Free energy difference with Jarzynski equality: Interfaces in the lattice ϕ^4 theory

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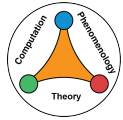


Trento ECT*, 5 / 12 / 2025

Outline

1. The model and the motivation
   - ϕ^4 phase diagram
   - Interfaces
   - string behavior
2. Jarzynski
   - out-of-equilibrium trajectories
   - heat and work
   - the equality
   - proof
   - metrics
   - scaling
3. Some results
   - conclusions

Phase diagram of ϕ^4

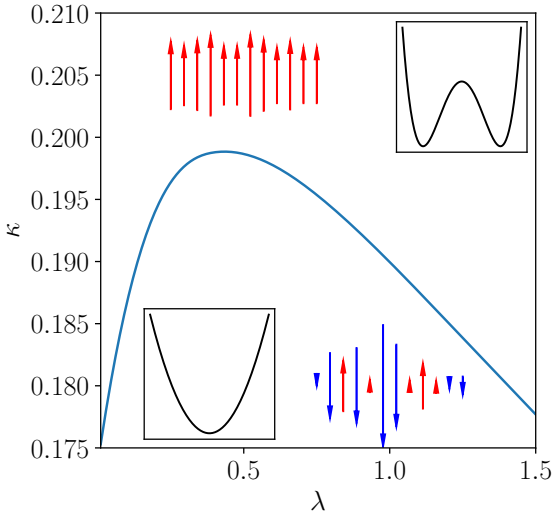
We will consider ϕ^4 theory in three space-time dimensions:

$$S = \sum_x \left\{ \phi_x^2 + \lambda \left(\phi_x^2 - 1\right)^2 - 2\,\kappa \sum_\mu \phi_x\, \phi_{x+\hat{\mu}} \right\}$$

For each λ at large enough κ:
system is **spontaneously magnetized**

We will be interested in this phase
especially in the region near the **critical line**
which is in the $3D$ **Ising** universality class

[Hasenbusch, 1999]



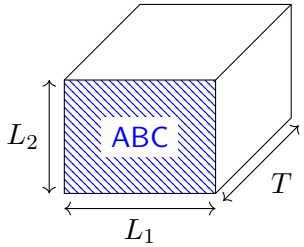
Inducing an Interface

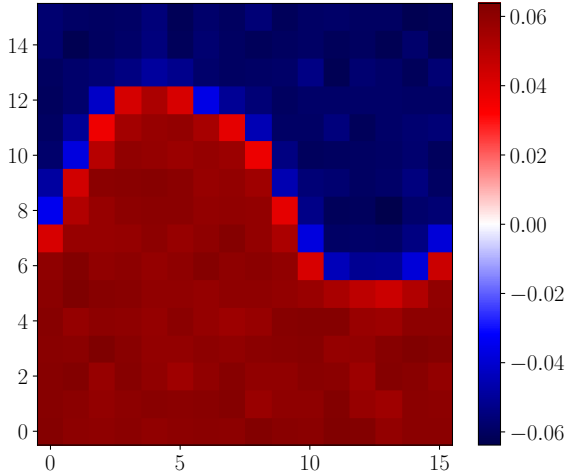
Anti-periodic boundary condition (ABC)
frustrates the ferromagnetic order

Somewhere in the lattice
an **interface** is induced

The interface will contribute to
the free energy in two ways:

$$\Delta F = F_s(L_1, L_2) - \log T$$

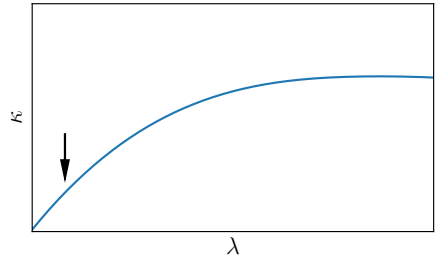


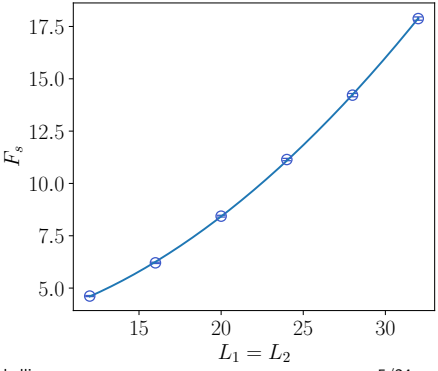


String Behavior of the Free Energy

$$F_s = \sigma\, L_1\, L_2 + \dots$$

- Corrections depend on the geometry
  e.g. Lüscher term when $L_1 \gg L_2$
- Corrections to Nambu-Gotō start at order $1/\sigma^3$
- Leading correction is compatible with Ising result in [Caselle *et al.*, 2007]
- From universality: $\sigma/m^2 = 0.1040(8)$ at criticality from [Caselle *et al.*, 2023] (m: mass in the bulk)
- At small λ attraction from Gaussian fixed point
- Can we find $\sigma \gg m^2$ and compare to [Aharony *et al.*, 2024]?





