Calculation of the running coupling in non-Abelian gauge theories from Jarzynski's equality

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LATTICE 2021
The XXXVIII International Symposium on Lattice Field Theory
26.-30. July 2021

Based on: JHEP 07 (2020) 233 **[arXiv:2003.13734]**

Introduction and motivation

- Since the 1990's, various fluctuation- and entropy-production theorems have been formulated in non-equilibrium statistical mechanics **[Evans, Cohen, and Morriss, 1993] [Gallavotti and Cohen, 1995] [Jarzynski, 1997] [Crooks, 1998]**
- In addition to giving deep mathematical insights into irreversibility and non-equilibrium phenomena, they provide the basis for a novel type of Monte Carlo calculations
- Applications include the evaluation of interface tensions in spin systems **[Chatelain, 2007]** and the equation of state in lattice gauge theory **[Caselle et al., 2016] [Caselle, Nada and M.P., 2018]**
- Here, we present another application: the evaluation of the running coupling in $\mathrm{SU}(N)$ Yang-Mills theories in the Schrödinger-functional scheme

Jarzynski's theorem

- Jarzynski's theorem **[Jarzynski, 1997]**: For a thermodynamic system driven out of equilibrium by a variation $\lambda(t)$ of the parameters of its Hamiltonian H (for $t_{\mathrm{in}} \le t \le t_{\mathrm{fin}}$), the exponential average of the work W done on the system in units of the temperature T equals the ratio of the partition functions for *equilibrium* states with parameters $\lambda(t_{\mathrm{fin}})$ and $\lambda(t_{\mathrm{in}})$:

$$\overline{\exp\left(-W/T\right)} = \frac{Z_{\lambda(t_{\mathrm{fin}})}}{Z_{\lambda(t_{\mathrm{in}})}}$$

- A relation between equilibrium and non-equilibrium quantities
- t can either be real time (e.g. in experiments), or Monte Carlo time in a simulation
- The average on the left-hand side is taken over all possible trajectories that the system can follow, when its parameters are modified according to the *arbitrary* and *fixed* $\lambda(t)$ protocol
- Combining Jarzynski's theorem with Jensen's inequality, the second law of thermodynamics follows
- Jarzynski's equality reduces to known results in two different limits:
  1. $t_{\mathrm{fin}} - t_{\mathrm{in}} \to \infty$: the system remains in thermodynamic equilibrium, $W = \Delta F$
  2. $t_{\mathrm{fin}} - t_{\mathrm{in}} \to 0$: parameters instantaneously switched from $\lambda(t_{\mathrm{in}})$ to $\lambda(t_{\mathrm{fin}})$, Jarzynski's equality reduces to *statistical reweighting*

Sketch of (one, constructive) proof

- We assume that the transition probabilities $P[\phi \to \phi']$ satisfy detailed balance

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

where $\pi = \exp\left(-H/T\right)/Z$ is the Boltzmann distribution

- The exponential of minus the work (over T) along a generic trajectory is

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

- The statistical average over non-equilibrium trajectories can be written as

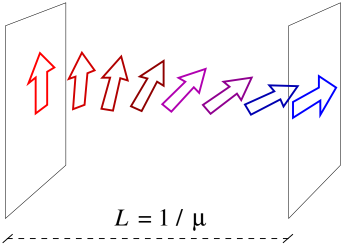
$$\lim_{N\to\infty} \sum_{\{\phi(t)\}} \pi_{\lambda(t_{\rm in})}\left[\phi(t_{\rm in})\right] \prod_{n=0}^{N-1} \left\{ \frac{Z_{\lambda(t_{n+1})}}{Z_{\lambda(t_n)}} \cdot \frac{\pi_{\lambda(t_{n+1})}\left[\phi\left(t_n\right)\right]}{\pi_{\lambda(t_n)}\left[\phi\left(t_n\right)\right]} \cdot P_{\lambda(t_{n+1})}\left[\phi(t_n) \to \phi(t_{n+1})\right] \right\}$$

- Simple algebraic manipulations allow one to iteratively sum over configurations at all times t, with the result:

$$\overline{\exp\left(-W/T\right)} = \frac{Z_{\lambda(t_{\rm fin})}}{Z_{\lambda(t_{\rm in})}}$$

Running coupling in the Schrödinger-functional scheme

- Consider the Euclidean-time evolution of a gauge theory, with bare coupling g_0, between initial ($\tau = 0$) and final ($\tau = L$) Euclidean times, with fixed boundary conditions
- This induces a classical field configuration with Euclidean action $S^{\mathrm{cl}} \propto 1/g_0^2$
- In the *Schrödinger-functional scheme* **[Symanzik, 1981] [Lüscher et al., 1992]** the running coupling $g(L)$ is defined from the *quantum effective action* $S^{\mathrm{eff}} \propto 1/g^2(L)$
- We computed $g^2(L)$ with Jarzynski's equality, through Monte Carlo simulations in which the system is driven out of equilibrium by changing the boundary conditions



Implementation in $\mathrm{SU}(2)$ Yang-Mills theory

- Field configurations for the spatial link matrices at the boundaries $U = \exp(iaC_{x_0})$ with

