Approximate Validity of the Jarzynski Relation for Non-Gibbsian Initial States in Isolated Systems

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Quantum Jarzynski relation for a Gibbsian initial state

The generalization of the Jarzynski relation (JR) (*Jarzynski, PRL 78, 2690, 1997*) for quantum systems must follow a proper "two-measurement scheme" (*Campisi et al., RMP 83, 771, 2011*). If the system has initially an energy E_{ini} before undergoing a force process $\lambda(t)$, then there is a conditional probability $P(E_{fin}|E_{ini},\lambda(t))$ for the system to have an energy E_{fin} after the process. Let $W=E_{fin}-E_{ini}$ denote the work associated with this process and $P(W)=P(E_{fin}|E_{ini},\lambda(t))P_{ini}(E_{ini})$ the work probability. The average of the exponential of the work then reads $\langle e^{-\beta W}\rangle=\sum_W e^{-\beta W}P(W)$, where β is the inverse temperature.

If the initial state is a Gibbsian state, i.e., $P_{ini}(E_{ini})=e^{-\beta E_{ini}}/Z_{ini}$ (where $Z_{ini}=\sum_{E_{ini}}e^{-\beta E_{ini}}$), the quantum JR follows immediately (*Mukamel, PRL 90, 170604, 2003*)

$$\langle e^{-\beta W}\rangle=\sum_{E_{fin},E_{ini}}e^{-\beta(E_{fin}-E_{ini})}P(E_{fin}|E_{ini},\lambda(t))e^{-\beta E_{ini}}/Z_{ini}=\frac{Z_{fin}}{Z_{ini}}=e^{-\beta\Delta F},$$

where ΔF is the difference of the free energies of the initial and final state at the same inverse temperature β. A special property of the conditional probability is used in the derivation, namely $\sum_{E_{fin}}P(E_{fin}|E_{ini},\lambda(t))=\sum_{E_{ini}}P(E_{fin}|E_{ini},\lambda(t))=1$.

Quantum Jarzynski relation for a non-Gibbsian initial state

A natural question arises whether or not the JR still holds if the initial state is a non-Gibbsian state, such as a state narrowly centered at energy E'_{ini}? Obviously, a direct theoretical analysis is not feasible as it depends on the details of the work probability $P(W)$. Therefore, we resort to the numerical simulation on a quantum spin-1/2 ladder system to see if the JR still holds for non-Gibbsian states.

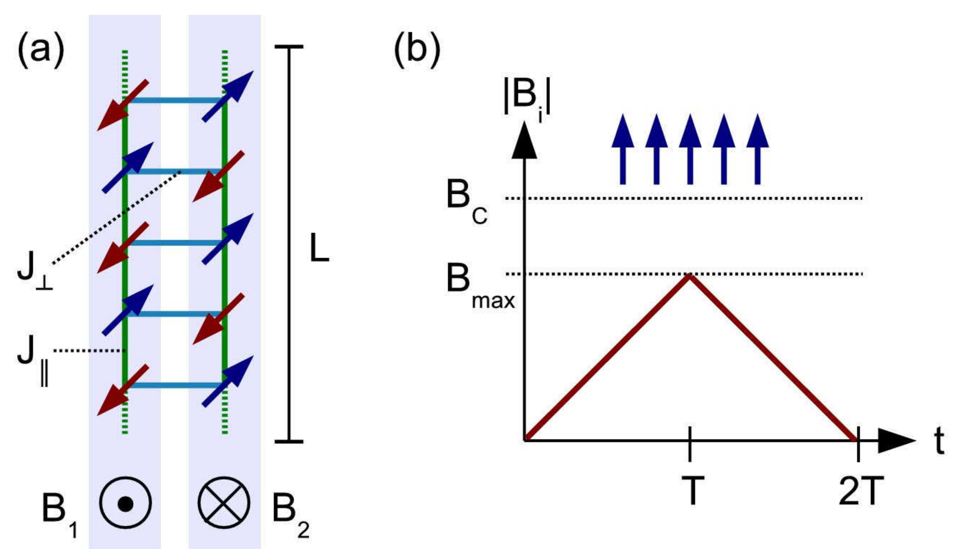
The Hamiltonian and force process

$$H=J_\parallel H_\parallel+J_\perp H_\perp$$

$$H_\parallel=\sum_{i=1}^{L-1}\sum_{k=1}^{2}S^x_{i,k}S^x_{i+1,k}+S^y_{i,k}S^y_{i+1,k}+\Delta S^z_{i,k}S^z_{i+1,k}$$

