The equation of state with non-equilibrium methods

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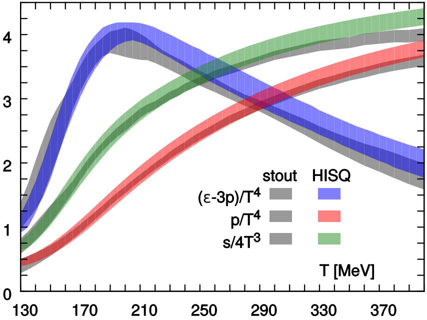
In lattice gauge theories the expectation values of a large set of physical quantities is *naturally* related to the computation (via Monte Carlo simulations) of free-energy differences (or, equivalently, of ratios of partition functions).

- free-energy of interfaces, 't Hooft loops, magnetic susceptibility, entanglement entropy...
- the **pressure** ($\rightarrow$ the equation of state)



Continuum results with $2+1$ dynamical quark flavours at physical quark masses with HISQ **[HotQCD, 2014]** and stout **[Wuppertal-Budapest, 2014]** actions

Free-energy differences in LGTs

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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
$$f \sim \int \mathrm{d}\lambda \frac{\partial \log Z}{\partial \lambda}$$
- reweighting
- snake algorithm
$$\frac{Z(\lambda')}{Z(\lambda)} = \frac{Z(\lambda')}{Z(\lambda_N)} \ldots \frac{Z(\lambda_{i+1})}{Z(\lambda_i)} \ldots \frac{Z(\lambda_1)}{Z(\lambda)}$$

Jarzynski's equality may provide a more efficient and intuitive method

The Second Law of Thermodynamics

We start from the 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. Partition function and free energy are

$$Z_\lambda(T) = \int \mathrm{d}\Gamma e^{-\beta H_\lambda(\Gamma)} \qquad F_\lambda(T) = -\beta^{-1} \ln Z_\lambda(T)$$

The transformation is defined as an evolution of the system driven by a discrete/continuous variation of λ between the initial and final 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)

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

Jarzynski's equality

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

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

- It relates the exponential statistical average of the work done on a system over several realizations of the (non-equilibrium) transformation with the difference between the initial and the final free energy of the system.
- 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

- 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 driven **out of equilibrium**

This result can be derived for

- Langevin evolution
- molecular dynamics
- Monte Carlo simulations

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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 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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Two special cases

Two insightful limits of Jarzynski's equality:

- 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** $\to$ a common way to estimate p 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.

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The equation of state with non-equilibrium methods

Pressure on the lattice

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.

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

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

On the lattice, the temperature T is the inverse of the temporal extent,

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

and it can be controlled by the inverse coupling β_g.

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

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 $W_{\mathrm{SU}(N_c)}$ 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.

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

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

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Equilibrium thermodynamics in Yang-Mills theories

For YM thermodynamics highly precise determinations are relatively easy and available at high temperatures

→ precision studies can be performed and compared with other theoretical tools

- *low-temperature phase* ($T < T_c$) → description in terms of a gas of massive, non-interacting hadrons → HRG model in QCD

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

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

The most recent determinations have been obtained

- using a variant of the integral method **[Engels et al., 1990]** in **[Borsànyi et al., 2012]**

  $\rightarrow$ the primary observable is the **trace of the energy-momentum tensor**, results up to $1000\,T_c$

