

Free energy of interfaces in the ϕ^4 theory

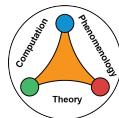
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DI TORINO



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- 1 The model and the motivation
 - ϕ^4 phase diagram
 - Interfaces
 - Free energy and Strings
- 2 Compute free energy with Jarzynski
- 3 Results
 - fitting the free energy
 - going far from Ising
- 4 Speculation
 - digression on $U(1)$
 - comparison
- 5 Conclusions

Phase diagram of ϕ^4

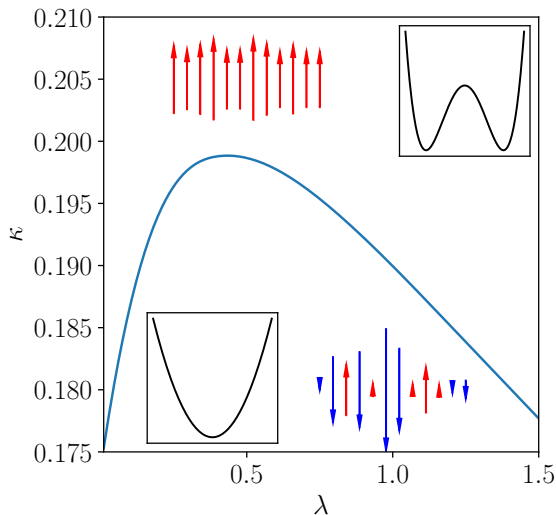
We will consider ϕ^4 theory in three space-time dimensions:

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

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]



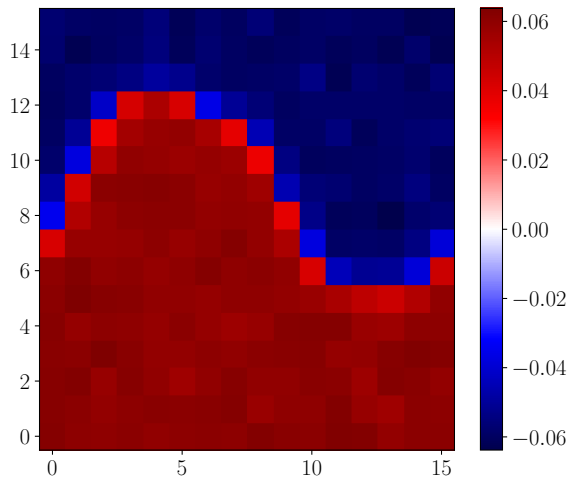
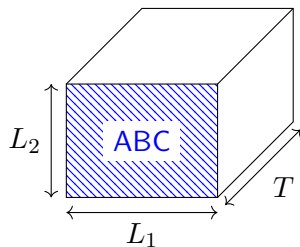
Inducing an Interface

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

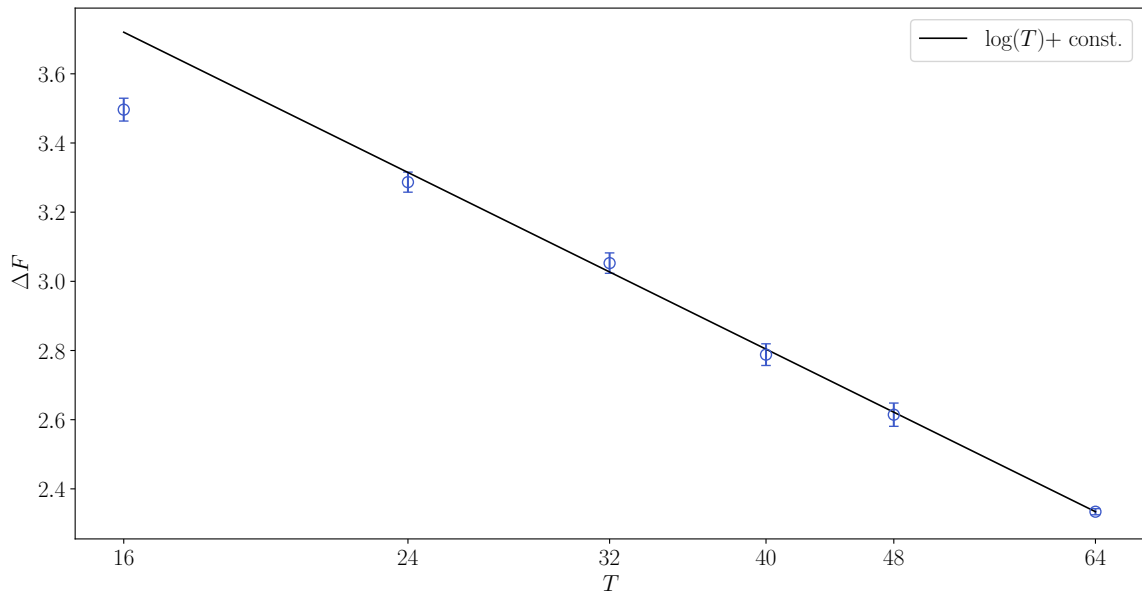
Somewhere in the lattice
an **interface** is induced

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

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



Logarithmic in T ($L_1 \times L_2 = 20 \times 20$)