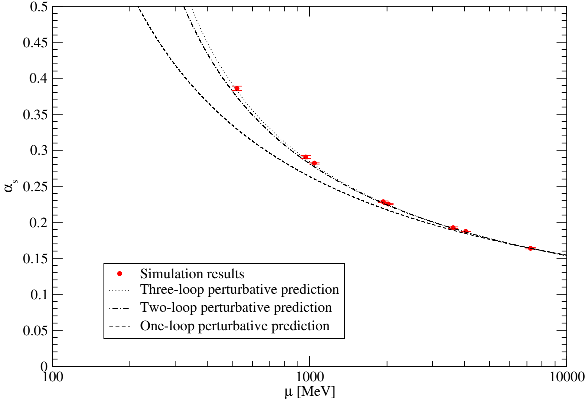
$$C_0 = \frac{1}{L}\,\mathrm{diag}\,(-\eta, \eta)\,, \qquad C_L = \frac{1}{L}\,\mathrm{diag}\,(\eta - \pi, \pi - \eta)$$

- η is varied from $\eta(t_{\mathrm{in}}) = \pi/4$ to $\eta(t_{\mathrm{fin}}) = \eta(t_{\mathrm{in}}) + \Delta\eta$ through a sequence of "quenches" in Monte Carlo time
- Defining the effective action $\Gamma = -\ln Z$, the running coupling in the Schrödinger-functional scheme is obtained as

$$g^2(L) = -\lim_{\Delta\eta \to 0} \frac{24\Delta\eta}{\Delta\Gamma} \left(\frac{L}{a}\right)^2 \sin\left[\frac{\pi}{2}\left(\frac{a}{L}\right)^2\right]$$

- Coupling evolution determined iteratively, through a step-scaling function $\sigma(s, g^2(L)) = g^2(sL)$ **[Lüscher, Weisz and Wolff, 1991]** (an integrated version of the β function of the theory)

Running coupling in $\mathrm{SU}(2)$ Yang-Mills theory



Results for $\alpha_s = g^2/(4\pi)$ in $\mathrm{SU}(2)$ Yang-Mills theory, *vs.* the momentum scale $\mu = 1/L$, and comparison with weak-coupling expansions at one, two and three loops

Implementation in $\mathrm{SU}(3)$ Yang-Mills theory

- The implementation for $\mathrm{SU}(3)$ theory is similar to $\mathrm{SU}(2)$, but boundary matrices $U = \exp(iaC_{x_0})$ are defined through

$$C_0 = \frac{1}{L}\,\mathrm{diag}\left(\eta - \frac{\pi}{3}, \eta\left(\nu - \frac{1}{2}\right), -\eta\left(\nu + \frac{1}{2}\right) + \frac{\pi}{3}\right),$$

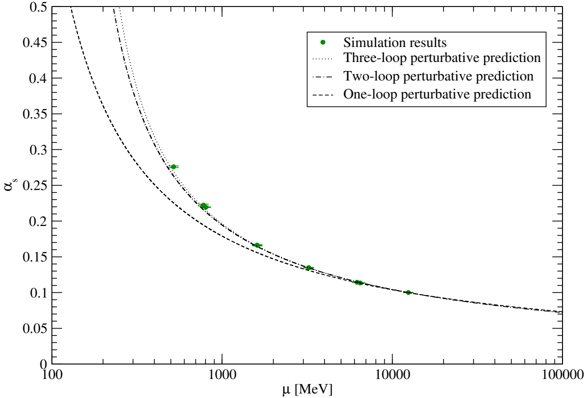
$$C_L = \frac{1}{L}\,\mathrm{diag}\left(-\eta - \pi, \eta\left(\nu + \frac{1}{2}\right) + \frac{\pi}{3}, -\eta\left(\nu - \frac{1}{2}\right) + \frac{2\pi}{3}\right)$$

- Running coupling obtained as

$$g^2(L) = \lim_{\Delta\eta \to 0} \frac{12\Delta\eta}{\Delta\Gamma}\left(\frac{L}{a}\right)^2 \left\{\sin\left[\frac{2\pi}{3}\left(\frac{a}{L}\right)^2\right] + \sin\left[\frac{\pi}{3}\left(\frac{a}{L}\right)^2\right]\right\}$$

by varying η from $\eta(t_{\mathrm{in}}) = 0$ to $\eta(t_{\mathrm{fin}}) = \eta(t_{\mathrm{in}}) + \Delta\eta$ (for $\nu = 0$)

Running coupling in $\mathrm{SU}(3)$ Yang-Mills theory



Results for $\alpha_s = g^2/(4\pi)$ in $\mathrm{SU}(3)$ Yang-Mills theory, *vs.* the momentum scale $\mu = 1/L$, and comparison with weak-coupling expansions at one, two and three loops

Summary

- Jarzynski's equality provides a rigorous basis for versatile and computationally efficient non-equilibrium Monte Carlo simulations in lattice field theory
- As a case study, in this work we reproduced the results for the running coupling in the Schrödinger-functional scheme for $\mathrm{SU}(2)$ **[Lüscher et al., 1992]** and $\mathrm{SU}(3)$ Yang-Mills theories **[Lüscher et al., 1993]**
- Extension to full QCD is straightforward, generalization to other physical observables is possible