Is the Jarzynski Equation Valid for Non-Gibbsian Pure Initial Quantum States?

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Overview

This talk mainly consists of the presentation of numerical experiments on dynamics of spin-systems .

These numerical investigations indicate that the Jarzynski-equality may approximately hold in many cases, even if the initial state is masively non-thermal.

Our (or at least my) understanding of the numerical findings is moderate.

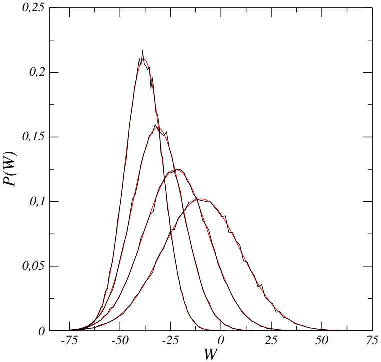
All presented results are publisehd in: *Phys. Rev. E 94, 012125 (2016)* and *Phys. Rev. E, 89, 012131, (2014)*

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

remember: $P(W)$ may depend heavily on the protocol

- very general statement(s), valid far from equilibrium
- statment 1: l.h.s. independent of process protocol
- statement 2: l.h.s. equals an equilibrium property

illustration of “standard Jarzynski”



J. Stat. Mech. (2006) P06005, C. Chatelain and D. Karevski

Questions:

What is “work” W in the quantum context? $\Rightarrow$
Not so simple since there is no trajectory

Under which condition is the Jarzynski equation valid?

quantum work P. Talkner and P. Hanggi, Phys. Rev. E, 93, 022131 (2016)

So far there is no generally accepted definition of work in the quantum context. However, a very popular approach is the "two-energy-measurements-scheme"

- 1. Do a first projective measurement of the full system energy $\Rightarrow E_{ini}$
- 2. Perform a process by means of a time dependent Hamiltonian $\hat{H}(\lambda(t))$
- 3. Do second projective measurement of the full system energy $\Rightarrow E_{fin}$

The difference between the second and first energy measurement is work, i.e., $W = E_{fin} - E_{ini}$

validity of Jarzynski M. Campisi, P. Hanggi, and P. Talkner, Rev. Mod. Phys. 83, 771 (2011)

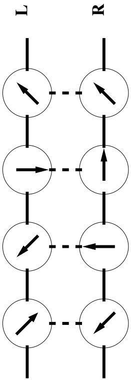
It has been shown that Jarzynski is generally valid if the initial state of the full system is Gibbsian, i.e.,

$$\hat{\rho}_{ini} \propto e^{-\beta(\hat{H}_{sys}+\hat{H}_{env}+\hat{H}_{int})}$$

- Details of $\hat{\rho}_{ini}$ matter. It cannot be replaced by requiring the equivalence of ensembles, etc.
- Preparing $\hat{\rho}_{ini}$ requires a "superbath". What if there is none?

May extrinsic thermal relaxation be replaced by some intrinsic mechanism ?

“spin-ladder”



Heisenberg-type Hamiltonian:

$$\hat{H} = \sum_{ij} J_{ij}(\hat{\sigma}_x^i \hat{\sigma}_x^j + \hat{\sigma}_y^i \hat{\sigma}_y^j + 0.6\ \hat{\sigma}_z^i \hat{\sigma}_z^j),$$

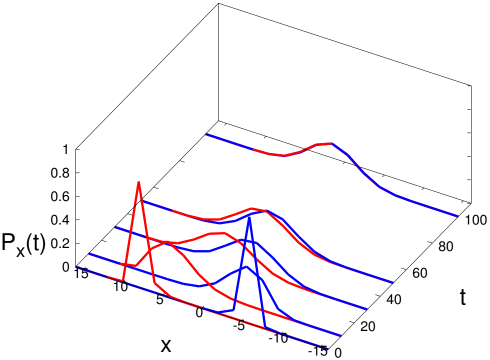
Observable

$$\hat{x} = \frac{1}{2}\left(\sum_{l \in L} \hat{\sigma}_z^l - \sum_{r \in R} \hat{\sigma}_z^r\right)$$

Roughly this may be viewed as particles hopping between the junctions of a ladder. The particles may hop along the legs and along the rungs. The particles interact. X counts the difference of particles between the legs leg. There are 16 rungs (32 spins) and 16 particles (“half filling”).

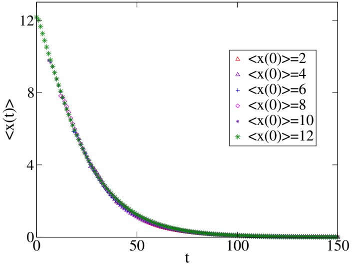
We solved the Schrödinger equation for a pure state as concentrated in X and energy, as we could possibly prepare:

$P_X(t)$: probability to find a certain X

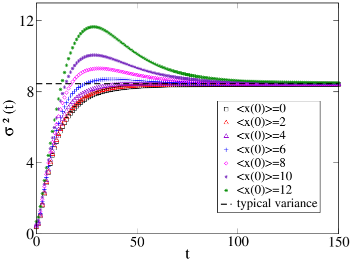


The particle difference essentially behaves like a Brownian particle in parabolic potential.

