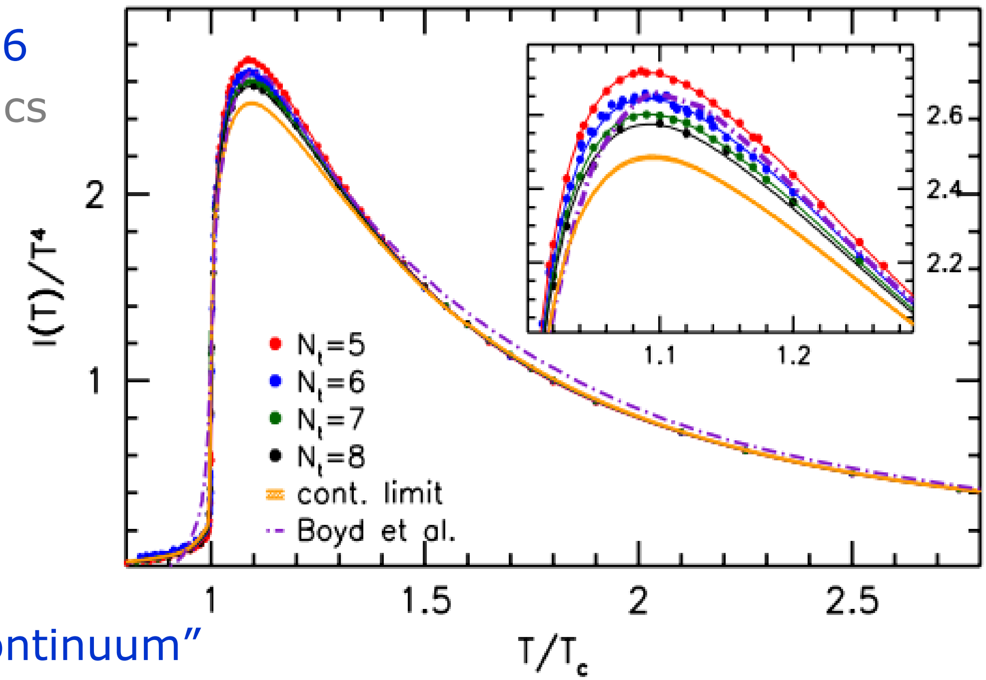
$$\frac{\epsilon - 3p}{T^4} = \left(\frac{1}{VT^3}\right) a\frac{d\beta}{da}\left\langle \frac{dS}{d\beta}\right\rangle_{sub}$$

Reference data

S. Borsanyi et al., JHEP 07 (2012) 056

Precision SU(3) lattice thermodynamics for a large temperature range

- N_s/N_t = 8 near T_c
- small N_t dependence at T>1.3Tc
- peak height at Nt=6 is about 7% higher than continuum value
- assuming T_c=293MeV

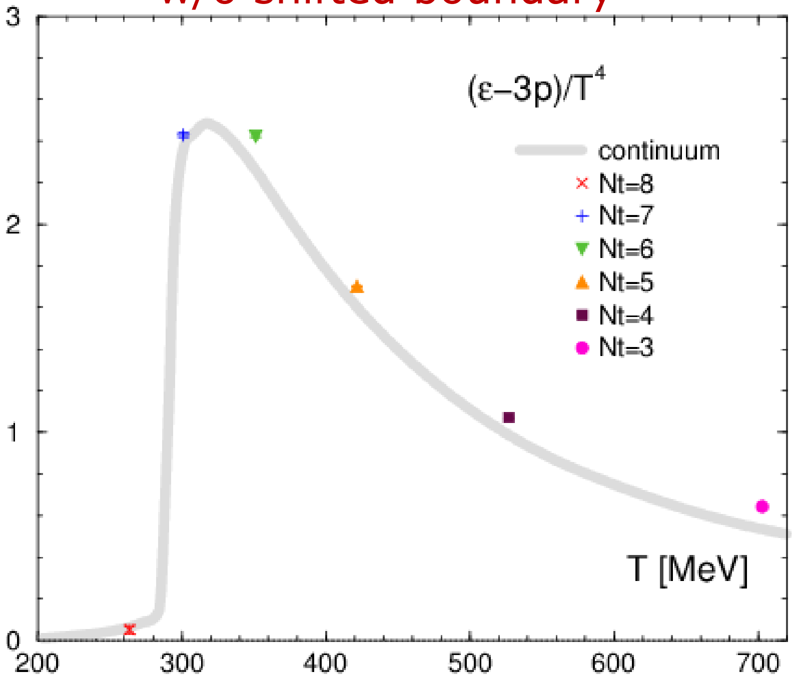


The continuum values referred as “continuum”

