The equation of state with non-equilibrium methods

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in collaboration with

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Free-energy differences in LGTs

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).

- the **pressure** ($\rightarrow$ equilibrium thermodynamics)
- but also: free-energy of interfaces, 't Hooft loops, magnetic susceptibility, entanglement entropy...

In general, the calculation of ΔF is a **computationally challenging** problem, since it usually cannot be performed directly.

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

Motivations to look for more efficient and intuitive methods

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Jarzynski's equality

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 (depending on some parameter $\lambda \rightarrow$ e.g. the coupling) with free energy $F(\lambda, T) = -\beta^{-1} \ln Z(\lambda, T)$.

We are interested in an evolution of the system driven during which λ **is changed** from an initial value λ_i to a final one λ_f.

We can state non-equilibrium equality **[C. 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 processes such as

- Langevin evolution
- molecular dynamics
- **Monte Carlo simulations**

The evolution 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.

The initial state must be at equilibrium, but all the following ones do not!

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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

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

and using *Jensen's inequality*

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

(valid for averages on real x) we get

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

from which we have

$$\langle W\rangle \geq \Delta F$$

In this sense Jarzynski's relation can be seen as a **generalization** of the Second Law.

Jarzynski's equality in Monte Carlo simulations

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

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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Two special cases

Let's look at two insightful 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

$$W = \Delta F$$

  $\to$ this is the case of **thermodynamic integration**

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The equation of state with non-equilibrium methods

Pressure on the lattice

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]**

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

where the integrand is calculated from plaquette expectation values and the temperature T is controlled by the inverse coupling β_g by the usual relation $T = \frac{1}{a(\beta_g) N_t}$.

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Pressure with Jarzynski's relation

The **difference in 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 between T_0 and T:

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

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

Trace of the energy-momentum tensor, energy density and entropy density are obtained by

$$\frac{\Delta}{T^4} = T\frac{\partial}{\partial T}\left(\frac{p}{T^4}\right) \qquad \epsilon = \Delta + 3p \qquad s = \frac{\Delta + 4p}{T}$$

A test for the $\mathrm{SU}(2)$ pressure in the proximity of the deconfining transition yielded excellent results **[Caselle et al.,2016]**.

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]**

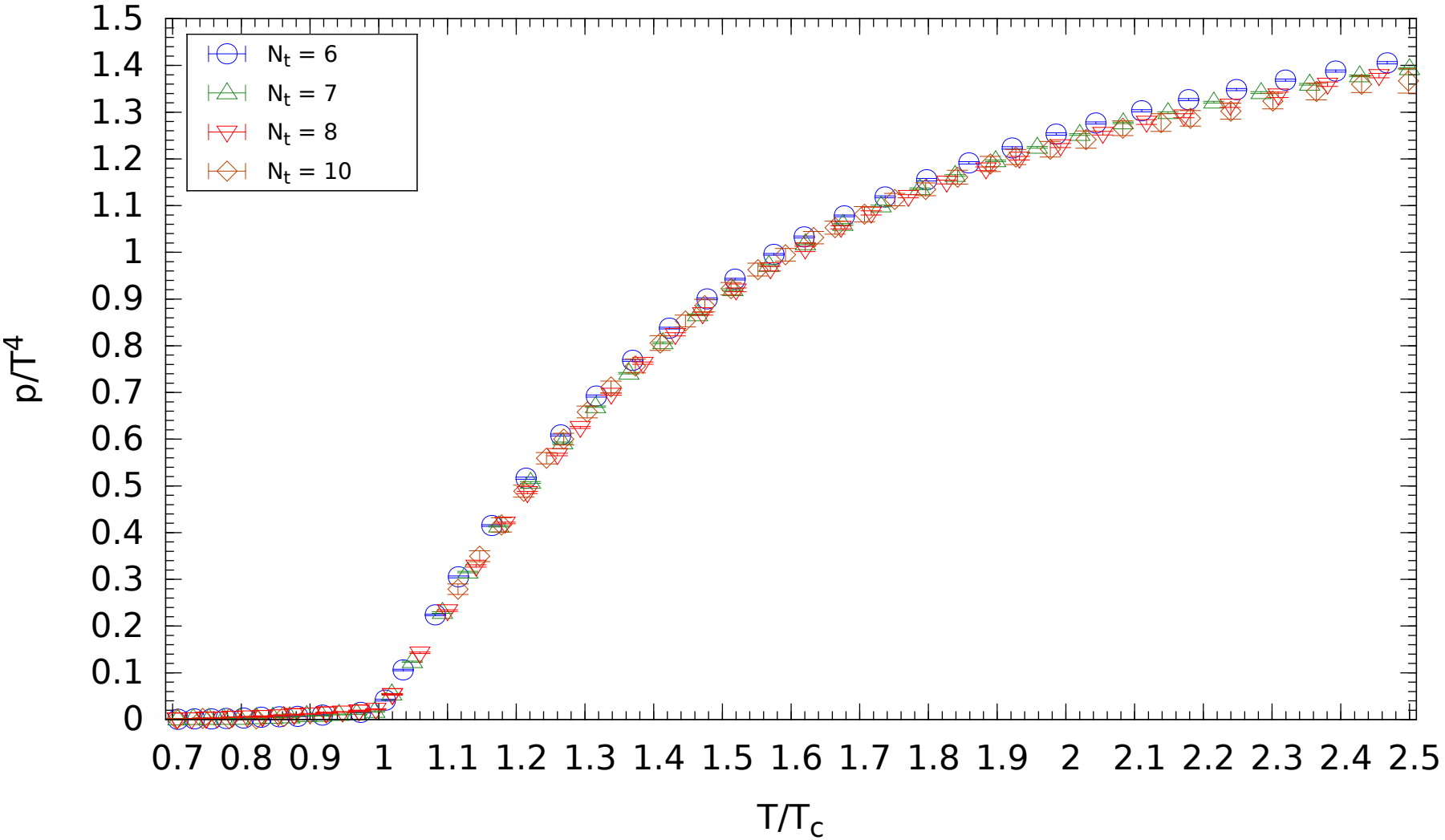
  $\rightarrow$ the primary observable is the **entropy density** (extracted from the spacetime components of the energy-momentum tensor)