Jarzynski so far: Free energy

Jarzynski's theorem for lattice gauge theory
Caselle *et al.*, 2016

QCD thermodynamics from lattice calculations with nonequilibrium methods: The SU(3) equation of state
Caselle *et al.*, 2018

Strong coupling from non-equilibrium Monte Carlo simulations
Francesconi *et al.*, 2020

Entanglement entropy from non-equilibrium Monte Carlo simulations
Bulgarelli *et al.*, 2023

Flow-Based Sampling for Entanglement Entropy and the Machine Learning of Defects
Bulgarelli *et al.*, 2024

Casimir effect in critical $O(N)$ models from non-equilibrium Monte Carlo simulations
Bulgarelli *et al.*, 2025

Jarzynski so far: Sampling (mainly SNF)

Mitigating topological freezing using out-of-equilibrium simulations
Bonanno *et al.*, 2024

Stochastic normalizing flows as non-equilibrium transformations
Caselle *et al.*, 2022

Numerical determination of the width and shape of the effective string using Stochastic Normalizing Flows
Caselle *et al.*, 2024

Scaling of stochastic normalizing flows in SU(3) lattice gauge theory
Bulgarelli *et al.*, 2024

Scaling flow-based approaches for topology sampling in $\mathrm{SU}(3)$ *gauge theory*
Bonanno *et al.*, 2025

Annealed Importance Sampling
Neal, 1998

Out of Equilibrium MC

System with action $S_\lambda[\phi]$ explicitly depending on a parameter λ

For each value of λ, can device a transition probability $\mathcal{P}_\lambda(\phi \to \phi')$

We can lead the system **out-of-equilibrium** changing λ during the Markov Chain:

$$\phi_0 \xrightarrow{\mathcal{P}_{\lambda(1)}} \phi_1 \xrightarrow{\mathcal{P}_{\lambda(2)}} \phi_2 \xrightarrow{\mathcal{P}_{\lambda(3)}} \dots \xrightarrow{\mathcal{P}_{\lambda(N_{\text{step}})}} \phi_{N_{\text{step}}}$$

We will assume detailed balance to hold for each $\mathcal{P}_\lambda$

Heat and Work

In general:

$$S_{\lambda(0)}[\phi_0] \neq S_{\lambda(N_{\text{step}})}[\phi_{N_{\text{step}}}]$$

We will call **Work**[1] the change in the action due to change in parameters:

$$\delta W_k = S_k[\phi_{k-1}] - S_{k-1}[\phi_{k-1}]$$

And **Heat** the change in the action due to change of the configuration:

$$\delta Q_k = S_k[\phi_k] - S_k[\phi_{k-1}]$$

So that

$$\Delta S = \sum_{k=1}^{N_{\text{step}}} \left(\delta W_k + \delta Q_k\right) = W + Q$$

$$\phi_k \xrightarrow{\mathcal{P}_{\lambda(k+1)}} \phi_{k+1}$$

[1] done on the system

Jarzynski Equality

$$\langle e^{-W} \rangle_{\mathrm{f}} = e^{-\Delta F}$$

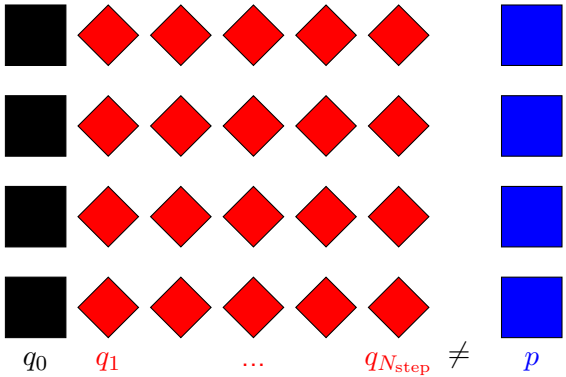
[Jarzynski, 1996]

$\langle \cdot \rangle_{\mathrm{f}}$ is the average over **forward trajectories**

ΔF is the **free energy difference** between $\lambda(0)$ and $\lambda(N_{\mathrm{step}})$

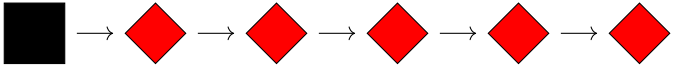
Let the **prior** be $q_0 \sim e^{-S_{\lambda(0)}}$
And the **target** be $p \sim e^{-S_{\lambda(N_{\mathrm{step}})}}$

ΔF is the difference in free energy between the q_0 and p **equilibrium distribution**



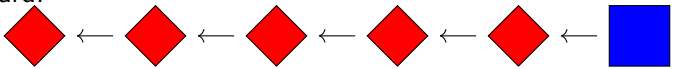
Forward and Reverse Process

Besides the forward process



$$P_{\mathrm{f}} = q_0(\phi_0) \prod_{k=1}^{N_{\mathrm{step}}} \mathcal{P}_{\lambda(k)}(\phi_{k-1} \to \phi_k)$$

Consider the backward:



$$P_{\mathrm{r}} = p(\phi_{N_{\mathrm{step}}}) \prod_{k=1}^{N_{\mathrm{step}}} \mathcal{P}_{\lambda(k)}(\phi_k \to \phi_{k-1})$$

Crooks Fluctuation Theorem

Let us compute

$$\log \frac{P_{\mathrm{f}}}{P_{\mathrm{r}}} = \log \frac{q_0(\phi_0)}{p(\phi_{N_{\mathrm{step}}})} \sum_{k=1}^{N_{\mathrm{step}}} \log \frac{\mathcal{P}_{\lambda(k)}(\phi_{k-1} \to \phi_k)}{\mathcal{P}_{\lambda(k)}(\phi_k \to \phi_{k-1})} = S_{N_{\mathrm{step}}}(\phi_{N_{\mathrm{step}}}) - S_0(\phi_0) - \Delta F - Q$$

since

$$\sum_{k=1}^{N_{\mathrm{step}}} \log \frac{\mathcal{P}_{\lambda(k)}(\phi_{k-1} \to \phi_k)}{\mathcal{P}_{\lambda(k)}(\phi_k \to \phi_{k-1})} = \sum_{k=1}^{N_{\mathrm{step}}} (S_k(\phi_k) - S_k(\phi_{k-1})) = Q$$

by detailed balance [Crooks, 1999]

