Lattice QCD averages from non-equilibrium transformations

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M. Caselle, G. Costagliola, A. Nada, M. P. and A. Toniato
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Outline

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Motivation

- In lattice calculations for QCD and QCD-like theories, the expectation values of a large class of physical quantities have a *natural* interpretation in terms of ratios of partition functions

$$\langle \mathcal{O} \rangle = \frac{\int \mathcal{D}\phi \mathcal{O} \exp(-S)}{\int \mathcal{D}\phi \exp(-S)} = \frac{Z_{\mathcal{O}}}{Z}$$

- By "natural" we mean, that $Z_{\mathcal{O}}$ can be easily written as a partition function of a physical system with a well-defined set of local fields and (generalized) couplings
- Examples:
  - Equilibrium thermodynamic observables (p, ϵ, s, ...)
  - Some non-local operators (e.g. 't Hooft loops, Wilson loops and Polyakov loop correlators in a dual formulation of the theory, etc.)
- The numerical evaluation of $\langle \mathcal{O} \rangle$ becomes challenging, whenever an *overlap problem* between the simulated and target ensemble exists
- Under certain circumstances, the computation can be simplified, by factoring $\langle \mathcal{O} \rangle$ into a product of simpler terms **[de Forcrand et al., 2001]**

$$\frac{Z_{\mathcal{O}}}{Z} = \frac{Z_1}{Z} \cdot \frac{Z_2}{Z_1} \cdot \frac{Z_3}{Z_2} \cdot \dots \cdot \frac{Z_{\mathcal{O}}}{Z_{n-1}}$$

- However, the possibility of performing this reformulation in a *computationally efficient* way is highly non-generic

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Non-equilibrium methods for Monte Carlo simulations

- The factorization of $\langle \mathcal{O} \rangle$ into a product of partition-function ratios requires the existence of a sequence of well-defined intermediate equilibrium ensembles
- An alternative computational strategy completely bypasses this requirement, and allows one to evaluate $\langle \mathcal{O} \rangle$ through a statistical average over realizations of *non-equilibrium transformations*

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Jarzynski's theorem in a nutshell

- Jarzynski's theorem **[Jarzynski, 1997]** states the equality of the exponential average of the work done on a system in non-equilibrium processes, and the ratio of the partition functions of the final (Z_{fin}) and initial (Z_{in}) ensembles, respectively realized at "times" t_{f} and t_{i}

$$\left\langle \exp\left(- \int_{\mathrm{in}}^{\mathrm{fin}} \frac{\delta W}{T} \right) \right\rangle = \frac{Z_{\mathrm{fin}}}{Z_{\mathrm{in}}}$$

- The average is over a large number of realizations of non-equilibrium evolutions from the initial to the final ensembles
- "Time" can either refer to
  - Monte Carlo time in a numerical simulation
  - Real time in an experiment
- Related ideas date back to the 1970's **[Bochkov and Kuzovlev, 1977]**
- Connection to entropy-production fluctuation theorems **[Evans et al., 1993]** encoded in a generalization **[Crooks, 1999]**

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Proof – I: Notation

- Consider a statistical system of degrees of freedom ϕ, described by the partition function Z

$$Z = \sum_{\phi} \exp\left(-\frac{H}{T}\right)$$

- Consider the normalized Boltzmann distribution $\pi = \exp\left(-H/T\right)/Z$ and assume the detailed-balance condition
- Let λ denote the parameters (Hamiltonian couplings, temperature, et c.) on which π and Z depend
- Take λ to be time-dependent: $\lambda = \lambda(t)$, for $t_{\mathrm{i}} \leq t \leq t_{\mathrm{f}}$, and discretize $\Delta t = t_{\mathrm{f}} - t_{\mathrm{i}} = N \cdot \tau$
- The exponential of minus the work (over T) from t_{i} to t_{f} is obtained as

$$\lim_{N\to\infty} \exp\left(-\sum_{n=0}^{N-1}\left\{\frac{H_{\lambda(t_{n+1})}\left[\phi\left(t_n\right)\right]}{T\left(t_{n+1}\right)} - \frac{H_{\lambda(t_n)}\left[\phi\left(t_n\right)\right]}{T\left(t_n\right)}\right\}\right)$$

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$$\pi[\phi]P[\phi \to \phi'] = \pi[\phi']P[\phi' \to \phi]$$

  where $P[\phi \to \phi']$ denotes the transition probability from ϕ to ϕ'
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$$t_n = t_{\mathrm{i}} + n\tau \quad \text{for } n \in \{0, 1, 2, \dots, N-1, N\}$$

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Proof – II: Manipulations

- Since the Boltzmann distribution π is such that $Z \cdot \pi = \exp\left(-H/T\right)$, the previous expression can be rewritten as the $N \to \infty$ limit of

$$\prod_{n=0}^{N-1} \frac{Z_{\lambda(t_{n+1})} \cdot \pi_{\lambda(t_{n+1})}\left[\phi\left(t_n\right)\right]}{Z_{\lambda(t_n)} \cdot \pi_{\lambda(t_n)}\left[\phi\left(t_n\right)\right]}$$

