The equation of state with non-equilibrium methods

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in collaboration with

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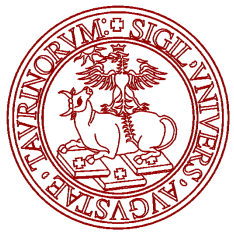

In lattice gauge theories the expectation values of a large set of physical quantities is *naturally* related to the computation (via Monte Carlo simulations) of free-energy differences (or, equivalently, of ratios of partition functions).

For example:

- equilibrium thermodynamics (pressure)
- free-energy of interfaces between center domains
- 't Hooft loops
- magnetic susceptibility of strongly-interacting matter

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- "integral method": computing first the *derivative* of the free energy with respect to some parameter, and then integrate
- reweighting
- snake algorithm

Good motivations to search new methods and algorithms.

Indeed, we want to introduce in LGTs a **novel** method to calculate *directly* ΔF based on a recent but well-established result from non-equilibrium statistical mechanics.

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1. Jarzynski's equality

2. From SM to LGTs: interface free energy in $\mathbb{Z}_2$ gauge model

3. The equation of state with non-equilibrium methods
   - The pressure from Jarzynski's equality
   - Results for $\mathrm{SU}(3)$ Yang-Mills theory

The Second Law of Thermodynamics

We start from Clausius inequality

$$\int_A^B \frac{\mathrm{d}Q}{T} \leq \Delta S$$

that for isothermal transformations becomes

$$\frac{Q}{T} \leq \Delta S$$

If we use

$$\begin{cases} Q = & \Delta E - W \quad \text{(First Law)} \\ F \stackrel{\text{def}}{=} & E - ST \end{cases}$$

the Second Law becomes

$$W \geq \Delta F$$

where the equality holds for reversible processes.

Moving from thermodynamics to statistical mechanics we know that the former relation (valid for a *macroscopic* system) becomes

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Let's consider a system with Hamiltonian H_λ parametrized by λ. Its partition function is

$$Z_\lambda(T) = \int \mathrm{d}\Gamma e^{-\beta H_\lambda(\Gamma)}$$

and the free energy is

$$F_\lambda(T) = -\beta^{-1} \ln Z_\lambda(T)$$

Now we are interested in letting the system evolve in time by varying the parameter λ between two values.
The crucial quantity is the **work** performed on the system

$$W = \int_{t_i}^{t_f} \mathrm{d}t \dot{\lambda} \frac{\partial H_\lambda}{\partial \lambda}$$

(this is not arbitrary: $\dot{H} = \dot{\lambda}\frac{\partial H}{\partial \lambda} + \dot{\Gamma}\frac{\partial H}{\partial \Gamma}$ can be identified with the First Law of Thermodynamics)

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Jarzynski's equality

Now we can precisely state the non-equilibrium equality [Jarzynski, 1997]

$$\left\langle \exp\left(-\frac{W(\lambda_i, \lambda_f)}{T}\right)\right\rangle = \exp\left(-\frac{F(\lambda_f) - F(\lambda_i)}{T}\right)$$

Jarzynski's equality relates the exponential statistical average of the work done on a system during a non-equilibrium process with the difference between the initial and the final free energy of the system.

This result can be derived for different kinds of processes

- Langevin evolution
- molecular dynamics
- Monte Carlo simulations

In general, the evolution of the system is performed by changing continuously (as in real time experiments) or discretely (as in MC simulations) a chosen set of one or more parameters, such as the couplings of the system.

At the beginning of each transformation the system must be at equilibrium.

In each step of the process the value of λ is changed and the system is brought **out of equilibrium**.

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Relation with the Second Law

It is instructive to see how this result is connected with the Second Law of Thermodynamics

Starting from Jarzynski's equality

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and using *Jensen's inequality*

$$\langle \exp x\rangle \geq \exp\langle x\rangle$$

(valid for averages on real x) we get

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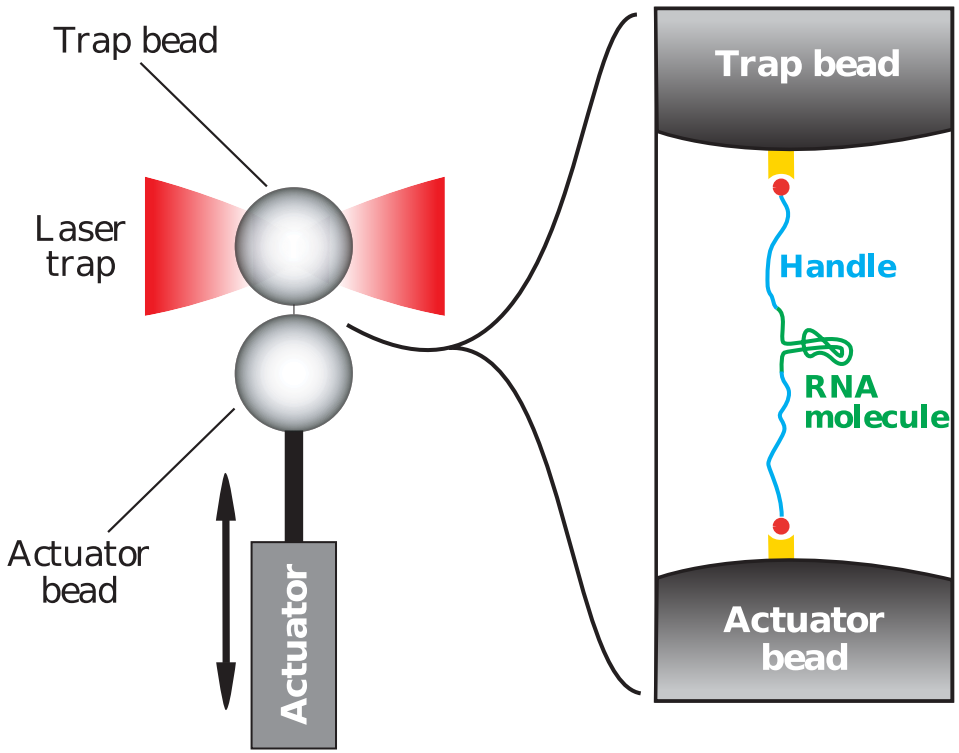
An experimental test

An experimental test of Jarzynski's equality was performed in 2002 by Liphardt *et al.* by mechanically stretching a single molecule of RNA between two conformations.

The irreversible work trajectories (via the non-equilibrium relation) provide the result obtained with reversible stretching.



Jarzynski's equality in a Monte Carlo simulation

$$\left\langle \exp\left(-\frac{W(\lambda_0,\lambda_N)}{T}\right)\right\rangle = \exp\left(-\frac{\Delta F}{T}\right)$$

1. the non-equilibrium transformation begins by changing λ with some prescription (e.g. a linear one)
$$\lambda_0 \to \lambda_1 = \lambda_0 + \Delta\lambda$$
2. we compute the "work"
$$H_{\lambda_{n+1}}[\phi_n] - H_{\lambda_n}[\phi_n]$$
3. after each change, the system is updated using the new value $\to$ driving the system out of equilibrium!
$$[\phi_n] \xrightarrow{\lambda_{n+1}} [\phi_{n+1}]$$
4. the **total work** $W(\lambda_0,\lambda_N)$ made on the system to change λ using N **steps** is
$$W(\lambda_0,\lambda_N) = \sum_{n=0}^{N-1}\left(H_{\lambda_{n+1}}[\phi_n] - H_{\lambda_n}[\phi_n]\right)$$
5. at the end, we create a new initial state ϕ_0 and we repeat this transformation for n_r **realizations**

The $\langle\ldots\rangle$ indicates that we have to take the **average on all possible realizations** of the transformation $\to$ it must be repeated several times to obtain **convergence** to the correct answer!