time shifted $\langle \hat{x}(t) \rangle$



variances of x



initial state:

$$|\Psi(a, E_{\text{ini}})\rangle \propto e^{-a(\hat{H}-E_{\text{ini}})^2}\, |\Phi\rangle$$

$|\Phi\rangle$: "Haar measure random state"

protocol:

$$\hat{H}(t) = \hat{H} - h_{\text{max}}\, f(t)\, \hat{x}$$

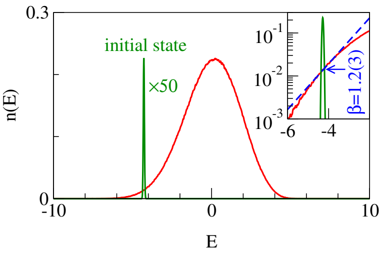
with

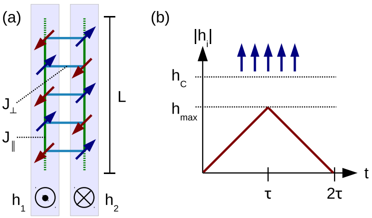
$$f(t) = \begin{cases} t/\tau\,, & 0 < t \leq \tau\,, \\ 2 - t/\tau\,, & \tau < t \leq 2\tau\,. \end{cases}$$

"temperature"

$$\beta = \frac{\mathrm{d}}{\mathrm{d}E} \ln n(E)$$

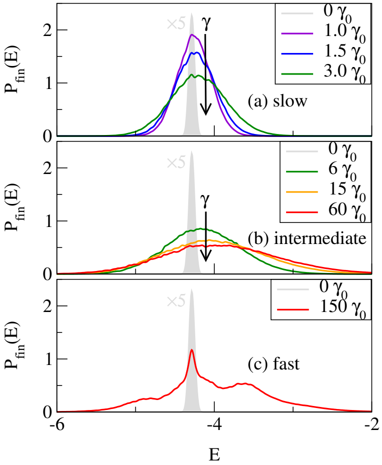
$n(E)$: density of states



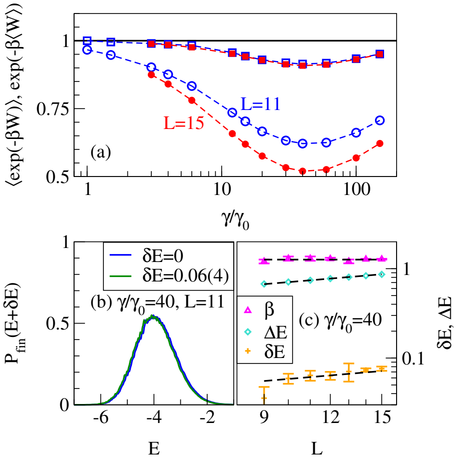


Pure Quantum Jarzynski: Results

work pdf's



"Jarzynski quantifiers"



This suggests that Jarzynski may approximately hold for pertinent systems and protocols, even if the initial state is not Gibbsian.

What may be inferred from this numerical experiment?

Why Jarzynski cannot (approximately) hold for all systems, protocols and non-Gibbsian initial states: $\Rightarrow$ Counter examples are easy to construct.

Why Jarzynski could hold for very many systems, protocols and non-Gibbsian initial states (Michele's idea):

$$\langle e^{-\beta W} \rangle = \langle e^{-\beta H^{H}_{\text{fin}}} e^{\beta H_{\text{ini}}} \rangle_{\text{diag}} \qquad \text{always true}$$

P. Talkner, P. Hanggi, and M. Morillo, Phys. Rev. E 77, 051131 (2008)

$$\langle e^{-\beta W} \rangle = \langle e^{-\beta H^{H}_{\text{fin}}} e^{-\beta H_{\text{ini}}} \rangle_{\text{can}} = e^{-\beta \Delta F} \qquad \text{always true}$$

$$\langle e^{-\beta H^{H}_{\text{fin}}} e^{\beta H_{\text{ini}}} \rangle_{\text{eigenstate}} \stackrel{?}{=} \langle e^{-\beta H^{H}_{\text{fin}}} e^{\beta H_{\text{ini}}} \rangle_{\text{can}} \qquad \text{true if ETH holds}$$

- The last equation is a form of the "Eigenstate Thermalization Hypothesis" (ETH) countless papers on the ETH written by many people starting with Deutschin 1991
- If the latter holds for all (!) $e^{-\beta H^{H}_{\text{fin}}} e^{\beta H_{\text{ini}}}$, Jarzynski holds for initial energy eigenstates
- However, $e^{-\beta H^{H}_{\text{fin}}} e^{\beta H_{\text{ini}}}$ is a rather exotic operator in the context of the ETH.
- The previous numerics may be viewed as a rough check of the ETH.

bottom line: There are people out there trying to show that thermal initial sates are not at the heart of the Jarzynski-relation.

The talk itself as well as the papers on which it is based are (hopefully) already accessible through our homepage.

Thank you for your attention !