$$H_\perp=\sum_{i=1}^{L}S^x_{i,1}S^x_{i+1,2}+S^y_{i,1}S^y_{i+1,2}+\Delta S^z_{i,1}S^z_{i+1,2}$$

$$h(t)=h\lambda(t)(S^z_1-S^z_2)$$



The initial state

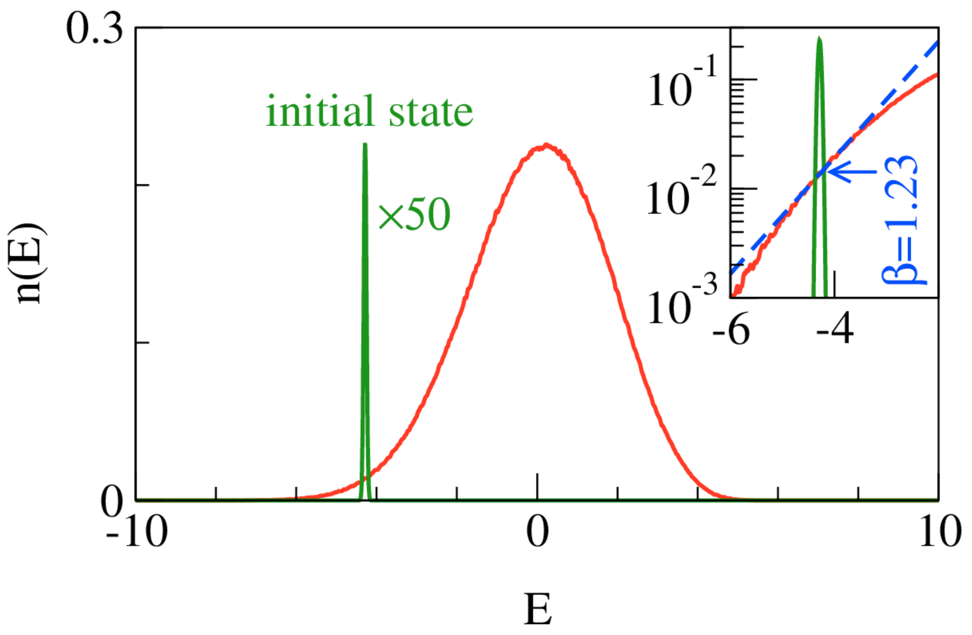
The initial state is obtained by a Gaussian projection on a random state $|\Phi\rangle$ drawn according to the Haar measure from the total Hilbert space of the system,