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

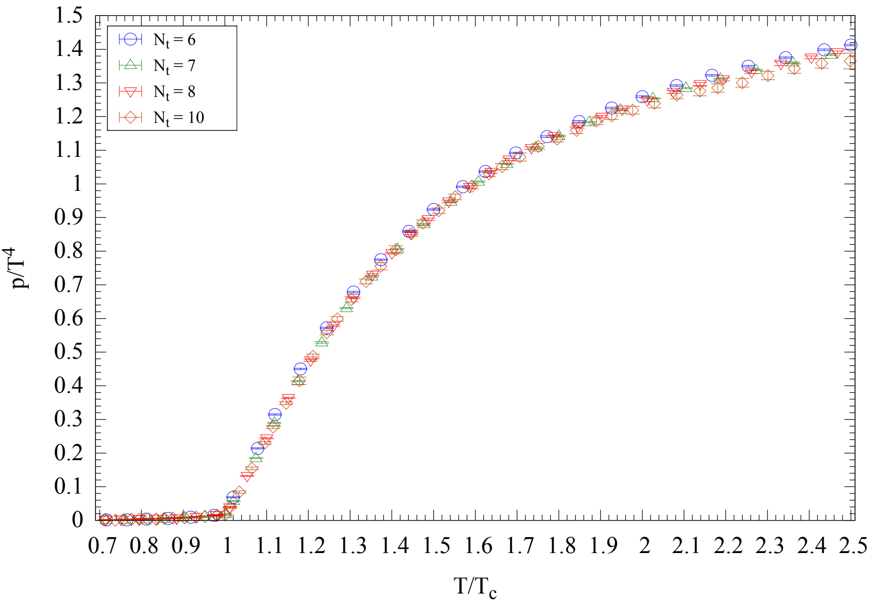
  $\rightarrow$ the primary observable is the **entropy density** (extracted from the off-diagonal components of the energy-momentum tensor computed with shifted boundary conditions), results up to $230\,T_c$

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

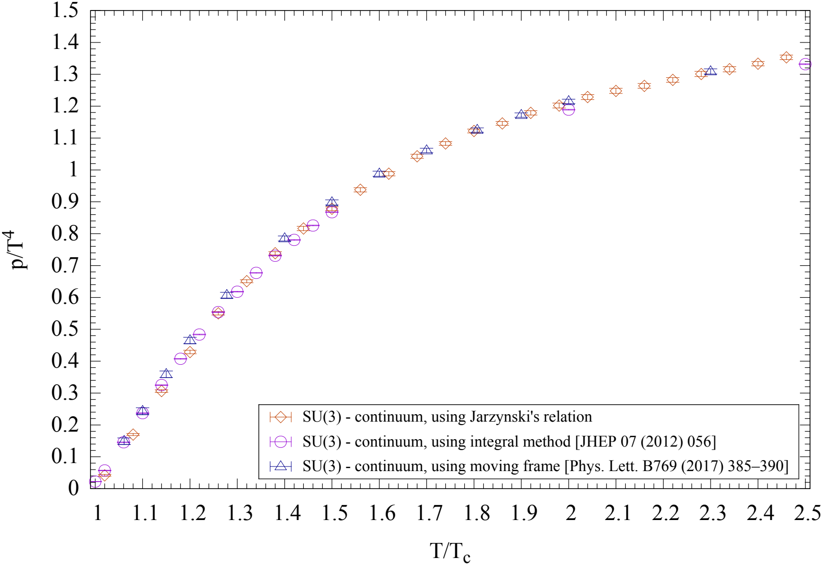
  $\rightarrow$ the components of $T_{\mu\nu}$ are directly accessible

An high-precision determination of the $\mathrm{SU}(3)$ e.o.s. is an excellent benchmark for any new technique

