Applications of Jarzynski's theorem in lattice gauge theories[1]

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*Speaker

[1] M. Caselle *et al.*, arXiv:1604.05544 [hep-lat]

Free-energy differences in LGTs

In lattice gauge theories the computation of free-energy differences is involved in the calculation (via Monte Carlo simulations) of a large set of physical quantities, for example:

- the pressure and the phase diagram in QCD/QCD-like theories
- interfaces between center domains
- the magnetic susceptibility in a strong magnetic field

In many cases the calculation of ΔF is a **computationally challenging** problem, especially in brute-force approaches: this motivates the search for new methods and algorithms.

The purpose of this talk is to present a **novel** (at least in LGTs) method to calculate the (exponential of the) free-energy difference. In general it will be applicable to any case in which we compute the ratio of partition functions of **physical systems**, i.e. expressed in terms of **well-defined** variables and couplings.

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Summary

Jarzynski's equality - I

Jarzynski's equality[1][2] puts in relation the exponential average of the work done on a system in a non-equilibrium process with the free energy difference between the initial and the final state of the system.

This evolution of the system is performed by changing (continuously or discretely) a set λ of one or more parameters, which can be the couplings or even the temperature of the system itself.
In each step of the process λ is changed and the system (in general) is brought **out of equilibrium**.

[1] C. Jarzynski, *Nonequilibrium Equality for Free Energy Differences*, Phys. Rev. Lett. 78 (1997) 2690–2693
[2] C. Jarzynski, *Equilibrium free-energy differences from nonequilibrium measurements: A master-equation approach*, Phys. Rev. E56 (1997) 5018–5035

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Jarzynski's equality - II

Jarzynski's equality can be written (for an isothermal transformation) as

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

- the left side is the ratio of the partition functions: $\exp\left(-\frac{\Delta F}{T}\right) = \frac{Z(T,\lambda_f)}{Z(T,\lambda_i)}$ where $\Delta F = F(\lambda_f) - F(\lambda_i)$
- $W(\lambda_i,\lambda_f)$ is the **work** made on the system to change the control parameter from λ_i to λ_f. If the transformation is discrete (like a Markov chain in MC simulations), then

$$W(\lambda_i,\lambda_f) = \sum_{n=0}^{N-1} [H(\lambda_{n+1},\phi_n) - H(\lambda_n,\phi_n)]$$

  where ϕ_n is the variable configuration at the n-th step of the transformation
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Parameters

Using Jarzynski's relation in Monte Carlo simulations we have to deal essentially with two parameters:

- N, the number of steps for each transformation between initial and final value of the parameter λ
- n_r, the number of "trials", i.e. realizations of the non-equilibrium transformation

A **systematic error** is expected as the change of the λ parameter in each transformation is not continuous, but discretized on a finite number of steps.
This error can be estimated by looking at discrepancies between the results of the 'direct' ($\lambda_i \to \lambda_f$) and the 'reverse' ($\lambda_f \to \lambda_i$) transformation.

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Benchmark study I: 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
- related to flux tubes in confining gauge theories

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 low values of the inverse coupling β_g.

Moreover it can be exactly rewritten as the 3-dimensional Ising model on the **dual** lattice:

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

with the new parameter

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

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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 partition functions of two different configurations:

- one in which all couplings are set to $J_{x,\mu} = 1$ (periodic boundary conditions)
- another one in which the couplings between the first and last slice in a specific direction μ are set to $J_{x,\mu} = -1$ (antiperiodic boundary conditions)

We can introduce the interface free energy as

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

where N_0 is the size of the lattice in the μ direction.
An improved definition can be used to account for multiple interfaces in finite-size systems.[1]

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

In order to compute the Z_a/Z_p ratio we can apply the Jarzynski's relation by gradually varying the $J_{x,\mu}$ parameter of the chosen slice from 1 to -1 (and viceversa):

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

where N is the total number of steps between periodic ($J_{x,\mu}(0) = 1$) and antiperiodic ($J_{x,\mu}(N) = -1$) boundary conditions.

