



BERGISCHE  
UNIVERSITÄT  
WUPPERTAL

# PARALLEL TEMPERING ALGORITHM APPLIED TO THE DECONFINEMENT TRANSITION OF QUENCHED QCD

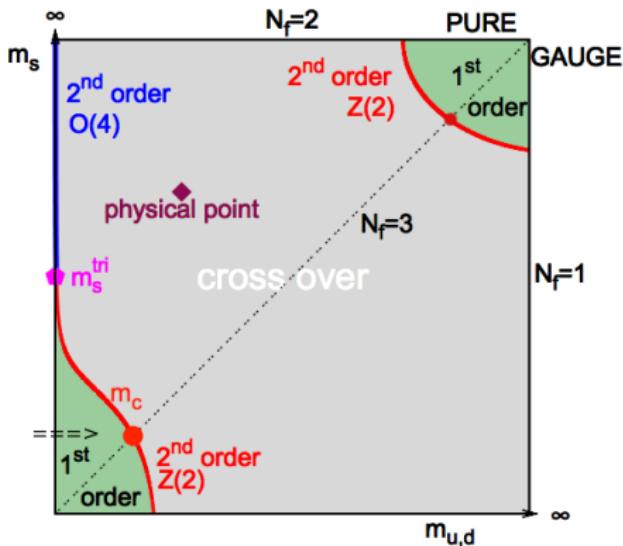
Ruben Kara

and

S. Borsányi, Z. Fodor, D. Godzieba, P. Parotto, A. Pásztor,  
D. Sexty

Lattice 2022

Based on arXiv:2202.05234



Forcrand et. al. 1702.00330

## Columbia Plot for $\mu = 0$

- $m_q \rightarrow \infty$  : Pure gauge theory (quenched case)
- Latent heat in cont. lim. Shirogane PRD 16, Borsanyi, R.K. PRD 22  $\Rightarrow$  1st order
- Phys. quark masses and  $\mu = 0$ : Crossover
- Which value takes the (heavy) critical mass  $m_c$ ?

# The (never) ending story? A small selection...

## Latest studies regarding the heavy mass region

- Suzuki PTEP 2013
- Ejiri et. al. PRD 2016
- Ejiri et. al. PRD 2020
- Ejiri et. al. PTEP 2021
- Cuteri, Philipsen et. al. PRD 2021

## Lower mass region

- Pisarski, Wilczek PRD 1984
- Cuteri, Philipsen, Sciarra JHEP 2021
- Dini, Karsch et. al. PRD 2022

What are the reasons for the structures?

### QCD Lagrangian

$$\mathcal{L} = \bar{\psi}(i\gamma^\mu D_\mu - m)\psi - \frac{1}{4}F_{\mu\nu}^a F_a^{\mu\nu}$$

- Exact global and local SU(3) gauge theory

What are the reasons for the structures?

### QCD Lagrangian

$$\mathcal{L} = \bar{\psi}(i\gamma^\mu D_\mu - m)\psi - \frac{1}{4}F_{\mu\nu}^a F_a^{\mu\nu}$$

- Exact global and local  $SU(3)$  gauge theory

### Center Symmetry $\mathcal{Z}_3$ for $m \rightarrow \infty$

- Invariance under  $U_4(\vec{x}, t_0) \rightarrow zU_4(\vec{x}, t_0)$ ,  $z \in \{1, e^{\pm i2\pi/3}\}$ ,  $U \in SU(3)$
- SSB at high temperatures (deconfinement)
- Order parameter Polyakov loop:  $|\langle P \rangle| \sim e^{-F/T}$

# What are the reasons for the structures?

## QCD Lagrangian

$$\mathcal{L} = \bar{\psi}(i\gamma^\mu D_\mu - m)\psi - \frac{1}{4}F_{\mu\nu}^a F_a^{\mu\nu}$$