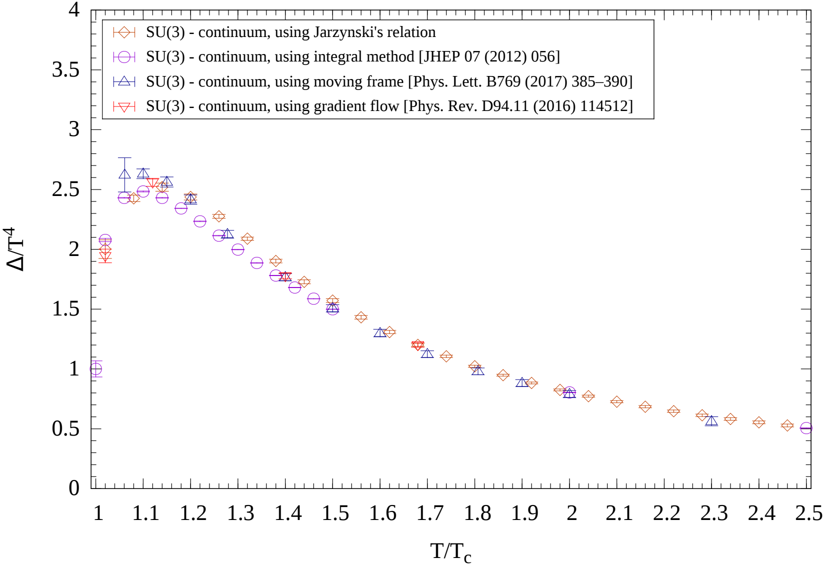
SU(3) pressure across the deconfinement transition, for different values of N_t, with Jarzynski's equality



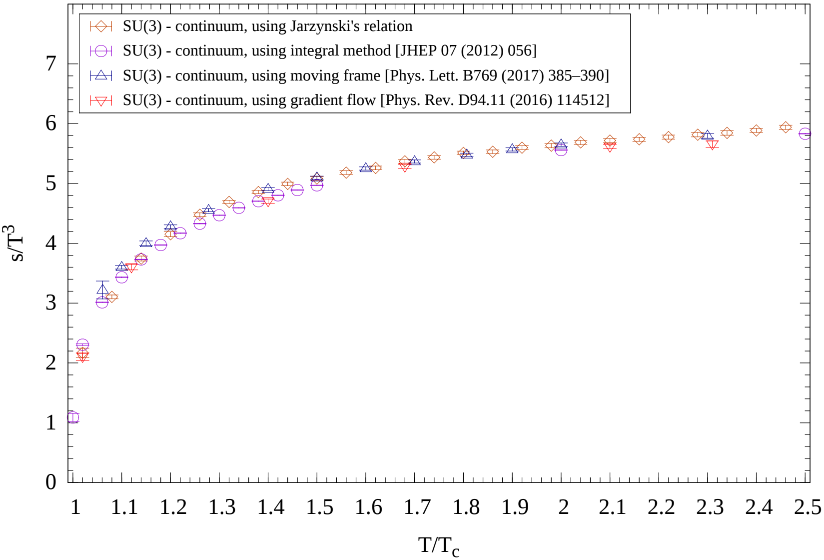
SU(3) pressure - continuum extrapolation