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

F_s can be described with
an *Effective String Theory*

At large λ : everything like **Ising**

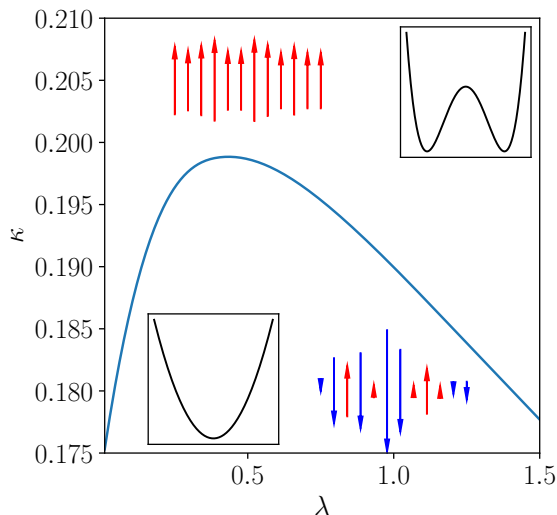
The **Universality Class** imposes

$$\sigma = 0.1040(8) m^2 \text{ [Caselle } et al., 2007]$$

m : mass of the particle in the bulk

Effective String Theory \sim Nambu-Gotō

Corrections begin at order $1/\sigma^3$



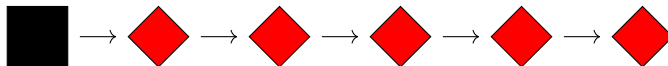
Out of Equilibrium MC

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

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

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}_λ

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

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

¹done on the system

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

$$\langle e^{-W} \rangle_f = e^{-\Delta F}$$

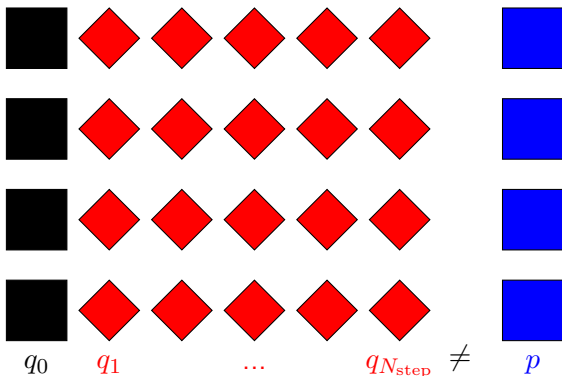
[Jarzynski, 1996]

$\langle \cdot \rangle_f$ is the average over **forward trajectories**

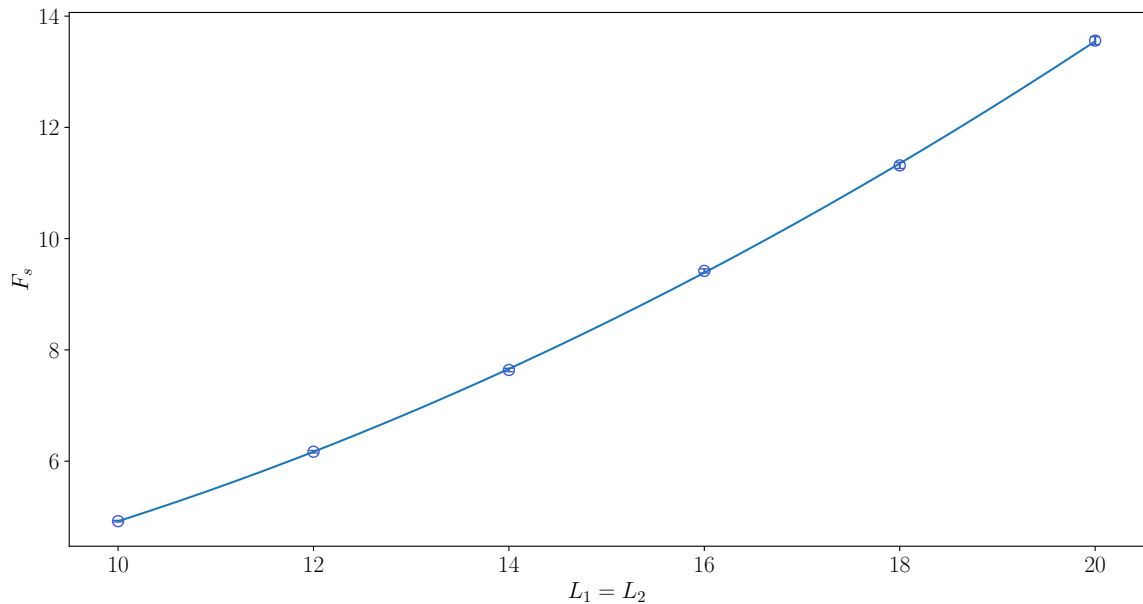
ΔF is the **free energy difference**
between $\lambda(0)$ and $\lambda(N_{\text{step}})$

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

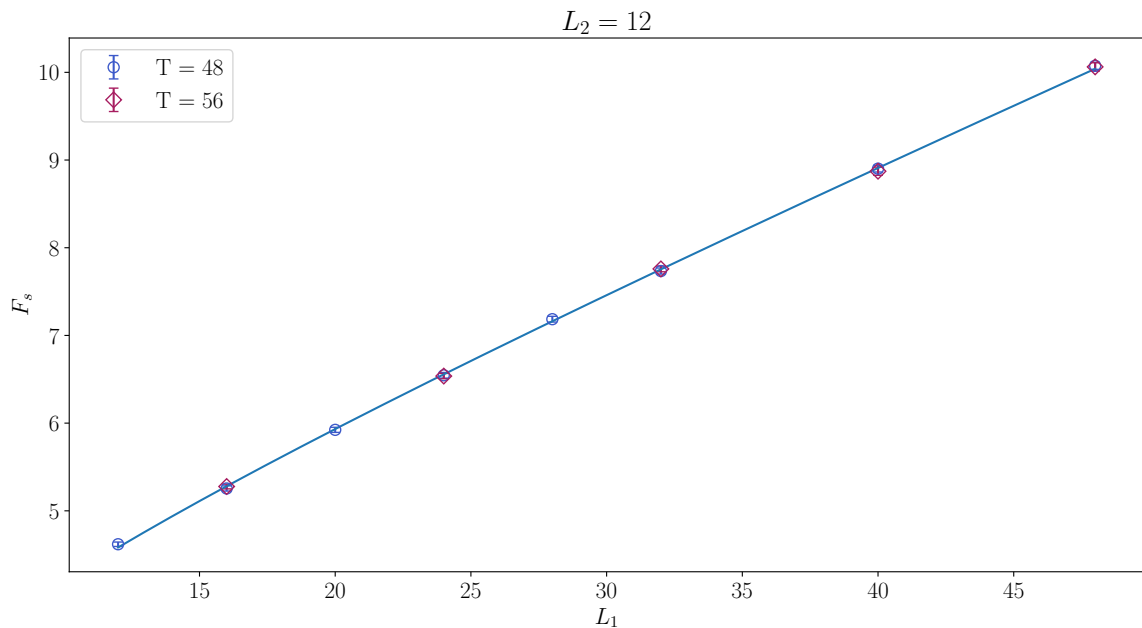
ΔF is the difference in free energy between
the q_0 and p **equilibrium distribution**