Trace anomaly (e-3p)/T^4

$$\frac{\epsilon - 3p}{T^4} = \left(\frac{1}{VT^3}\right) a \frac{d\beta}{da} \left\langle \frac{dS}{d\beta} \right\rangle_{sub}$$

w/o shifted boundary



beta-function: Boyd et al. (1998)

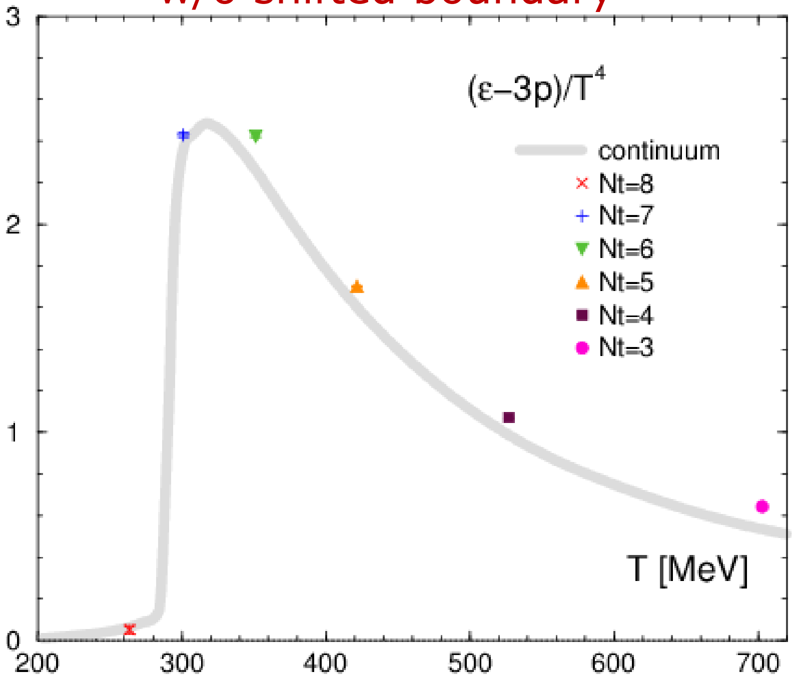
Trace anomaly (e-3p)/T^4

$$\frac{\epsilon - 3p}{T^4} = \left(\frac{1}{VT^3}\right) a\frac{d\beta}{da}\left\langle\frac{dS}{d\beta}\right\rangle_{sub}$$

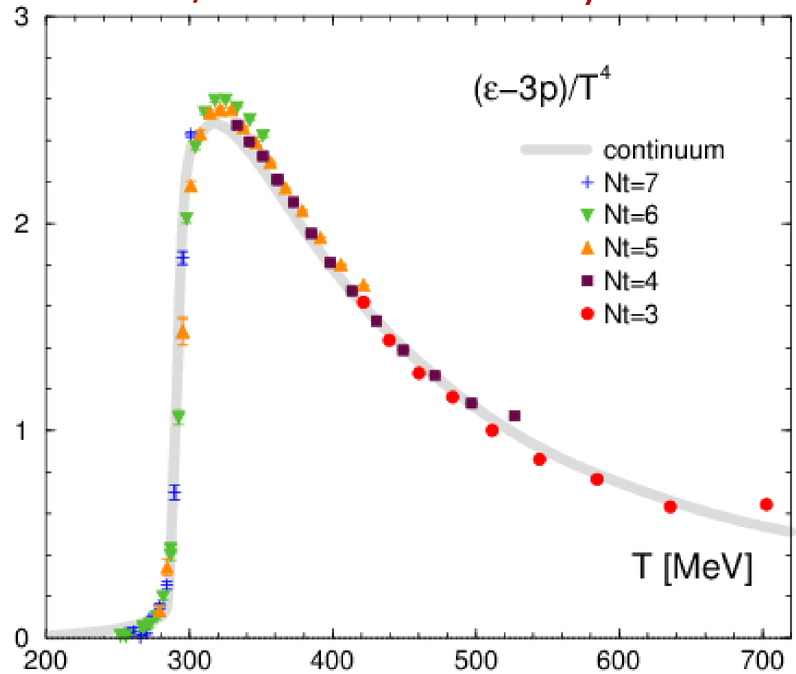
$$\mathrm{T} = \frac{1}{a\sqrt{N_t^2 + \vec{n}^2}}$$