- using the gradient flow **[Asakawa et al., 2014]**

- see also **posters by S. Ejiri and D. Laubach**

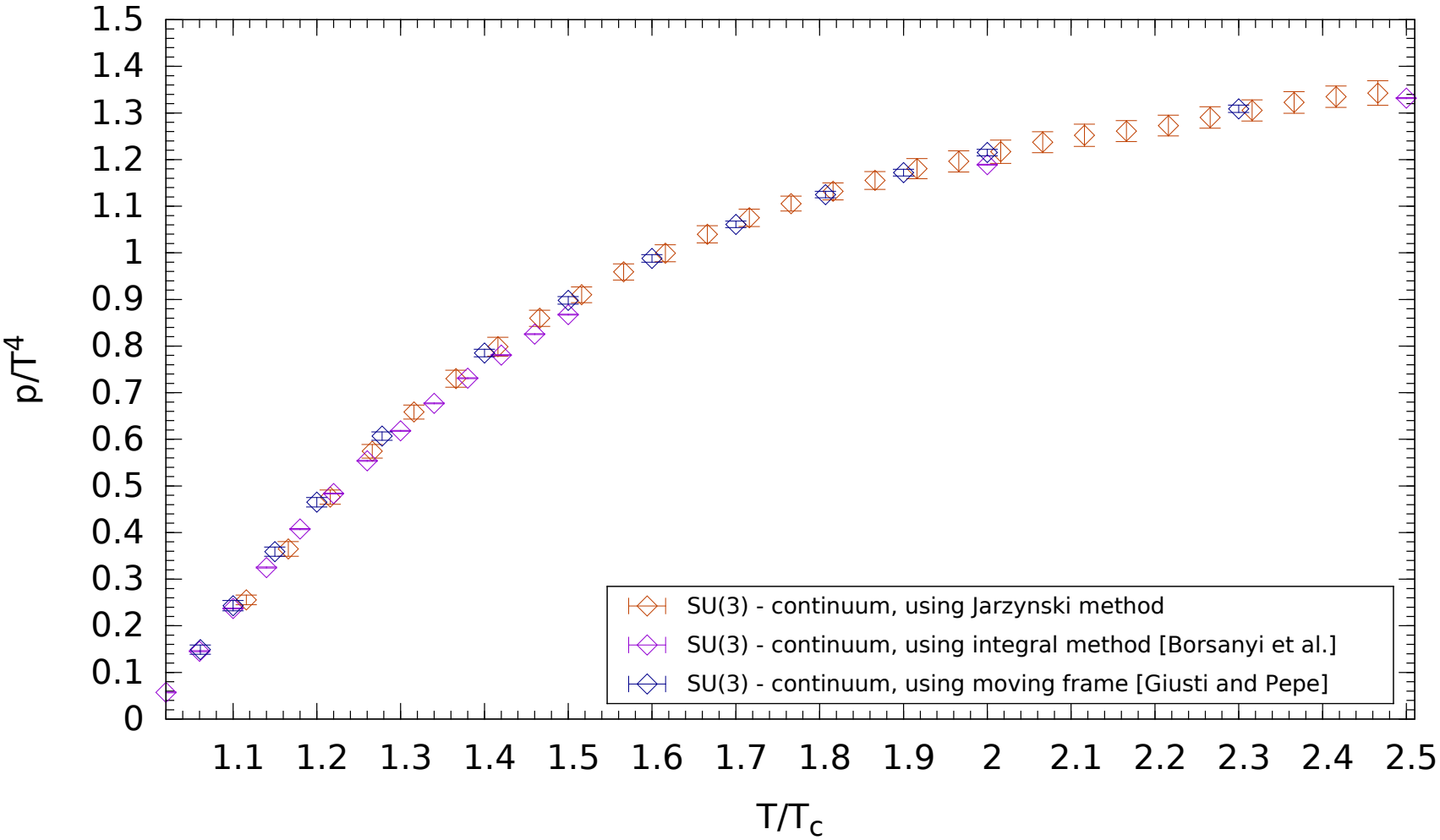
An high-precision determination of the $\mathrm{SU}(3)$ e.o.s. is an excellent benchmark for the **efficiency** of a technique based on non-equilibrium transformations.

SU(3) pressure across the deconfinement transition, for different values of N_t (preliminary)



SU(3) pressure - continuum extrapolation (preliminary)

$\sim$ 700k configurations across all values of N_t were used in this region



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** $\rightarrow$ very useful when the signal is small or when increasing the volume
- trivial to implement; plus, in practice we are only computing plaquette expectation values

Moreover,

- 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

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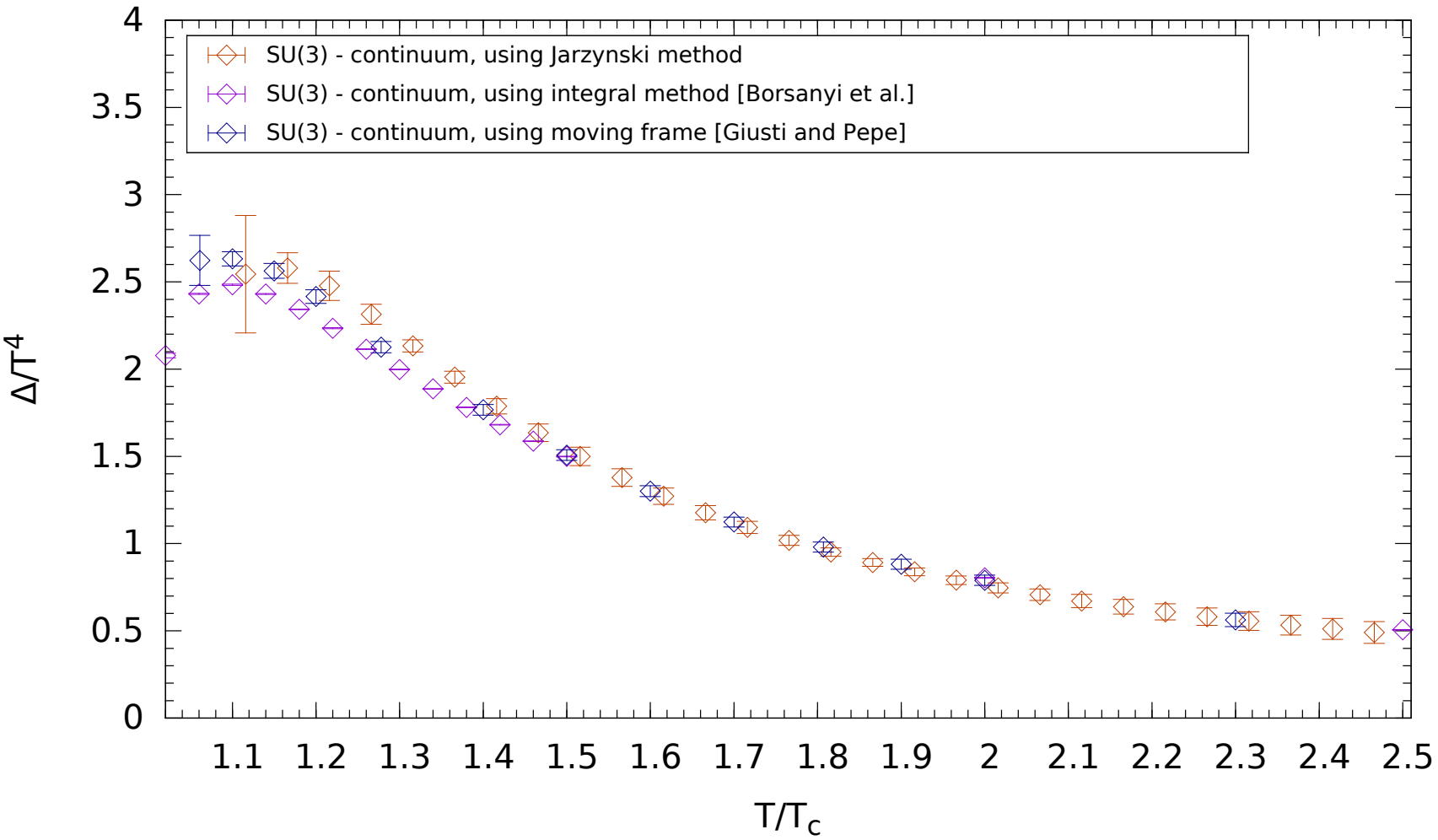
Conclusions