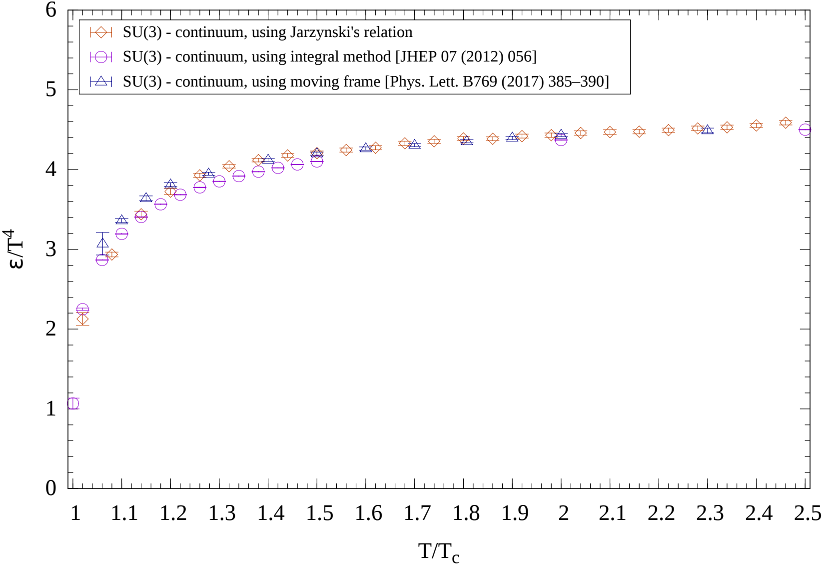
SU(3) trace anomaly



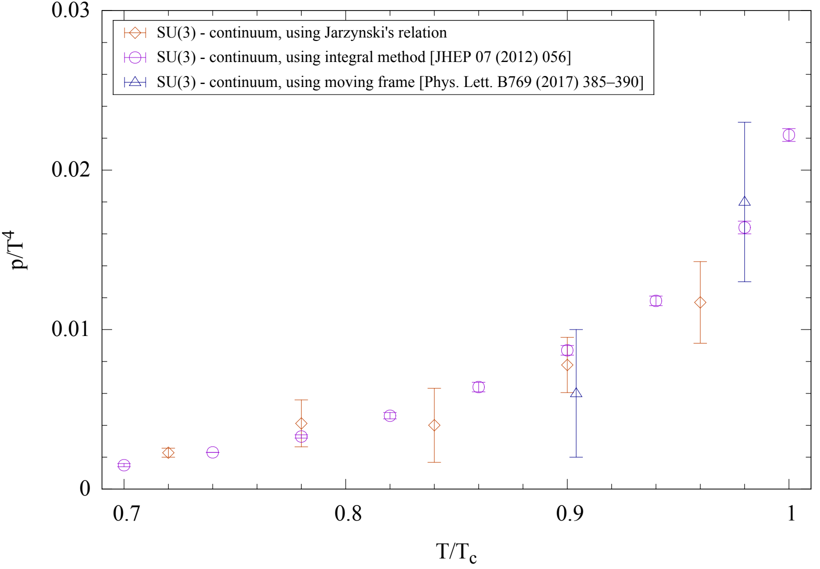
SU(3) entropy density



SU(3) energy density



SU(3) pressure - confining phase



Conclusions

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

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

Good agreement with former $\mathrm{SU}(3)$ e.o.s. determinations (with completely different methods!), although errors are very small and so some **discrepancies** are quite severe

- possibly due to a combination of (technical) factors

State of the art computations in **full QCD** (with *staggered* quarks) are very precise and already available for a large range of T, but several challenges remain!

- a determination with physical quark masses using *Wilson* fermions is still beyond current capabilities
- new techniques will provide independent checks and may have a central role in improving the efficiency of lattice calculations

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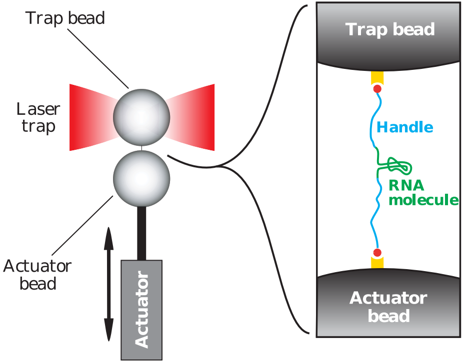
Thank you for your attention!

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.



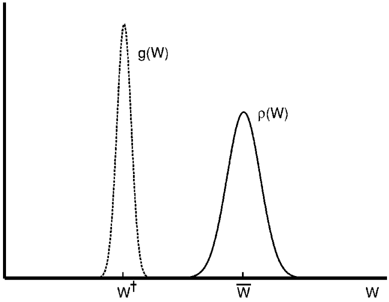
Extended to non-isothermal transformations [Chatelain, 2007] (the temperature takes the role of λ)

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

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.