We call the difference $S_{N_{\mathrm{step}}}(\phi_{N_{\mathrm{step}}}) - S_0(\phi_0) - Q - \Delta F$ **dissipated work**:

$$\log \frac{P_{\mathrm{f}}}{P_{\mathrm{r}}} = W - \Delta F = W_d$$

Unbiased Sampling and Proving Jarzynski

$$P_\mathrm{r} = P_\mathrm{f}\, e^{-W_d} = P_\mathrm{f}\, e^{\Delta F - W}$$

We would like to sample the target p:

$$\langle \mathcal{O} \rangle_p = \int \mathcal{D}\phi\, p(\phi)\, \mathcal{O}(\phi) = \int \prod_{k=0}^{N_\mathrm{step}} \mathcal{D}\phi_k\, P_\mathrm{r}\, \mathcal{O}(\phi_{N_\mathrm{step}}) = \int \prod_{k=0}^{N_\mathrm{step}} \mathcal{D}\phi_k\, P_\mathrm{f}\, e^{-W_d}\, \mathcal{O}(\phi_{N_\mathrm{step}})$$

or shortly

$$\langle \mathcal{O} \rangle_p = \langle e^{-W_d}\, \mathcal{O}(\phi_{N_\mathrm{step}}) \rangle_\mathrm{f}$$

Take the special case $\mathcal{O} = 1$:

$$1 = \langle e^{-W_d} \rangle_\mathrm{f} \qquad \text{or} \qquad e^{-\Delta F} = \langle e^{-W} \rangle_\mathrm{f}$$

Metrics of Jarzynski: the Dissipated Work

$$\langle \mathcal{O} \rangle_p = \langle e^{-W_d} \, \mathcal{O}(\phi_{N_{\text{step}}}) \rangle_{\text{f}}$$

looks dangerously like a **reweighting formula**...

We need to make sure W_d does not grow with the "size" of the system

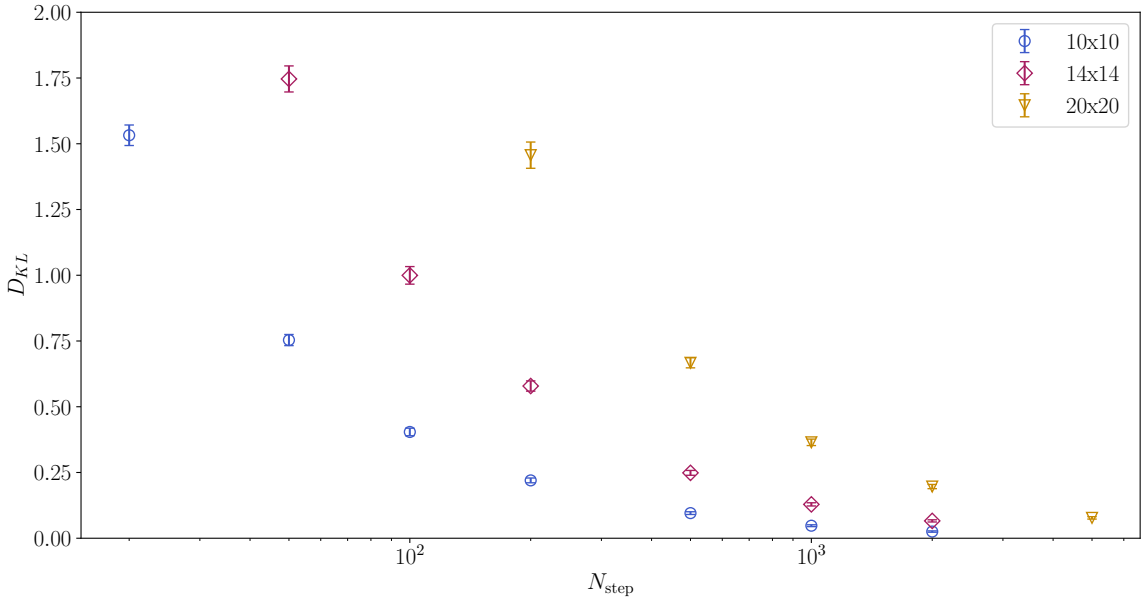
Let us make an observation:

$$0 \leq D_{\text{KL}}(P_{\text{f}} || P_{\text{r}}) = \langle \log \frac{P_{\text{f}}}{P_{\text{r}}} \rangle_{\text{f}} = \langle W_d \rangle_{\text{f}}$$

Where $D_{\text{KL}}(q||q')$ is the **Kullback-Leibler divergence**, greater or equal to 0
It is a measure of how much two distributions differ

This also shows $\langle W \rangle_{\text{f}} \geq \Delta F$

Metrics of Jarzynski: the Dissipated Work



Metrics of Jarzynski: the ESS

For each observable we would define the **Effective Sample Size** as

$$\mathrm{ESS}_{\mathcal{O}} = \frac{\mathrm{Var}(\mathcal{O})_p}{\mathrm{Var}(\mathcal{O}\, e^{-W_d})_{\mathrm{f}}}$$