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

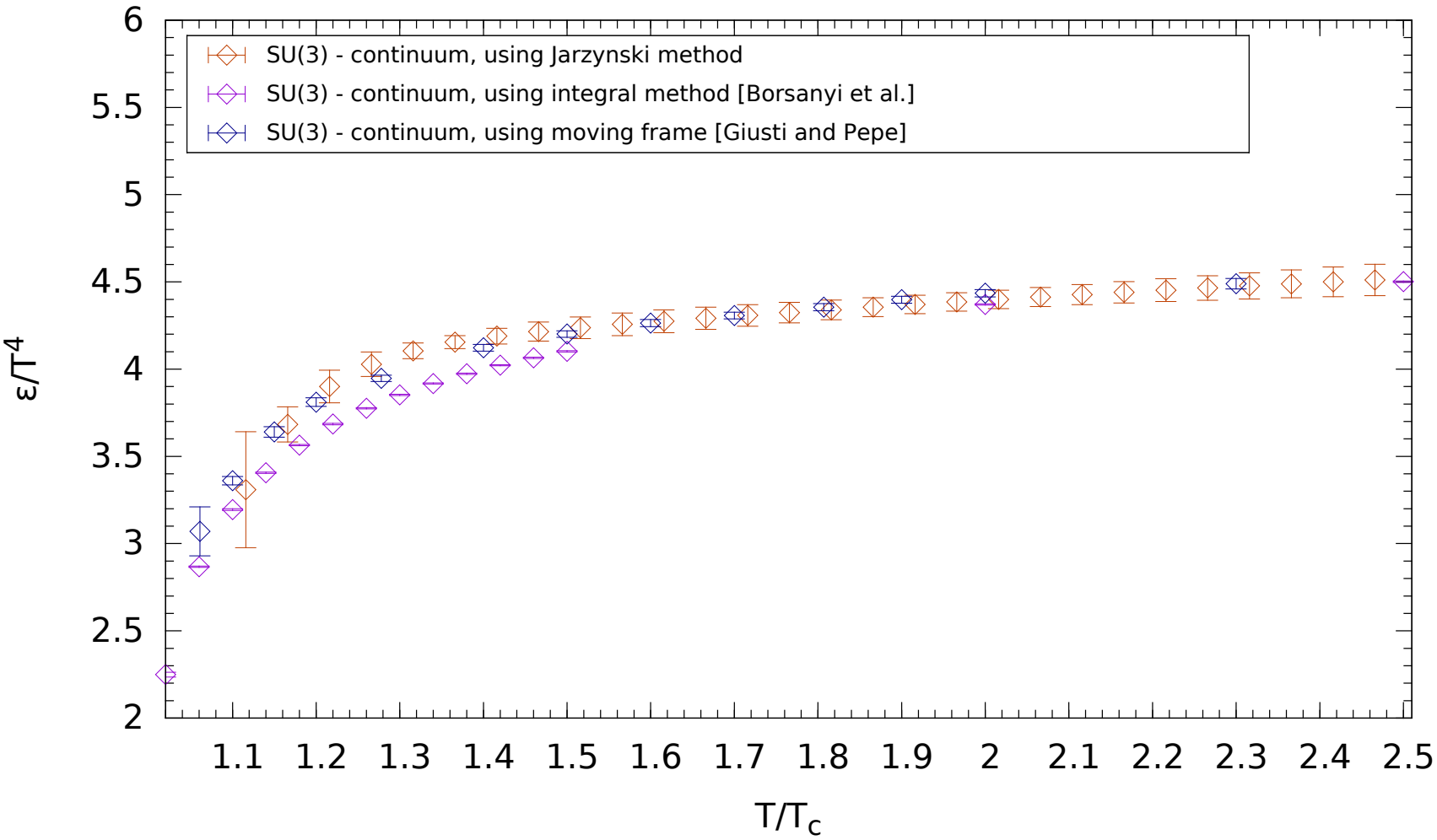
- suitable choices of N and n_r provide high-precision results while keeping the expected discrepancies under control
- even with a limited amount of configurations it is possible to extract precise results
- results are still preliminary: an accuracy check is being performed in the $[T_c, 1.2\,T_c]$ region where discrepancies between different methods arise
- an implementation for the full theory with the inclusion of dynamical quarks is rather natural and a test for full QCD is in preparation

Thank you for your attention!

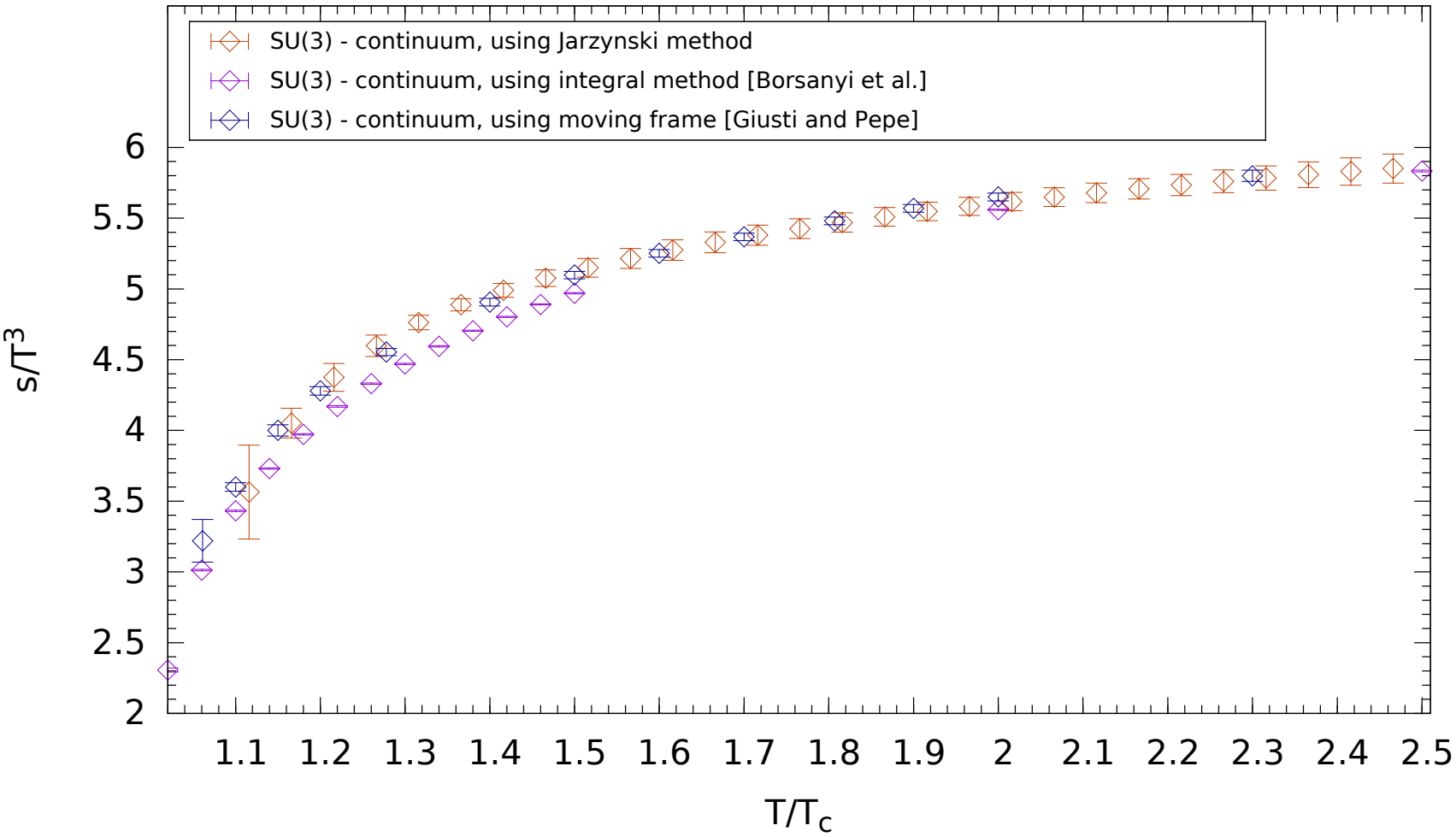
SU(3) trace anomaly - continuum extrapolation (preliminary)



SU(3) energy density - continuum extrapolation (preliminary)



SU(3) entropy density - continuum extrapolation (preliminary)



Applications beyond the equation of state

- 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.