- Exact global and local SU(3) gauge theory

## Center Symmetry $\mathcal{Z}_3$ for $m \rightarrow \infty$

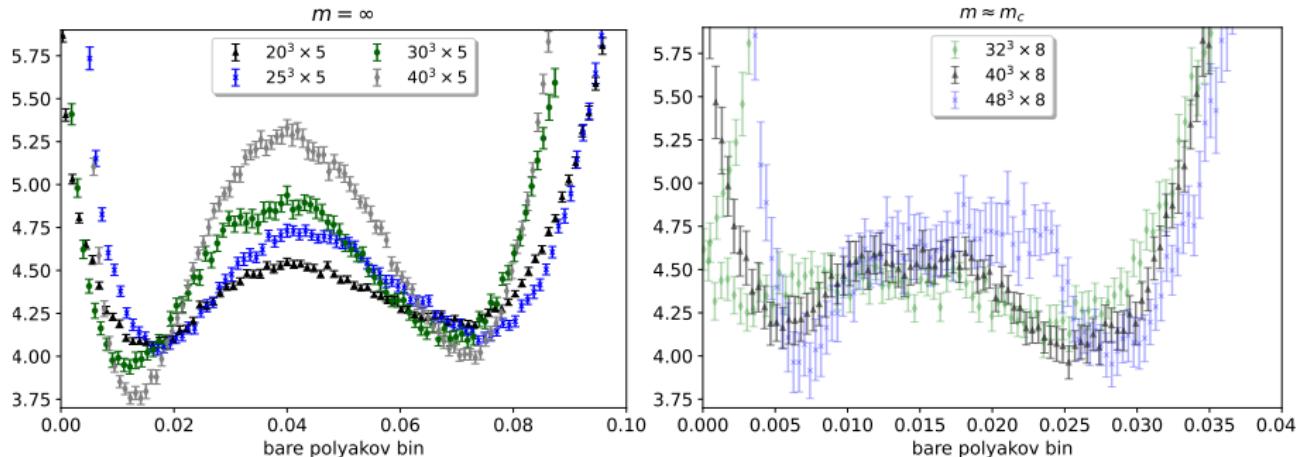
- Invariance under  $U_4(\vec{x}, t_0) \rightarrow zU_4(\vec{x}, t_0)$ ,  $z \in \{1, e^{\pm i2\pi/3}\}$ ,  $U \in \text{SU}(3)$
- SSB at high temperatures (deconfinement)
- Order parameter Polyakov loop:  $|\langle P \rangle| \sim e^{-F/T}$

## Chiral symmetry for $m \rightarrow 0$

- $\mathcal{L}_F = \bar{\psi}_L iD\!\!\!/ \psi_L + \bar{\psi}_R iD\!\!\!/ \psi_R$
- SSB at moderate temperatures
- Order parameter chiral condensate  $\langle \bar{\psi}\psi \rangle = \langle \bar{\psi}_L\psi_R + \bar{\psi}_R\psi_L \rangle$

# Facing (super-)critical slowing down: $\beta \approx \beta_c$

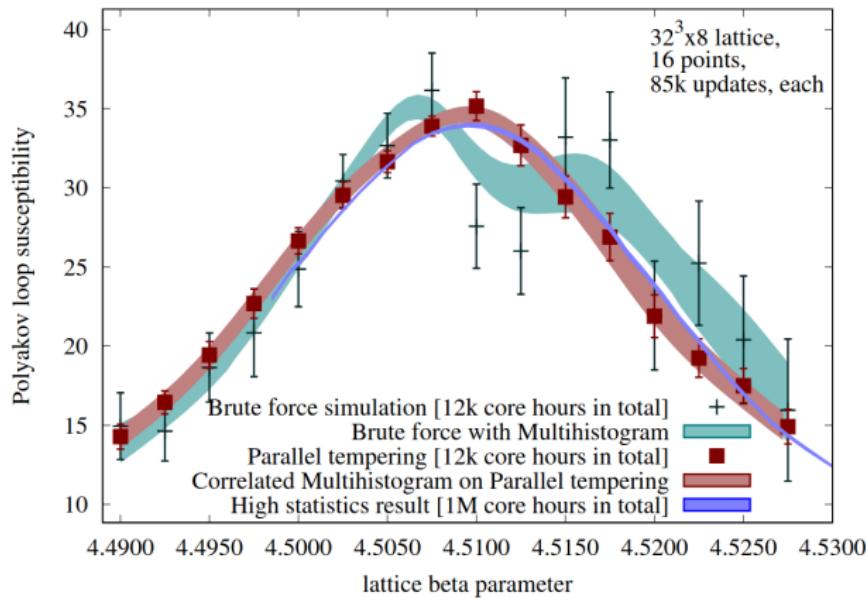
"Effective" Polyakov loop potential from the histogram