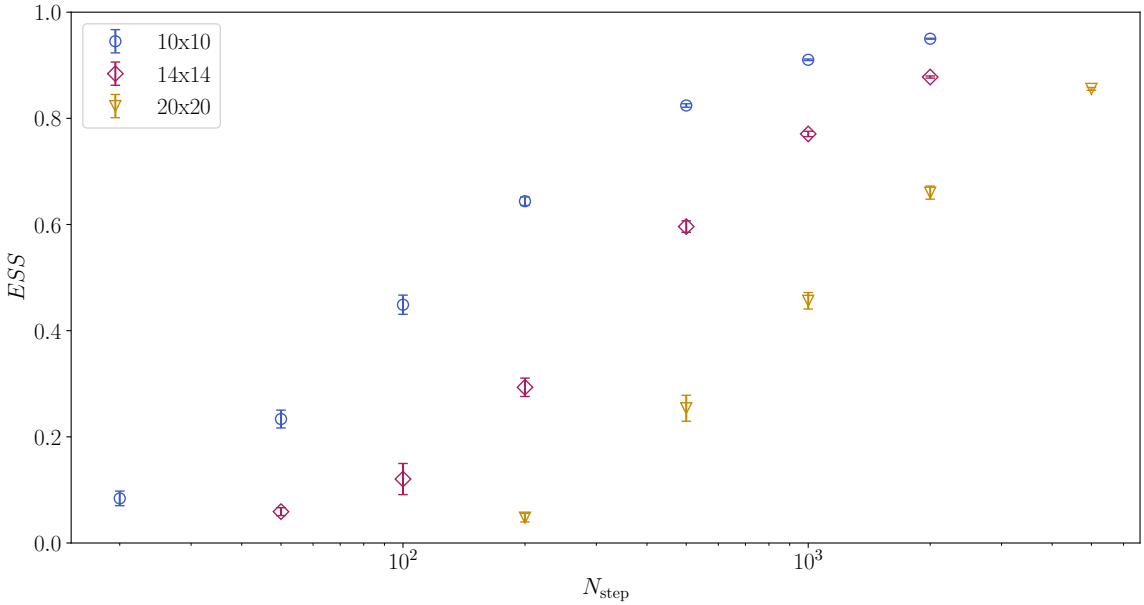
Neglecting the correlations between $\mathcal{O}$ and e^{-W_d}, we define a "generic" ESS

$$\mathrm{ESS} = \frac{\langle e^{-W} \rangle_{\mathrm{f}}^{\,2}}{\langle e^{-2W} \rangle_{\mathrm{f}}} = \frac{1}{\langle e^{-2W_d} \rangle_{\mathrm{f}}}$$

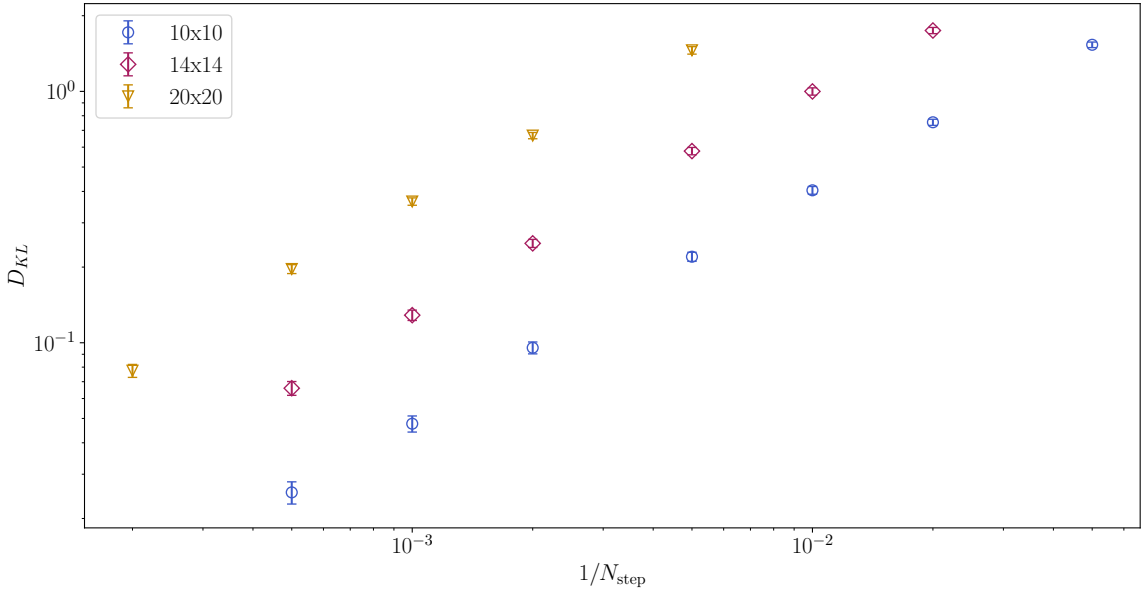
This is an estimation of the quality of the sampling

