Stiffness of probability distributions of work and Jarzynski relation for initial microcanonical and energy eigenstates

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(Received 11 June 2020; revised 3 March 2021; accepted 1 April 2021; published 23 June 2021)

We consider closed quantum systems which are driven such that only negligible heating occurs. If driving only affects small parts of the system, it may nonetheless be strong. Our analysis aims at clarifying under which conditions the Jarzynski relation (JR) holds in such setups, if the initial states are microcanonical or even energy eigenstates. We find that the validity of the JR for the microcanonical initial state hinges on an exponential density of states and on stiffness. The latter indicates an independence of the probability density functions (PDFs) of work of the energy of the respective microcanonical initial state. The validity of the JR for initial energy eigenstates is found to additionally require smoothness. The latter indicates an independence of the work PDFs of the specific energy eigenstates within a microcanonical energy shell. As the validity of the JR for pure initial energy eigenstates has no analog in classical systems, we consider it a genuine quantum phenomenon.

DOI: 10.1103/PhysRevE.103.062139

I. INTRODUCTION

The long-standing question regarding whether, and in what way, closed finite quantum systems approach thermal equilibrium has recently gathered renewed attention. On the theoretical side, thermalization and equilibration have been investigated, e.g., for rather abstract settings [1–6] and also for more specific condensed-matter-type systems [7–10]. In these works major concepts are the eigenstate thermalization hypothesis and typicality, both of which will also play certain roles in the present paper. The developments on experiments on ultracold atoms now allow for testing what had been merely theoretical results before (see, e.g., Refs. [11–13]).

Rather than just the existence of equilibration within closed quantum systems, the very peculiarities of the dynamical approach to equilibrium have moved to the center of interest [11,14]. Questions addressed in this context include limits on relaxation time scales and agreement of unitary quantum dynamics of closed quantum systems with standard statistical relaxation principles, such as Fokker-Planck equations [15–18] or more general standard stochastic processes [19,20]. Also, the emergence of universal nonequilibrium behavior involving work and driven systems is currently under discussion [21].

To a large extent, universal nonequilibrium behavior may be captured by fluctuation theorems (see, e.g., Ref. [22] and references therein). The Jarzynski relation (JR), a general statement on work that has to be invested to drive processes also and especially far from equilibrium, is a prime example of such a fluctuation theorem. Many derivations of the JR from various starting grounds have been presented. These include classical Hamiltonian dynamics, stochastic dynamics such as Langevin or master equations, and quantum mechanical starting points [22–27]. However, all these derivations (except for Ref. [28]) assume that the system, which is acted on with some kind of force, is strictly in a Gibbsian equilibrium state before the process starts. (The notion of the system here routinely includes the bath.) Thus, this starting point differs significantly from the progress in the field of thermalization: There, the general features of thermodynamic relaxation are found to emerge entirely from the system itself without any necessity of evoking external baths or specifying initial states in detail. Clearly, the preparation of a strictly Gibbsian initial state requires the coupling to a (super)bath prior to starting the process.

This situation renders the question whether or not the standard JR also holds for systems starting in other than Gibbsian states (e.g., microcanonical states) rather exigent. Note that, other than for Gibbsian initial states, the answer to this question is expected to depend on specific properties of the considered systems.

In this context, a property (which we call stiffness) of work distributions has been suggested as a key ingredient for the validity of the JR for microcanonical initial states in Ref. [28]. In this pioneering work, the validity of the JR is proven for classical systems initialized in microcanonical initial states given the systems feature stiffness and microreversibility. Moreover, for a classical Lorentz gas, stiffness and the validity of the JR for microcanonical initial states are numerically demonstrated. Furthermore, the JR was found to hold for microcanonical initial states for some quantum spin models exhibiting stiffness in Ref. [29] in a numerical study. The present work extends this line of research in various directions: We examine the validity of the JR not only for microcanonical initial states but also for initial pure energy

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eigenstates; the latter is conceptually beyond the scope of Ref. [28]. It is also important to note that stiffness is a sufficient but not a necessary condition for the validity of the JR; thus the practical relevance of stiffness is challenged. The numerical modeling in the present paper allows us to address this practical relevance by means of an investigation of the validity of the JR in the presence of stiffness, as well as in its absence (the latter, to the best of our knowledge is, lacking in the literature).

The present paper is organized as follows. In Sec. II we introduce our basic hypothesis of the probability density function (PDF) of work being largely independent of the respective energy for microcanonical initial states. We call this property stiffness. The validity of the JR for microcanonical initial states is shown to follow from this assumption (together with the routinely applied assumption of an exponentially growing density of energy eigenstates). With an additional assumption about the system dynamics, which we call smoothness, we derive the validity of the JR even for energy eigenstates. In Sec. III we introduce our modeling, which is partly based on random matrices. In Sec. IV we provide numerical results for microcanonical initial states, indicating a very strong correspondence between the validity of the JR and stiffness of the system dynamics. In Sec. V we numerically show that also the aforementioned smoothness assumption is fulfilled for our modeling in the limit of large systems. This completes the demonstration of the existence of a class of systems which exhibits both stiffness and smoothness and thus fulfills the JR even for energy eigenstates. We close with a summary and discussion in Sec. VI.

II. STIFFNESS AND SMOOTHNESS OF WORK PDFS AND JARZYNSKI RELATION FOR INITIAL MICROCANONICAL STATES AND ENERGY EIGENSTATES

The present analysis focuses on closed systems. It focuses furthermore on setups in which the driving (which gives rise to consumption or release of work) only acts on a small part of the entire system. This specialization is intended to guarantee isothermality: Even if the driving is strong, the overall temperature of the full system (according to a definition given below) is to remain constant; the reasoning below will rely on this feature. It may appear as if this setting would return one to the standard case of the driven part being initially in a canonical state; however, there is a pivotal difference: In the present analysis we do not impose a limit to the strength of the interaction between the small driven part and the large rest. If this coupling is so small that its effect can be neglected during the driving, one may indeed employ the standard reasoning based on canonical initial states. Indeed, in this weak-coupling limit we numerically recover the validity of the JR without any further condition like the stiffness introduced below (cf. Fig. 3, $\alpha \to 0$). However, our analysis goes beyond this limit: If stiffness is present the JR holds at all interaction strengths, as may be inferred from Fig. 3. To put all this into a catchy picture, consider the paradigmatic unfolding of proteins in a solvent [30]. Using standard reasoning, the validity of the JR can be inferred if (i) the full compound of protein and solvent is initially strictly in a canonical Gibbs state or (ii) the influence of the solvent on the protein is negligible during the unfolding process. In contrast, the below reasoning establishes the validity of the Jarzynski equation, even if the full compound state is in an microcanonical state (or energy eigenstate) and the influence of the solvent on the protein is non-negligible during the unfolding. This is achieved on the basis of stiffness (and smoothness).