## Features

- Quenched (l.h.s): Potential barrier grows by increasing volume
- $m \approx m_c$  (r.h.s) : "Flat" potential barrier
- Both phases have to be sampled  $\Rightarrow$  High auto-corr. time in simulations

# Quenched case: (Super-)critical slowing down



## Tempering algorithms

- Multiple simulations at different  $\beta$  [Marinari 9205018] [Joó 9810032]
- Swap configurations between subensembles  $\Rightarrow$  reduced auto. corr.

# Parallel tempering: Two kinds of Markov transitions

## Independent Markov processes

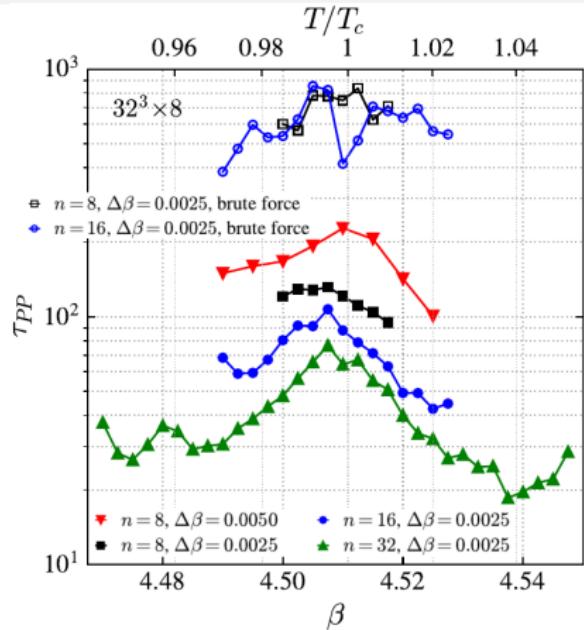
- Phase space  $\Gamma_{\text{PT}}$  product of sub-ensemble phase spaces  $\Gamma_i$
- (R)HMC for transition within single ensemble
- Transition between  $i$  and  $j$ : Swap config.  $a$  and  $b$  ?