We can check the convergence by looking for discrepancies between the 'direct' ($\lambda_i \to \lambda_f$) and 'reverse' ($\lambda_f \to \lambda_i$) transformations

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- in a Monte Carlo simulation we can control
  - N, the number of **steps** for each transformation between initial and final value of the parameter λ
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- in general, a systematic **discrepancy** appears between 'direct' ($\lambda_i \to \lambda_f$) and 'reverse' ($\lambda_f \to \lambda_i$) transformations when n_r is finite. In practice, one has to choose a suitable combination of N and n_r in order to obtain convergence.

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Two special cases

There are two particularly interesting limits of this relation

- the limit of $N \to \infty$: now the transformation is infinitely *slow* and the the system is always at equilibrium. The switching process is reversible: no energy is dissipated and thus

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  This is the case of **thermodynamic integration**

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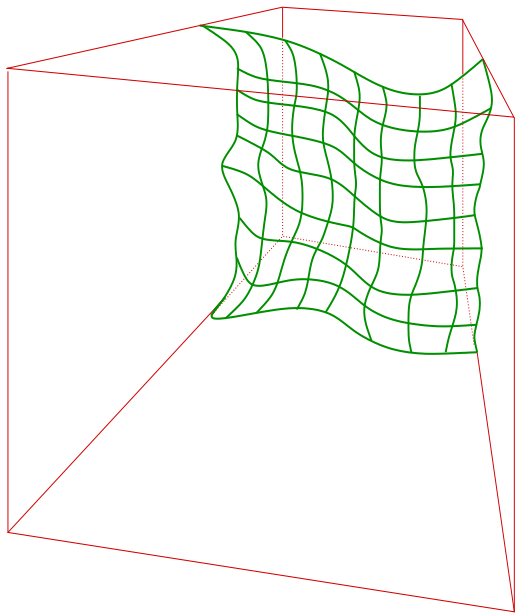
From SM to LGTs: interface free energy in $\mathbb{Z}_2$ gauge model

Interfaces in the $\mathbb{Z}_2$ gauge model

Why study interfaces?

- experimental applications in condensed matter systems
- appear in many contexts also in HEP ("domain walls" at finite T, 't Hooft loops)
- also related to flux tubes in confining gauge theories which can be studied with string-theory tools



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The $\mathbb{Z}_2$ gauge model in 3 dimensions is the simplest lattice gauge theory in which to study interfaces: it is described by a Wilson action with $\mathbb{Z}_2$ variables and possesses a **confining** phase for small values of the inverse coupling β_g.

It can be exactly rewritten through the Kramers-Wannier duality as the 3-dimensional Ising model on the **dual** lattice:

$$H = -\beta \sum_{x,\mu} J_{x,\mu}\, \sigma_x\, \sigma_{x+a\hat{\mu}}$$

where

$$\beta = -\frac{1}{2} \ln \tanh \beta_g$$

Interface free energy

To create an interface we induce a **frustration** on the system, by imposing $J_{x,\mu} = -1$ only for the couplings in a specific slice of the lattice (and only in one direction) and setting the remaining ones to 1.

The **free energy** associated with this interface can be expressed as the ratio between two partition functions:

- one with **periodic** boundary conditions (all $J_{x,\mu} = 1$)
- one with **antiperiodic** boundary conditions ($J_{x,\mu} = -1$ on a slice)

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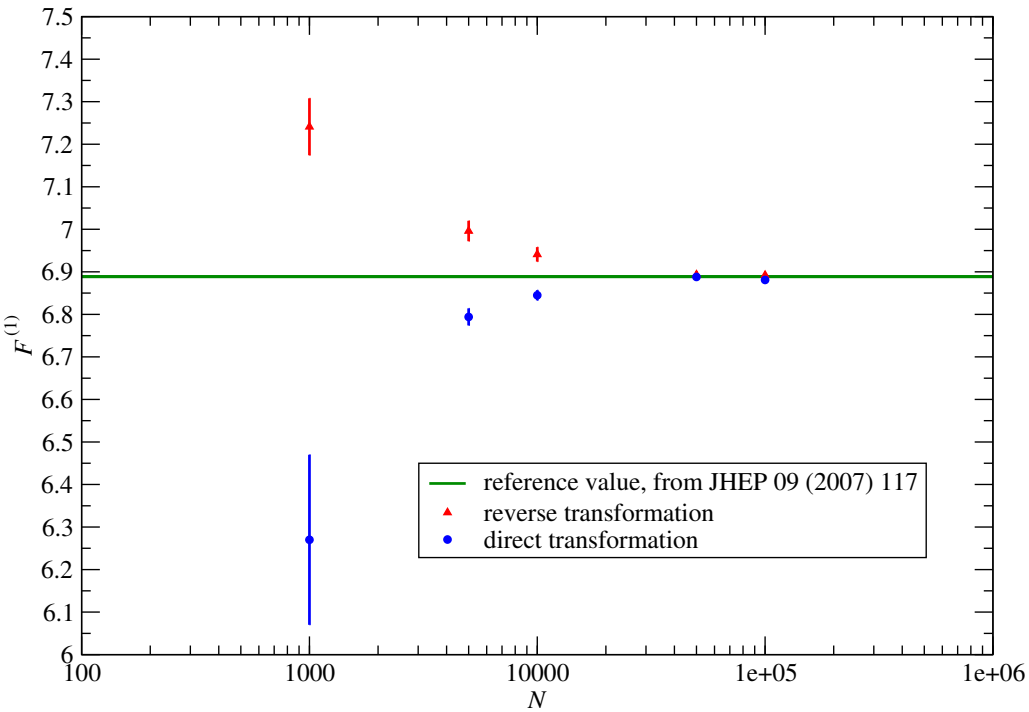
Results in the $\mathbb{Z}_2$ gauge model

In order to compute the Z_a/Z_p ratio we applied Jarzynski's relation by gradually varying the $J_{x,\mu}$ parameter with a linear prescription:

$$J_{x,\mu}(n) = 1 - \frac{2n}{N}$$

where N is the total number of steps between periodic and antiperiodic b.c.

$$\beta = 0.223102, \quad N_0 = 96, N_1 = 24, N_2 = 64$$



The equation of state with non-equilibrium methods

Equilibrium thermodynamics in non-Abelian gauge theories

- The thermal properties of QCD and QCD-like theories are particularly well suited for being studied on the lattice, due to *non-perturbative* nature of the deconfinement transition.

- *low-temperature phase* ($T < T_c$) $\rightarrow$ description in terms of a gas of massive, non-interacting hadrons.

- Even more dramatic for pure Yang-Mills theories - lattice data in the confining region have been compared in detail with the prediction of a glueball gas with an Hagedorn spectrum **[Meyer, 2009; Borsányi et al., 2012; Caselle et al., 2015, Alba et al., 2016]**.

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Pressure on the lattice

On an hypercubic lattice of size $N_t \times N_s^3$, the temperature is determined by

$$T = \frac{1}{a(\beta_g) N_t}$$

In practice, the temperature is controlled by the inverse coupling $\beta_g = \frac{2N_c}{g^2}$.

The **pressure** p in the thermodynamic limit equals the opposite of the **free energy density**

$$p \simeq -f = \frac{T}{V} \log Z(T, V)$$

and a common way to estimate it on the lattice is by the "integral method" **[Engels et al., 1990]**

$$p(T) = \frac{1}{a^4} \frac{1}{N_t N_s^3} \int_0^{\beta_g(T)} d\beta_g' \frac{\partial \log Z}{\partial \beta_g'}$$

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Pressure with Jarzynski's relation

Jarzynski's relation gives us a **direct** method to compute the pressure: we can change temperature T by controlling the parameter β_g in a non-equilibrium transformation!