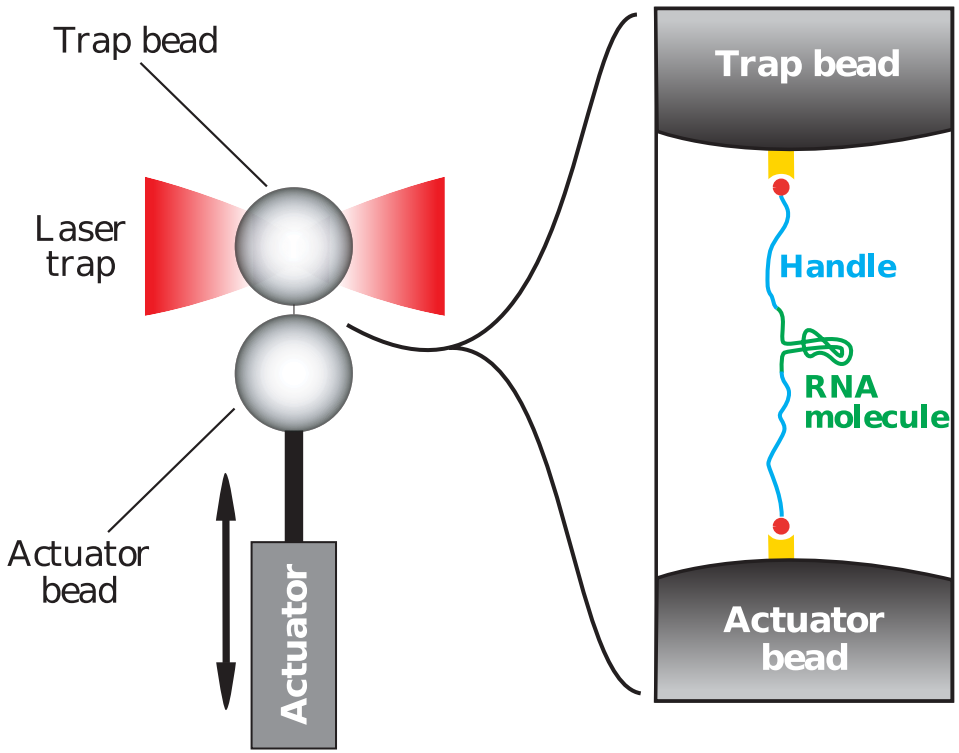
- the **entanglement entropy** in $\mathrm{SU}(N_c)$ gauge theories

- 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.

An experimental test

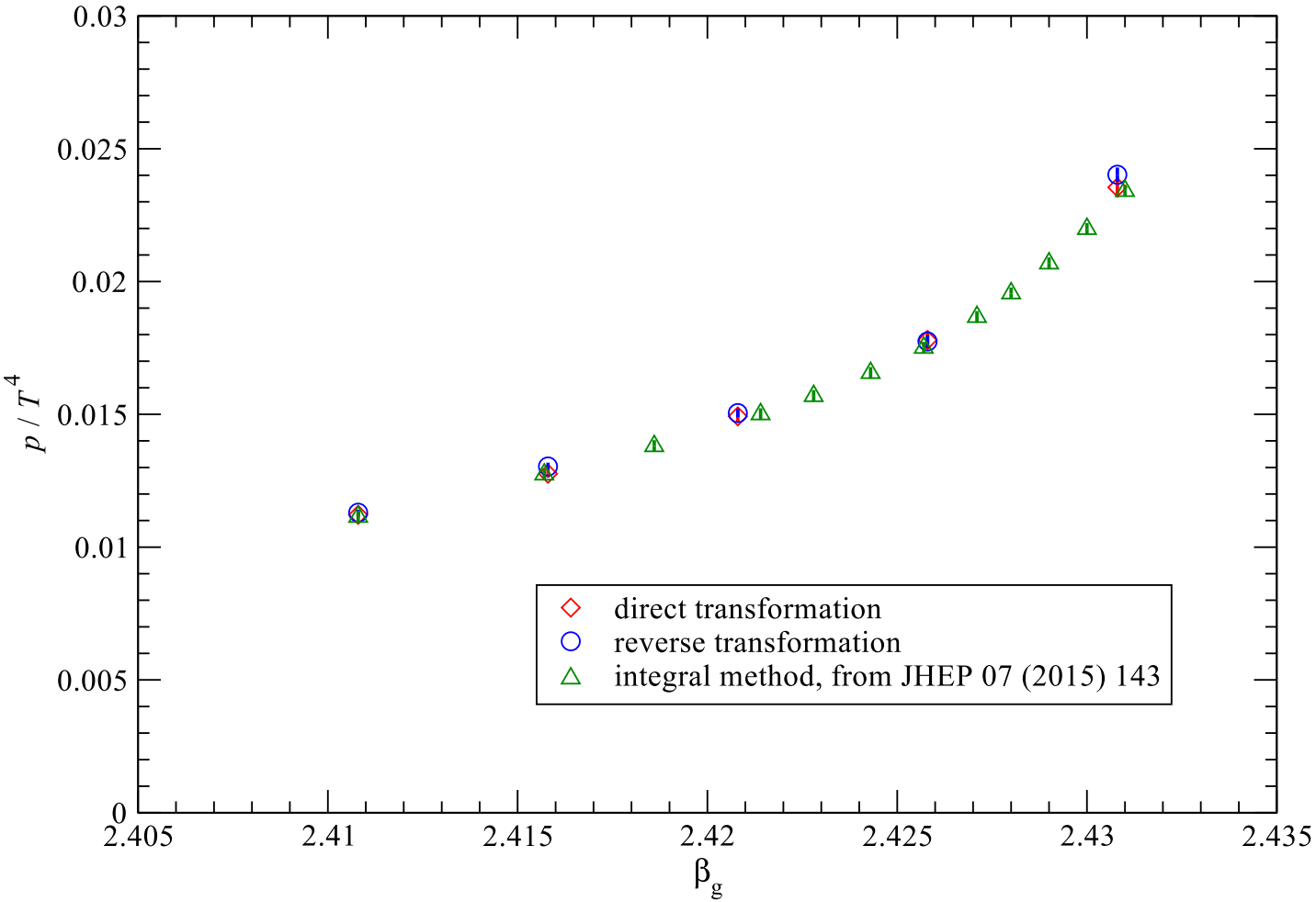
An experimental test of Jarzynski's equality was performed in 2002 by Liphardt *et al.* by mechanically stretching a single molecule of RNA between two conformations.

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



Preliminary results for the SU(2) model

Finite T simulations performed on $72^3 \times 6$ lattices. Temperature range is $\sim [0.9\,T_c,\, T_c]$.