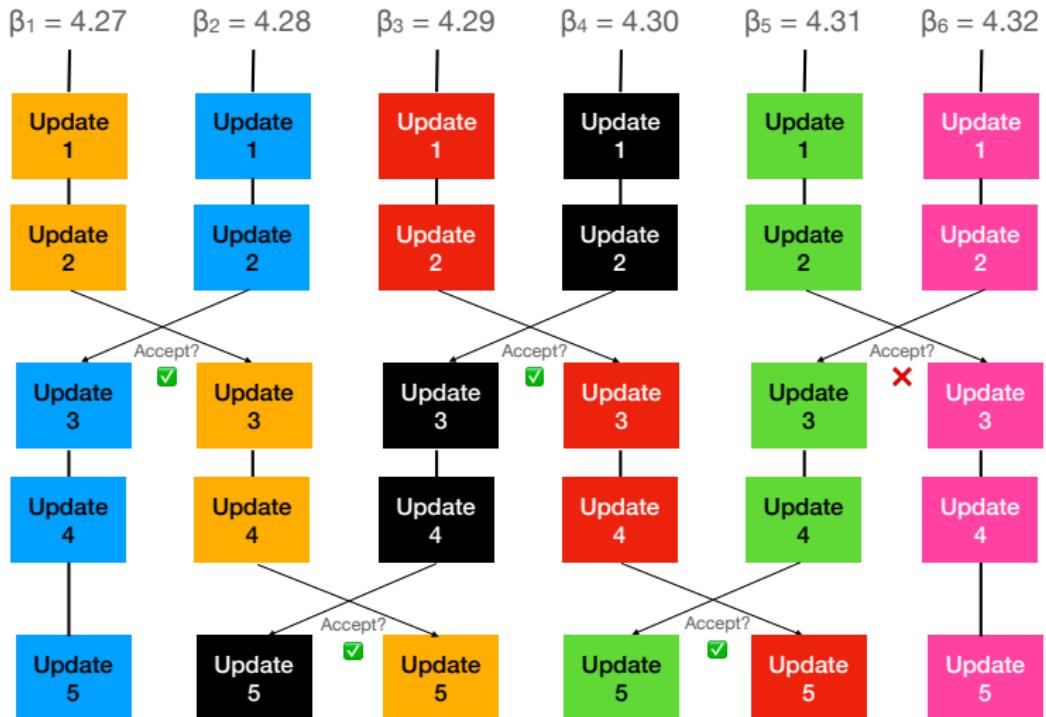
## Detailed balance condition

$$P_s(i, j) e^{-\mathcal{H}_i(a)} e^{-\mathcal{H}_j(b)} = P_s(j, i) e^{-\mathcal{H}_j(a)} e^{-\mathcal{H}_i(b)}$$

$$P_s(i, j) = \min \left( 1, e^{\Delta \mathcal{H}} \right)$$

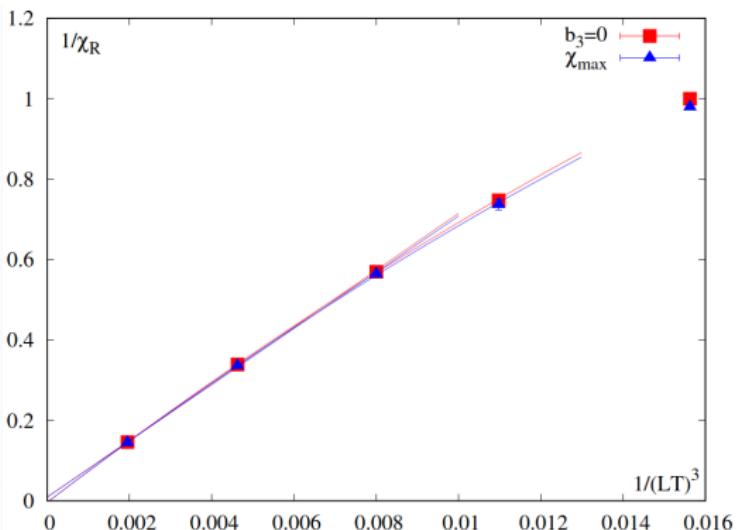
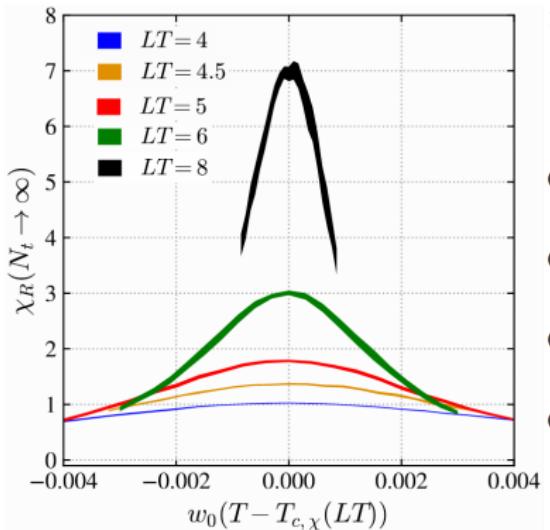
$$\Delta \mathcal{H} = \{\mathcal{H}_j(a) + \mathcal{H}_i(b)\} - \{\mathcal{H}_i(a) + \mathcal{H}_j(b)\}$$