Fitting the String



Fitting the String



Going far from Ising

Ising universality class:

$$\sigma = 0.1040(8) m^2$$

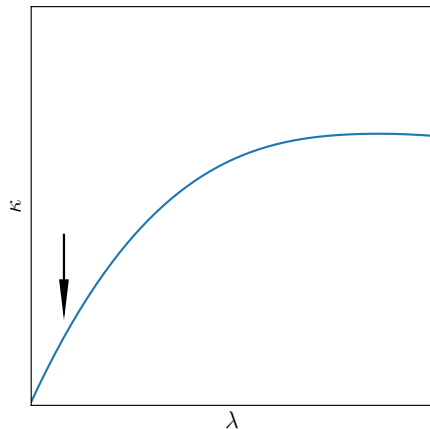
At very small λ :

attraction from the **Gaussian fixed point**

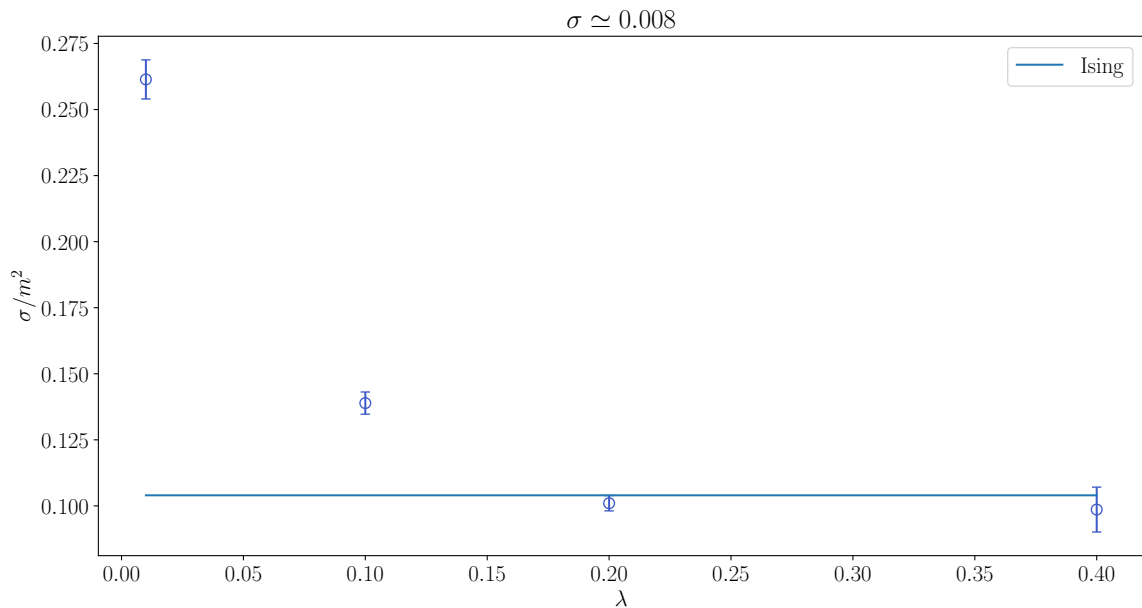
Violent corrections to the universal scaling

Unless we take κ very close to κ_c

We will see a **different value of σ/m^2**



Going far from Ising: some results for σ/m^2



A different regime for the string?

Interestingly: the attraction from the Gaussian fixed point makes σ/m^2 **larger**

Can we make it very large?

How would the effective string theory look in that scenario?

Can we reach a scenario similar to $U(1)$ in $2 + 1D$?

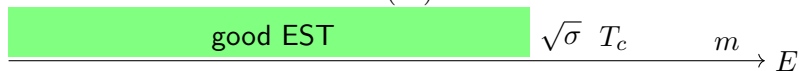
Here approaching the continuum limit we have $\sigma \gg m^2$

[Aharony *et al.*2024]

The case of U(1)

Why is EST a good effective theory?

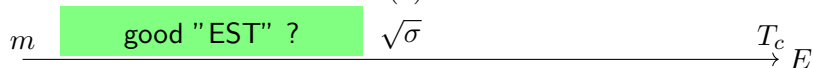
Usual SU(N) case:



Only one mass-scale (Λ_{QCD} if you want), lot of space below!

That is not always the case...

The U(1) case:



Other kinds of string? The U(1) "effective string"

The U(1) case:

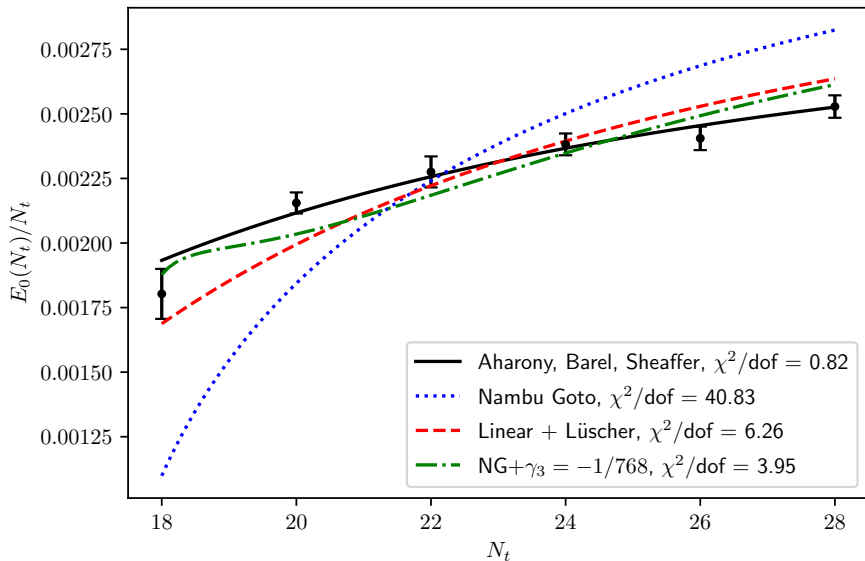
$$m \quad \text{good "EST" ?} \quad \sqrt{\sigma} \quad \xrightarrow{T_c} E$$