- Assume that the configuration at time $t = t_{n+1}$ is obtained by Markov evolution of the one at $t = t_n$ with transition probability $P_{\lambda(t_{n+1})}\left[\phi(t_n) \to \phi(t_{n+1})\right]$
- Then the statistical average can be written as
- In this expression, the sum over $\phi(t_i)$ can be carried out explicitly, because it appears only in $P_{\lambda(t_1)}\left[\phi(t_1) \to \phi(t_i)\right]$
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having simplified the intermediate $Z_{\lambda(t_n)}$ factors and used detailed balance

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Proof – III: Comments

- The theorem holds under very general conditions, no strong assumptions are needed
- For finite τ, the non-symmetric rôles of t_n and t_{n+1} in the Markov evolution induces a discrepancy between "forward" ($\lambda_{\text{in}} \to \lambda_{\text{fin}}$) and "reverse" ($\lambda_{\text{fin}} \to \lambda_{\text{in}}$) realizations of the non-equilibrium transformation
- The impact of this systematic effect is in general non-negligible, but it vanishes for $N \to \infty$
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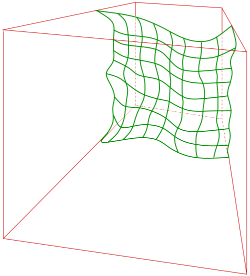
Interfaces in physics

- Fluctuating interfaces have countless physical realizations of interest in mesoscopic physics, in chemistry, in biophysics, ...
- In high-energy physics, they appear as various types of "domain walls" in high-temperature QFT, in cosmology, in the study of 't Hooft loops, et c.
- Of particular interest are interfaces whose fluctuations can be described in terms of $c = 1$ conformal field theory, using string-theory tools



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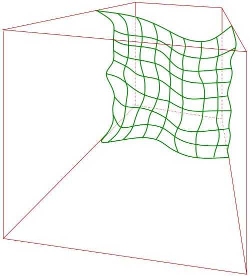

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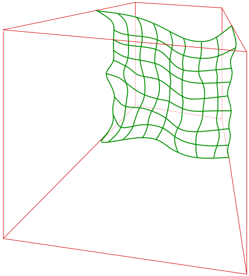

Interface free energy in a toy gauge theory

- Here we study the interface free energy in a toy model: $\mathbb{Z}_2$ lattice gauge theory in three dimensions

$$S_{\mathbb{Z}_2} = -\beta_{\mathrm{g}} \sum_{x\in\Lambda} \sum_{0\le\mu<\nu\le 2} \sigma_\mu(x)\sigma_\nu(x+a\hat{\mu})\sigma_\mu(x+a\hat{\nu})\sigma_\nu(x)$$

- Kramers–Wannier duality maps this theory to the 3D Ising model; the confining regime of the gauge theory corresponds to the ordered phase of the spin model
- An (odd number of) interface(s) can be enforced by antiperiodic boundary conditions
- The results from Jarzynski's algorithm converge to those obtained from different methods **[Caselle et al., 2007]**
- Our numerical results from interfaces of linear size L confirm the predictions of low-energy effective string theory **[Aharony and Karzbrun, 2009]**
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$$F^{(2)} = -\ln \operatorname{arctanh}(Z_{\mathrm{a}}/Z_{\mathrm{p}}) + \ln(L_0/a).$$

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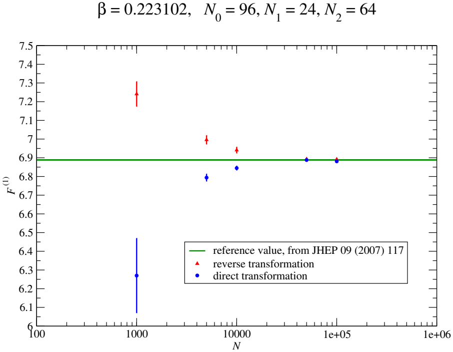

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QCD (and QCD-like theories) at finite temperature

- The thermal properties of QCD at temperatures T of hundreds MeV have major implications for the evolution of the early Universe—particularly during the *quark epoch* (approximately 10^{-12} to 10^{-6} s after the Hot Big Bang)
- These properties are being studied at the LHC and at other experimental facilities, through ultrarelativistic collisions of heavy nuclei
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- Similar studies for other strongly coupled non-Abelian gauge theories may be of relevance for New Physics models

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Equation of state (EoS) in the confining phase

- The sudden increase in pressure, energy and entropy densities at $T \sim 160$ MeV indicates liberation of a large number of light degrees of freedom
- By contrast, in the low-temperature phase, the EoS can be modelled by a gas of massive, essentially non-interacting, hadrons; exponential suppression of all equilibrium-thermodynamics quantities
- This is most dramatic in the pure-glue theory **[Meyer, 2009] [Borsányi et al., 2012] [Caselle et al., 2015]**, due to the existence of a large mass gap ($M_{0^{++}} \gg M_\pi$)
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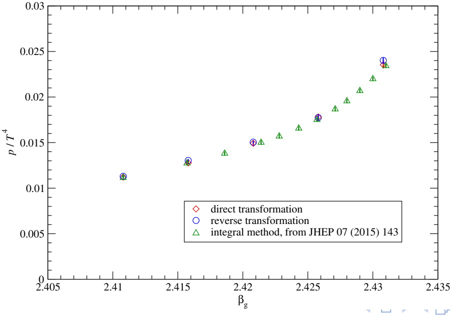

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Summary and future work

- Jarzynski's theorem provides a very versatile method to compute observables in Monte Carlo simulations on the lattice
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Thanks for your attention!