$$V = \prod_{i=1}^{3} \frac{aN_s}{\sqrt{1 + (\frac{n_i}{N_t})^2}}$$

w/o shifted boundary

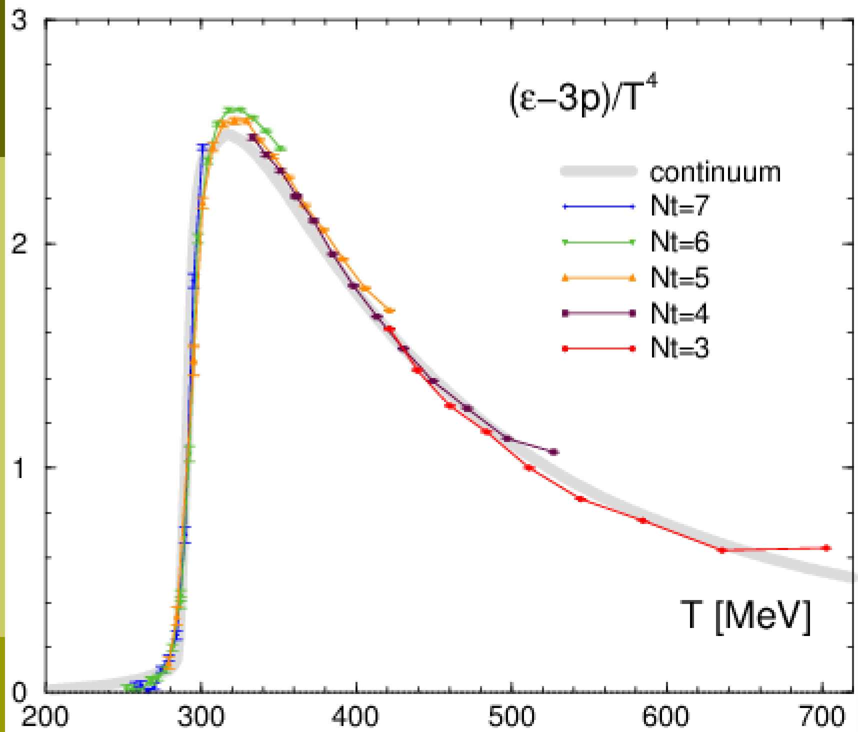


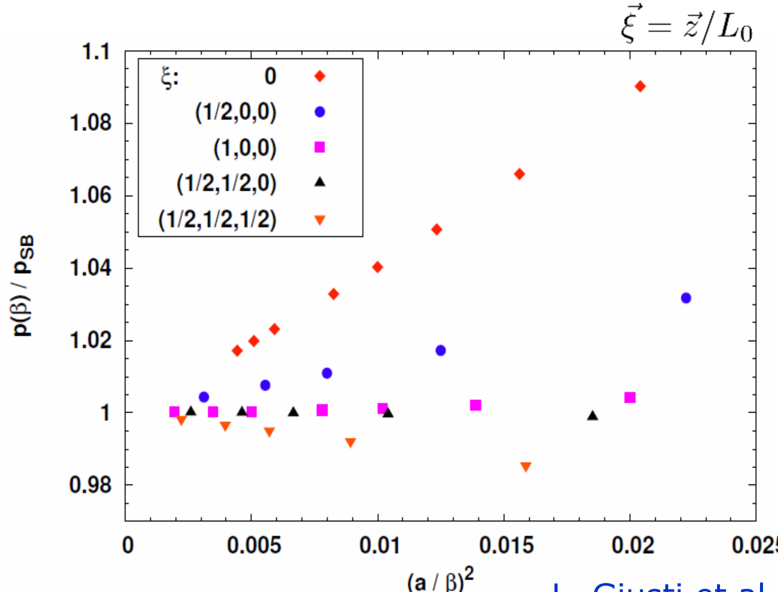
w/ shifted boundary



beta-function: Boyd et al. (1998)