As the system is closed, there is no external source or sink of heat; any energy change of the full system is to be counted as work W (for an overview of different perspectives, see, e.g., Ref. [31]). The measurement of the inner energy is described by a two-point projective measurement scheme. In this respect we choose the same starting point as employed in derivations of the JR as described, e.g., in Ref. [32] and references therein.

We consider a system described by a time-dependent Hamiltonian $H(t)$ during the time $t \in [0, T]$, which induces a nonequilibrium process. The corresponding unitary time-propagation operator U is defined by

$$U := \mathcal{T} \exp\left(-i \int_0^T H(t')dt'\right), \tag{1}$$

where $\mathcal{T}$ is the time-ordering operator and we tacitly set $\hbar = 1$.

Let $|i\rangle$ be the eigenstates of $H(0)$ and $|f\rangle$ the eigenstates of $H(T)$ and further let ϵ_i and ϵ_f be the corresponding eigenvalues, respectively. Starting from the initial state $|i\rangle$, $p_{f\leftarrow i}$ denotes the probability to make a transition into $|f\rangle$:

$$p_{f\leftarrow i} = \mathrm{Tr}(|f\rangle\langle f|U|i\rangle\langle i|U^\dagger). \tag{2}$$

The average over the work PDFs $\langle h(W)\rangle_W$ starting from an initial state $\rho(0)$ can be calculated for an arbitrary function $h(W)$ of the work W:

$$\langle h(W)\rangle_W = \sum_{i,f} \mathrm{Tr}[\rho(0)|i\rangle\langle i|]p_{f\leftarrow i}h(\epsilon_f - \epsilon_i). \tag{3}$$

Here $\mathrm{Tr}[\rho(0)|i\rangle\langle i|]$ is the probability to find the system after the first projective measurement in the initial state $|i\rangle$ and $W = \epsilon_f - \epsilon_i$ is the work performed with the transition $i \to f$.

One can easily show that these transition probabilities $p_{f\leftarrow i}$ are doubly stochastic:

$$\sum_i p_{f\leftarrow i} = \sum_f p_{f\leftarrow i} = 1. \tag{4}$$

In general, these transition probabilities vary from eigenstate to eigenstate. We thus define the probability $p_{F\leftarrow i}$ to transition from an eigenstate $|i\rangle$ into an energy interval E_F:

$$p_{F\leftarrow i} = \sum_{f|\epsilon_f\in E_F} p_{f\leftarrow i}, \quad E_n = [n\delta, (n+1)\delta], \quad n = I, F. \tag{5}$$

Here δ is to be chosen large compared to the level spacing of the full system, but small compared to the involved energy scales of E and W. Note that I and F are integers used to address the initial (E_I) and final energy intervals (E_F), respectively. This construction serves as a coarse graining of the energy scale.

In a similar way, we define the average probability to make a transition from an initial state $|i\rangle$ from the energy interval E_I

into an energy interval E_F:

$$p_{F\leftarrow I} = \sum_{i|\epsilon_i\in E_I} \frac{p_{F\leftarrow i}}{\Omega_I}. \tag{6}$$

Here Ω_I and Ω_F denote the number of eigenstates of $H(0)$ in the interval E_I and of $H(T)$ in the interval E_F, respectively, with

$$\Omega_n = \mathrm{Tr}(\Pi_n), \quad \Pi_I = \sum_{i|\epsilon_i\in E_I} |i\rangle\langle i|, \quad \Pi_F = \sum_{f|\epsilon_f\in E_F} |f\rangle\langle f|. \tag{7}$$

Hence, $p_{F\leftarrow I}$ is the average over all $p_{F\leftarrow i}$ with $\epsilon_i \in E_I$.

Note that these transition probabilities depend on the energy width δ. Closely related to these transition probabilities is the so-called work probability density function, which describes the probability to perform the work $W = (F - I)\delta$ starting from an initial energy $E = I\delta$:

$$P_E(W) = \frac{1}{\delta} p_{F\leftarrow I}. \tag{8}$$

The transition probabilities and the work PDFs are essentially the same, up to a constant rescaling factor. However, in large systems these work PDFs typically become independent of the concrete choice of δ [29].

Starting from Eq. (3), the average over the work PDFs $\langle h(W)\rangle_W$ for a function $h(W)$, which does not vary significantly on the scale of δ, can be calculated from $p_{F\leftarrow I}$:

$$\langle h(W)\rangle_W = \sum_{I,F} \mathrm{Tr}[\rho(0)\Pi_I] p_{F\leftarrow I} h(\bar{E}_F - \bar{E}_I). \tag{9}$$

Here $\bar{E}_n = n\delta$ is an approximation of the energies in the initial ($n = I$) interval E_I and of the final ($n = F$) interval E_F. From Eq. (4) we derive the following properties of $p_{F\leftarrow i}$ and $p_{F\leftarrow I}$:

$$\sum_i p_{F\leftarrow i} = \Omega_F, \tag{10}$$

$$\sum_I \Omega_I p_{F\leftarrow I} = \Omega_F. \tag{11}$$

Up to now we have only defined various quantities and derived general statements, but have not made any assumptions. We now arrive at the derivation of the JR for microcanonical initial states. To begin with, we define the latter as

$$\rho^I_{\mathrm{mc}}(0) = \Pi_I \Omega_I^{-1}. \tag{12}$$

In order to derive the JR for microcanonical initial states we make two assumptions. First, we assume that the probability to make a transition from a state from the energy interval E_I to the energy interval E_F only depends on the difference of F and I:

$$p_{F\leftarrow I} = p(F - I). \tag{13}$$

We call this assumption stiffness. For a discussion of the conditions on its occurrence, at least in a regime in which Fermi's golden rule applies, see Appendix A. This assumption can also be expressed in terms of work PDFs $P_E(W)$. If these work PDFs are independent of the initial energy E, then Eq. (13) is fulfilled.