- Peculiar scenario: gapless in a continuum limit ($m \rightarrow 0$)
- It is possible to build effective theory [Aharony *et al.*2024]:
for $m \gg \mu \gg \sqrt{\sigma}$
- At large distances still have $\langle P P^\dagger \rangle \sim K_0(E_0 R)$
- but now

$$E_0 = \sigma L - \frac{\pi}{6L} + \frac{1}{\pi L} \text{Li}_2(e^{-mL})$$

Note $\text{Li}_2(z) \rightarrow 0$ when $z \rightarrow 0$,
so the new term vanishes for large m_0 .

U(1): numerical results



[Caselle and Mariani, 2025]

Comparing ϕ^4 to U(1)

Interestingly both strings are "**solitonic**"

- in ϕ^4 is the kink between the two vacua
- in U(1) is the Condensation of monopoles [Polyakov, 1976]

The solitonic nature of the U(1) string is actually more evident in a dual model
Which is again a **scalar interacting theory** with effective $\cos(\phi)$ potential

$$S_W \rightarrow \frac{1}{4\pi^2 \beta} \sum_x \left[\frac{1}{2} (\nabla \phi)^2 + 8\pi^2 \beta e^{-k\beta} \cos(\phi) \right]$$

And $m^2 = 8\pi^2 \beta e^{-k\beta}$

In U(1) we can only tune β and go closer to or farther from the continuum limit

In ϕ^4 tuning **two parameters** (λ and κ) we can vary m and σ independently
(although it is less obvious how)

- We can reliably measure the free energy due to interfaces
- In $2 + 1D$ ϕ^4 theory it can be described by an EST
- Close to the critical line σ/m^2 is predicted by the universality class
- The Gaussian fixed point induces strong corrections that make σ larger
- How close should we go to the Gaussian fixed point to see $\sigma \gg m^2$?
- Will we find exactly the same phenomenology as in the $U(1)$ case?
- We know exactly the shape of the soliton in ϕ^4 as well as in $U(1)$

Thank you for your attention!

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 $SU(3)$ gauge theory

Bonanno *et al.*, 2025

Annealed Importance Sampling

Neal, 1998

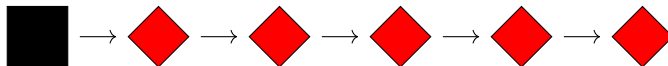
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Jarzynski Equality

$$\langle e^{-W} \rangle_f = e^{-\Delta F}$$

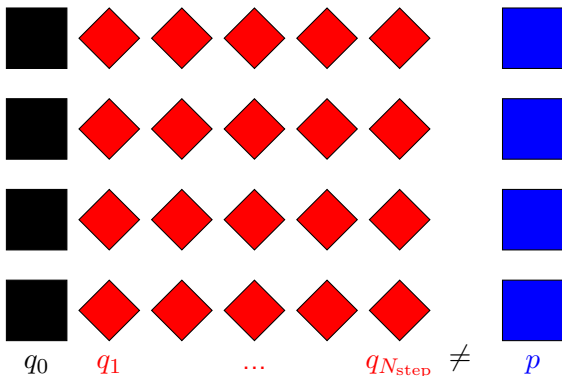
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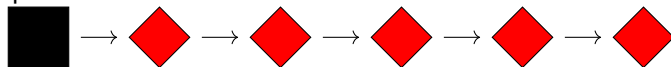
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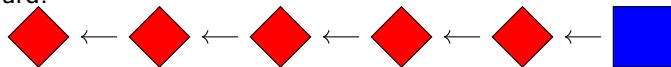
Forward and Reverse Process

Besides the forward process



$$P_f = q_0(\phi_0) \prod_{k=1}^{N_{\text{step}}} \mathcal{P}_{\lambda(k)}(\phi_{k-1} \rightarrow \phi_k)$$

Consider the backward:



$$P_r = p(\phi_{N_{\text{step}}}) \prod_{k=1}^{N_{\text{step}}} \mathcal{P}_{\lambda(k)}(\phi_k \rightarrow \phi_{k-1})$$

Crooks Fluctuation Theorem

Let us compute

$$\log \frac{P_f}{P_r} = \log \frac{q_0(\phi_0)}{p(\phi_{N_{\text{step}}})} \sum_{k=1}^{N_{\text{step}}} \log \frac{\mathcal{P}_{\lambda(k)}(\phi_{k-1} \rightarrow \phi_k)}{\mathcal{P}_{\lambda(k)}(\phi_k \rightarrow \phi_{k-1})} = S_{N_{\text{step}}}(\phi_{N_{\text{step}}}) - S_0(\phi_0) - \Delta F - Q$$

since

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

by detailed balance

[Crooks, 1999]

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

$$\log \frac{P_f}{P_r} = W - \Delta F = W_d$$

Unbiased Sampling and Proving Jarzynski

$$P_r = P_f e^{-W_d} = P_f e^{\Delta F - W}$$

We would like to sample the **target** p :

$$\langle \mathcal{O} \rangle_p = \int \mathcal{D}\phi p(\phi) \mathcal{O}(\phi) = \int \prod_{k=0}^{N_{\text{step}}} \mathcal{D}\phi_k P_r \mathcal{O}(\phi_{N_{\text{step}}}) = \int \prod_{k=0}^{N_{\text{step}}} \mathcal{D}\phi_k P_f e^{-W_d} \mathcal{O}(\phi_{N_{\text{step}}})$$

or shortly

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

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

$$1 = \langle e^{-W_d} \rangle_f$$

or

$$e^{-\Delta F} = \langle e^{-W} \rangle_f$$

Metrics of Jarzynski: the Dissipated Work

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

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:

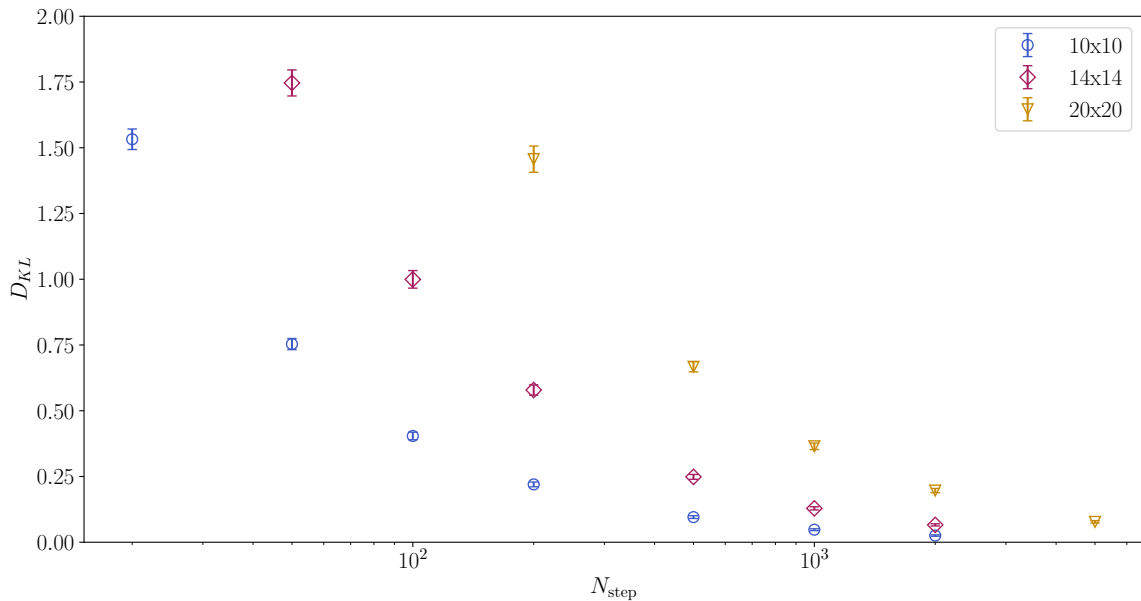
$$0 \leq D_{\text{KL}}(P_f || P_r) = \langle \log \frac{P_f}{P_r} \rangle_f = \langle W_d \rangle_f$$

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 $\langle W \rangle_f \geq \Delta F$
(Second law of thermodynamics)

Metrics of Jarzynski: the Dissipated Work



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

$$\text{ESS}_{\mathcal{O}} = \frac{\text{Var}(\mathcal{O})_p}{\text{Var}(\mathcal{O} e^{-W_d})_f}$$

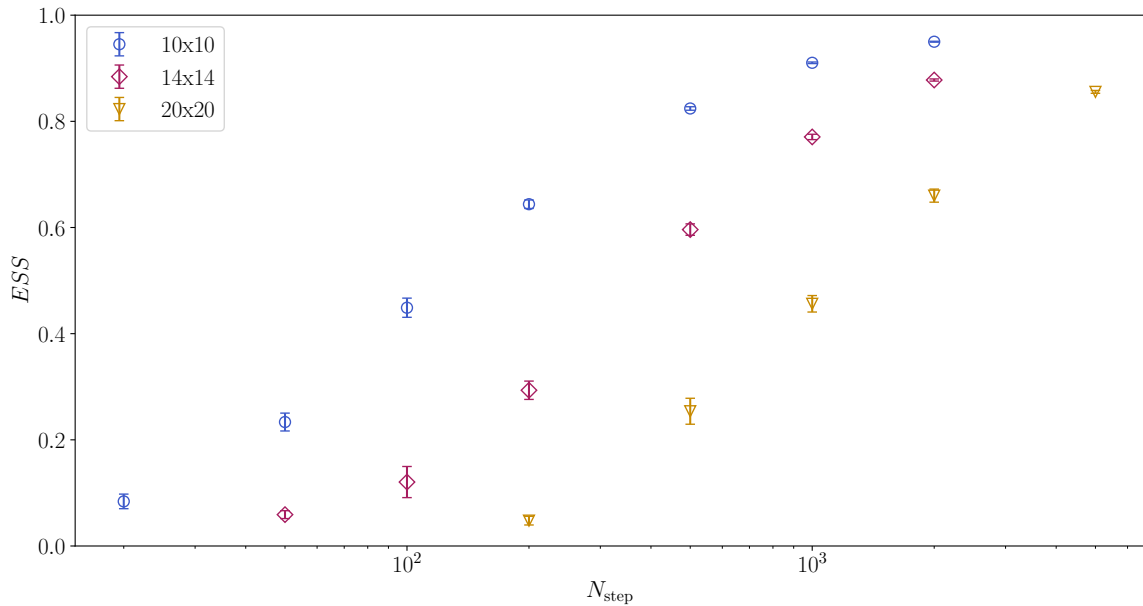
Neglecting the correlations between \mathcal{O} and e^{-W_d} , we define a "generic" ESS

$$\text{ESS} = \frac{\langle e^{-W} \rangle_f^2}{\langle e^{-2W} \rangle_f} = \frac{1}{\langle e^{-2W_d} \rangle_f}$$

