Is the Jarzynski Equation Generically Valid, Even for Strongly Non-Gibbsian, Pure Initial Quantum States?

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Instead of an Outline

- The decision that this talk would happen was reached rather late, too late to prepare it carefully.
- Thus, this talk is an enlarged version of 15-min talk just given at the DPG-spring meeting, Dresden
- Most people in the audience likely know more about the Jarzynski relation than I do. I apologize for nevertheless talking about it. Any expert input is welcome !
- Numerical data, especially in the second part of this talk is rather preliminary and comes with absolutely no warranty...

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

What is work in the quantum world ?

P. Talkner et al., Phys. Rev. E, 93, 022131 (2016),
Gallego et al., New J. Phys. 18, 103017 (2016), etc.

Here we employ the "two-energy-measurements-scheme":

measure energy: E_{ini} $\Rightarrow$ "move" Hamiltonian $\Rightarrow$ measure energy again: E_{fin} .
work: $W = E_{fin} - E_{ini}$

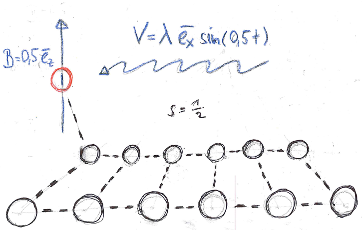
When is the Jarzynski equation guaranteed to be valid ?
$\Rightarrow$ If the initial state of the full system is Gibbsian, i.e.,

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

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

- 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 Jarzynski possibly also hold for $\hat{\rho}_{ini} = |\epsilon_0\rangle\langle\epsilon_0|$, with $|\epsilon_0\rangle$ being an energy eigenstate of the full system? (For pertinent systems, of course)



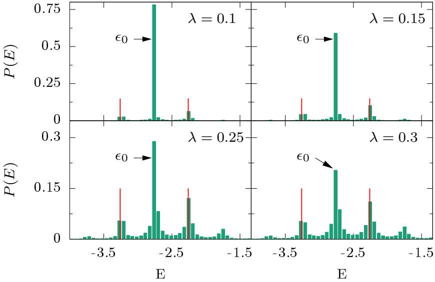
The ladder plays the role of a bath, to which the spin is weakly coupled.
We irradiate resonantly for six sine-periods (cyclic protocol):

$$\hat{H} = \hat{H}_0 + \lambda \hat{V}(t)$$
$$\hat{H}_0 = B\hat{s}_z + \hat{H}_{SL} + \hat{H}_L$$
$$\hat{V}(t) = \sin(Bt)\hat{s}_x$$

initial state is an energy eigenstate of $\hat{H}_0$

energy probability distribution after irradiation

$(N = 17\,,\ B = 0.5\,,\ \omega = 0.5\,,\ p = 6)$

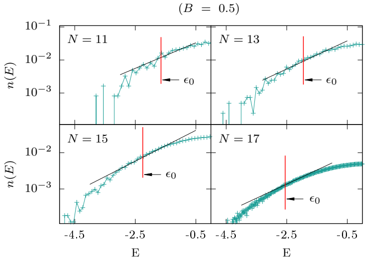


Is this outcome in accord with the Jarzynski equation?

And if so, what is the pertinent temperature?

Spin Resonance as Jarzynski Experiment

density of states of the total system around the initial energy

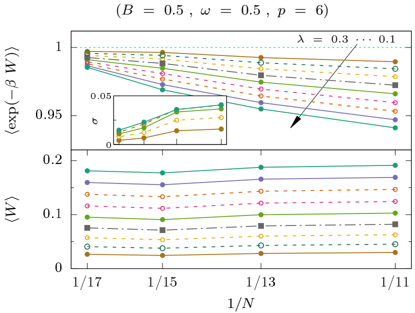


We start at an energy at which the density of states is nicely described by an exponential:

$$n(E) \approx e^{\beta E},$$

from this fit we take the inverse temperature β

scaling of "Jarzynski-quantifier" $\langle e^{-\beta W} \rangle$ with system size



Apparently the Jarzynski equation may hold in the limit of large (pertinent) systems even for extremely non-thermal initial states !