Lattice artifacts from shifted boundaries





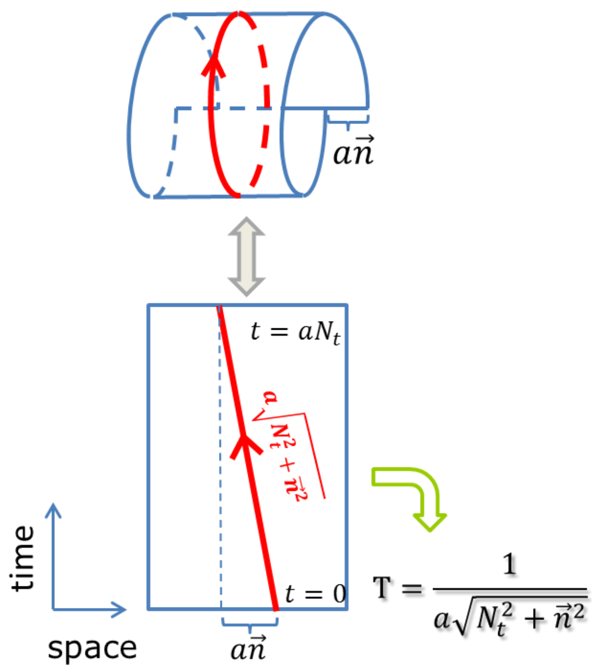
L. Giusti et al. (2011)

Figure 2: Pressure at finite lattice spacing for the SU(N) Yang–Mills theory in the non-interacting limit. The discretization used is the Wilson action and the 'clover' form of the lattice field strength tensor. The inverse temperature is given by $\beta = L_0\sqrt{1+\xi^2}$, and a is the lattice spacing.

- Lattice artifacts are suppressed at larger shifts
- Non-interacting limit with fermions should be checked

Critical temperature T_c

Polyakov loop is difficult to be defined because of misalignment of time and compact directions



$$T = \frac{1}{a\sqrt{N_t^2+\vec{n}^2}}$$

Dressed Polyakov loop

E. Bilgici et al., Phys. Rev. D77 (2008) 094007

Polyakov loop defined with light quarks

$$\Sigma_n(m,V) = \int_0^{2\pi} \frac{d\phi}{2\pi} \frac{e^{-i\phi n}}{V} \langle Tr[(m+D_\phi)^{-1}]\rangle_G$$