The **difference of pressure** between two temperatures T and T_0 is

$$\frac{p(T)}{T^4} - \frac{p(T_0)}{T_0^4} = \left(\frac{N_t}{N_s}\right)^3 \log\langle e^{-W_{\mathrm{SU}(N_c)}}\rangle$$

with $W_{SU(N_c)}$ being the *"work"* made on the system:

$$W_{\mathrm{SU}(N_c)} = \sum_{n=0}^{N-1} \left[S_W(\beta_g^{(n+1)}, \hat{U}) - S_W(\beta_g^{(n)}, \hat{U})\right];$$

here S_W is the standard Wilson action and $\hat{U}$ is a configuration of $\mathrm{SU}(N_c)$ variables on the links of the lattice.

A test for the $\mathrm{SU}(2)$ pressure in the proximity of the deconfining transition yielded excellent results.

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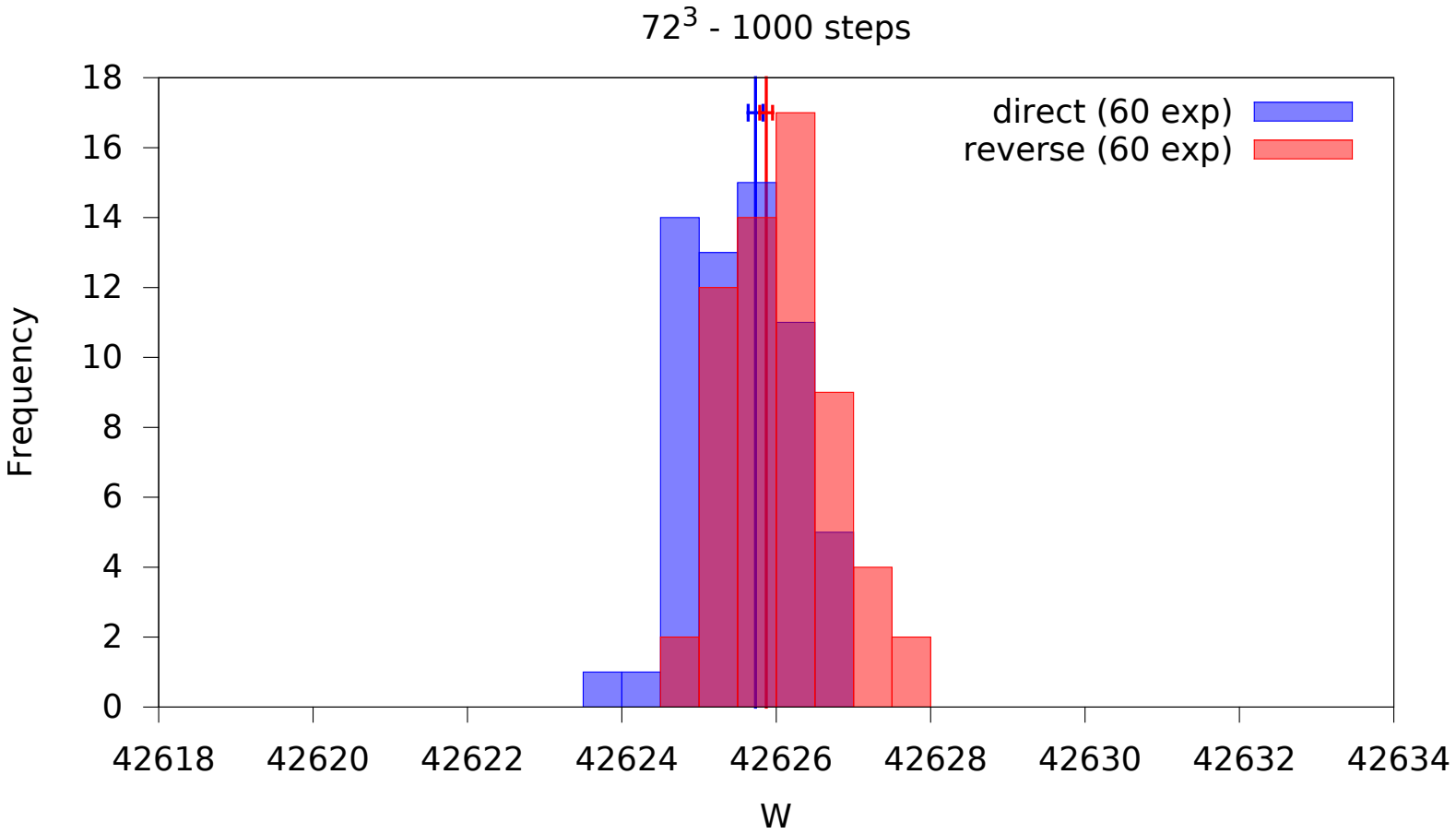
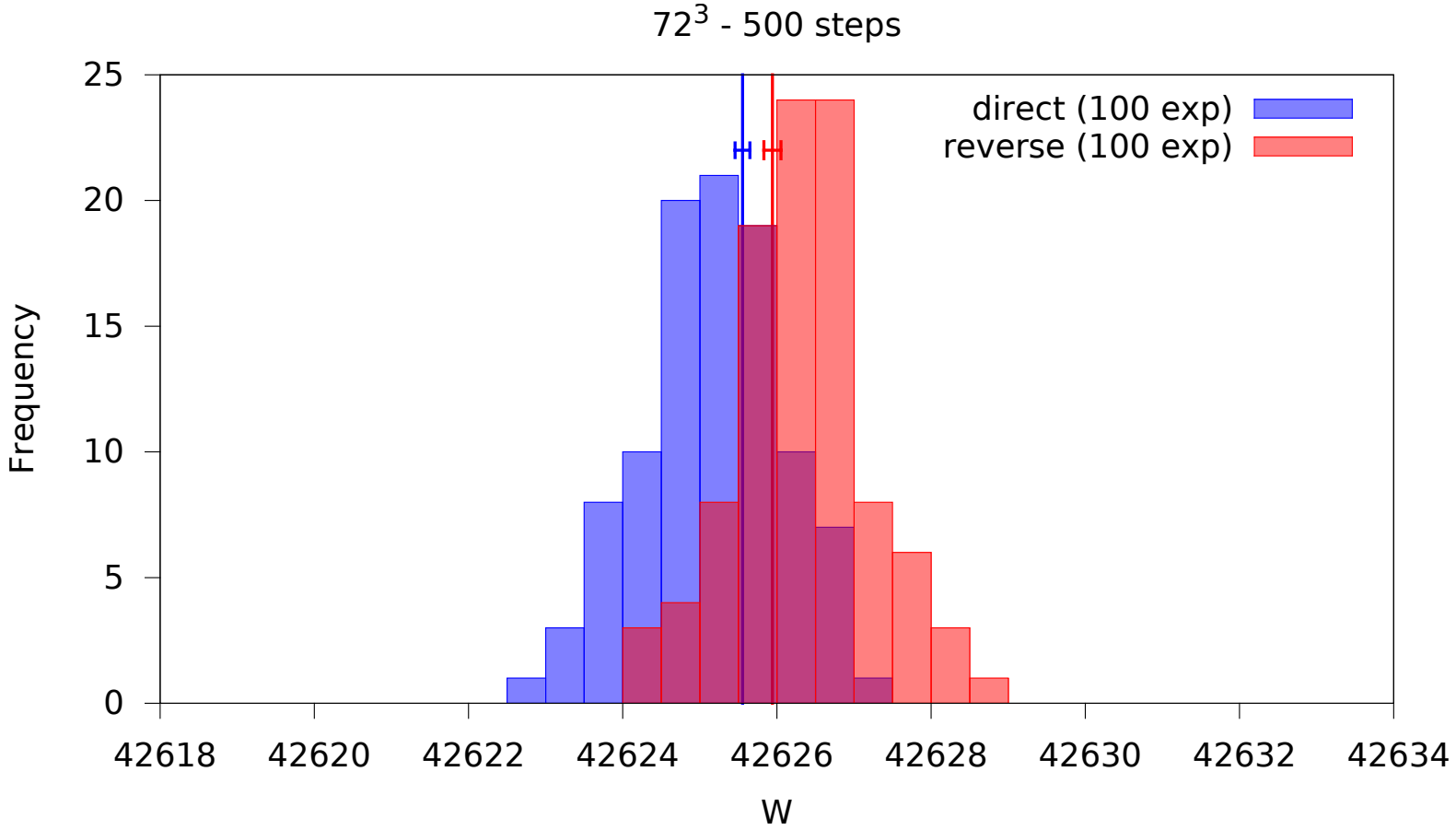
Work distributions



Total work W distributions for realizations of the transformation: $\beta = 2.4158 \leftrightarrow 2.4208$.