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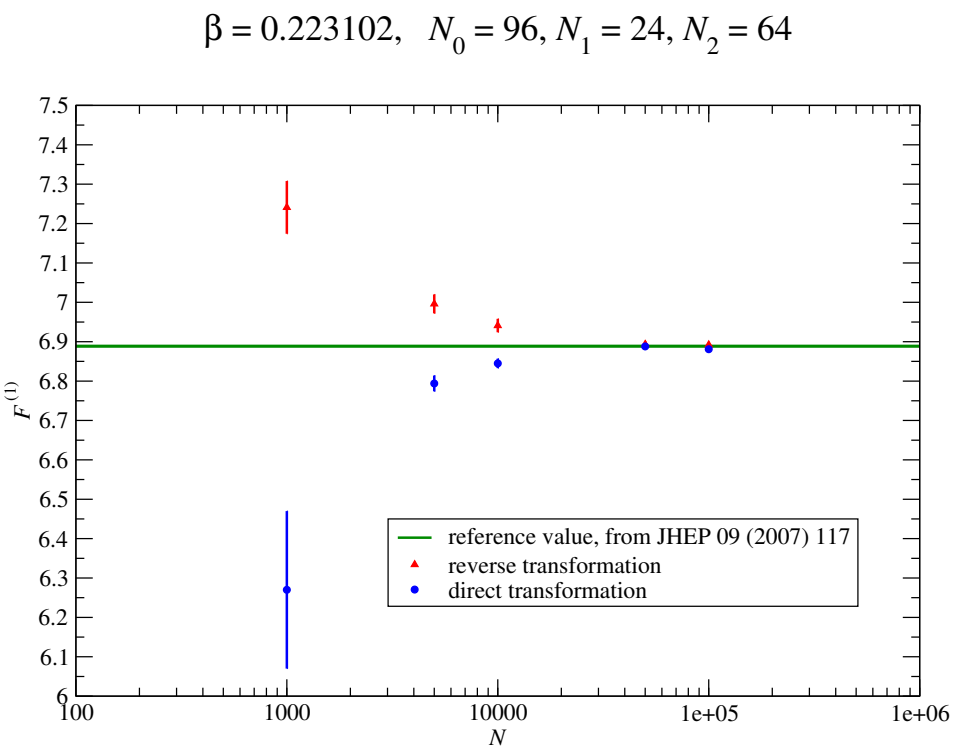

The results from 'direct' and 'reverse' transformations converge to older results when N is large enough

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With this method (using $N = 10^6$ steps and $n_r = 10^3$ trials) we obtained high-precision results at fixed β and various interface sizes.

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 of the interface, in order to understand the nature of the terms that do not arise from the NG low-energy expansion.

Benchmark study II: pressure in $\mathrm{SU}(2)$ gauge theory

Pressure on the lattice

On an hypercubic lattice of size $N_t \times N_s^3$, the temperature is determined by the inverse of the temporal extent (with periodic boundary conditions): $T = (aN_t)^{-1}$. In practice, the temperature can be controlled by the lattice spacing a, i.e. by changing the inverse of the coupling constant $\beta_g = \frac{2N_c}{g^2}$.

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 it is usually estimated on the lattice using the so-called "integral method" [1]:

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

where the integrand is calculated from plaquette expectation values on finite T lattices. The result is normalized to the value of $p(T)$ at $T = 0$ in order to remove the contribution of the vacuum.

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Pressure with Jarzynski's relation

Jarzynski's relation gives us a direct method to compute the pressure: now the parameter β_g controls the temperature T and so we can vary it in a non-equilibrium transformation!

In practice the **difference of pressure** between two temperatures T_f and T_i is given by

$$\frac{p(T_f)}{T_f^4} - \frac{p(T_i)}{T_i^4} = \left(\frac{N_t}{N_s}\right)^3 \ln\langle e^{-A}\rangle$$

with A being the 'work' made on the system:

$$A = \sum_{t=0}^{N-1} \left[S_W(\beta_g(t+1), \hat{U}) - S_W(\beta_g(t), \hat{U}) \right];$$

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.

Several values of this difference have been computed with this algorithm in the proximity of the deconfining transition (for temperatures $T < T_c$), using either $N = 1000$ or $N = 2000$ steps and $n_r = 30$ transformations.