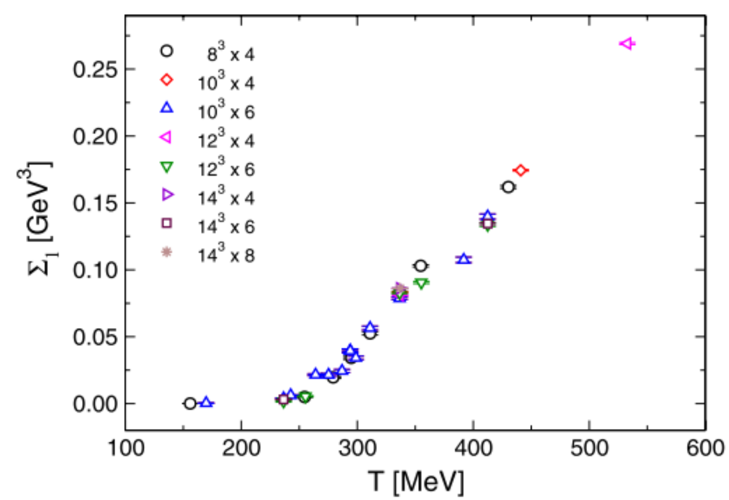
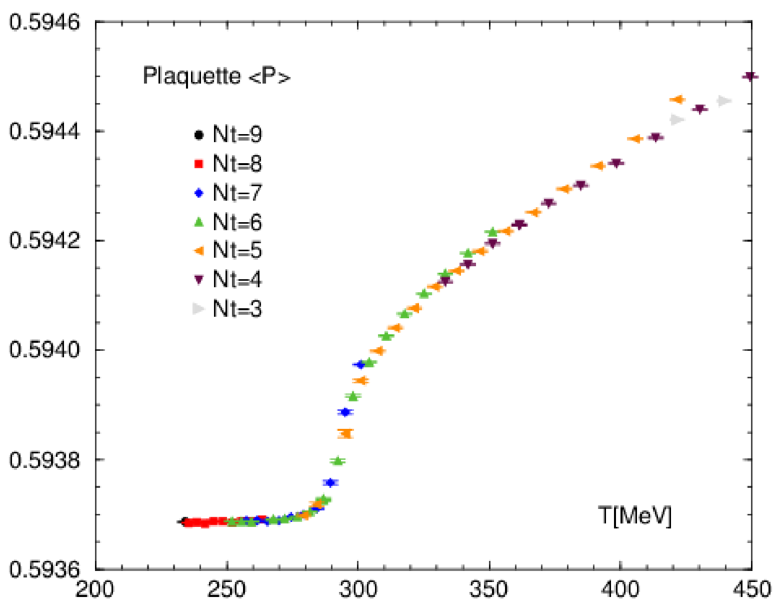


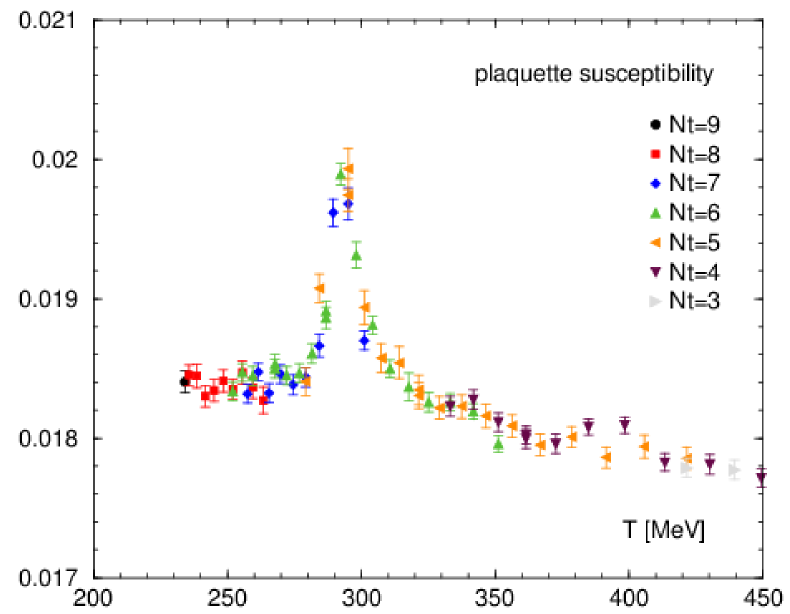
FIG. 2 (color online). The dressed Polyakov loop at $m = 100$ MeV in units of GeV^3 as a function of the temperature T in MeV.

Critical temperature Tc

Plaquette value $\langle P \rangle = \frac{1}{6N_s^3 N_t} \sum_P \langle 1 - \frac{1}{3} ReTrU_P \rangle$

Plaquette susceptibility $\chi_P = N_s^3 N_t \left(\langle P^2 \rangle - \langle P \rangle^2 \right)$