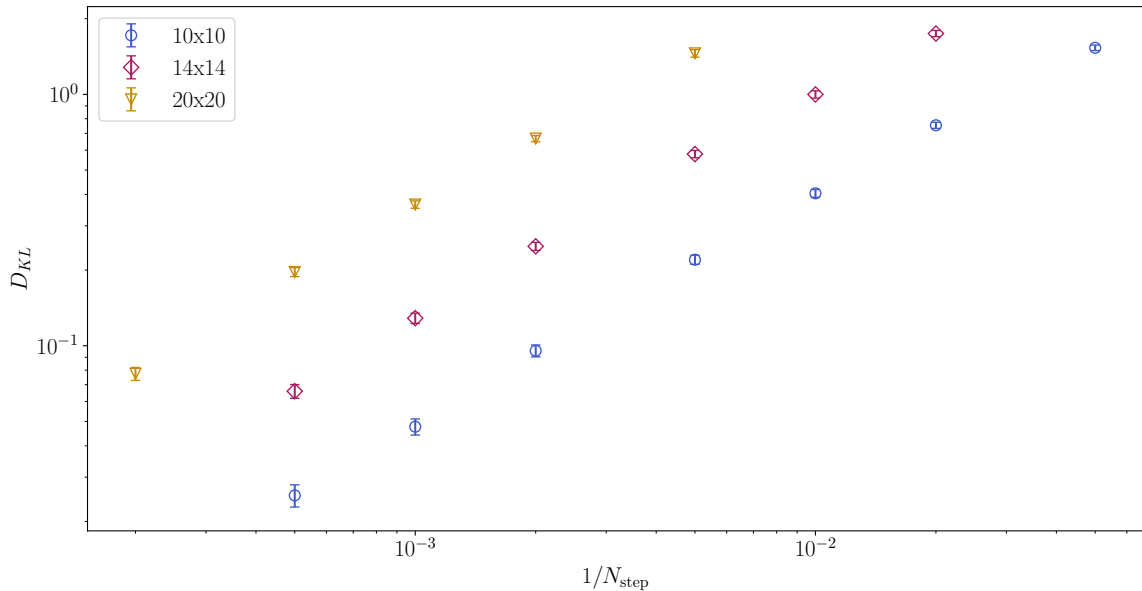
This is an estimation of the quality of the sampling