Our second assumption states that the densities of states (DOSs) of the initial $D_{\mathrm{ini}}(\bar{E}_I) := \delta^{-1}\Omega_I$ and final Hamiltonians $D_{\mathrm{fin}}(\bar{E}_F) := \delta^{-1}\Omega_F$ grow exponentially:

$$D_{\mathrm{ini}}(\bar{E}_I) = Z_{\mathrm{ini}} \exp(\beta \bar{E}_I),$$
$$D_{\mathrm{fin}}(\bar{E}_F) = Z_{\mathrm{fin}} \exp(\beta \bar{E}_F). \tag{14}$$

Up to now β, Z_{ini}, and Z_{fin} are just some positive real numbers. In the discussion below (16) these numbers are interpreted in terms of standard statistical thermodynamics. Equations (14) implement two assumptions. (i) The DOSs of the inital Hamiltonian and the final Hamiltonian are both exponentially growing at the respective energies. We elaborate on the physical implication of this assumption in Sec. III. (ii) The (inverse) temperatures β initially and finally are the same. This corresponds to the no-heating condition introduced at the beginning of this section.

Of course Eqs. (13) and (14) are not expected to hold for all energies E. Here we only require that these relations hold at least for an energy interval which is large enough to comprise almost the entire work PDF.

To arrive at the JR for microcanonical initial states, we start by calculating the average of $\exp(-\beta W)$ over the work PDFs according to Eq. (9),

$$\begin{aligned}\langle \exp(-\beta W)\rangle_W &= \sum_{I',F} \mathrm{Tr}\big[\rho^I_{\mathrm{mc}}(0)\Pi_{I'}\big] p_{F\leftarrow I'} \exp[-\beta(\bar{E}_F - \bar{E}_{I'})] \\ &= \sum_F p(F - I)\exp[-\beta(\bar{E}_F - \bar{E}_I)].\end{aligned} \tag{15}$$

In the last step we evaluated the sum over I' by using $\mathrm{Tr}(\Omega_I^{-1}\Pi_I\Pi_{I'}) = \delta_{I,I'}$ and used the stiffness assumption (13). By replacing F by $F' + I - I'$, with I' the new summation index and F' an arbitrary but fixed integer, we get

$$\begin{aligned}\langle \exp(-\beta W)\rangle_W &= \sum_{I'} p(F' - I')\exp[-\beta(\bar{E}_{F'} - \bar{E}_{I'})] \\ &= \frac{1}{\Omega_{F'}} \frac{Z_{\mathrm{fin}}}{Z_{\mathrm{ini}}} \sum_{I'} p_{F'\leftarrow I'}\Omega_{I'} = \frac{Z_{\mathrm{fin}}}{Z_{\mathrm{ini}}}.\end{aligned} \tag{16}$$

In the second step we used that the DOSs of the initial and the final Hamiltonians exponentially grow according to Eq. (14). In the last step we used Eq. (11).

Equation (16) formally is a JR for the work PDFs obtained by starting from microcanonical initial states, with the temperature replaced by a parameter describing the exponential growth of the DOS of the full system. As such Eq. (16) already represents the main result of the present section. Note that Eq. (16) holds for arbitrary processes and its right-hand side only contains static, process-independent model parameters.

Formally, the JR could be fulfilled for microcanonical initial states, even if Eqs. (13) and (14) do not hold. In this sense these assumptions are stronger than the validity of the JR; to rephrase, these assumptions represent sufficient but not necessary conditions. This peculiarity will be investigated in detail below.

In an analogous way we can derive Eq. (16) for initial energy eigenstates $\rho(0) = |i\rangle\langle i|$ if we additionally assume that

$$p_{F\leftarrow i} \approx p_{F\leftarrow I} \tag{17}$$

holds for all $i \in \mathbb{N}$ with $\epsilon_i \in E_I$. This additional assumption means that the transition probabilities from an eigenstate $|i\rangle$ to

an energy interval E_F are smooth functions of the initial and final energies. We therefore call it smoothness. The validity of this assumption is investigated in Sec. V for a finite-size scaling.

To demonstrate an even closer analogy of Eq. (16) with the standard JR, it remains to be explained in what sense the right-hand side of Eq. (16) may be considered as the familiar right-hand side of the standard JR, $e^{-\beta\Delta F}$, where F is the free energy. Such an identification would hold if

$$-\frac{\ln Z_\alpha}{\beta} \stackrel{?}{=} F_\alpha. \tag{18}$$

In order to judge whether or not Eq. (18) is justified, consider the logarithm of Eq. (14),

$$\ln D_\alpha(U) = \ln Z_\alpha + \beta U. \tag{19}$$

The index $\alpha \in \{\text{ini}, \text{fin}\}$ signals whether the equation refers to the initial or final Hamiltonian, respectively. Moreover, the discrete average energies $\bar{E}_I$ and $\bar{E}_F$ are replaced by the continuous parameter U.

If one identifies, along the lines of Boltzmann's original approach, the entropy S_α as

$$\ln D_\alpha := S_\alpha \tag{20}$$

(where we tacitly set $k_B = 1$), one may convert Eq. (19) into

$$-\frac{\ln Z_\alpha}{\beta} = U - \frac{S_\alpha}{\beta}. \tag{21}$$

Note that, in accordance with Eq. (14), $\partial_U S_\alpha = \beta$; hence β has the meaning of inverse temperature and the right-hand side of Eq. (21) is, accordingly, the free energy F as introduced in standard textbooks on phenomenological thermodynamics. In this sense Eq. (18) indeed holds, which entails the rewriting of Eq. (16) in a form closer to the familiar one,

$$\langle e^{-\beta W}\rangle_E = e^{-\beta\Delta F}, \tag{22}$$

where $\langle\cdots\rangle_E$ denotes the microcanonical expectation value corresponding to energy E. This concludes our consideration of the validity of a JR for microcanonical initial states under the assumption of stiff work PDFs.

III. MODELS AND DRIVING PROTOCOL

With the following numerical investigations we ascertain the pivotal relevance of stiff work PDFs for the validity of the JR for microcanonical initial states. We therefore introduce a model that is partly based on random matrices. Within this model we can control the stiffness of the resulting work PDFs via a single parameter ξ. This allows us to observe the influence of stiffness on the JR for microcanonical initial states.