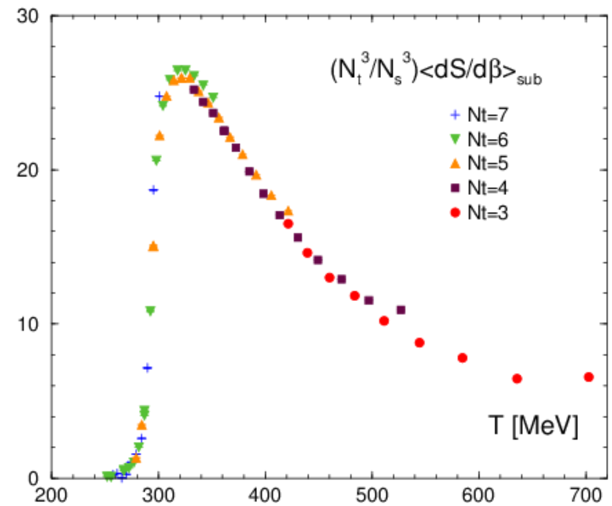




Plaq. suscep. has a peak around T = 293 MeV

Beta-functions (in case of quenched QCD)

$$\frac{\epsilon - 3p}{T^4} = \left(\frac{1}{VT^3}\right) a \frac{d\beta}{da} \left\langle \frac{dS}{d\beta} \right\rangle_{sub}$$

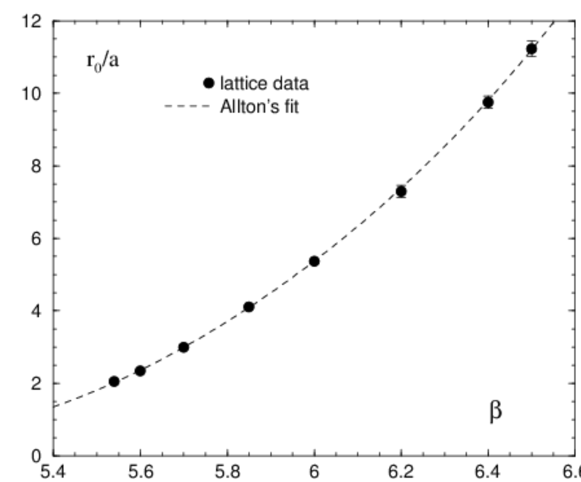


In the fixed scale approach
beta-func at the simulation point is required

However, T=0 simulations near the point are necessary to calculate the beta-function

We are looking for
new methods to calculate beta-function

- Reweighting method
- Shifted boundary condition



Entropy density from shifted boundaries

Entropy density s/T^3

from the cumulant of the momentum distribution

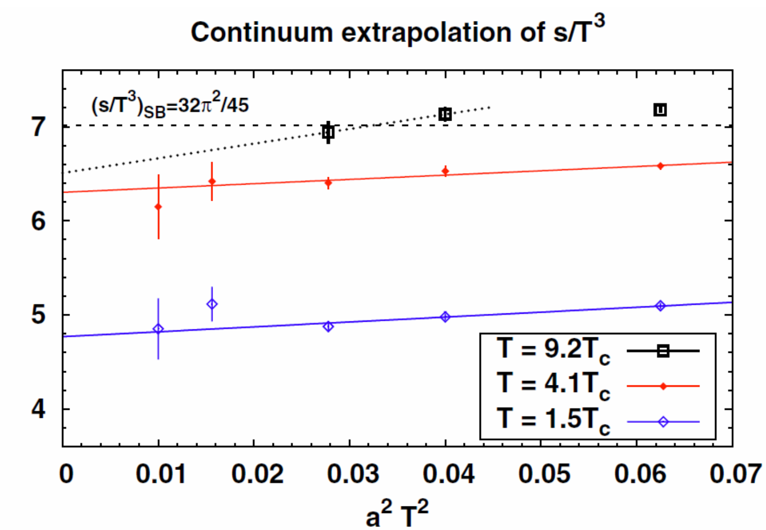
L. Giusti and H. B. Meyer, Phys. Rev. Lett. 106 (2011) 131601

$$\frac{s(T)}{T^3} = \lim_{a\to 0} \frac{2K(T,\vec{z},a)}{|\vec{z}|^2 T^5 V}$$

$$K(T,\vec{z},a) = -\ln \frac{Z(T,\vec{z},a)}{Z(T,\vec{0},a)}$$

$Z(T,\vec{z},a)$: partition function with shifted boundary

where $\vec{z} = (0,0,n_z a)$, n_z being kept fixed when a→0



L. Giusti et al. (2011)

FIG. 1 (color online). Scaling behavior of s/T^3; see Eq. (15). The Stefan-Boltzmann value reached in the high-T limit is also displayed.