It is a measure of the variance of the weights in the reweighting

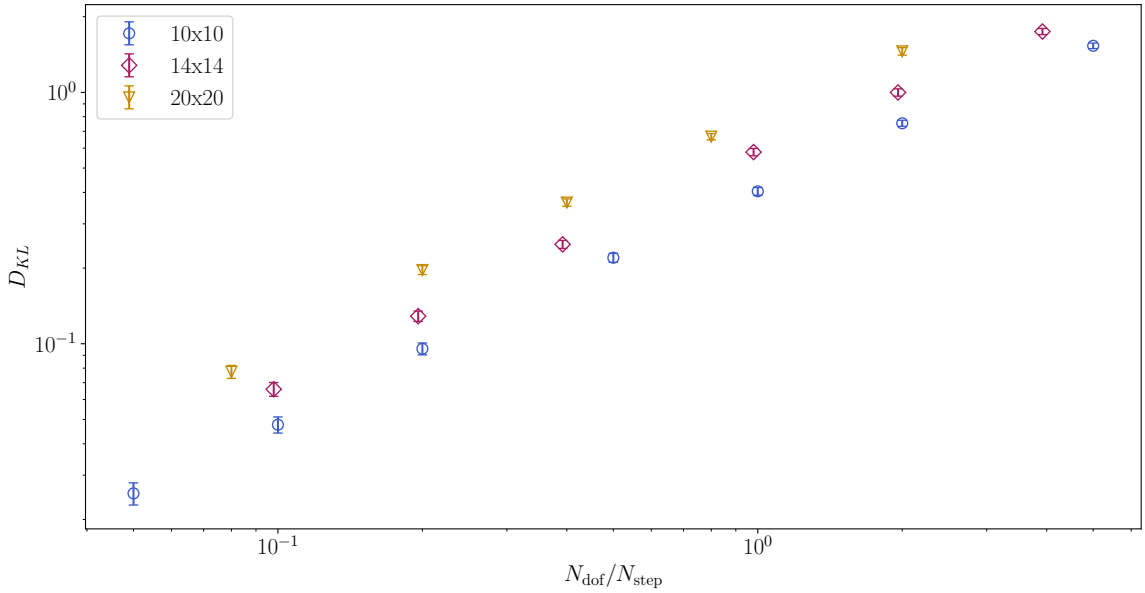
Metrics of Jarzynski: the ESS



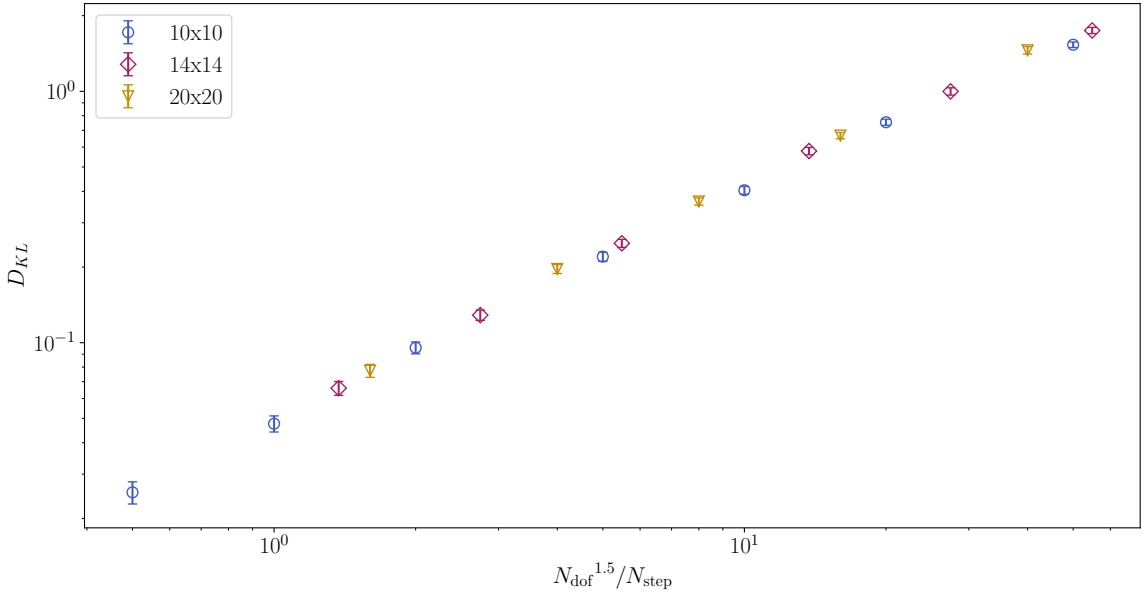
Scaling



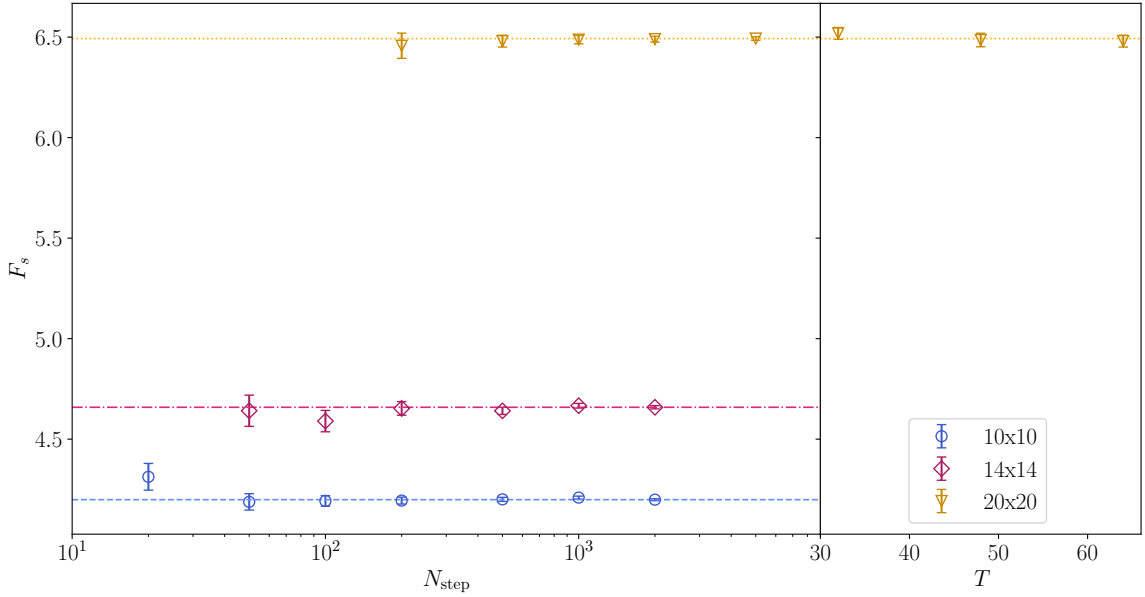
Scaling


10x10
14x14
20x20
10^0
10^{-1}
D_{KL}