We consider an isolated system comprising a relatively small subsystem H_{sys} and a bigger part serving as the heat bath H_{bath}. Both parts may interact via H_{int}; the strength of this interaction is not limited. Finally, a time-dependent force periodically drives the system H_{prot}. Concretely, we choose the small subsystem to be a spin and the time-dependent force to be a kind of microwave field such that the whole model allows for an interpretation in terms of a spin-resonance

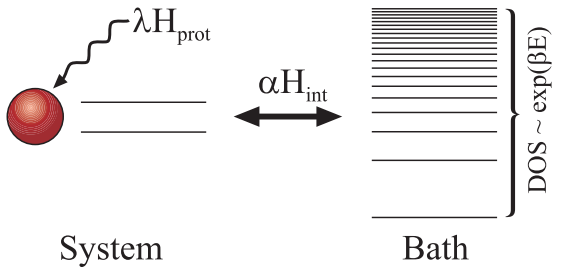

FIG. 1. Schematic structure of the numerical model. A two-level system is coupled via a random interaction to a bath with an exponentially growing DOS. The structure of the interaction influences the resulting work PDFs.

experiment with a finite lifetime of the spin excitation (see Fig. 1). A very similar model (the spin–Gaussian orthogonal random matrix model) was previously used to study relaxation in finite environments [33]. The bath is only specified by a relatively large and exponentially growing DOS; these are the features that make the bath much "larger" than the system.

Specifically, the Hamiltonian of the full system reads

$$H(t) = H_{\text{sys}} + H_{\text{bath}} + \alpha H_{\text{int}} + \lambda H_{\text{prot}}(t). \tag{23}$$

The small subsystem is a simple two-level system, e.g., a spin-$\frac{1}{2}$ particle in a magnetic field B_z. The Hamiltonian of this subsystem is characterized as

$$H_{\text{sys}}\left|E_j^{\text{sys}}\right\rangle = E_j^{\text{sys}}\left|E_j^{\text{sys}}\right\rangle, \quad E_{1|2}^{\text{sys}} = \mp\frac{B_z}{2}. \tag{24}$$

The $|E_j^{\text{sys}}\rangle$ obviously denote the eigenstates of H_{sys}. We choose $B_z = 0.5$ throughout this paper.

The bath part is also defined by its energy levels,

$$H_{\text{bath}}\left|E_j^{\text{bath}}\right\rangle = E_j^{\text{bath}}\left|E_j^{\text{bath}}\right\rangle,$$
$$E_j^{\text{bath}} = \frac{1}{\beta}\ln\left\{\frac{j}{N}\exp\left(\beta E_{\text{max}}^{\text{bath}}\right) + \left(1-\frac{j}{N}\right)\exp\left(\beta E_{\text{min}}^{\text{bath}}\right)\right\}, \tag{25}$$

while N denotes the dimension of the bath. This definition yields a (strictly) exponentially growing DOS $\Omega_{\text{bath}}(E) \propto \exp\beta E$ comprising energies from $E_{\text{min}}^{\text{bath}} = 0$ to $E_{\text{max}}^{\text{bath}} = 4.5$. The constant β (which takes the role of a temperature here) is chosen to be 1. This modeling corresponds to a bath with infinite heat capacity, i.e., the temperature is always $1/\beta$, regardless of the actual bath energy (as is well known, practically all sufficiently large real systems with short-range interactions approximately feature this property [34]). The below choice of the interaction guarantees that the exponentially growing DOS of the bath induces an approximately exponentially growing DOS of $H_{\text{sys}} + H_{\text{bath}} + \alpha H_{\text{int}}$ for all parameters.

We now define the interaction between the system and the bath. This is the most subtle part of our modeling. We introduce the following notation:

$$\left|E_m^{\text{sys}}, E_n^{\text{bath}}\right\rangle := \left|E_m^{\text{sys}}\right\rangle \otimes \left|E_n^{\text{bath}}\right\rangle. \tag{26}$$

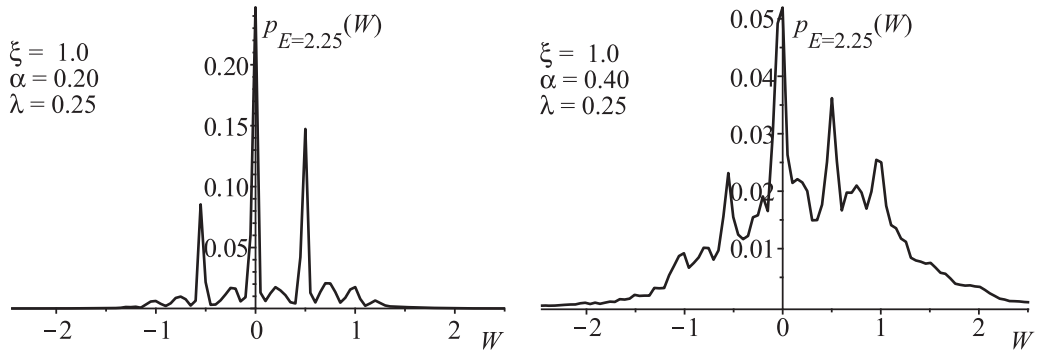

FIG. 2. Work PDFs for two different bath couplings α. For the weaker coupling we see two sharp peaks at $W = \pm B_z$, resulting from spin flips induced by the resonant irradiation. For the stronger coupling the work PDF is much broader.

Regarding this product basis, we define the interaction part

$$\begin{aligned}&\langle E_m^{\rm sys}, E_n^{\rm bath}|H_{\rm int}|E_k^{\rm sys}, E_l^{\rm bath}\rangle \\ &\quad = (1-\delta_{mk})g\big(E_n^{\rm bath}+E_l^{\rm bath}\big)f\big(|E_n^{\rm bath}-E_l^{\rm bath}|\big)R_{nl}, \quad (27)\end{aligned}$$

$$g(\bar{E}) = \exp\left(-\frac{\beta\xi\left(\bar{E}-E_{\rm max}^{\rm bath}\right)}{4}\right),$$

$$f(\omega) = \exp\left(-\frac{\omega^2}{2\sigma_{\rm int}^2}\right). \quad (28)$$

Here $R_{nl} = R_{ln}$ denote normally distributed random numbers with zero mean and unit variance.