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

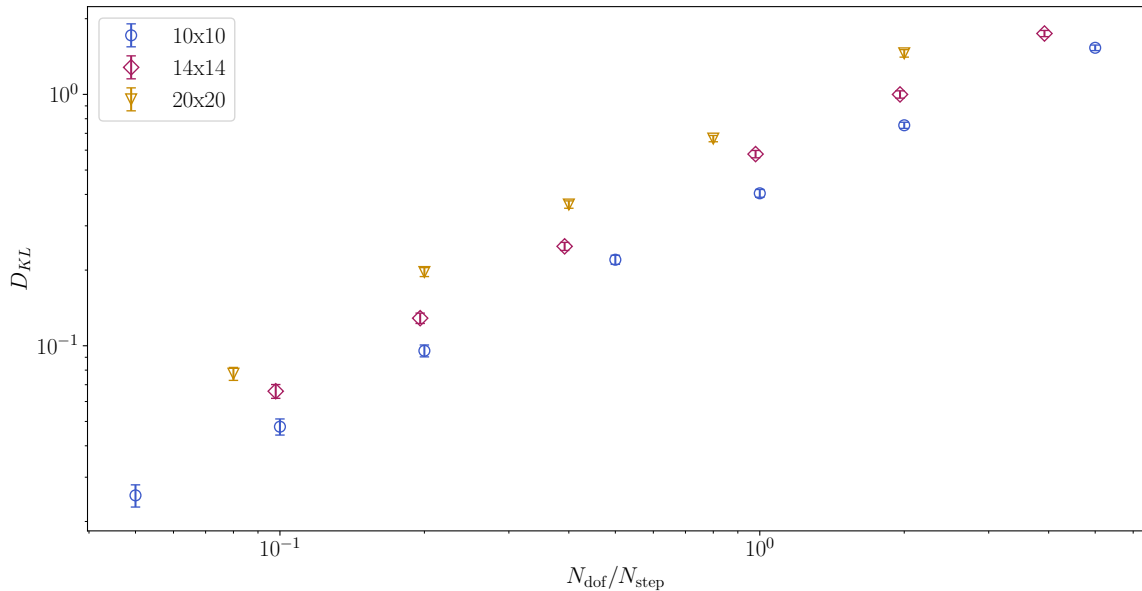
Metrics of Jarzynski: the ESS



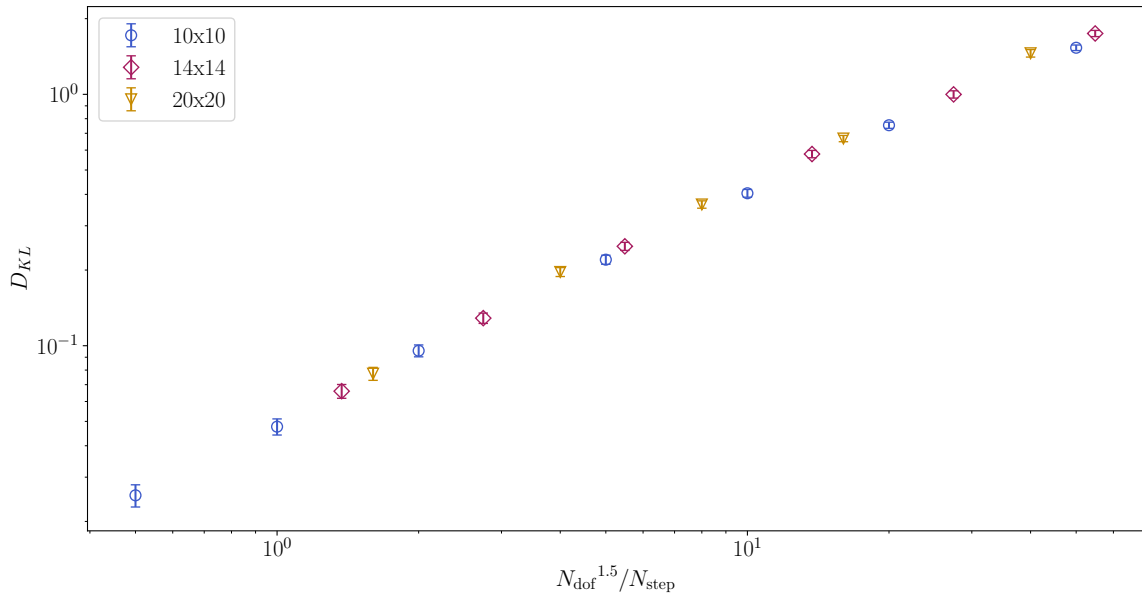
Scaling



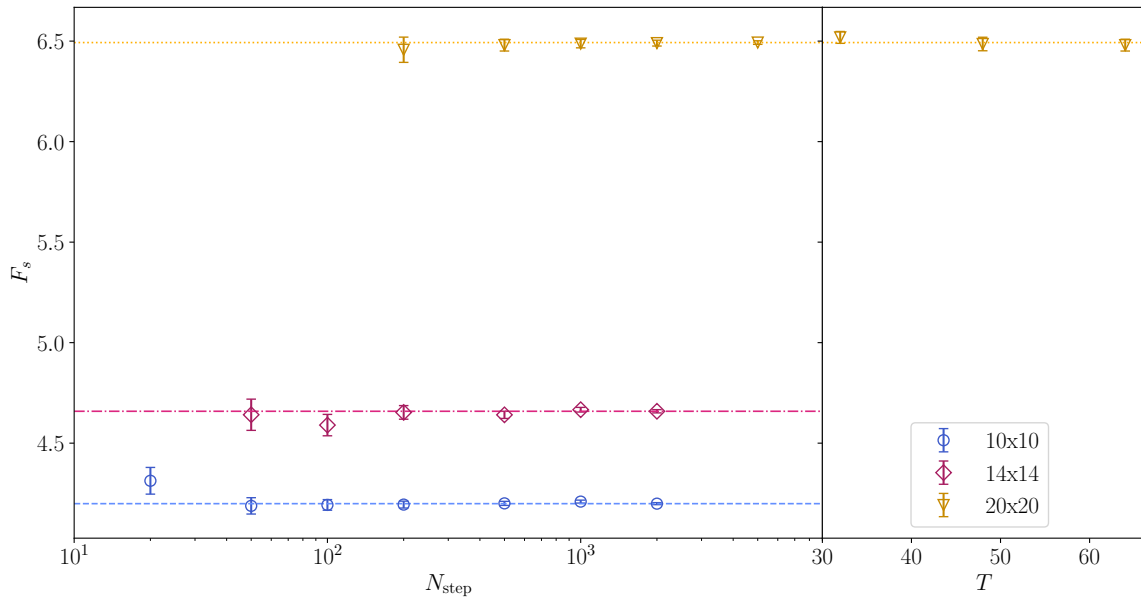
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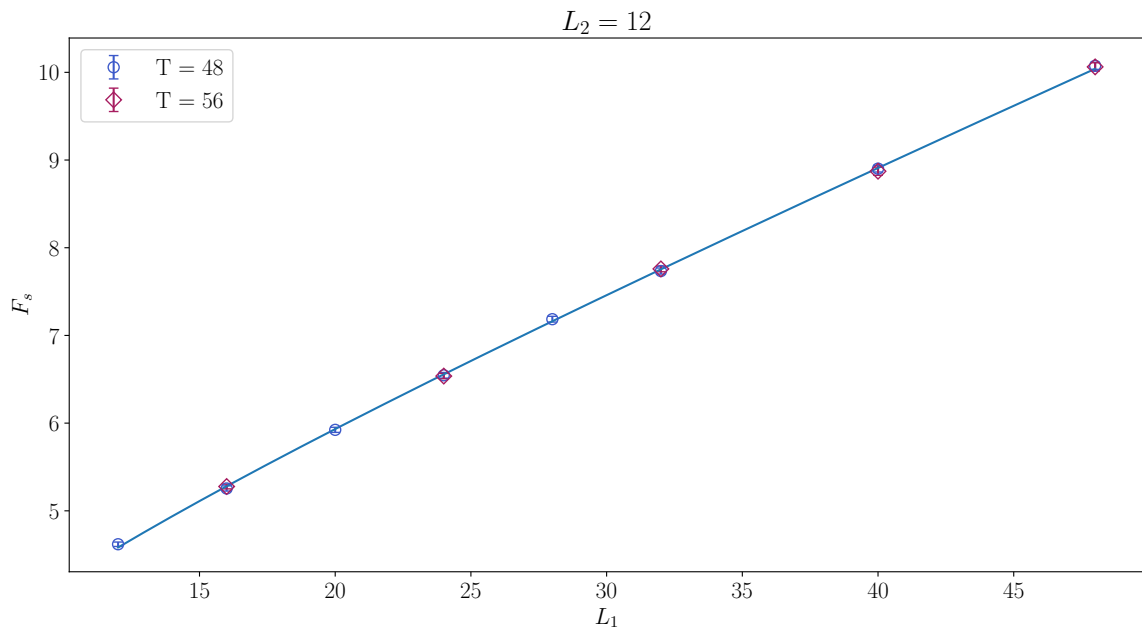
Scaling



Some Results: F_s only depends on L_1 and L_2



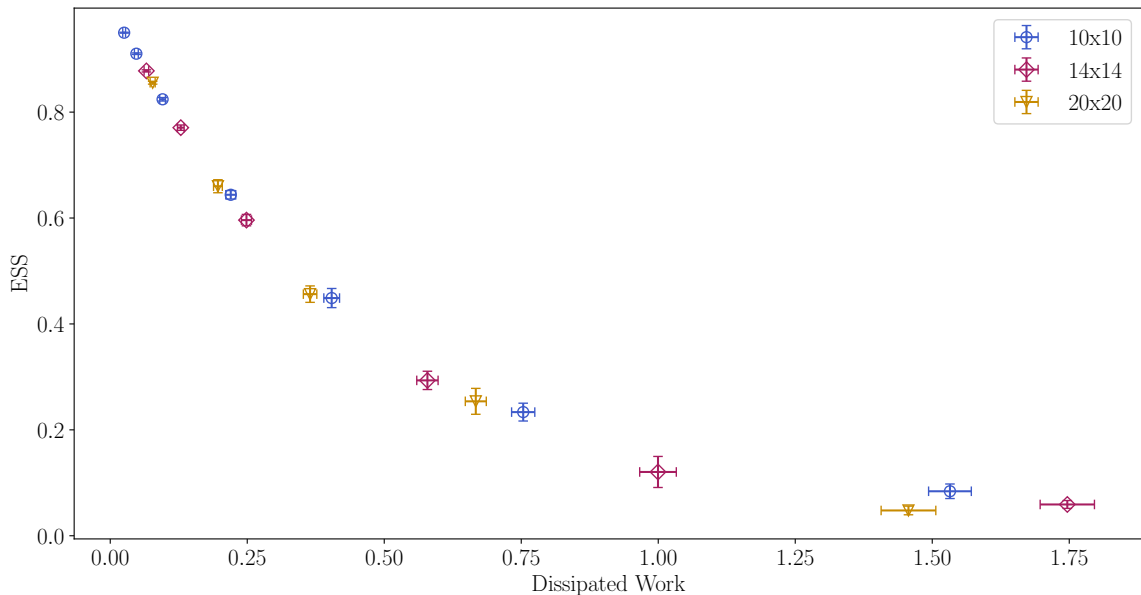
Some Results: F_s and Effective String Model