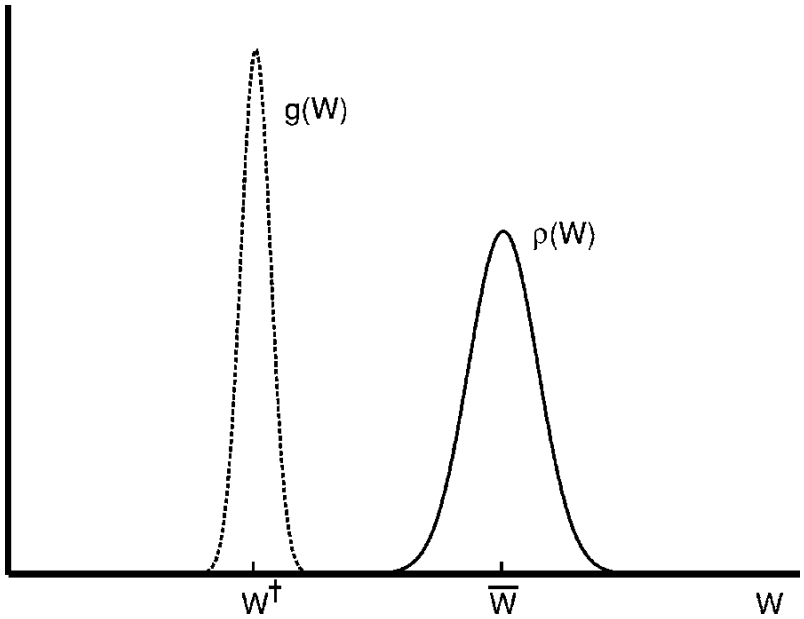
Excellent agreement with integral method data [Caselle et al., 2015]

SU(3) statistics

N_t	N_s	N_0	T/T_c range	n_{conf}
6	96	48	$[0.7, 1.02]$	220k
6	96	48	$[1.02, 2.5]$	320k
7	108	48	$[0.7, 1.02]$	250k
7	108	48	$[1.02, 2.5]$	320k
8	120	48	$[0.7, 1.02]$	270k
8	120	48	$[1.02, 2.5]$	110k
10	120	48	$[0.7, 1.02]$	230k
10	160	48	$[1.02, 2.5]$	65k

Lattice sizes and statistics for a given temperature range (thermalization not included)

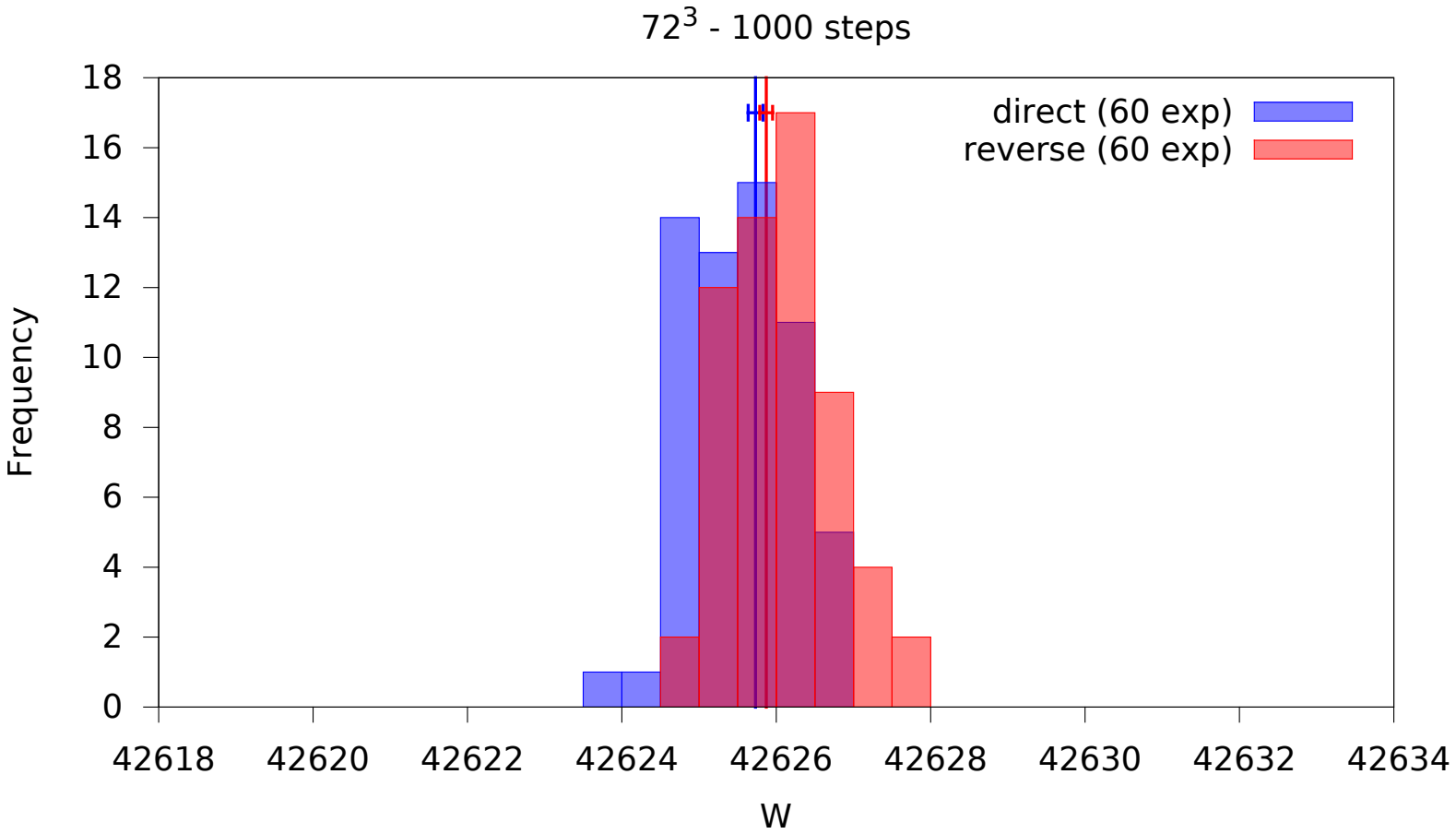
Dominant realizations



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.