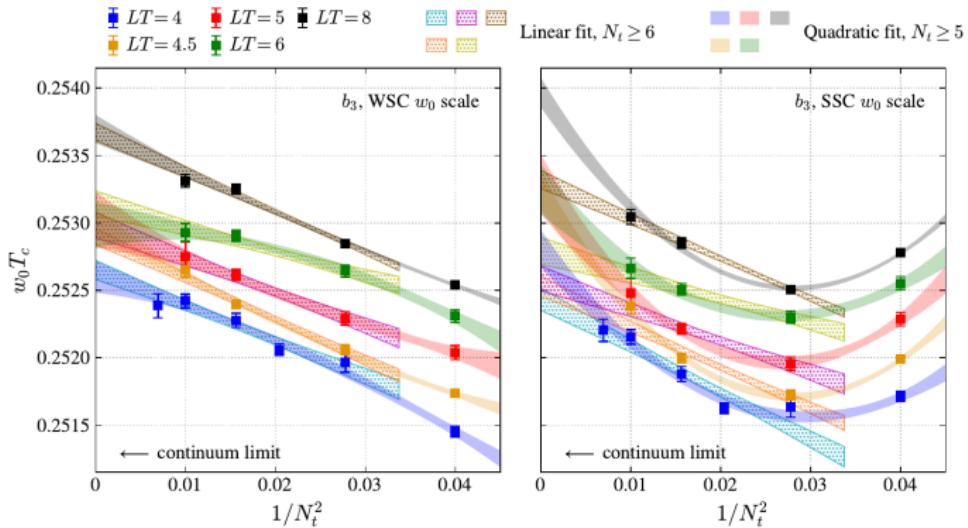
# Polyakov loop and its susceptibility

$$P = \frac{1}{N_s^3} \sum_{\vec{x}} P_{\vec{x}} = \frac{1}{N_s^3} \sum_{\vec{x}} \text{tr} \left[ \prod_{\tau} U_4(\vec{x}, \tau) \right] \quad \chi = N_s^3 \left( \langle |P|^2 \rangle - \langle |P| \rangle^2 \right)$$



Borsanyi, R.K. et. al. PRD (2022)

# Transition temperature $w_0 T_c$



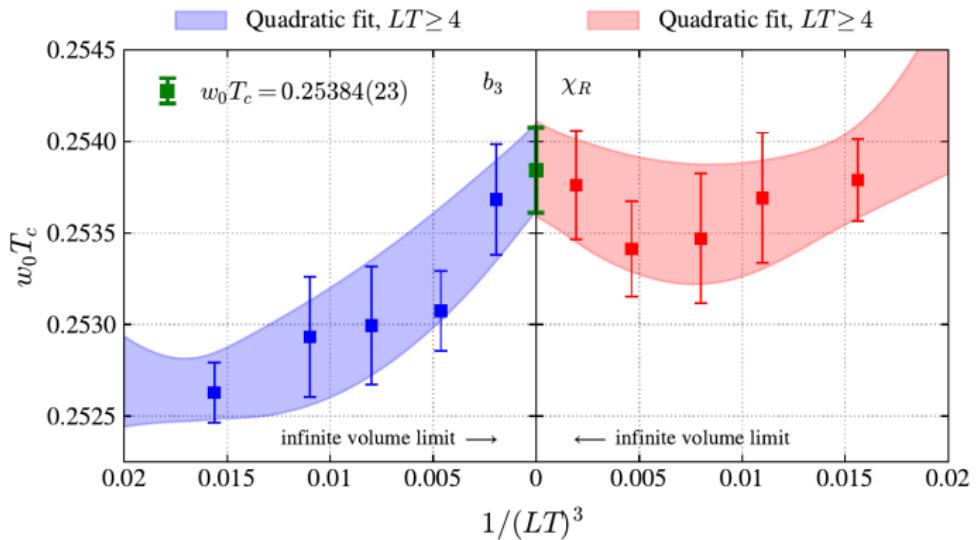
Scale setting based on Wilson flow

$$t \frac{d}{dt} [t^2 E(t)]_{t=w_0^2} = 0.3 \quad \frac{w_0}{a(\beta) N_t} = w_0 T$$