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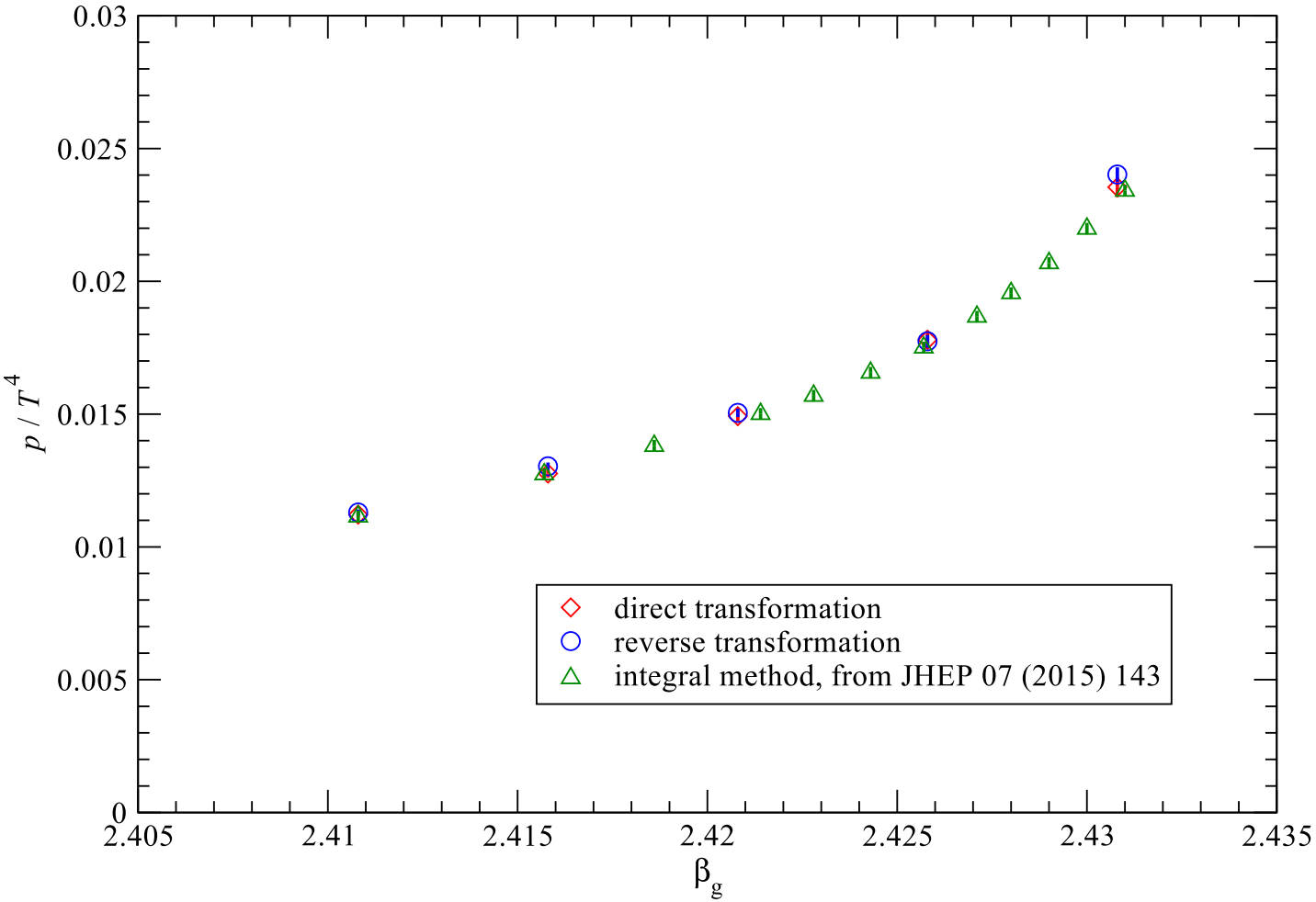
Preliminary results for the SU(2) model

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



Excellent agreement with older data[1] using a fraction of CPU time.

[1] M. Caselle, A. N. and M. Panero, , *JHEP* **07** (2015) 143

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

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

  Methods based on Jarzynski's relation can be applied in order to perform non-equilibrium transformations in which the field B itself is changed gradually.

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

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Conclusions

Jarzynski's equality allows for new methods to compute free-energy differences in lattice gauge theories. Methods based on this relation have been tested on the computation of two different physical quantities:

- the free energy of an interface in the $\mathbb{Z}_2$ gauge model
- the pressure in the confining region of the $\mathrm{SU}(2)$ gauge model

In both cases the method proved to be perfectly reliable with a suitable choice of the parameters (N and n_r); moreover the computational efficiency is at least similar and in many cases even superior to standard methods.

Eliminating the vacuum contribution

Using the 'integral method' the pressure can be rewritten (relative to its $T = 0$ vacuum contribution) as

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

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 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.

Lattice regularization

For $\mathrm{SU}(N_c)$ pure gauge theories on the lattice the dynamics is described by the standard Wilson action

$$S_W = -\frac{\beta}{N_c} \sum_p \mathrm{ReTr} U_p$$

where U_P is the product of four U_μ $\mathrm{SU}(N_c)$ variables on the space-like or time-like plaquette P and $\beta = \frac{2N_c}{g^2}$.

The partition function is

$$Z = \int \prod_{x,\mu} \mathrm{d}U_\mu(x) e^{-S_W}$$

the expectation value of an observable $\mathcal{O}$

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \prod_{n,\mu} \mathrm{d}U_\mu(n)\, \mathcal{O}(U_\mu(n))\, e^{-S_W}$$