10^{-1}
10^0
$N_{\mathrm{dof}}/N_{\mathrm{step}}$

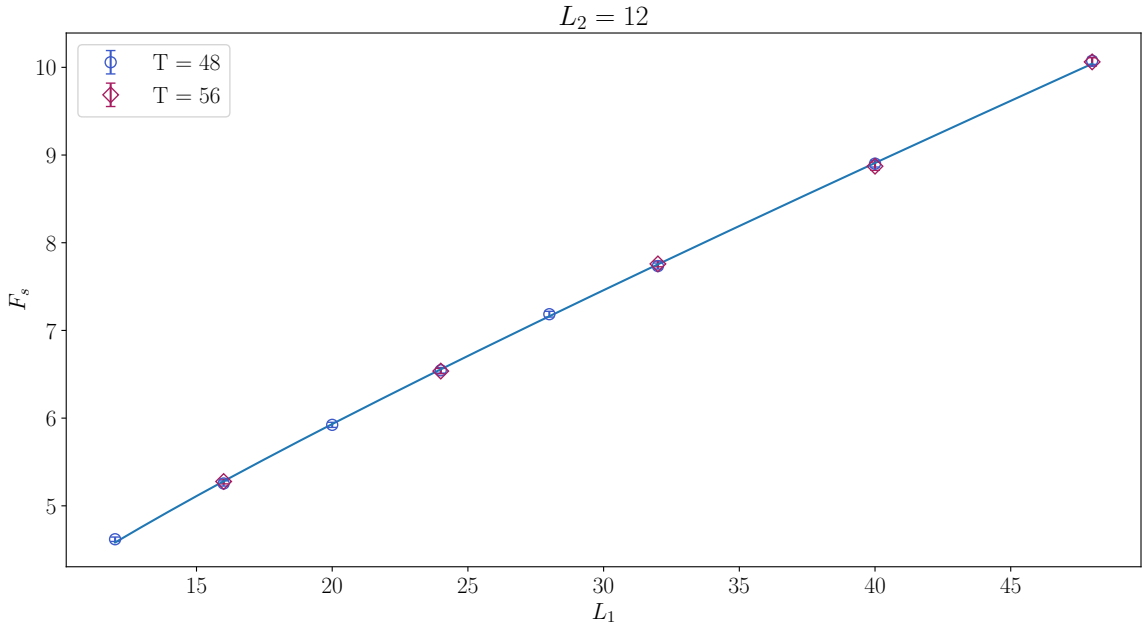
Scaling


10x10
14x14
20x20
10^0
10^{-1}
D_{KL}
10^0
10^1
$N_{\mathrm{dof}}{}^{1.5}/N_{\mathrm{step}}$

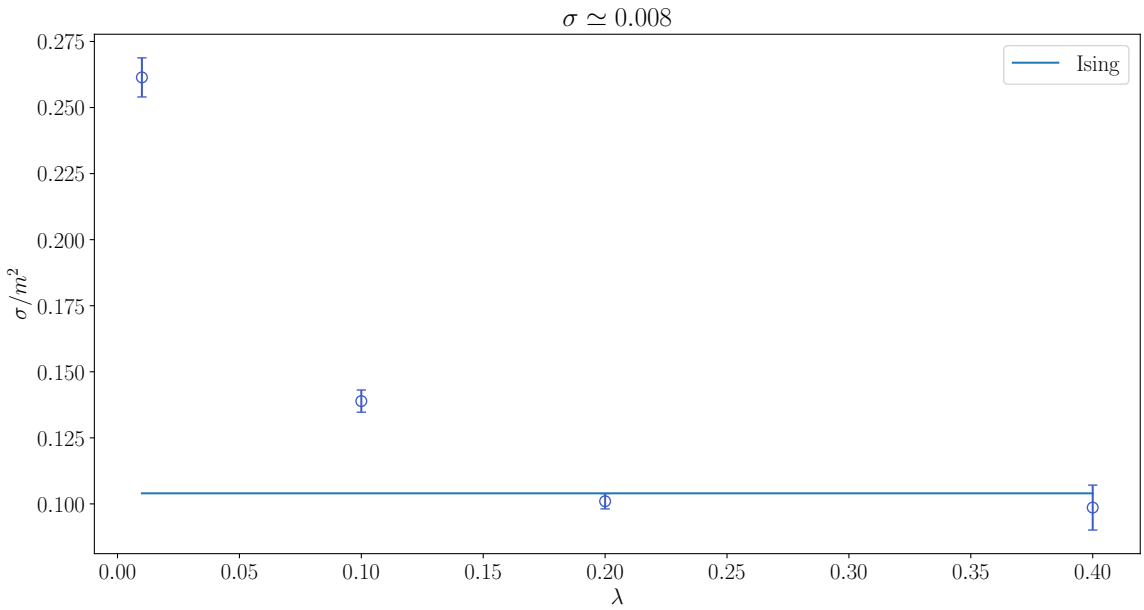
Some Results: F_s only depends on L_1 and L_2