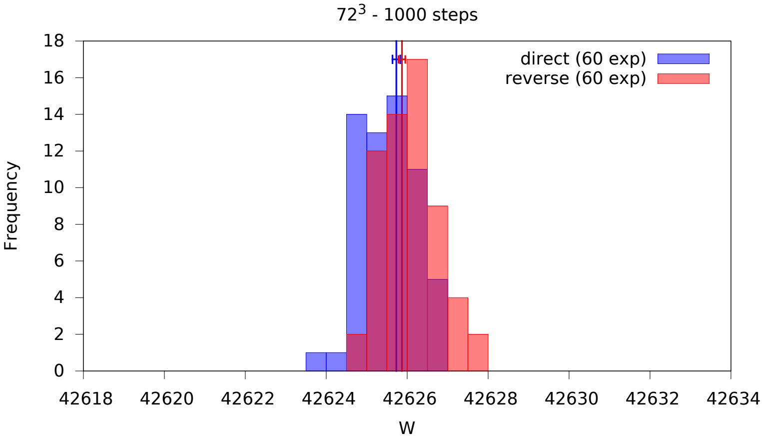
Dominant realizations



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.

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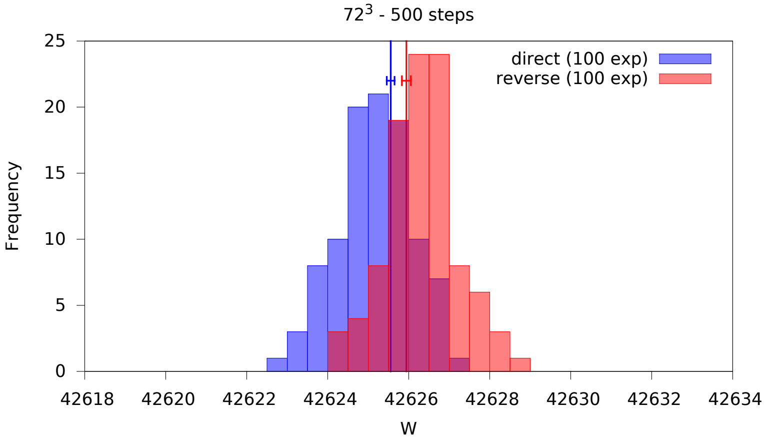

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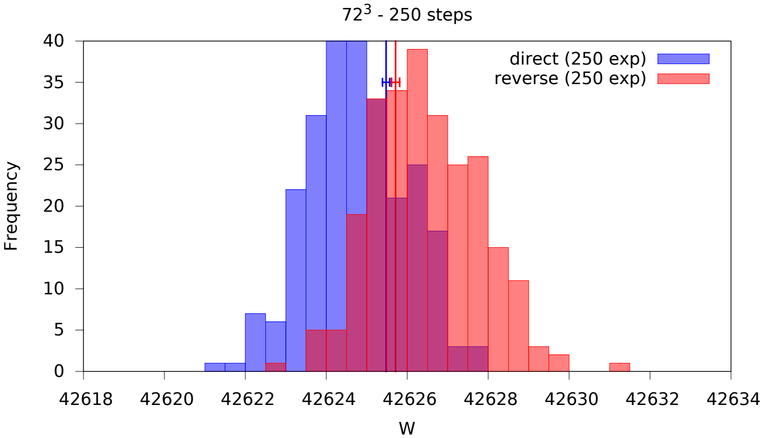

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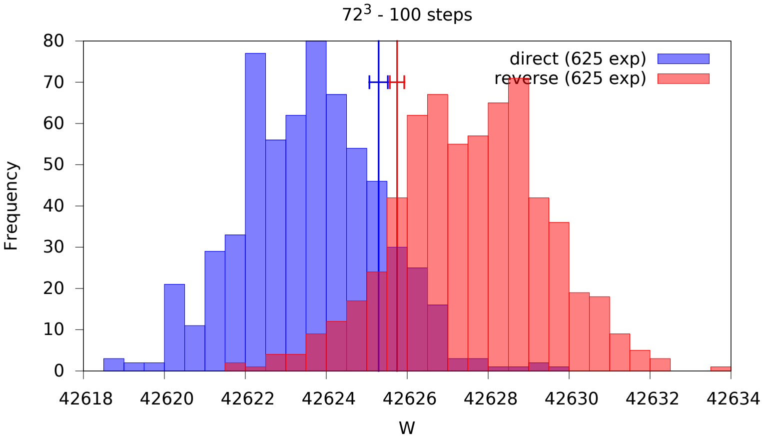

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Pressure renormalization

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

A few more observations:

- 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

The integral method

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

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

A widely used technique to estimate it on the lattice is 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.