Vertical lines indicate the value of ΔF obtained from these trials.

Work distributions



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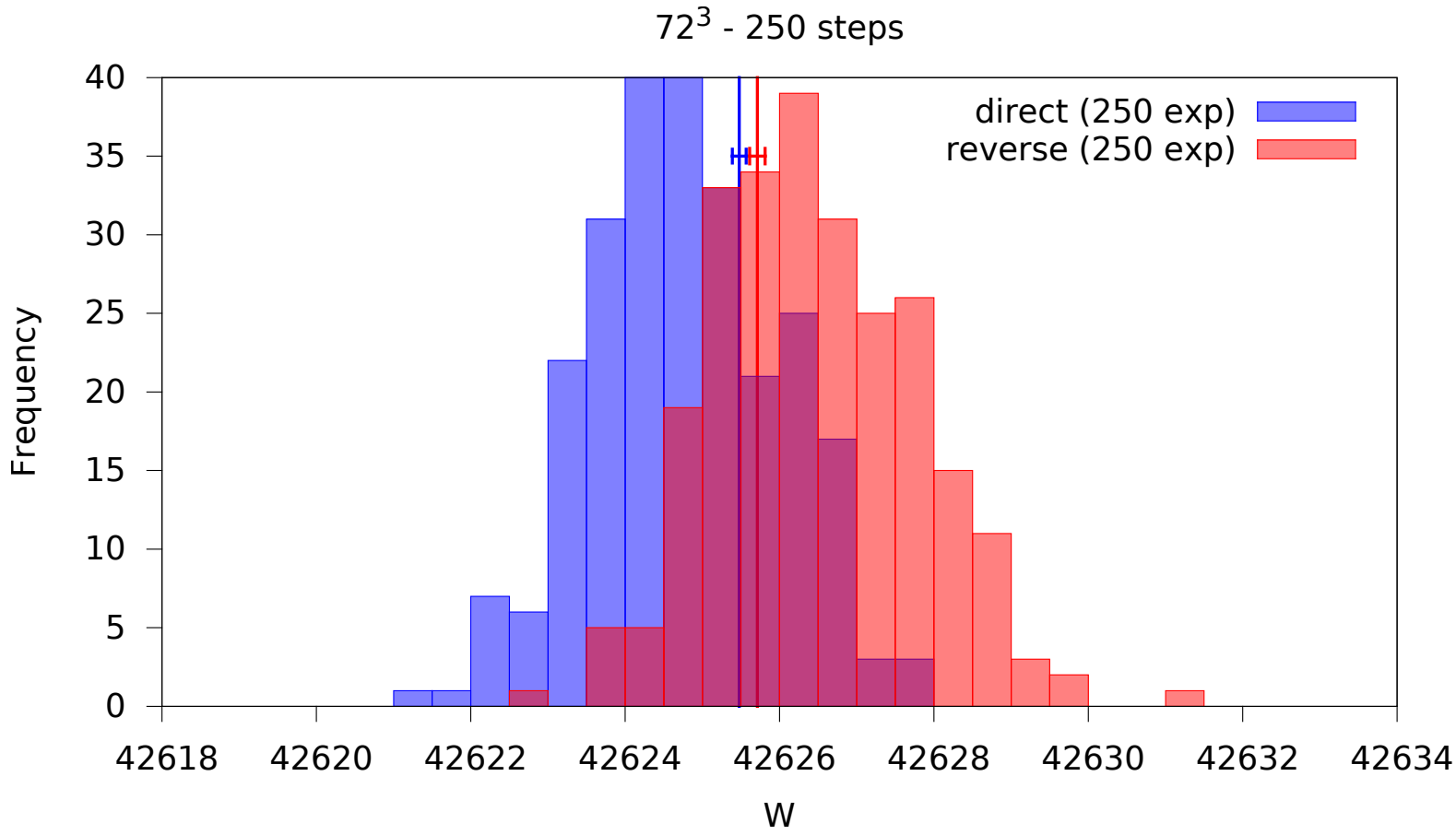

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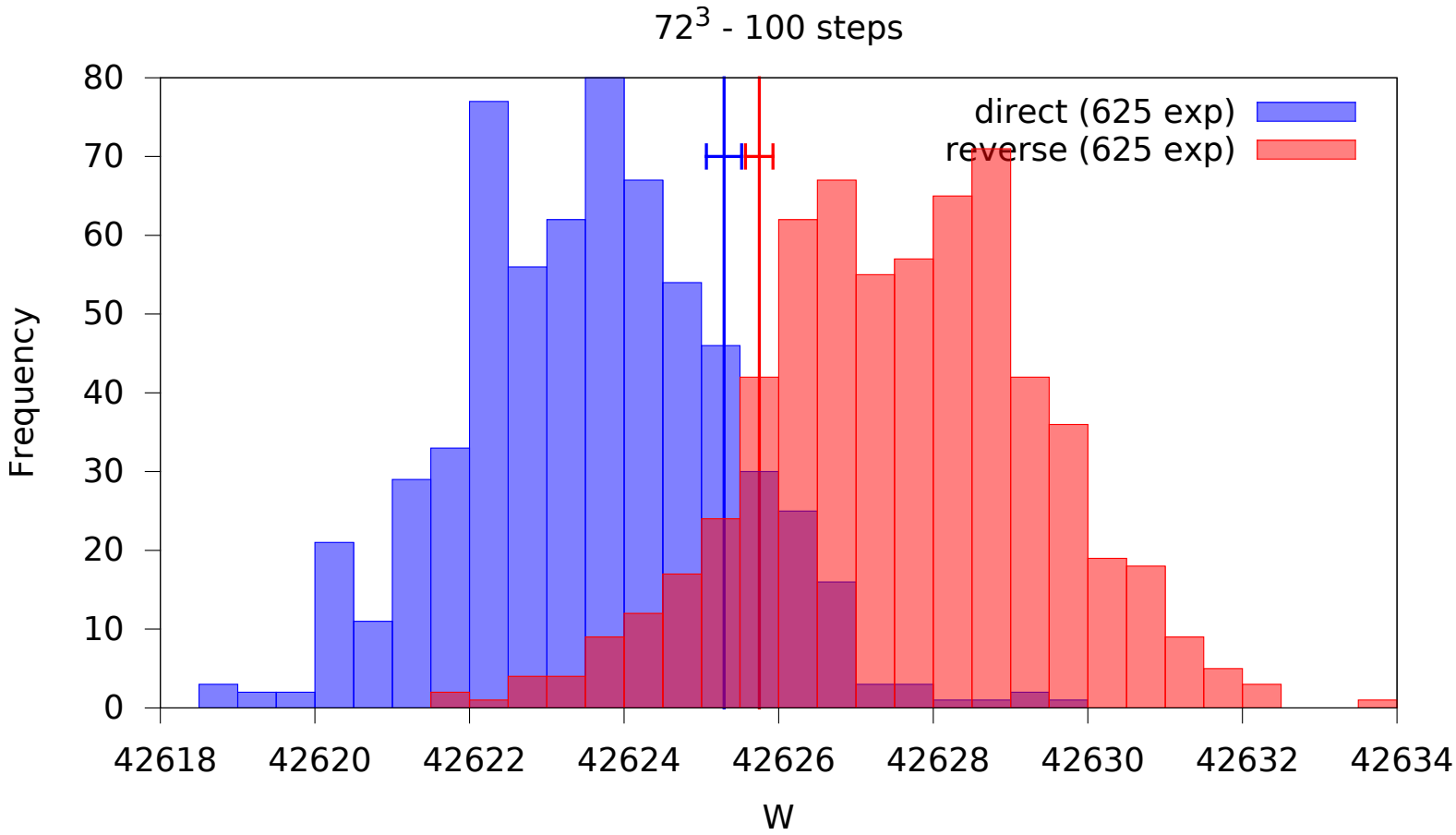