Entropy density from shifted boundaries

- Entropy density at a temperature (T_0)
  by the new method with shifted b.c.

$$s(T_0)$$

- Entropy density w/o beta-function
  by the T-integral method

$$s(T)/a\frac{d\beta}{da}$$

$$\frac{\epsilon - 3p}{T^4} = \left(\frac{N_t^3}{N_s^3}\right) a\frac{d\beta}{da}\left\langle\frac{dS}{d\beta}\right\rangle_{sub}$$

$$\frac{p}{T^4} = \int_0^T dT' \, \frac{\epsilon - 3p}{T'^5}$$

$$\Rightarrow \quad Ts = \epsilon + p$$

Beta-func is determined by
matching of entropy densities at T_0

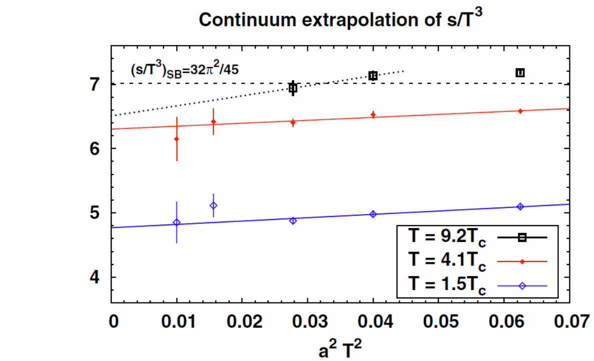
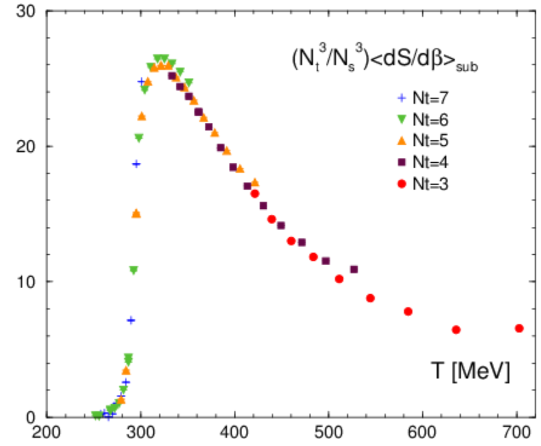


FIG. 1 (color online). Scaling behavior of s/T^3; see Eq. (15). The Stefan-Boltzmann value reached in the high-T limit is also displayed.



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momentum distribution

$$\frac{R(\vec{p})}{V} = \frac{Tr\{e^{-L_0 \hat{H}} \hat{P}(\vec{p})\}}{Tr\{e^{-L_0 \hat{H}}\}}$$

L_0 : Temporal extent

$\hat{H}$: Hamiltonian

$\hat{P}(\vec{p})$: projector onto states with total momentum p

The generating function K(z) of the cumulants of the mom. dist. is defined

$$e^{-K(\vec{z})} = \frac{1}{V} \sum_{\vec{p}} e^{i\vec{p}\cdot\vec{z}} R(\vec{p})$$

the cumulants are given by

$$k_{\{2n_1,2n_2,2n_3\}} = (-1)^{n_1+n_2+n_3+1} \frac{\partial^{2n_1}}{\partial \vec{z}_1^{2n_1}} \frac{\partial^{2n_2}}{\partial \vec{z}_2^{2n_2}} \frac{\partial^{2n_3}}{\partial \vec{z}_3^{2n_3}} \left. \frac{K(\vec{p})}{V} \right|_{\vec{z}=0}$$

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The generating func. K(p) can be written
with the partition function

$$e^{-K(\vec{p})} = \frac{Z(\vec{z})}{Z}$$

$$Z(\vec{z}) = Tr\{e^{-L_0 \hat{H}} e^{i\hat{p}\vec{z}}\}$$

Z(z) can be expressed as a path integral with the field satisfying the shifted b.c.