- For notation see Fodor JHEP (2014)

Measure of the skewness

$$B_3 = \frac{\langle (|P| - \langle |P| \rangle)^3 \rangle}{\langle (|P| - \langle |P| \rangle)^2 \rangle^{3/2}}$$

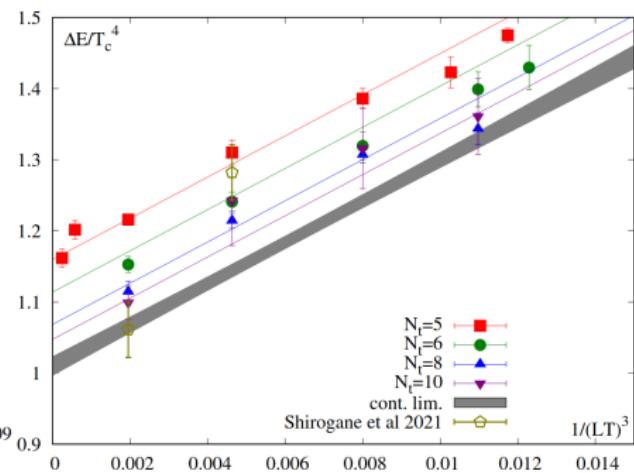
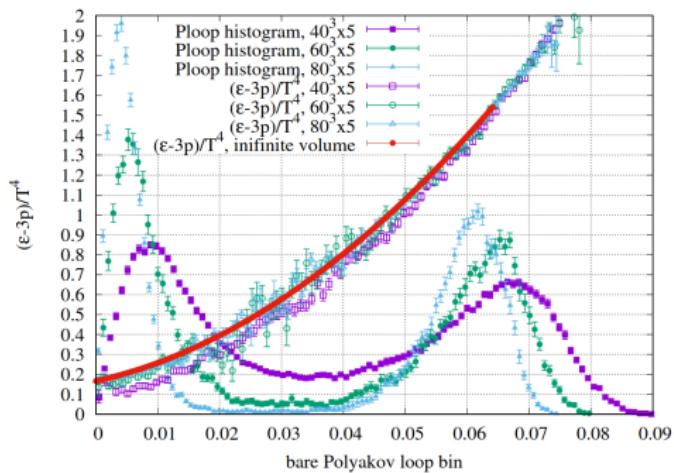


## Systematics

- $\underbrace{\chi_R, b_3}_{\text{2}} \cdot \underbrace{\text{deg. of poly. fits}}_{\text{4}} \cdot \underbrace{\text{cutoff}}_{\text{4}} \cdot \underbrace{\text{WSC/SSC}}_{\text{2}} \cdot \underbrace{\text{deg. of w}_0/\text{a fit}}_{\text{2}} \cdot \underbrace{\text{cont. lim. deg.}}_{\text{2}} = 256 \text{ different analyses}$