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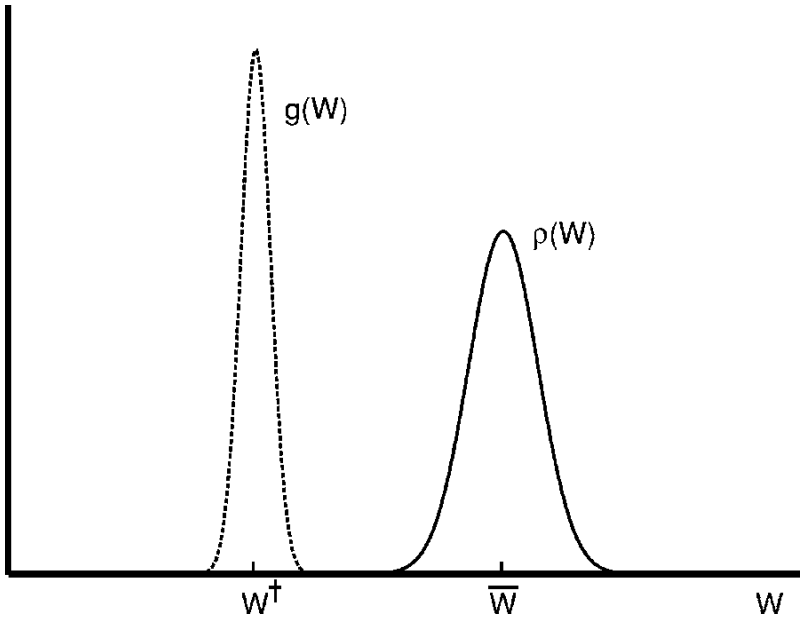
Dominant realizations



Picture taken from **[Jarzynski, 2006)]**

The work is statistically distributed on $\rho(W)$; however the trials that dominate the exponential average are in the region where $g(W) = \rho(W)e^{-\beta W}$ has the peak.

Crooks fluctuation theorem

Crooks discovered in 1998 another relation deeply connected with Jarzynski's equality

$$\frac{P_F(W)}{P_R(-W)} = e^{\beta(W-\Delta F)}$$

The $P_{F,R}$ indicate the probability distribution of the work performed in the forward and reverse realizations of the transformation.

$W_d = W - \Delta F$ is the **dissipated** work.

The $\mathrm{SU}(3)$ equation of state

The equation of state of the $\mathrm{SU}(3)$ Yang-Mills theory has been determined in the last few years using different methods.

- using a variant of the integral method **[Borsànyi et al., 2012]**

  $\rightarrow$ the primary observable is the **trace of the energy-momentum tensor**

- using a moving frame **[L. Giusti and M. Pepe, 2016]**

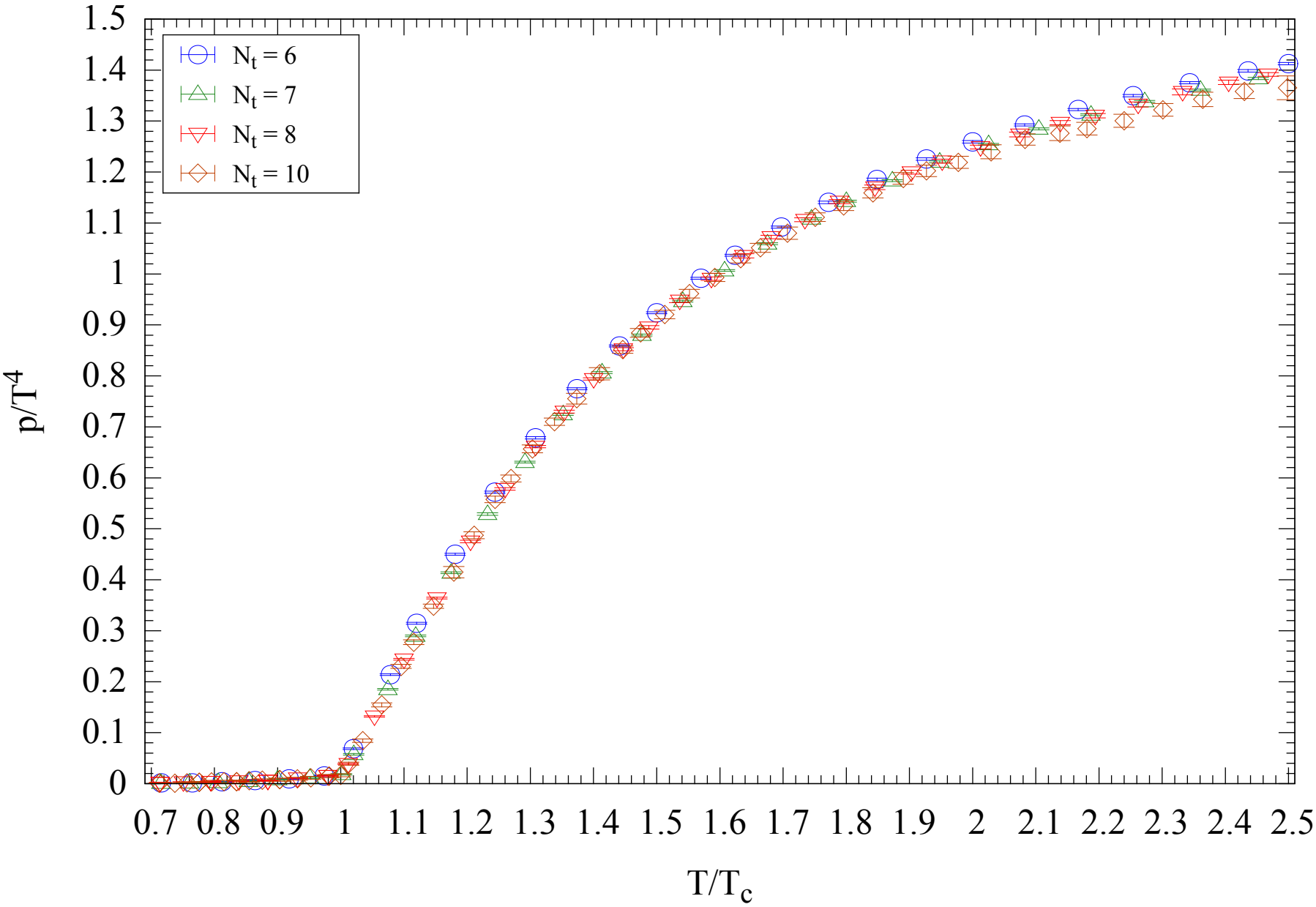
  $\rightarrow$ the primary observable is the **entropy density**