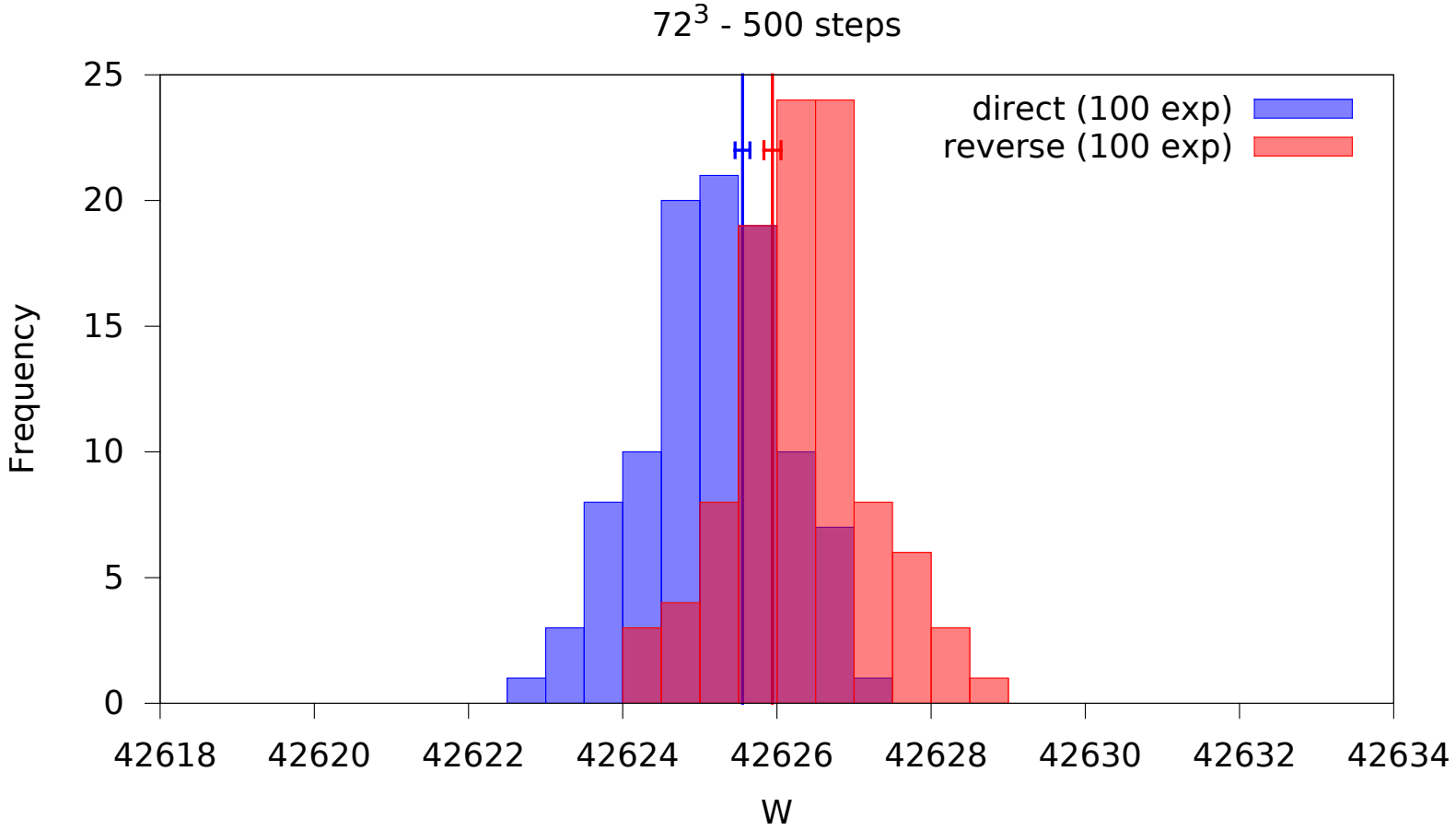
Work distributions



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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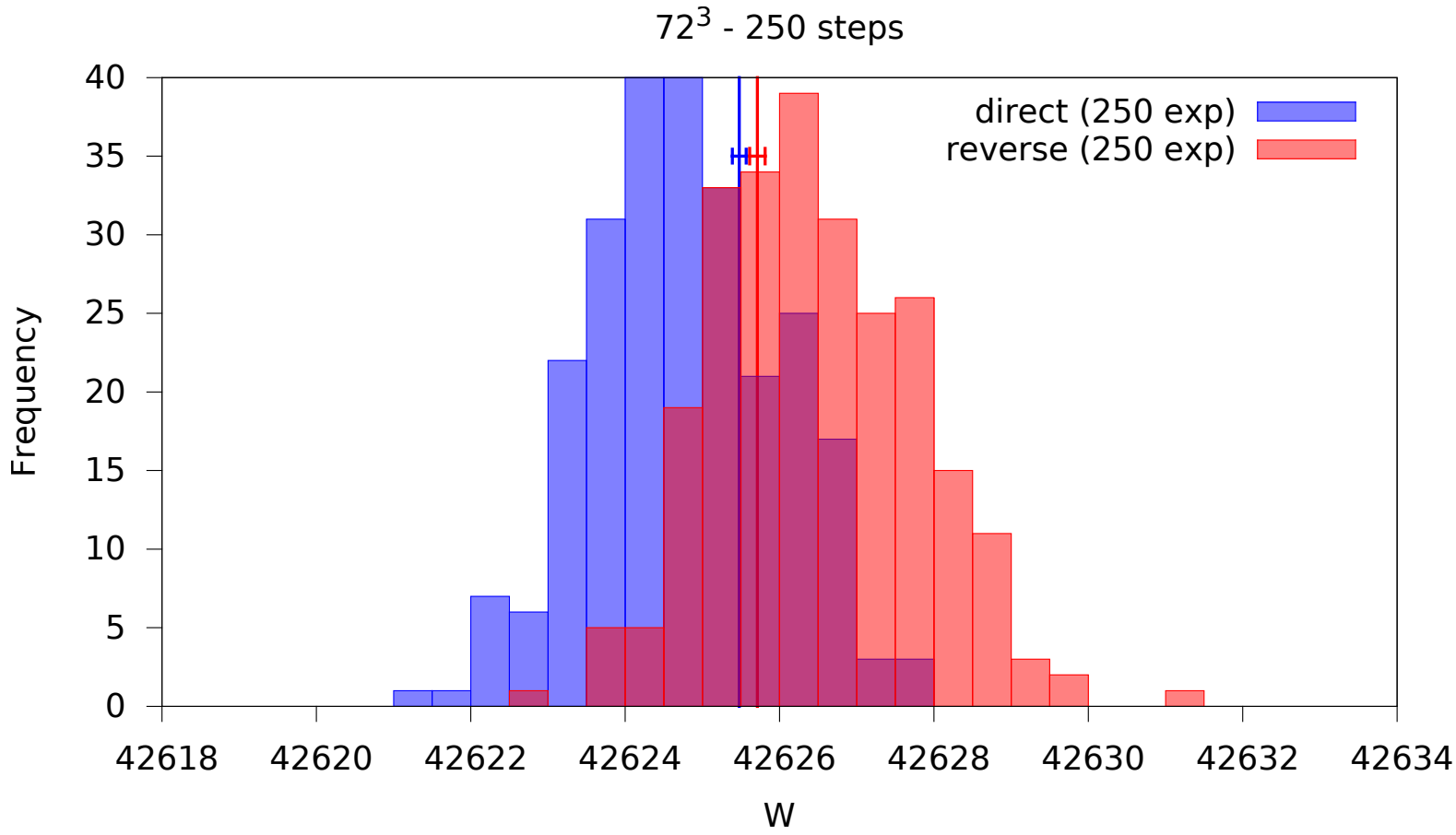