Some Results: F_s and Effective String Model



Some Results: σ/m^2 far from Ising

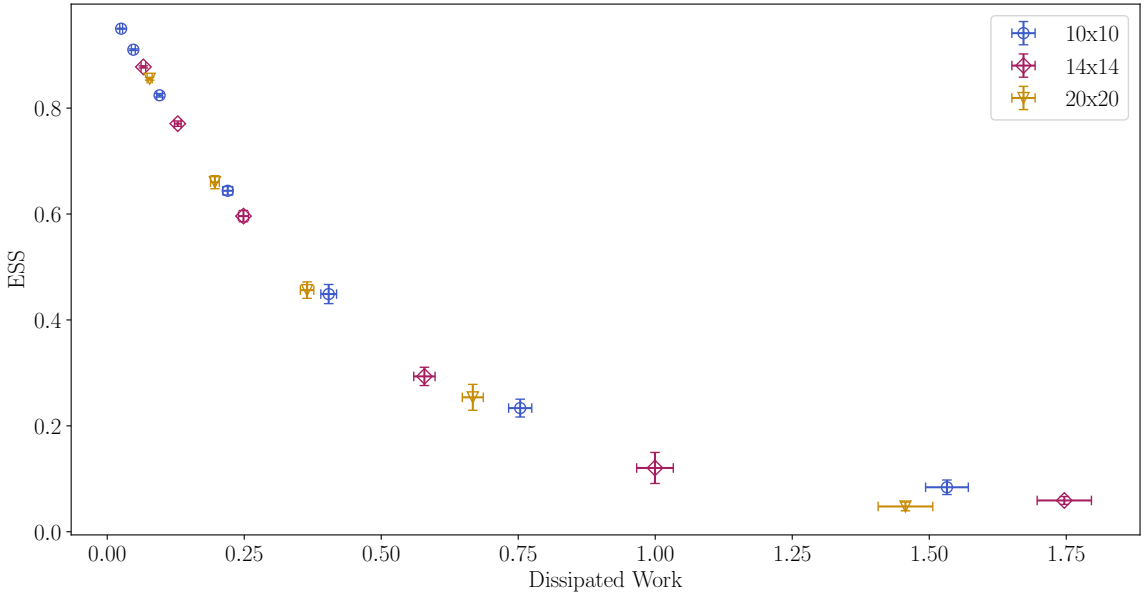


Concluding remarks

- Jarzinsky equality can be easily proven for Markov chains
- It offers a direct way for computing differences in **free energy**
- Jarzynski equality can be used to **sample** equilibrium distributions using out-of-equilibrium simulations
- ESS and dissipated work (D_{KL}) are important **metrics**
- **Scaling** the volume, performances can be retained with polynomial cost

Thank you for your attention!

ESS and Dissipated Work



A Note on F_s

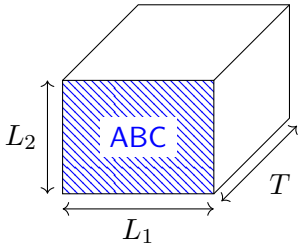
The free energy difference ΔF between ABC and PBC is

$$\Delta F = F_s(L_1, L_2) - \log T$$

Given that $1/m \ll T \ll L_{\text{gas}}$, F_s is a function of L_1 and L_2 only

- m is the mass of the bulk particle
- L_{gas} is an exponentially large scale ($\mathcal{O}\left(e^{F_s}\right)$)

For $T > L_{\text{gas}}$ a gas of interfaces is formed



More precisely

$$L_{\text{gas}} = \tfrac{1}{2} e^{F_s^{(2)}}$$

where $F_s^{(2)} \simeq F_s$ is the free energy of each interface in a pair of consecutive interfaces

Dissipated Work

By definition the dissipated work of a trajectory is

$$W_d = W - \Delta F$$

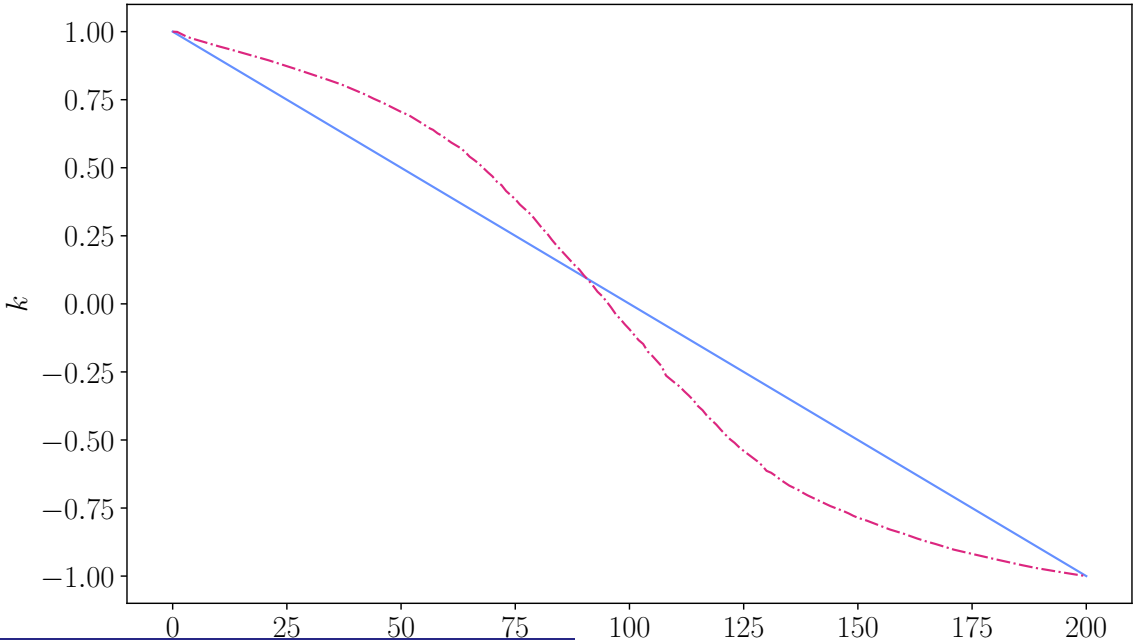
In practice, its average can be computed as follows:

$$\log \langle \exp(-W + \langle W \rangle) \rangle = \langle W \rangle + \log \langle \exp(-W) \rangle \stackrel{J}{=} \langle W \rangle - \Delta F = \langle W_d \rangle$$

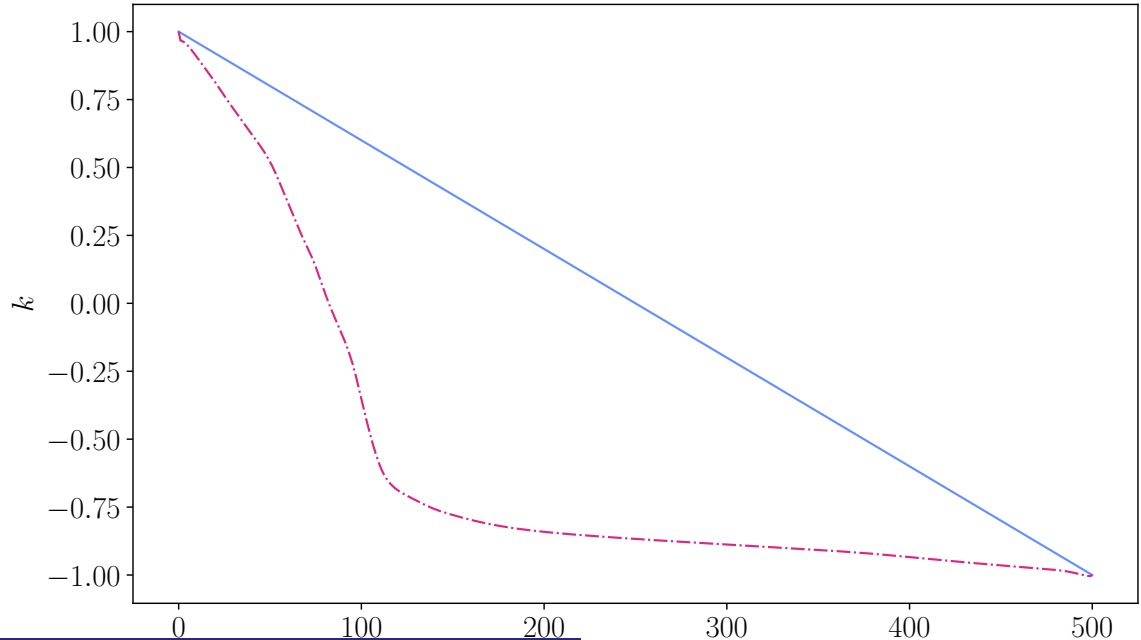
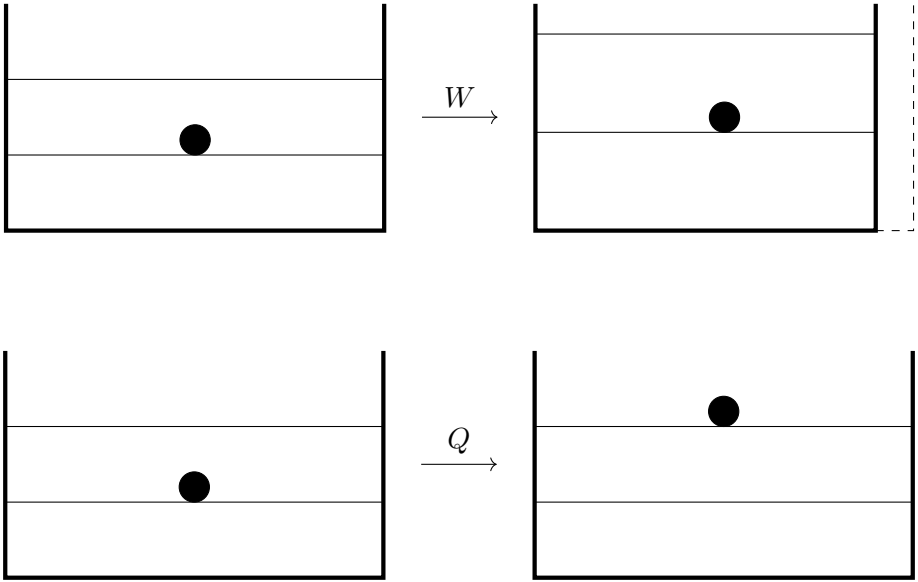
Where $\stackrel{J}{=}$ denotes Jarzynski Equality:

$$\langle e^{-W} \rangle \stackrel{J}{=} e^{-\Delta F}$$

Searching for Optimal Protocol



Protocol Bad



Work and Heat: by cartoons