To assess the rationale behind this modeling, consider the following. The interaction $H_{\rm int}$ only allows transitions (for the nondriven model, i.e., for $\lambda = 0$) between energetically similar bath states. Direct transitions between states with significantly different bath energies are suppressed by the Gaussian function $f(\omega)$, i.e., their suppression is controlled by the respective variance $\sigma_{\rm int}^2 = 0.5$. Within the validity of Fermi's golden rule, the decay rate γ of the z component of the magnetization of the spin for some initial bath energy $E^{\rm bath}$ can be estimated as $\gamma \propto \exp[\beta(1-\xi)E^{\rm bath}]$ for our model. In a physical system we would expect γ to depend on the temperature $1/\beta$ of the bath, but not on its actual energy within a regime of equal temperature. For $\xi = 1$ the rate γ actually becomes independent of the bath energy $E^{\rm bath}$. We thus consider this the most physical case.

While it is not obvious, it is an actual and most important fact that ξ also controls the stiffness of the model. It turns out that stiff work PDFs arise precisely at the above most physical case $\xi = 1$. For smaller and larger ξ stiffness is lost. For clarity of presentation, we do not discuss the inner workings of this stiffness control mechanism here, but simply present clear numerical evidence for its existence in Appendix B.

We finally introduce the time-dependent protocol exclusively acting on the system part:

$$H_{\rm prot}(t) = \sin(\omega_{\rm prot}t)(|E_1^{\rm sys}\rangle\langle E_2^{\rm sys}| + {\rm H.c.}). \quad (29)$$

Thinking again of the system in terms of a spin-$\frac{1}{2}$ particle, the protocol describes a sinusoidally modulated magnetic field in the x direction, as routinely used in spin resonance experiments. We choose $\omega_{\rm prot} = B_z = 0.5$, i.e., the irradiation is on resonance. The duration of the protocol is set to $T = 3.5\frac{2\pi}{\omega_{\rm prot}}$ throughout this paper. For small bath-couplings α the resulting work-PDFs comprises two sharp peaks, corresponding to Rabi-oscillations, while for larger values of α the resulting work-PDFs are much broader (see Fig. 2)

IV. JARZYNSKI RELATION FOR MICROCANONICAL INITIAL STATES AND VARIOUS SYSTEM CONFIGURATIONS

We consider a microcanonical $\rho_{\rm mc}^{I_0}(0)$ initial state from the center of the spectrum of the initial Hamiltonian $H(0)$ with an energetic width of about $\delta \approx 0.06$:

$$\rho_{\rm mc}^{I_0}(0) = \Omega_{I_0}^{-1}\Pi_{I_0}, \quad I_0 = \left\lfloor \frac{E_0}{\delta} \right\rfloor,$$

$$E_0 = \frac{\max(\epsilon_j)+\min(\epsilon_j)}{2}. \quad (30)$$

The dimension of the bath is set to $N = 4000$. For this initial state we numerically check the JR for three different stiffness parameters $\xi = 0.6, 1.0, 2.0$ with various bath couplings $\alpha = 0, 0.05, 0.1, \ldots, 0.5$ and irradiation strengths $\lambda = 0, 0.025, 0.05, \ldots, 0.25$.

In order to quantify deviations from the perfectly fulfilled JR [Eq. (22)], we introduce the following definition:

$$\begin{aligned}D_{\rm mc}(\xi,\alpha,\lambda) := {\rm Tr}\big(U\rho_{\rm mc}^{I_0}(0)U^\dagger \exp\{-\beta[H(T)-E_0]\}\big) \\ -\exp(-\beta\Delta F). \quad (31)\end{aligned}$$

Since we consider cyclic processes ΔF is equal to zero and $\exp(-\beta\Delta F)$ becomes equal to 1. If the JR holds for the considered set of parameters (ξ, α, and λ), the corresponding quantifier $D(\xi,\alpha,\lambda)$ vanishes.

The results for the microcanonical initial states are displayed in Fig. 3. Light green means that the JR is fulfilled, while other colors indicate deviations.

In the case of weak bath couplings α or weak irradiation strengths λ the JR is trivially fulfilled, even for microcanonical initial states and regardless of stiffness ($\xi \neq 0$): For $\lambda \approx 0$ we are in the limit of adiabatic following and thus no work will be performed. For $\alpha \approx 0$ the coupling between system and bath parts may be neglected during the driving. Nevertheless, the reduced initial $H_{\rm sys}$ state is a thermal state with the inverse temperature β. So the protocol acts on a system prepared in a Gibbsian state. For this scenario it is well known that the JR holds. In the center of interest are thus the regions of larger α and λ.

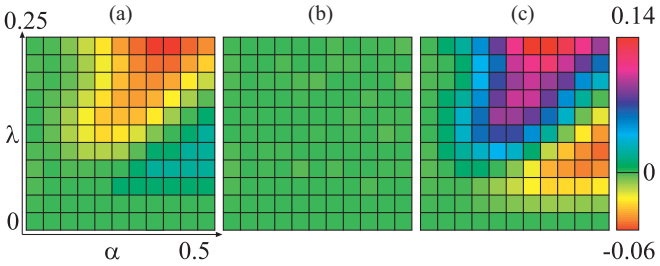

FIG. 3. Plot of $D_{\mathrm{mc}}(\xi, \alpha, \lambda)$ for various system configurations: (a) $\xi = 0.6$, (b) $\xi = 1.0$, and (c) $\xi = 2.0$. Light green (zero) indicates that the system complies with the JR, while other colors (nonzero values) quantify the deviations from the JR. Apparently, the JR is always fulfilled for $\xi = 1$, even for microcanonical initial states.

For $\xi = 1.0$ the resulting work PDFs are stiff, up to small fluctuations (see Appendix B). Since stiff work PDFs imply the JR for microcanonical initial states, the respective deviations in Fig. 3 are nearly zero, at all α and λ. This is our main numerical result.

For $\xi = 0.6, 2.0$ the resulting work PDFs are not stiff (see Appendix B). In principle, the JR could still be fulfilled for microcanonical initial states, since stiffness is formally not a necessary condition. However, at both values, i.e., $\xi = 0.6, 2.0$, we find deviations from the JR "to both sides" [$D_{\mathrm{mc}}(\xi, \alpha, \lambda)$ positive as well as negative]. These deviations appear to systematically depend on α and λ and are nonzero for most α and λ. However, there are a few combinations of α and λ for which the JR is fulfilled (see the corresponding light green corridors in Fig. 3).