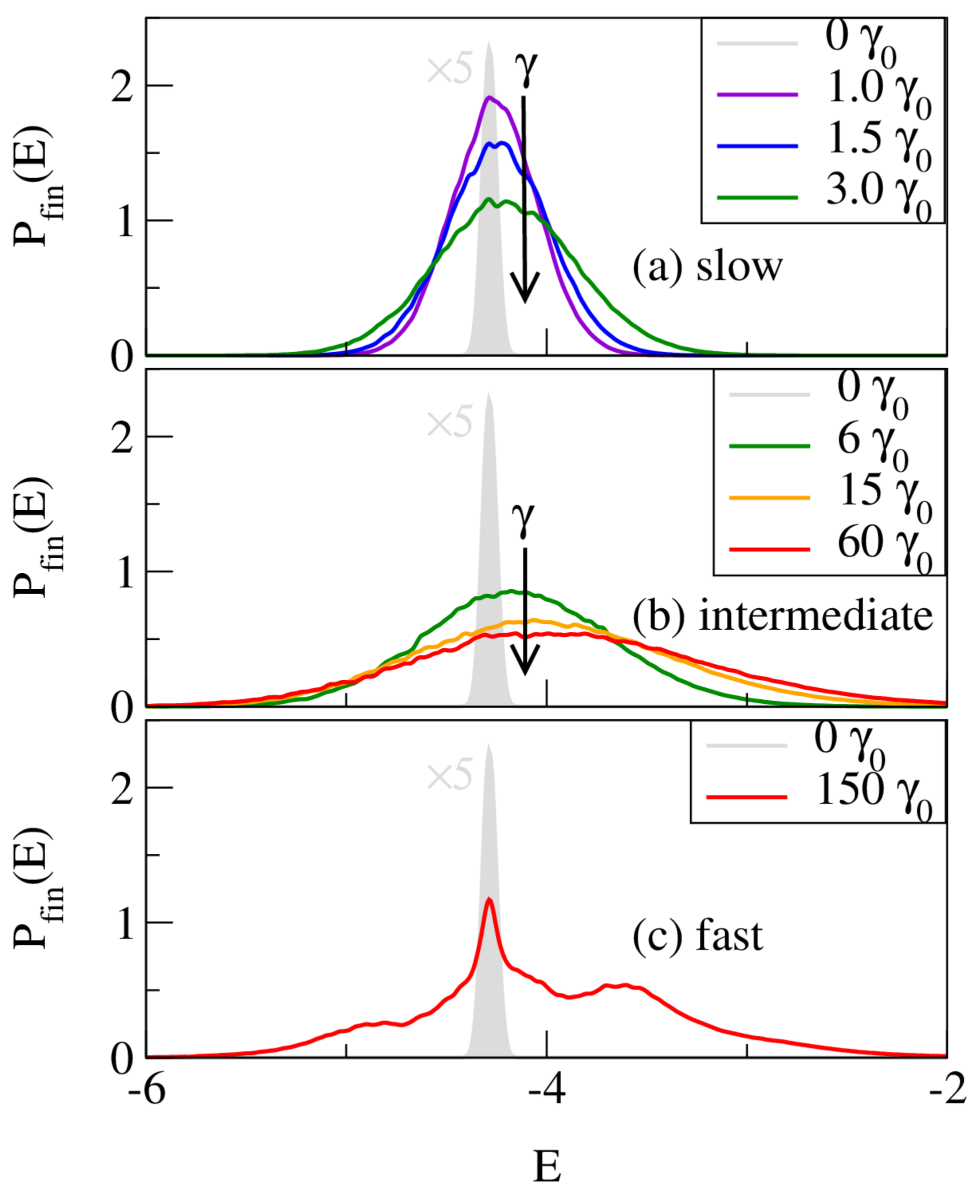
$$|\Psi(a,E)\rangle=\frac{e^{-a(H-E)^2/4}|\Phi\rangle}{\langle\Phi|e^{-a(H-E)^2/2}|\Phi\rangle}.$$

The corresponding inverse temperature for this state is obtained from

$$\beta=\frac{dS}{dE}=\frac{d\ln n(E)}{dE},$$

where $n(E)$ is the density of states (DOS) for H.





Numerical procedure

0. Calculate the DOS $n(E)$ for the initial Hamiltonian H (*Hams et al., PRE 67, 056702, 2003*);
1. Generate the initial state $|\Psi(a,E'_{ini},t=0)\rangle$ by the Chebyshev polynomial algorithm (*Tal-Ezer et al., JCP 81, 3967, 1984*);
2. Calculate the local density of states (LDOS) $P_{ini}(E)$ for the initial state $|\Psi(a,E'_{ini},t=0)\rangle$;
3. Solve the time-dependent Schrödinger equation for the Hamiltonian $H+h(t)$ by a second-order product formula algorithm (*De Raedt, CPR 7, 1, 1987*);
4. Calculate the LDOS $P_{fin}(E)$ for the final state $|\Psi(a,E'_{ini},t=2T)\rangle$;
5. Repeat from step 3 for different process rates $\gamma=1/2T$ (*γ_0 denotes the slowest rate used in the simulation*).

After the whole procedure, we collect the data sets of DOS $n(E)$, initial average energy $\langle E\rangle_{ini}$, LDOS $P_{ini}(E)$, final average energy $\langle E\rangle_{fin}$ and LDOS $P_{fin}(E)$ for further analysis.

Estimation of $\langle e^{-\beta W}\rangle$ and $e^{-\beta\langle W\rangle}$

As the simulation result for $P_{ini}(E)$ is not a δ-function (this would require $a=\infty$), we need to make an extra assumption to determine the work probability. The assumption is to relate $P_{fin}(E)$ and $P_{ini}(E)$ by a simple convolution rule