$$w_0 T_c = 0.25384(11)_{\text{stat}}(21)_{\text{sys}}$$

# Latent heat

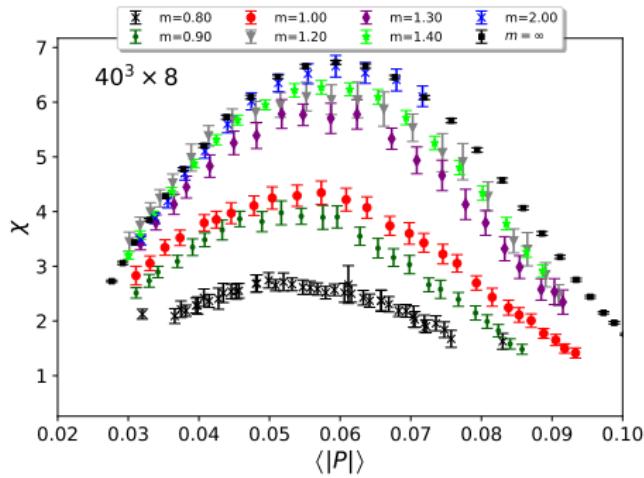
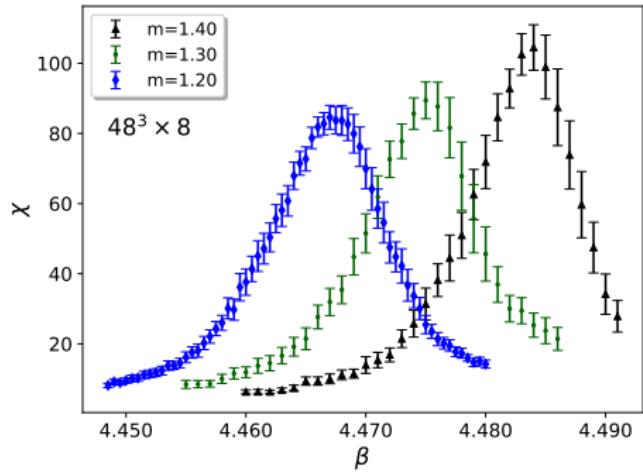


## Discontinuity of the trace anomaly

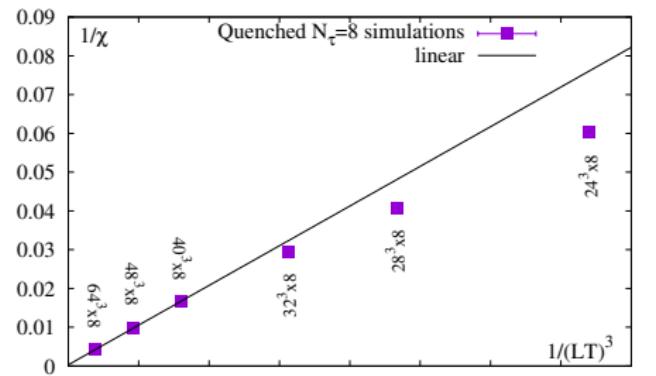
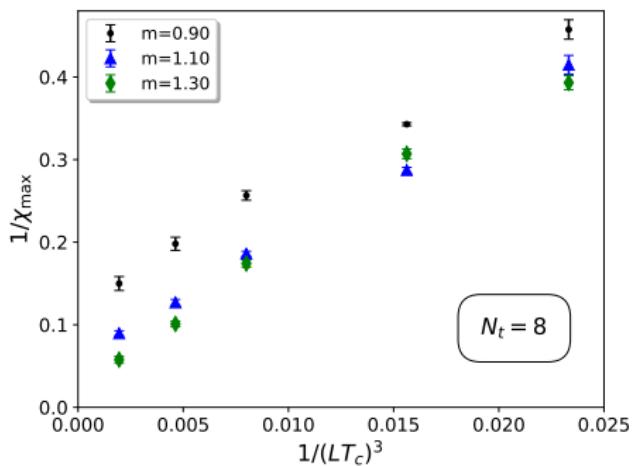
- Trace anomaly smooth function of  $|P|$
- Separation of cold and hot phase by min. between the peaks

$$\Delta \left[ \frac{\epsilon - 3p}{T^4} \right] = 1.025(21)_{\text{stat}}(27)_{\text{sys}}$$