By the Ward Identities, the cumulant is related to the entropy density "s"

$$k_{\{0,0,2\}} = T(\epsilon + p) = T^2 s$$

$$s = -\frac{1}{T^2} \lim_{V\to\infty} \frac{1}{V} \frac{d^2}{dz^2} \ln Z(\{0,0,z\})|_{z=0}$$

The specific heat and speed of sound can be also obtained in the method.

How to calculate $k_{\{0,0,2\}}$

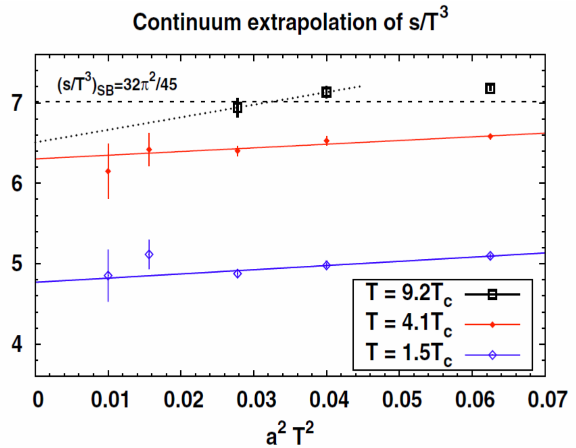
Evaluation of Z(z)/Z with reweighting method

$$\frac{Z(\vec{z})}{Z} = \prod_{i=1}^{n-1} \frac{\mathcal{Z}(r_i)}{\mathcal{Z}(r_{i+1})}$$

$$\bar{S}(U, r_i) = r_i S(U) + (1 - r_i) S(U^z)$$

$$\frac{\mathcal{Z}(r_i)}{\mathcal{Z}(r_{i+1})} = \langle e^{\bar{S}(U, r_{i+1}) - \bar{S}(U, r_i)} \rangle_{r_{i+1}}$$

$$K(\vec{z}) = -\ln \frac{Z(\vec{z})}{Z} = -\sum_{i=0}^{n-1} \ln \frac{\mathcal{Z}(r_i)}{\mathcal{Z}(r_{i+1})}$$



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Summary & outlook

We presented our study of the QCD Thermodynamics

by using Fixed scale approach

and Shifted boundary conditions

- Fixed scale approach
  - Cost for T=0 simulations can be largely reduced
  - first result in N_f=2+1 QCD with Wilson-type quarks
- Shifted boundary conditions are promising tool

  to improve the fixed scale approach
  - fine resolution in Temperature
  - suppression of lattice artifacts at larger shifts
  - Tc determination could be possible
  - New method to estimate beta-functions
- Test in full QCD → Nf=2+1 QCD at the physical point

Thank you for your attention !

L. Giusti and H. B. Meyer (2011) jhep1111, p10

$$\epsilon_\nu \langle \partial_\mu T_{\mu\nu}(x) O_1 \cdots O_n \rangle = -\sum_{i=1}^{n} \langle O_1 \cdots \delta_\epsilon^x O_i \cdots O_n \rangle$$

$$O(y) = T_{0k}(y)$$

$$\partial_0^x \left\{ \langle \bar{T}_{0k}(x_0) T_{0k}(y) \rangle - \delta(x_0 - y_0) \langle T_{kk} + \mathcal{L} \rangle \right\} = 0$$

$$\partial_k^w \left\{ \langle \tilde{T}_{0k}(w_0) T_{0k}(z) \rangle - \delta(w_k - z_k) \langle T_{00} + \mathcal{L} \rangle \right\} = 0$$

$$L_0 \langle \bar{T}_{0k}(x_0) T_{0k}(y) \rangle - L_k \langle \tilde{T}_{0k}(w_k) T_{0k}(z) \rangle = \langle T_{00} \rangle - \langle T_{kk} \rangle$$

$$V \to \infty \qquad L_0 \langle \bar{T}_{0k}(x_0) T_{0k}(y) \rangle = \langle T_{00} \rangle - \langle T_{kk} \rangle = -(e+p) = -Ts$$

$$\langle \bar{T}_{03}(x_0) T_{03}(y) \rangle = -k_{\{0,0,2\}}$$