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

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

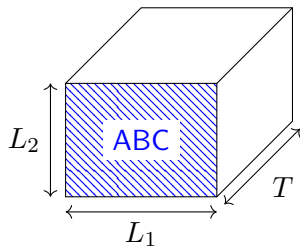
- m is the mass of the bulk particle
- L_{gas} is an exponentially large scale ($\mathcal{O}(e^{F_s})$)

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

More precisely

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

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

$$W_d = W - \Delta F$$

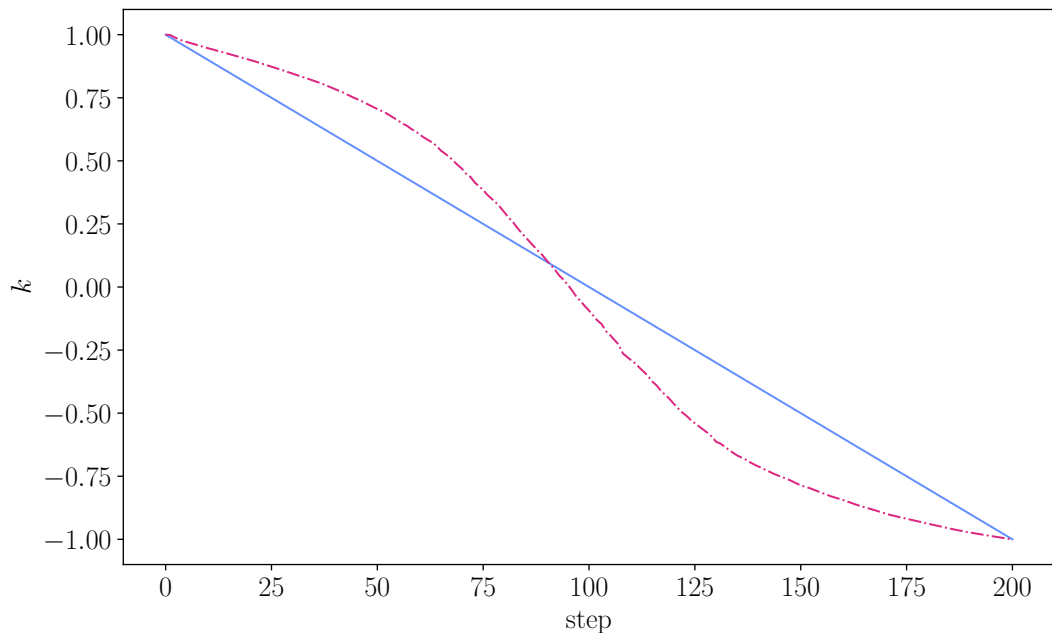
In practice, its average can be computed as follows:

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

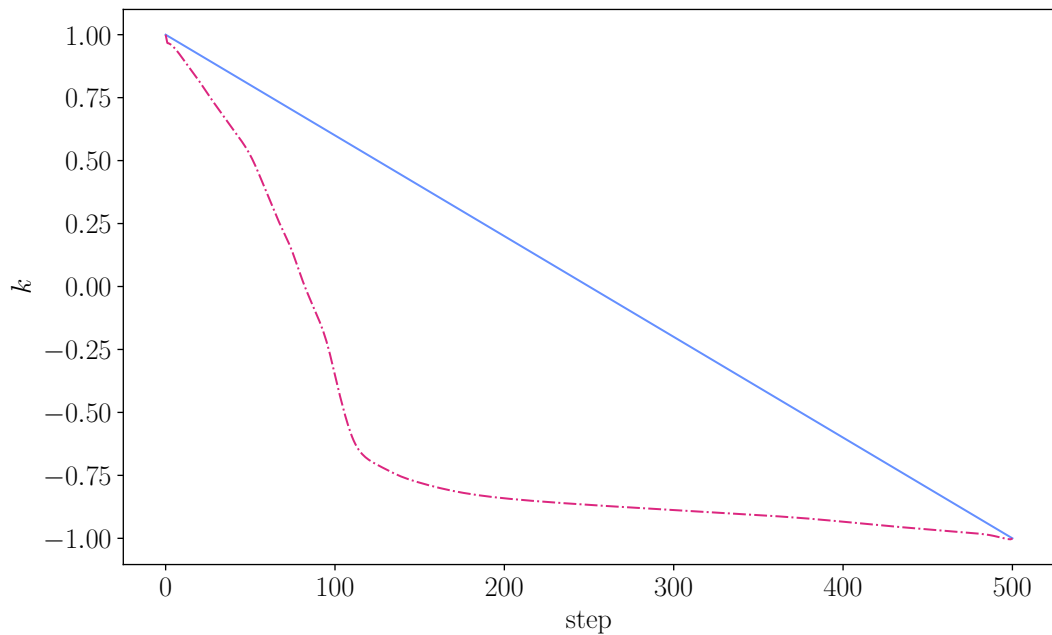
Where $\stackrel{J}{=}$ denotes Jarzynski Equality:

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

Searching for Optimal Protocol



Protocol Bad



Work and Heat: in cartoons