$\Rightarrow$ **Dresden ends, Bielefeld starts** $\Rightarrow$

Notes for Jochen Pisa 28 Aprile 2015

Microcanonical FT : $\frac{P_E(W)}{P_{E+W}(-W)} = \frac{\Omega_f(E+W)}{\Omega_i(E)}$

Consider cyclic protocol: then $H_i = H_f \Rightarrow \Omega_i = \Omega_f \Rightarrow \frac{P_E(W)}{P_{E+W}(-W)} = \frac{\Omega(E+W)}{\Omega(E)}$

Let's assume E and E+W are both in the exponential region of Ω where Ω can be written as : $\Omega(U) \doteq e^{\beta U}$

Then

$$\frac{P_E(W)}{P_{E+W}(-W)} = \frac{e^{\beta(E+W)}}{e^{\beta E}} \doteq e^{\beta W}$$

Hence $\langle e^{-\beta W}\rangle_E \doteq \int P_E(W)\, e^{-\beta W} dW = \int P_{E+W}(-W)\, dW \doteq N_\leftarrow(E)$.

$N_\leftarrow(E)$ generally differs from 1 M. Campisi, PRE 78 051123 (2008)

The question is then how much does $N_\leftarrow(E)$ differ from 1

“Stiff” Forward Probabilities

Consider the possibility that the work-pdf is essentially a function of the initial energy only, within a limited regime:

$$P(E_{fin}|E_{ini}) \stackrel{!}{=} f(E_{fin} - E_{ini})$$

for

$$\epsilon_- \leq E_{ini} \leq \epsilon_+$$

with

$$\int_{\epsilon_-}^{\epsilon_+} P(E_{fin}|\epsilon_0) dE_{fin} \approx 1,$$

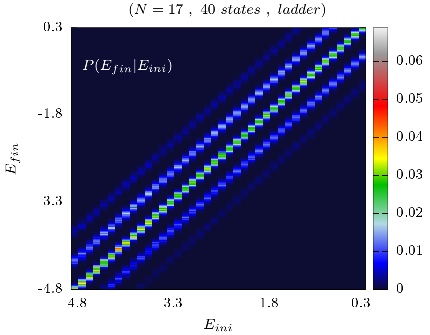
then,

$$\int_{\epsilon_-}^{\epsilon_+} P(\epsilon_0|E_{fin}) dE_{fin} =$$

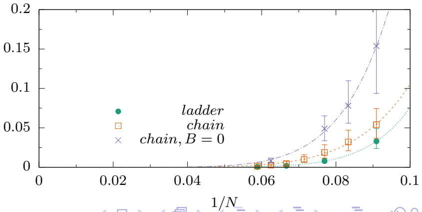
$$\int_{\epsilon_+}^{\epsilon_-} P(E_{fin}|\epsilon_0)(-dE_{fin}) \approx 1,$$

$\Rightarrow$ locally exponential density of states + locally stiff forward probabilities = Jarzynski equation holds

(grained) transition matrix $P(E_{fin}|E_{ini})$



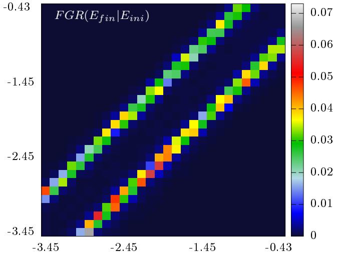
scaling of “stiffness” with system size



Coarse and Fine Structure of "Driving-Operator-Matrix"