- using the gradient flow **[Kitazawa et al., 2016]**

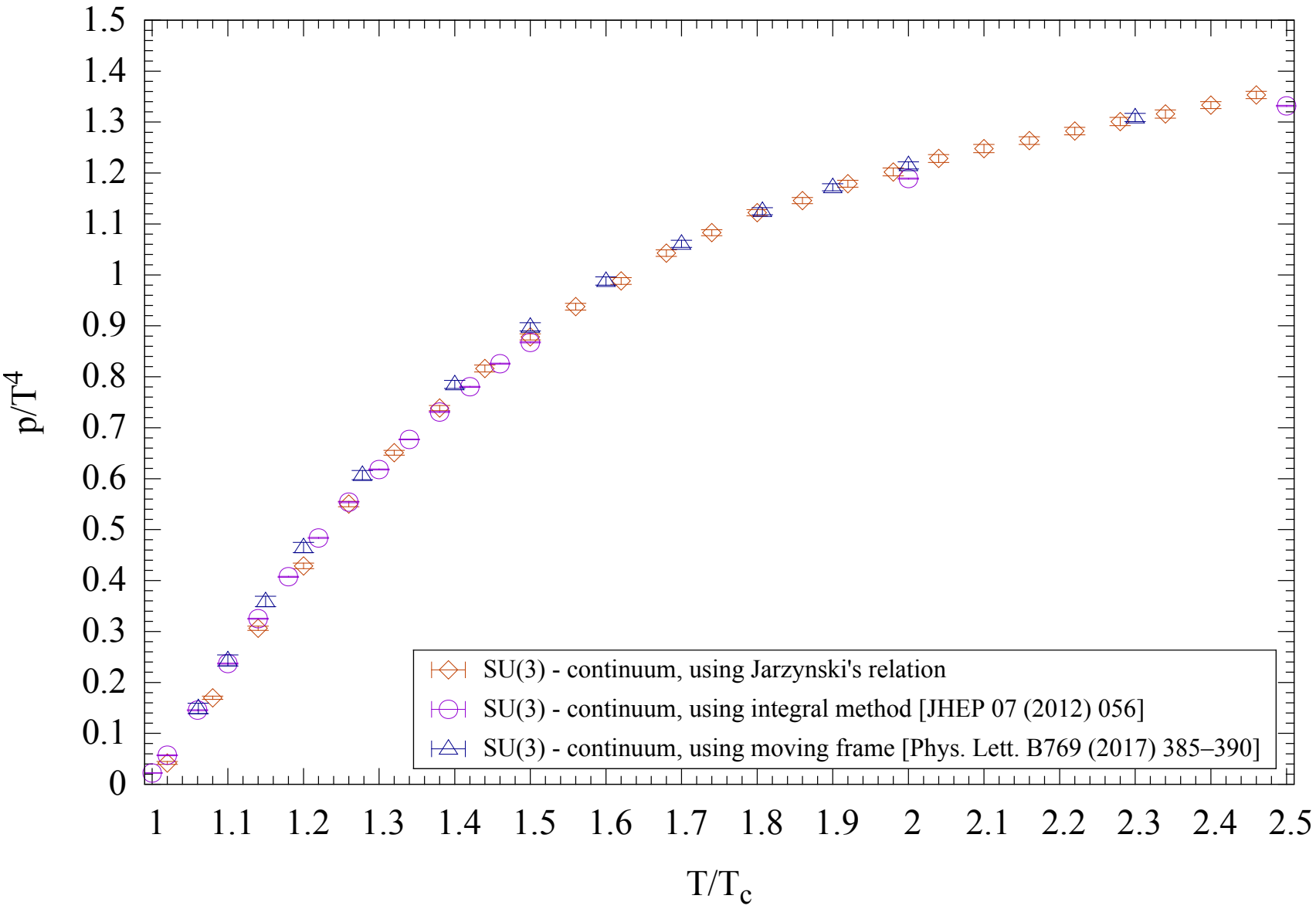
  $\rightarrow$ the primary observables are the **energy density** and the **pressure**

A high-precision determination of the $\mathrm{SU}(3)$ e.o.s. is an excellent benchmark for the **efficiency** of a technique based on non-equilibrium transformations.

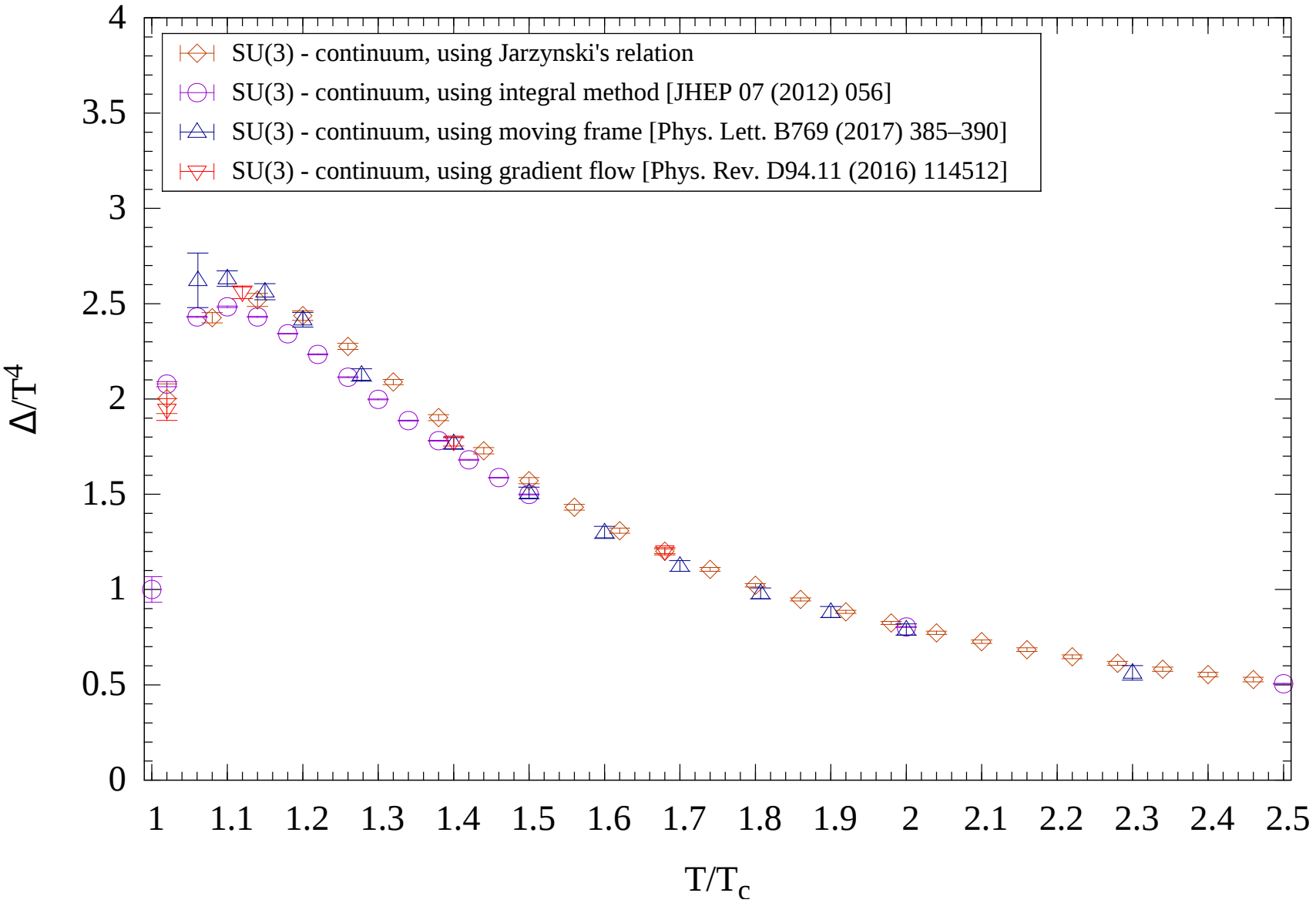
SU(3) pressure across the deconfinement transition, for different values of N_t, with Jarzynski's equality