In Appendix C the dependence of the deviations $D_{\mathrm{mc}}(\xi, \alpha, \lambda)$ on the initial energy E_0 is numerically investigated in more detail. We find that at $\xi \neq 1$ the initial energy plays a crucial role for the resulting deviations, but not so at $\xi = 1$. In particular, at the light green corridors in Figs. 3(a) and 3(c), the JR is violated for initial microcanonical states with energies other than E_0. These numerical finding suggests that the stiffness of work PDFs is crucial for the validity of the JR for microcanonical initial states.

V. VALIDITY OF THE JARZYNSKI RELATION FOR ENERGY EIGENSTATES AND FINITE-SIZE SCALING

Up to now we have investigated only the validity of the JR for microcanonical initial states (30). We now turn to initial states being eigenstates of the initial Hamiltonian $H(0)$. We define these initial states as

$$\rho^{i}_{\mathrm{es}}(0) = |i\rangle\langle i|. \tag{32}$$

The energetic width of these states is $\delta = 0$. In this sense they are fundamentally different from microcanonical initial states. However, in this section we will demonstrate that in the limit of large bath dimension, both behave similarly regarding the JR.

Again, we use Eq. (31) to check whether or not the JR is fulfilled. We define the corresponding deviations $D_{\mathrm{es}}(\xi, \alpha, \lambda)$ completely analogously to the $D_{\mathrm{mc}}(\xi, \alpha, \lambda)$ [cf. Eq. (31)] but with $\rho^{l_0}_{\mathrm{mc}}(0)$ replaced by $\rho^{i}_{\mathrm{es}}(0)$. Note that the average of the $D_{\mathrm{es}}(\xi, \alpha, \lambda)$ over a pertinent range of i equals a corresponding $D_{\mathrm{mc}}(\xi, \alpha, \lambda)$. Thus the following numerical results (Fig. 4) hold information not only about the sizes of the $D_{\mathrm{es}}(\xi, \alpha, \lambda)$ but also about the finite-size scaling of the $D_{\mathrm{mc}}(\xi, \alpha, \lambda)$.

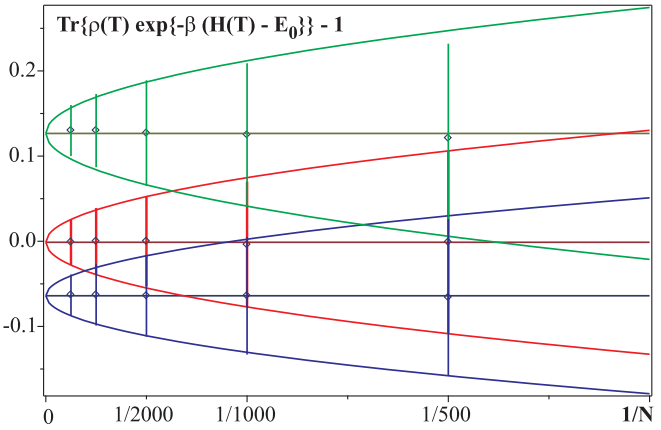

FIG. 4. Finite-size scaling of $D_{\mathrm{es}}(\xi, \alpha, \lambda)$ for eigenstates (from the center of the spectrum) of the respective initial Hamiltonians $H(0)$. Displayed are averages (symbols) and standard deviations (bars) for three different model parameter sets: ($\xi = 1, \alpha = 0.4, \lambda = 0.25$), red; ($\xi = 0.6, \alpha = 0.4, \lambda = 0.25$), blue; and ($\xi = 2.0, \alpha = 0.4, \lambda = 0.25$), green. The standard deviations are shown clearly by tilted parabolas. This suggests that the standard deviations decrease as $N^{-0.5}$.

A systematic survey of the $D_{\mathrm{es}}(\xi, \alpha, \lambda)$ for all α and λ is numerically very costly. We thus concentrate on cases where the violation of the JR is pronounced for $\xi \neq 1$, i.e., $\alpha = 0.4$ and $\lambda = 0.25$ (cf. Fig. 3).

Figure 4 shows statistical results of the $D_{\mathrm{es}}(\xi, \alpha, \lambda)$ for increasing bath sizes N. (For clarity, the results are displayed over the inverse bath size $1/N$.) Displayed are the averages (diamonds) and standard deviations (vertical error bars) for a stiff system $\xi = 1$ and two nonstiff systems $\xi = 0.6, 2$. The statistics encompass 100 different $D_{\mathrm{es}}(\xi, \alpha, \lambda)$ for adjacent i from the middle of the respective spectra for each parameter set.

The following principles may be inferred from Fig. 4. The averages appear to be independent of the system size N, and thus the $D_{\mathrm{mc}}(\xi, \alpha, \lambda)$ are independent of the system size; hence Fig. 3 provides a representative picture also for (larger) bath sizes other than $N = 4000$. The standard deviations of the $D_{\mathrm{es}}(\xi, \alpha, \lambda)$ decrease with bath size, presumably proportional to $N^{-0.5}$, as suggested by the tilted parabolas.

These findings strongly indicate that the JR is indeed fulfilled even for pure initial energy eigenstates for stiff systems in the limit of large bath (total system) sizes. Note that in this case the statistical character of the corresponding work PDFs is entirely due to pure quantum uncertainties. Furthermore, the JR appears to be always violated for pure initial energy eigenstates in the limit of large bath (total system) sizes if the system is nonstiff.

VI. CONCLUSION

In this article we have shown analytically that the Jarzynski relation holds for a broad class of non-Gibbsian initial states in

quantum systems under certain conditions. For microcanonical initial states these conditions are (i) an exponentially growing DOS with the same growth rate of the initial and final Hamiltonians in the relevant energy region (this no-heating condition may hold even at strong driving, if the driving only acts on a small part of the full system) and (ii) stiff work PDFs, i.e., work PDFs that are independent of the initial energy. Moreover, numerics indicate that the converse also holds: Systems that do not comply with the stiffness condition actually do violate the JR for microcanonical initial states, independent of the size of the system.

In order to analytically show the validity of the Jarzynski relation for initial energy eigenstates, we exploited an additional assumption about the work PDFs called smoothness, which is expected to hold for large systems. This expectation was supported by numerics for some examples, which showed that the Jarzynski relation is fulfilled in the limit of large systems for systems that do exhibit smoothness and violated for systems which do not.

To conclude, there appears to be a very tight link between the applicability of the Jarzynski relation and stiffness or smoothness for non-Gibbsian initial states which deserves further exploration.