$$P_{fin}(E_{fin})=\int P_{ini}(E_{ini})P_w(E_{fin}-E_{ini})dE_{ini}.$$

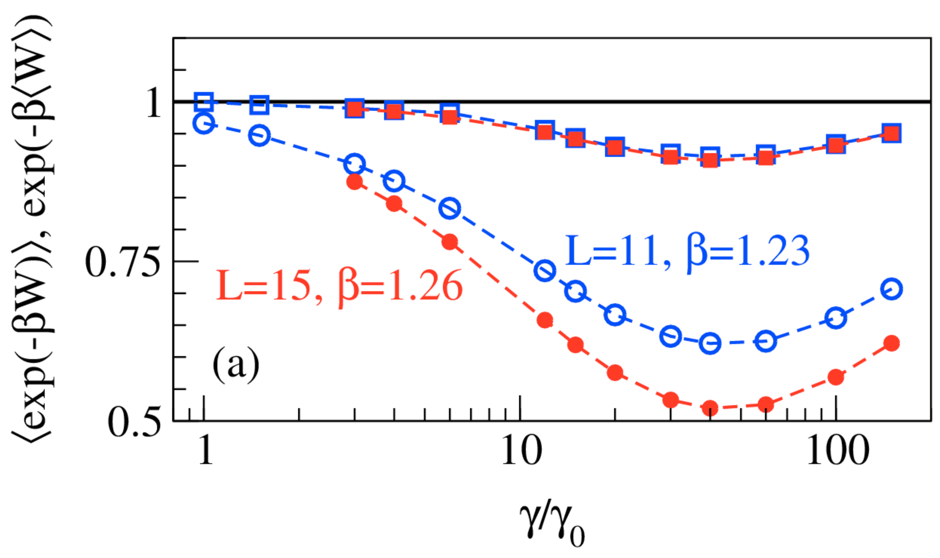
Then we have

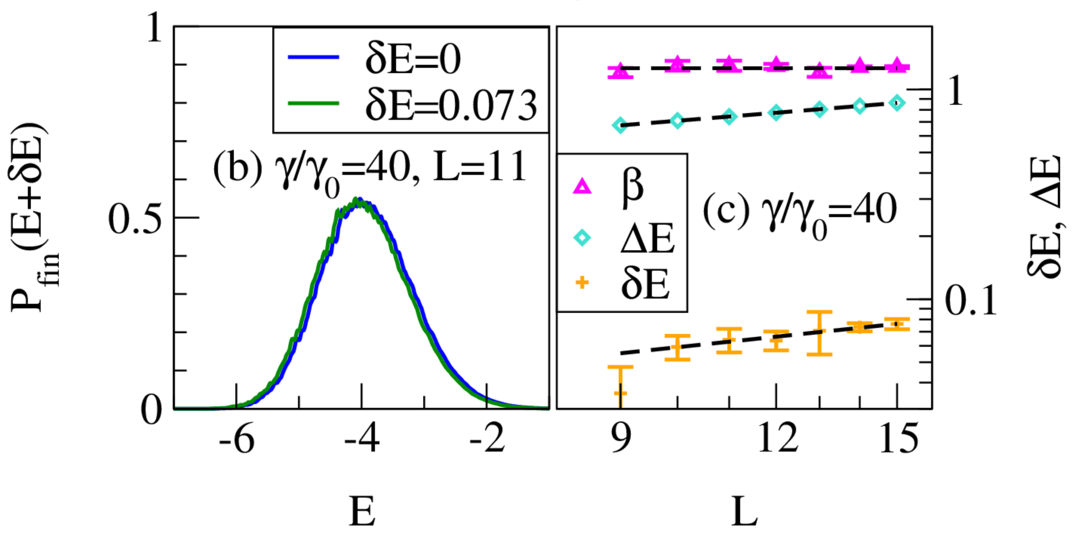
$$\langle e^{-\beta W}\rangle=\frac{\int P_{fin}(E_{fin})e^{-\beta E_{fin}}dE_{fin}}{\int P_{ini}(E_{ini})e^{-\beta E_{ini}}dE_{ini}},$$

and

$$e^{-\beta\langle W\rangle}=e^{-\beta(\langle E\rangle_{fin}-\langle E\rangle_{ini})}.$$

The simulation results of all the quantities are shown in the figures.





Conclusions

As our used force process is cyclic, which leads to $\Delta F=0$, we actually test the equality $\langle e^{-\beta W}\rangle=1$. Extensive tests on the ladder system with size $2L$ ranging from 18 to 30 spins are performed. We find that, for the nonintegrable system in quest, the Jarzynski relation is still fulfilled to good accuracy even if the initial state is beyond the Gibbsian state.
We will investigate the case with a non-cyclic force process in the future.

Acknowledgement: *The authors gratefully acknowledge the computing time granted by the JARA-HPC Vergabegremium and provided on the JARA-HPC Partition part of the supercomputer JUQUEEN at Forschungszentrum Jülich.*