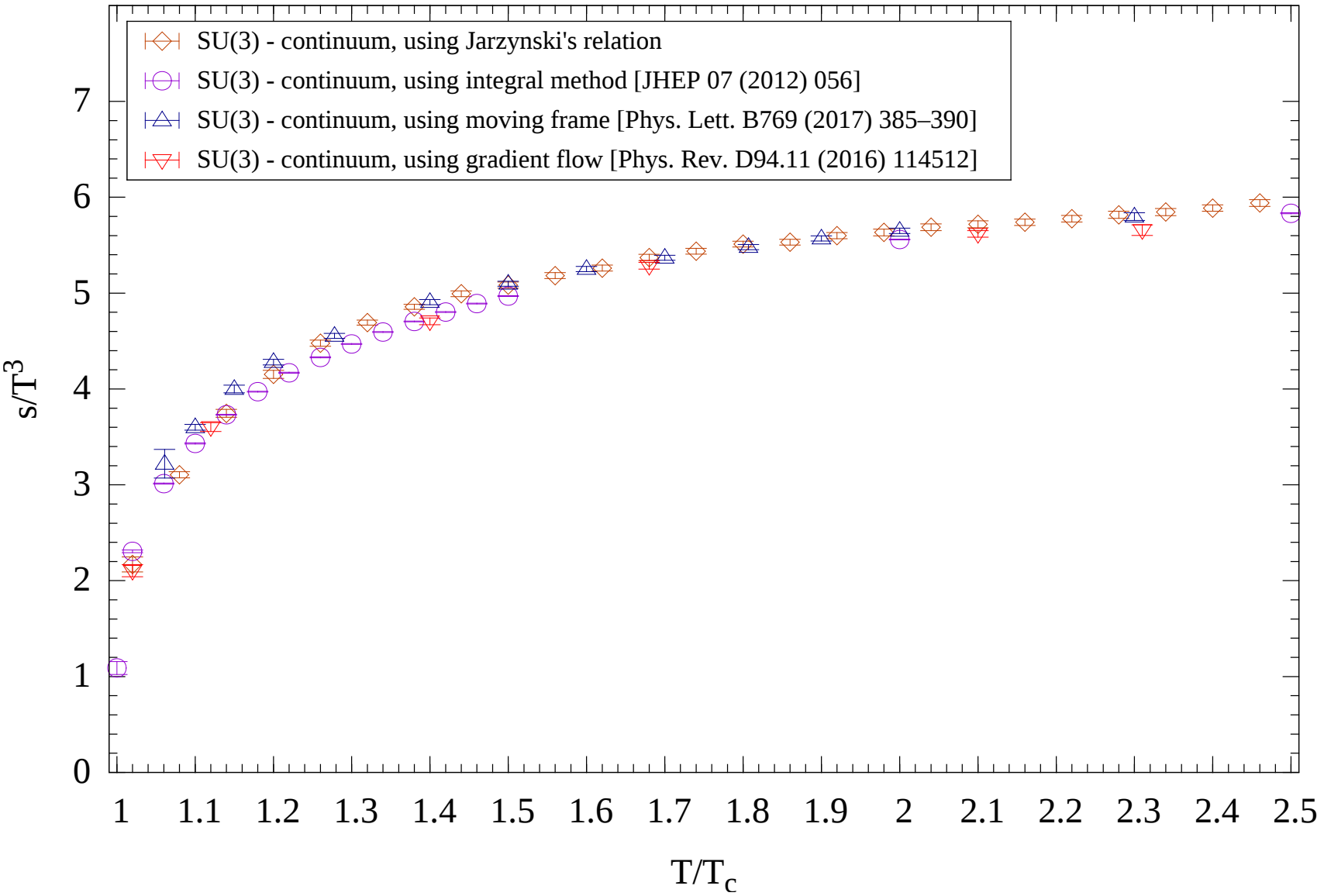
SU(3) pressure - continuum extrapolation