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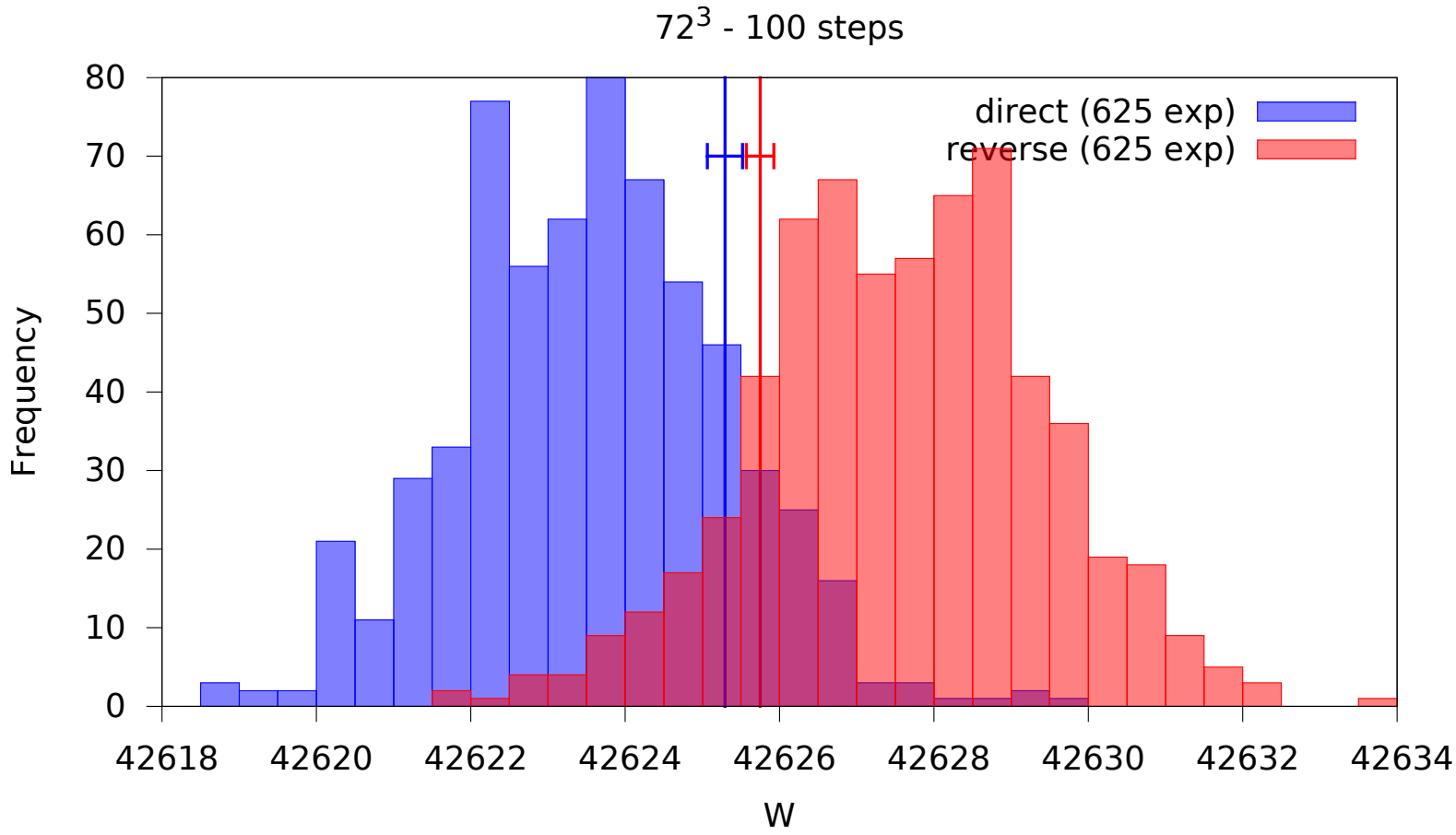

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Crooks fluctuation theorem

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.

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

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

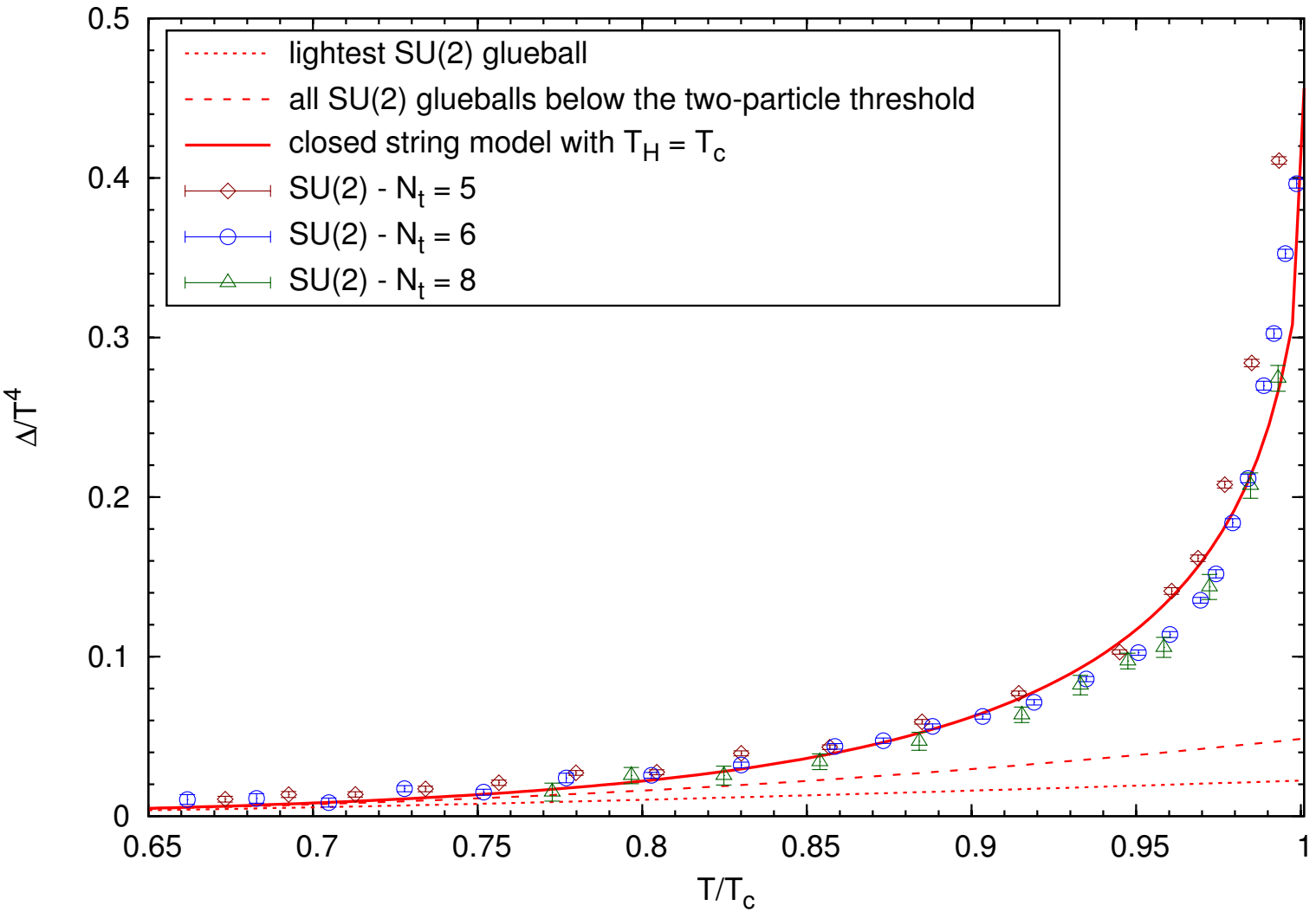
where P_σ and P_τ are the expectation values of spacelike and timelike plaquettes respectively and P_0 is the expectation value at zero T.

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.