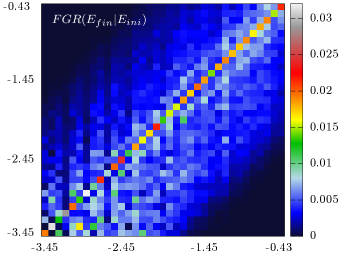
coarse: FGR - rates, ladder

$(N=13\ ,\ M=6|7\ ,\ ladder\ ,\ \kappa=0.2)$



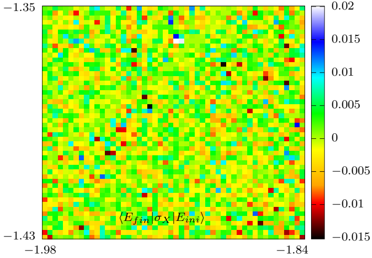
coarse: FGR - rates, chain

$(N=13\ ,\ M=6|7\ ,\ chain\ ,\ \kappa=1.0\ ,\ B=0)$



fine: individual matrix elements, ladder

$(N=13\ ,\ M=6\rightarrow M=7\ )$



fine: individual matrix elements, chain

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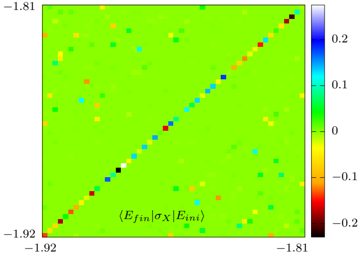
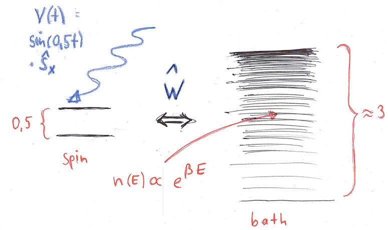


Random Matrix Based Model as a Convenient Testbed



"tailored" interaction $\hat{W}$

$$\langle E_f^B, 1|\hat{W}|E_i^B, 0\rangle = e^{\frac{\alpha(E_f+E_i)}{4}+i\phi}\cdot c(|E_f - E_i|)$$

$$\langle E_f^B, 0|\hat{W}|E_i^B, 0\rangle = \langle E_f^B, 1|\hat{W}|E_i^B, 1\rangle = 0$$

ϕ: independent random real numbers from $[0, 2\pi)$, $\alpha = \beta$ or else

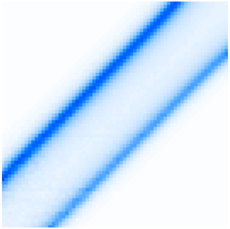
The model is essentially a spin coupled to an abstract environment with a strictly exponentially growing density of states. The system is again resonantly driven through $\hat{s}_x$. The interaction $\hat{W}$ is a matrix whose elements have tailored weights but random phases.

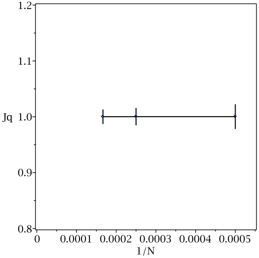
This model may be viewed as a driven and otherwise modified version of the "spin - GORM" model **Esposito et al. Phys. Rev. E 68, 066113**

FGR - rates

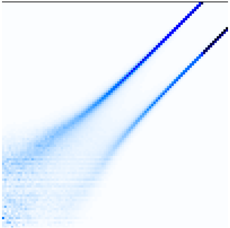
Jarzynski quantifier vs. bath size

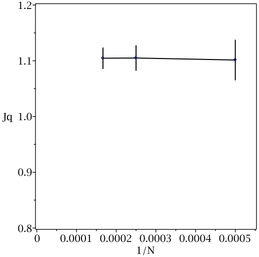
$\alpha = \beta$





$\alpha \neq \beta$





The End

- Initial thermal states as a prerequisite for the validity of the Jarzynski relation may be (widely) dispensable. This may be considered as being in line with the "quantum typicality" concept.
- The previous statement traces the validity of the Jarzynski relation back to the nature of the system, rather than to the nature of the initial state. Consequently the "strong validity" of the Jarzynski relation is system-dependent
- Among the conditions for the strong validity appear to be: exponential density of states of the bath, local "energy-shift-invariance" of the coarse structure of the driving operator,...
- THANK YOU FOR YOUR STAYING HERE UNTIL THE VERY END !