ACKNOWLEDGMENTS

This work was funded by the Deutsche Forschungsgemeinschaft (DFG) through Grants No. 397107022 (GE 1657/3-1) and No. 355031190 within the DFG Research Unit FOR 2692. This research was also supported in part by the National Science Foundation under Grant No. NSF PHY-1748958.

APPENDIX A: STIFFNESS CONDITION

The condition (13) may appear puzzling, since transition rates usually depend on the DOS at the final energy, but not on the DOS at the initial energy. So how can transition rates possibly depend only on the energy difference? In the following we try to elucidate under what conditions stiffness may nevertheless occur. The mere fact of the actual occurrence of stiffness in standard spin models may also be inferred from Ref. [29], where stiffness was boldly verified numerically.

Consider an $H_{\mathrm{prot}}(t)$ of the form

$$H_{\mathrm{prot}}(t) = V \sin \omega t. \tag{A1}$$

Let V_{fi} denote the elements of V in the energy eigenbasis of $H_0 := H_{\mathrm{sys}} + H_{\mathrm{bath}} + \alpha H_{\mathrm{int}}$. Assume for simplicity that V conforms with the eigenstate thermalization ansatz as suggested by Srednicki [35], i.e.,

$$V_{fi} = A(\epsilon)\delta_{if} + D(\epsilon)^{-1/2} f(\epsilon, |\omega|) R_{if}, \tag{A2}$$

where $\epsilon := (\epsilon_i + \epsilon_f)/2$ and $\omega := \epsilon_f - \epsilon_i$, with ϵ_i and ϵ_f eigenvalues of H_0; A and f are real and smooth functions of their arguments; D is the DOS of H_0; and "R_{if} is a numerical factor that varies erratically with i and f. It is helpful to think of the real and imaginary parts of R_{if} as random variables, each with zero mean and unit variance" [35]. To simplify even further we assume $A(\epsilon) \approx 0$ (this assumption may in principle be dropped, but it eases calculations significantly). A second, crucial assumption that is practically the same as Eq. (14) is the exponential form of $D(\epsilon)$, i.e.,

$$D(\epsilon) \overset{!}{\propto} e^{\beta\epsilon}. \tag{A3}$$

We are now set to calculate transitions rates as induced by $H_{\mathrm{prot}}(t)$, given that the whole setup is such that these rates may be calculated on the basis of Fermi's golden rule (FGR):

$$\gamma_{f\leftarrow i} \propto f^2(\epsilon, |\omega|) D(\epsilon)^{-1} D(\epsilon_f) \delta(|\omega|). \tag{A4}$$

Simplifying the product of the D's and taking Eq. (A3) into account as well as the definitions below Eq. (A2), we arrive at

$$\gamma_{f\leftarrow i} \propto f^2(\epsilon, |\omega|) \exp\left(\frac{\beta\omega}{2}\right) \delta(|\omega|). \tag{A5}$$

From this it is plain to be seen that this scenario will exhibit stiffness if

$$f(\epsilon, |\omega|) \overset{!}{=} f(|\omega|), \tag{A6}$$

since in this case the rates will only depend on ω, which is simply the difference between final and initial energies. Thus, in this FGR scenario, if and only if Eqs. (A3) and (A6) apply, stiffness occurs. Equation (A3) is likely fulfilled in a wide energy range for large and short-range interacting systems; Eq. (A6) plays also an important role in the dependence of expectation value dynamics on initial states [36]. As already mentioned, strong direct numerical evidence for the actual occurrence of stiffness in models like the present one with the bath being a kind of Heisenberg spin system is presented in Ref. [29].

APPENDIX B: STIFFNESS OF WORK PDFS

In the main text we varied the model parameter ξ and just claimed it would affect the stiffness of the work PDFs. In this Appendix we numerically check the actual influence of this model parameter on the work PDFs.

We therefore calculated the work PDFs $p_E(W)$ for various model parameters. In Fig. 5 we exemplarily present the data for $d = 4000$, $\alpha = 0.4$, $\lambda = 0.25$, and $\xi = 0.6, 1.0, 2.0$ for eigenstates of $H(0)$ with $E_0 \approx 2.25$.

Figure 5 shows the probabilities to perform zero work. For $\xi = 1.0$ the probabilities $p_E(0)$ appear to be approximately independent of E, while for $\xi = 0.6$ and 2.0 we find a significant dependence. While for larger bath dimensions d the work PDFs become smoother, the slope for $\xi = 0.6, 2.0$ appears to be independent of d.

APPENDIX C: JARZYNSKI RELATION FOR DIFFERENT INITIAL ENERGIES

In Sec. IV we considered deviations from the JR for various combinations of ξ, α, and λ but a fixed initial energy E_0 and found that for some combinations of these parameters the JR appeared to be fulfilled, even though the condition (13) is violated. We now consider the dependence of these deviations on the energy of the initial state $\rho(0)$ with the aforementioned parameters held constant. We consider microcanonical initial states, defined according to Eq. (30), with various energies E.