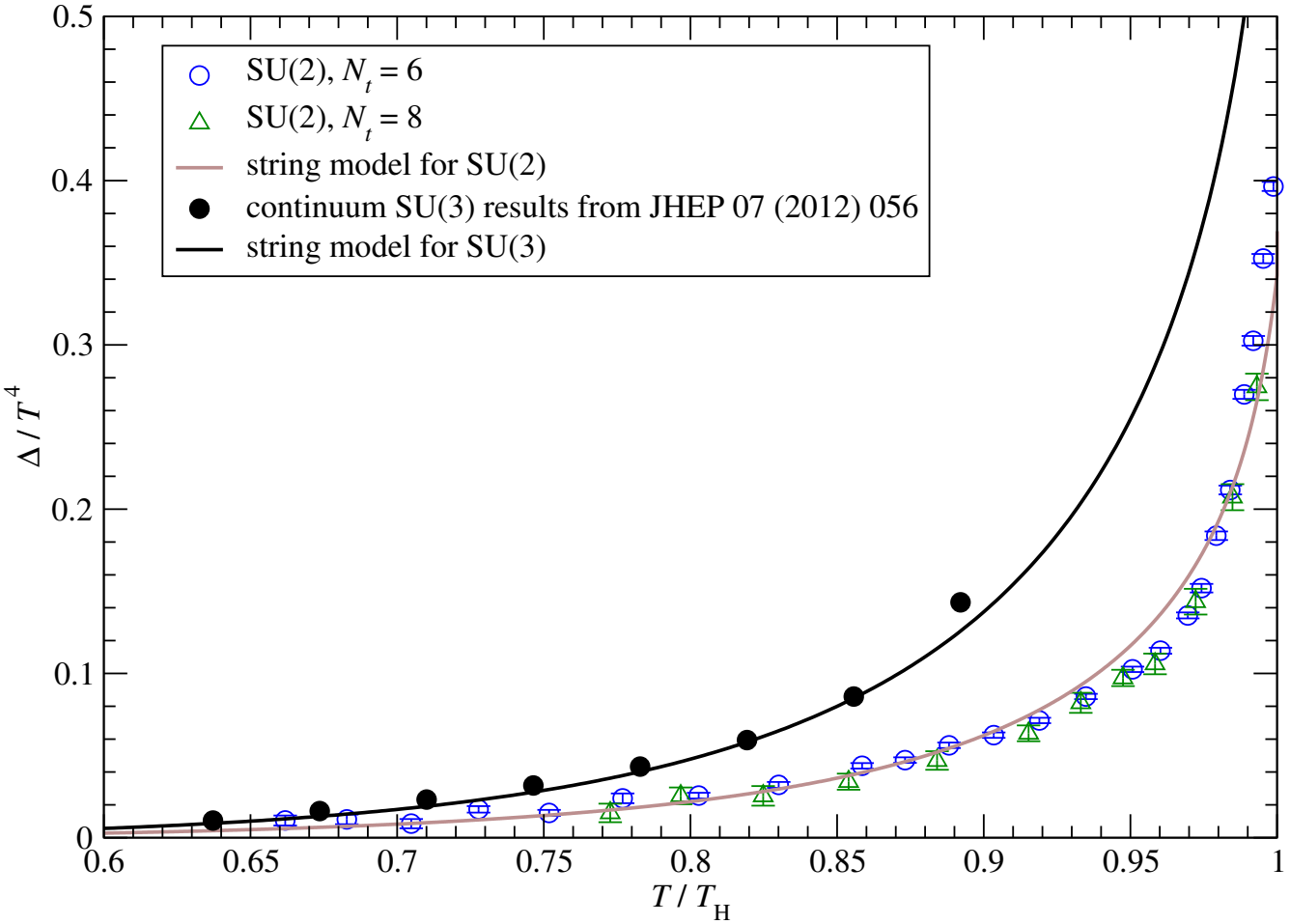
$$\frac{p(T)}{T^4} = \frac{p(T_0)}{T_0^4} + \left(\frac{N_t}{N_s}\right)^3 \ln \frac{\left\langle \exp\left[-W_{\mathrm{SU}(N_c)}(\beta_g^{(0)}, \beta_g)_{N_t \times N_s^3}\right]\right\rangle}{\left\langle \exp\left[-W_{\mathrm{SU}(N_c)}(\beta_g^{(0)}, \beta_g)_{\widetilde{N}^4}\right]\right\rangle^\gamma}$$

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

Hagedorn spectrum in $\mathrm{SU}(2)$ pure gauge theory



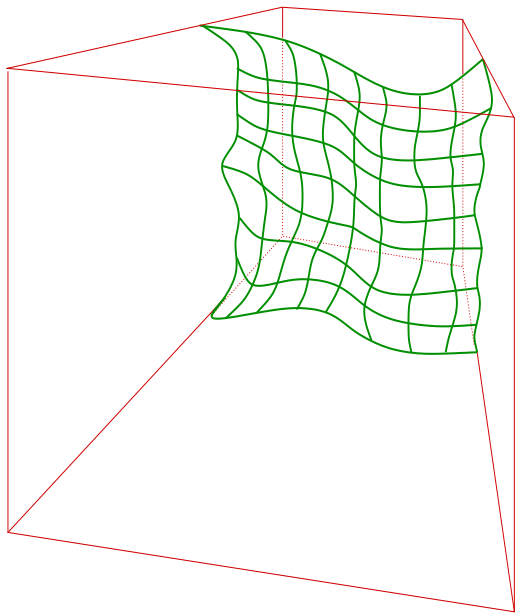
Hagedorn spectrum in SU(2) and SU(3) pure gauge theories



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)

$$\frac{Z_a}{Z_p} = N_0 \exp(-F^{(1)})$$

where N_0 is the size of the lattice in the μ direction

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.

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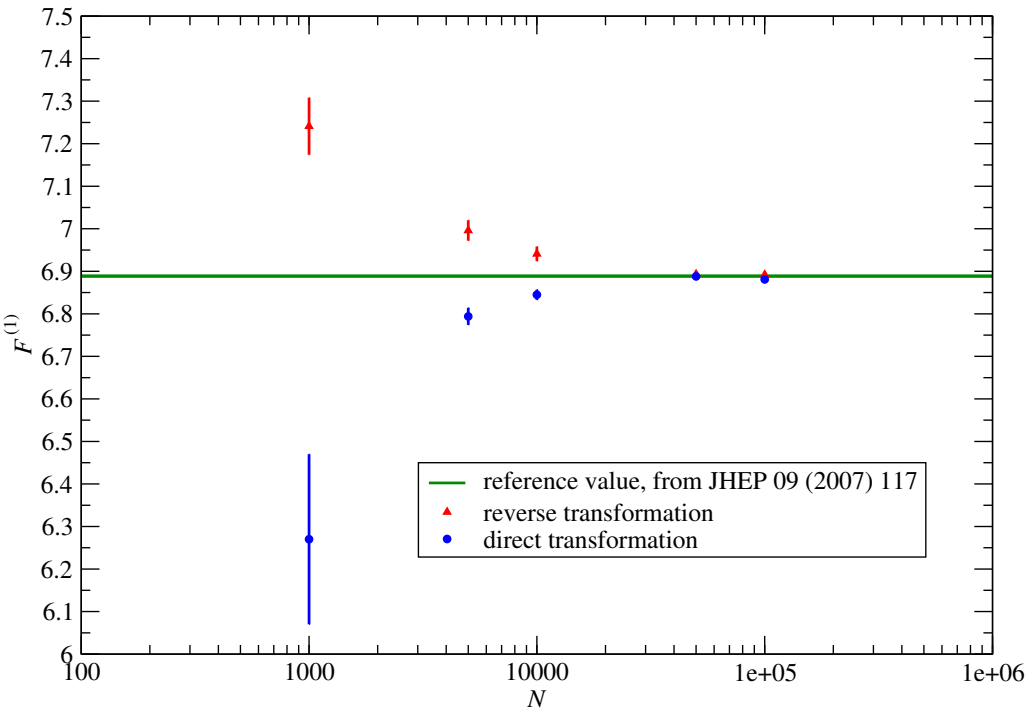
$\beta = 0.223102, \quad N_0 = 96, N_1 = 24, N_2 = 64$



The results from 'direct' and 'reverse' transformations converge to older results when N is large enough.

Effective string prediction

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.

The crucial quantity is the **work** performed on the system

$$W = \int_{t_{in}}^{t_{fin}} \mathrm{d}t \dot{\lambda} \frac{\partial H_\lambda}{\partial \lambda}$$

(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)

This is repeated in order to have an *ensemble* of realizations of this process: for each of them W is computed separately.