# Heavy but finite masses

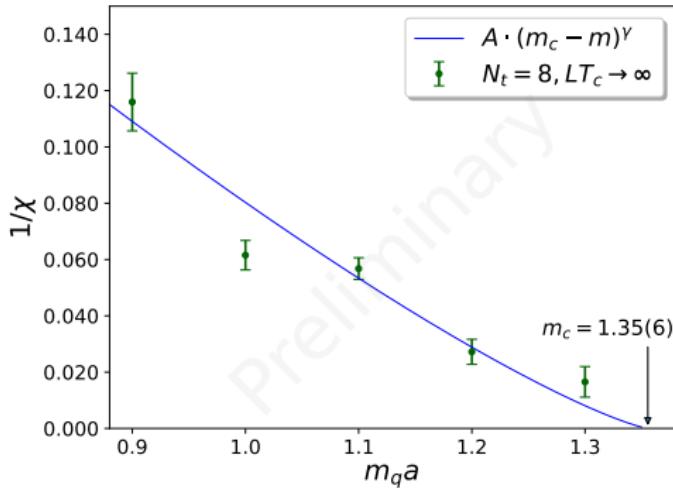
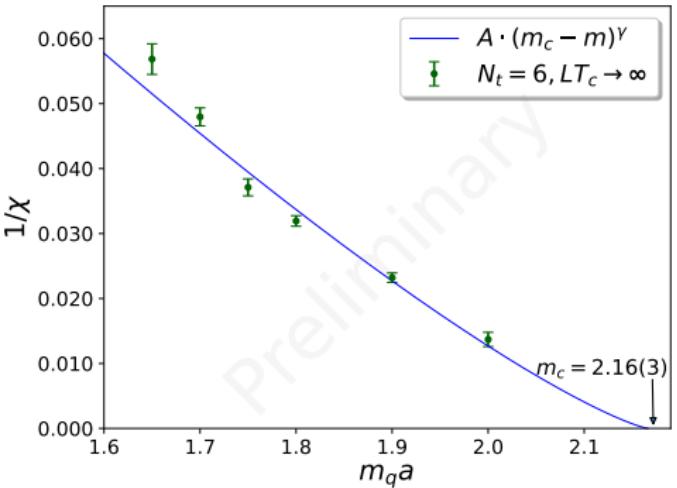


# Volume scaling for $N_t = 8$



Vol. scaling: Heavy mass region vs. quenched case

- Quenched (r.h.s.):  $LT > 4$  necessary to observe linear scaling



## Critical region

- $\chi_{\max}^{-1}$  follows a power law near the transition
- $m_q$  represents symmetry breaking field

$$\chi_{\max}^{-1}(LT_c \rightarrow \infty) = A \cdot (m_c - m)^\gamma$$

	$w_0 \cdot T_c$	$m_c$
$N_t = 6$	0.2531(2)	2.13(4)
$N_t = 8$	0.2477(4)	1.35(6)

# Summary

## Quenched QCD

- $\beta$  tempering algorithms to reduce auto-correlation
- $w_0 T_c = 0.25384(23)$  first per-mil accurate result in QCD thermodynamics
- $\Delta \left[ \frac{\epsilon - 3p}{T^4} \right] = 1.025(34) \implies$  1st order thermal transition

## Results of dynamical quark simulations

- $\chi(\langle |P| \rangle)$  allows precise peak determination
- Estimate of the critical mass:  $N_t = 6 \ m_c = 2.16$ ;  $N_t = 8 \ m_c = 1.35$

## Outlook

- Systematic error analysis
- Continuum limit of the critical mass

# Trace anomaly and latent heat

## Trace anomaly

- Measures deviation from an ideal gas

$$\epsilon - 3p = T^5 \frac{\partial}{\partial T} \left( -\frac{f}{T^4} \right)$$

- $\log Z$  can be expressed as integral over the gauge action  $S$

$$\frac{f}{T^4} = - \underbrace{\frac{1}{T^3 V}}_{(\frac{N_t}{N_x})^3} \int d\beta' \left[ S_0^{\text{per site}} - S_T^{\text{per site}} \right] = -N_t^4 \int d\beta' [S_0 - S_T]$$

- Taking into account  $T \frac{\partial}{\partial T} = -a \frac{\partial}{\partial a}$

$$\frac{\epsilon - 3p}{T^4} = -N_t^4 a \frac{\partial \beta}{\partial a} [S_0 - S_T]$$

- Latent heat:

$$\Delta \left( \frac{\epsilon - 3p}{T^4} \right) = N_t^4 a \frac{\partial \beta}{\partial a} [S_{\text{hot}} - S_{\text{cold}}]$$