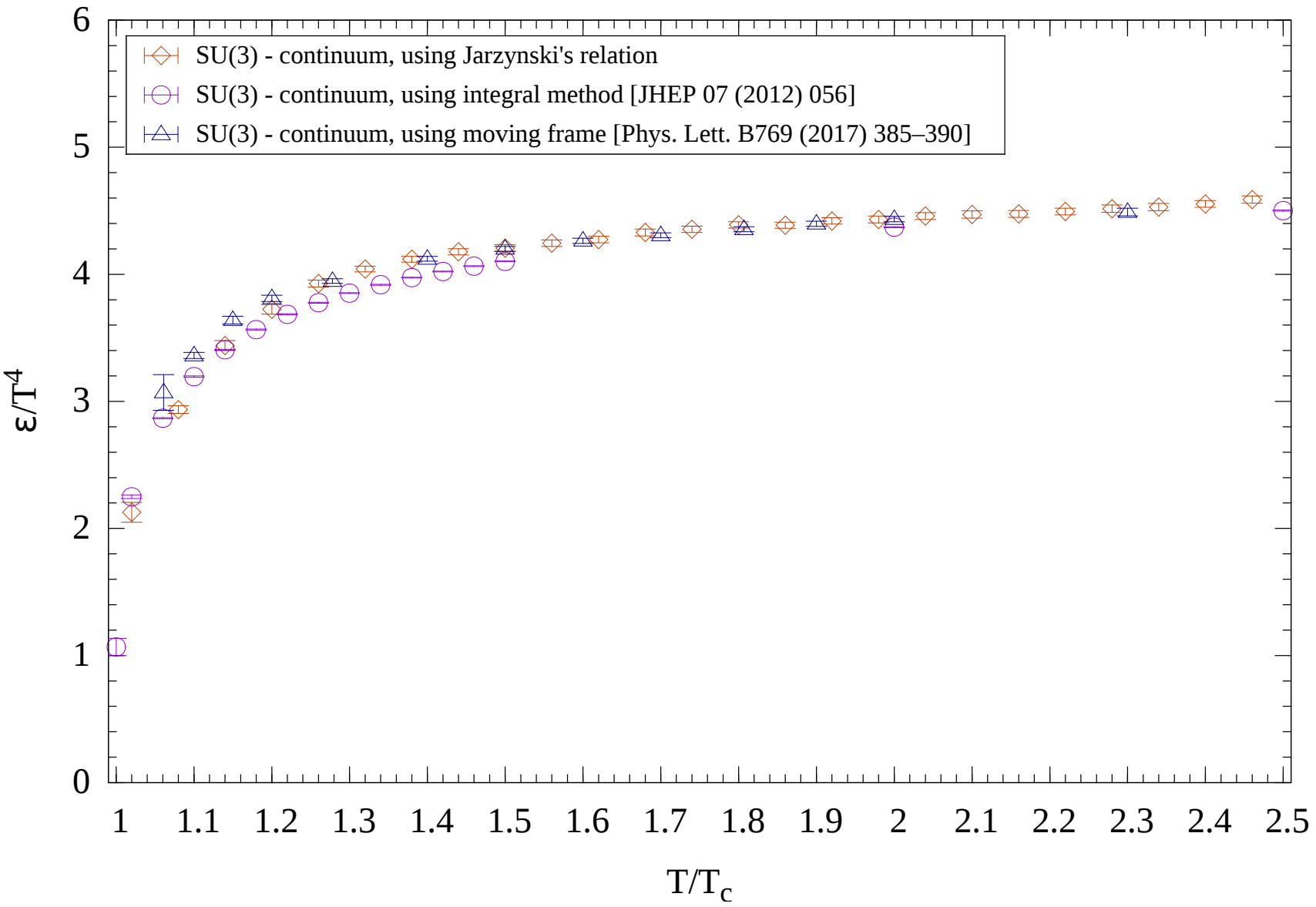
SU(3) trace anomaly



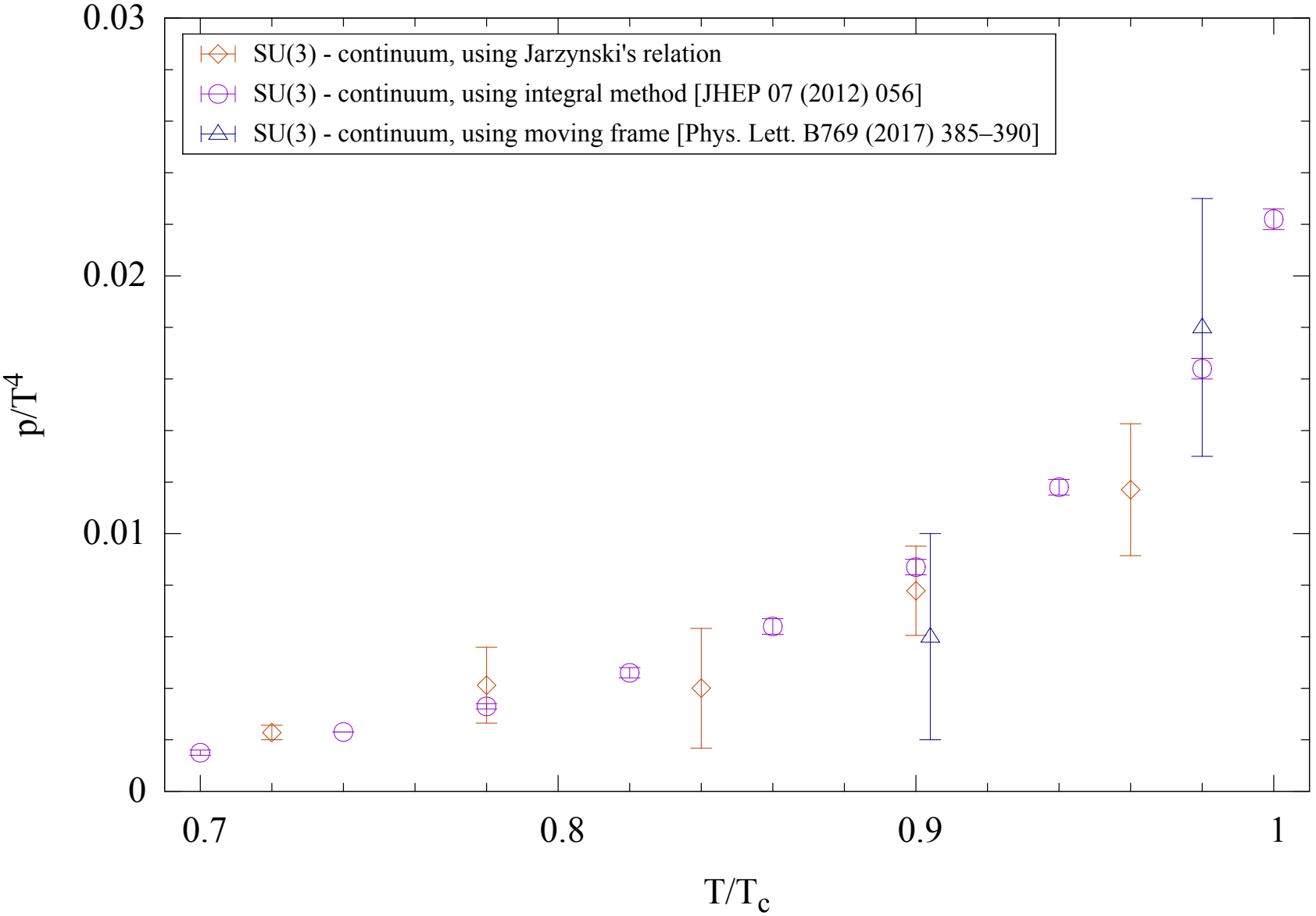
SU(3) entropy density



SU(3) energy density



SU(3) pressure - confining phase



Some potential applications

- In principle there are no obstructions to the derivation of numerical methods based on Jarzynski's relation for fermionic algorithms, opening the possibility for many potential applications in full QCD

- the free energy density in QCD with a **background magnetic field** B, to measure the magnetic susceptibility of the strongly-interacting matter.

- the **entanglement entropy** in $\mathrm{SU}(N_c)$ gauge theories

- studies involving the **Schrödinger functional**: Jarzynski's relation could be used to compute changes in the transition amplitude induced by a change in the parameters that specify the initial and final states on the boundaries.

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Conclusions

Jarzynski's equality provides a solid framework to compute **directly** the pressure on the lattice with Monte Carlo simulations.

- we can always verify the convergence of the method to the correct result by performing transformations in reverse and comparing the results
- with these checks we can look for systematic errors $\rightarrow$ especially useful close to the transition
- suitable choices of N and n_r provide high-precision results while keeping the expected discrepancies under control
- even with a limited amount of configurations it is possible to extract precise results

Why use it?

- very **efficient**: intuitively we are exploiting the autocorrelation, since the average is not taken across all configurations, but only on the different realizations
- to get more precise results we can not only increase n_r, but also N, i.e. we get closer to a **reversible transformation**

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Thank you for the attention!

Extended to non-isothermal transformations [Chatelain, 2007] (the temperature takes the role of λ)

$$\left\langle \exp\left(-\sum_{n=0}^{N-1} \left\{ \frac{H_{\lambda_{n+1}}[\phi_n]}{T_{n+1}} - \frac{H_{\lambda_n}[\phi_n]}{T_n} \right\} \right) \right\rangle = \frac{Z(\lambda_N, T_N)}{Z(\lambda_0, T_0)}$$

Pressure renormalization

The pressure is normalized to the value of $p(T)$ at $T = 0$ in order to remove the contribution of the vacuum. Using the 'integral method' the pressure can be rewritten (relative to its $T = 0$ vacuum contribution) as

$$\frac{p(T)}{T^4} = -{N_t}^4 \int_0^\beta d\beta' \left[3(P_\sigma + P_\tau) - 6P_0\right]$$

where P_σ and P_τ are the expectation values of spacelike and timelike plaquettes respectively and P_0 is the expectation value at zero T.

Using Jarzynski's relation one has to perform another transformation $\beta_i \to \beta_f$ but on a symmetric lattice, i.e. with lattice size $\widetilde{N}_s^4$ instead of $N_t \times N_s^3$. The finite temperature result is then normalized by removing the $T = 0$ contribution calculated this way.

$$\frac{p(T)}{T^4} = \frac{p(T_0)}{T_0^4} + \left(\frac{N_t}{N_s}\right)^3 \ln \frac{\left\langle \exp\left[-W_{\mathrm{SU}(N_c)}(\beta_g^{(0)}, \beta_g)_{N_t \times N_s^3}\right]\right\rangle}{\left\langle \exp\left[-W_{\mathrm{SU}(N_c)}(\beta_g^{(0)}, \beta_g)_{\widetilde{N}^4}\right]\right\rangle^\gamma}$$

with $\gamma = \left(N_s^3 \times N_0\right) / \widetilde{N}^4$.

Effective string prediction for the interface F

With this method (using $N \simeq 10^6$ steps and $n_r \simeq 10^3$ trials) we obtained high-precision results at fixed β and for different interface size L.

These results can be compared with the analytical prediction of the effective string model which describes the transverse fluctuations of the interface at low energy.

In particular, choosing the Nambu-Goto action as S_{eff}, one can look at the difference between numerical results and the NG prediction and examine its dependence on the size L of the interface, in order to understand the nature of the terms that do not arise from the NG low-energy expansion.