An additive renormalization in the form of a subtraction of $T = 0$ plaquette expectation values is required for each β

$$\frac{p(T)}{T^4} - \frac{p(T_0)}{T_0^4} = 6 {N_t}^4 \int_{\beta(T_0)}^{\beta(T)} \mathrm{d}\beta' \, \left(\langle U_\mathrm{p} \rangle_T - \langle U_\mathrm{p} \rangle_0 \right)$$

and so the primary observable is the **trace of the energy momentum tensor** $\Delta = T_{\mu\mu}$

$$\frac{\Delta(T)}{T^4} = -N_t^4 \frac{\partial \beta}{\partial \log a} \left[6 \left(\langle U_\mathrm{p} \rangle_T - \langle U_\mathrm{p} \rangle_0 \right) \right]$$

Thermodynamics from the gradient flow

Yang-Mills gradient flow **[Luscher, 2010], [Naranayan and Neuberger,2006]**

Small-t expansion relates non-zero t observables with the renormalized observables of the original theory **[Luscher and Weisz,2011]**

$$\tilde{O}(t,x) \underset{t\to 0}{\longrightarrow} \sum_i c_i(t) O_i^R(x)$$

In the case of the energy-momentum tensor (see also **[Del Debbio,Patella and Rago,2017]**), one can build **[Suzuki, 2013]**

$$T_{\mu\nu}(x,t) = \frac{1}{\alpha_{\tilde{U}}(t)} \tilde{U}_{\mu\nu}(t,x) + \frac{\delta_{\mu\nu}}{4\alpha_{\tilde{E}}(t)} \left(\tilde{E}(t,x) - \langle \tilde{E}(t,x) \rangle_0 \right)$$

where $\tilde{E}(t,x)$ and $\tilde{U}_{\mu\nu}(t,x)$ are dimension-4 gauge invariant operators.
From the $t \to 0$ extrapolation

$$T_{\mu\nu}^R = \lim_{t\to 0} T_{\mu\nu}(x,t)$$

one can extract, for example

$$\epsilon = -\langle T_{00}^R(x) \rangle \qquad p = \frac{1}{3} \sum_{i=1}^{3} \langle T_{ii}^R(x) \rangle$$

Double extrapolation (in a and t) is required.
First study with Wilson fermions available **[Taniguchi et al.,2017]**

Thermodynamics in a moving frame

Main idea: in relativistic thermal theories the entropy is proportional to the total momentum of the system as measured by a moving reference system

- shifted boundary conditions are imposed:

$$U_\mu(L_t, \vec{x}) = U_\mu(0, \vec{x} - L_t\vec{\xi})$$

- the temperature of the system is now given by

$$T = \frac{1}{L_t\sqrt{1+\vec{\xi}^2}}$$

- in this context new Ward identities can be derived (see also work on the renormalization of the energy-momentum tensor **[Giusti and Pepe,2015]**)

In particular one can extract the **entropy density** $s(T)$ **[Giusti and Meyer,2013]**

$$s(T) = -\frac{L_t(1+\vec{\xi}^2)^{\frac{3}{2}}}{\xi_k}\langle T_{0k}\rangle_{\vec{\xi}}\, Z_T$$

where Z_T is a renormalization constant that has to be computed separately

$$Z_T(g_0^2) = -\frac{\Delta f}{\Delta\xi_k}\frac{1}{\langle T_{0k}\rangle_{\vec{\xi}}}$$

opening the possibility for a study of the e.o.s. **[Giusti and Pepe, 2014]**

An implementation to fermionic degrees of freedom is ongoing **[Dalla Brida et al., 2017]**.

SU(3) pressure