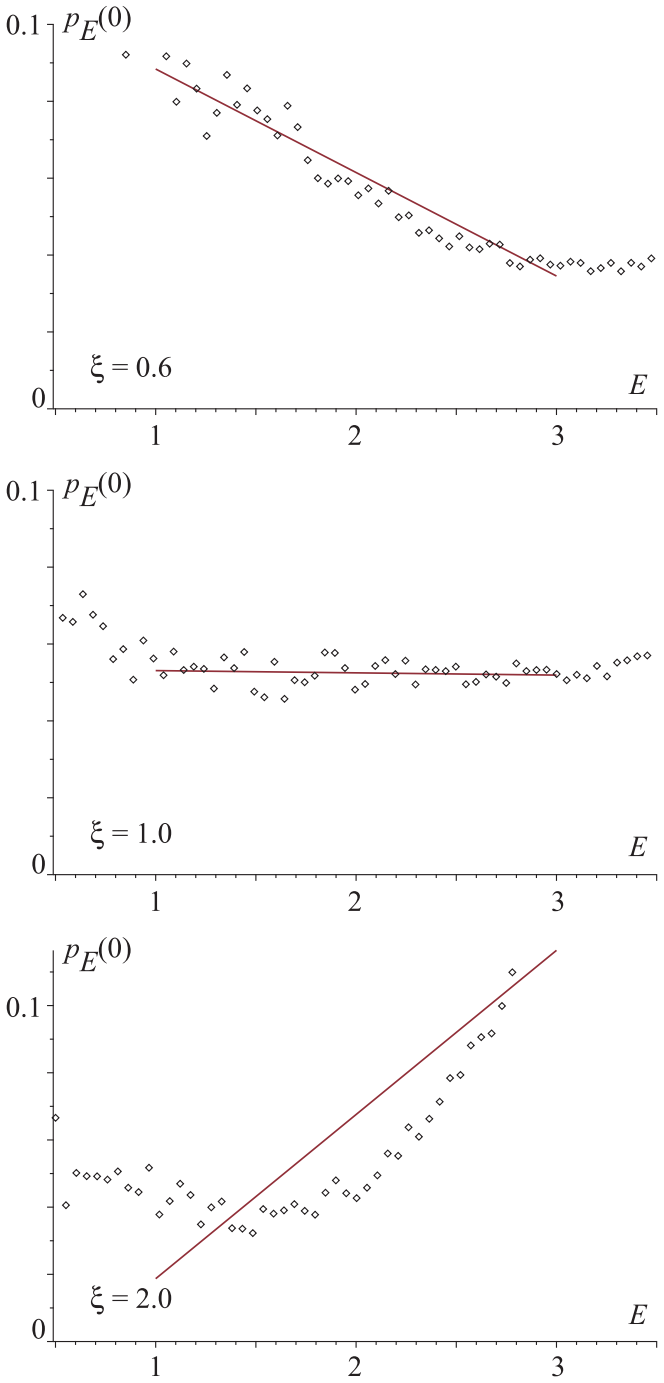

FIG. 5. For $\xi = 1.0$ the probability to perform zero work is approximately independent of the initial energy, while for $\xi = 0.6$ and 2.0 we find a significant dependence.

The resulting deviations $D(\xi = 2.0, \alpha = 0.45, \lambda = 0.15)$ are displayed in Fig. 6.

Note that for this parameter combination we found the JR fulfilled for the previously considered initial energy E_0. The data suggest that there is only a small energy range for which the JR is approximately fulfilled and E_0 coincidentally is within this region. The energy dependence for other α and λ looks quite similar. So we can find specific microcanonical initial states, which comply with the JR, even if the condition

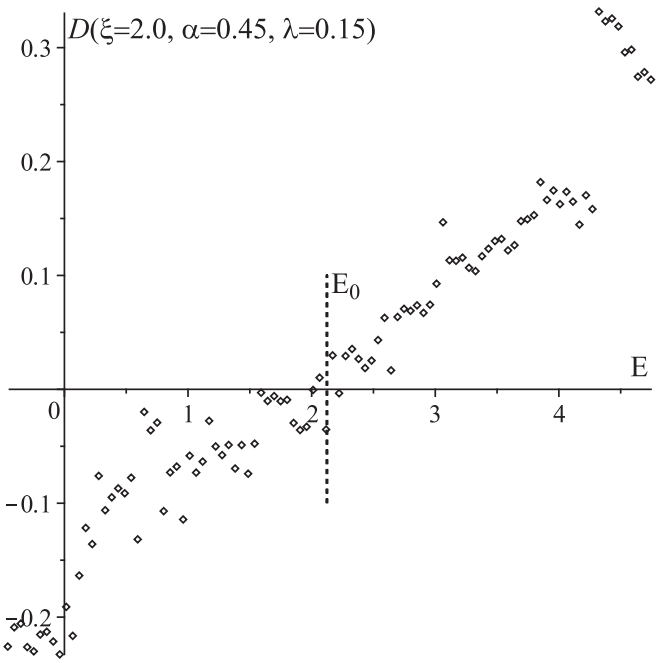

FIG. 6. Energy dependence of $D(\xi, \alpha, \lambda)$.

(13) is not fulfilled. However, since this is a feature of a very specific combination of system and initial state, we conclude that the JR is not fulfilled by this system and driving protocol in general. In contrast, for $\xi = 1$ there is a wide region of initial energies that fulfill the JR, which is a direct consequence of the conditions (13) and (14).

APPENDIX D: JARZYNSKI RELATION FOR NONDIAGONAL INITIAL STATES AND NONPROJECTIVE MEASUREMENTS

So far, only initial states that are diagonal in the energy eigenbasis of the initial Hamiltonian have been considered. However, some arguments related to "typicality" suffice to establish that, given the validity of Eq. (13), the validity of a JR will hold, even for a very large majority of pure states, which are not diagonal. These states also could be seen as a result of a nonprojective (weak) measurement of the initial energy. Consider to this end pure states $|\psi_E\rangle$ with the energy $E = \delta I$ which are drawn at random according to the unitary invariant Haar measure from the Hilbert space spanned by the projector Π_I. The corresponding work PDF is then given by

$$P_E(W) := \frac{1}{\delta}\langle\psi_E|U^\dagger \Pi_F U|\psi_E\rangle, \quad W = (F - I)\delta. \tag{D1}$$

Of course, here $P_E(W)$ technically depends on the specific $|\psi_E\rangle$. However, employing the methods and results of typicality [34,37], one finds for the Hilbert-space average HA$[\cdots]$ of $P_E(W)$ over the above $|\psi_E\rangle$,

$$\mathrm{HA}[P_E(W)] = \frac{1}{\delta}\mathrm{Tr}(\Pi_F U \rho^I_{\mathrm{mc}} U^\dagger), \tag{D2}$$

which equals the corresponding result for the mixed microcanonical initial state ρ^I_{mc} [cf. Eq. (8)]. While this finding points in the direction of the JR being fulfilled for the vast majority of the $|\psi_E\rangle$, it is, by itself, not sufficient

to conclude the latter. In order to do so, it remains to be shown that the corresponding Hilbert-space variance HV[$\cdots$] is small. Fortunately, expressions for such Hilbert-space variances may also be found in the literature [34,37]. Prior to computing these expressions for the present case we introduce some convenient notation. Let $\sigma^2(A)$ denote the variance of the spectrum of some operator A, with A being Hermitian, i.e., featuring real eigenvalues. Then the Hilbert-space variance for the work PDF is given by [34,37]

$$\mathrm{HV}[P_E(W)] = \frac{\sigma^2(\Pi_I U^\dagger \Pi_F U \Pi_I)}{\mathrm{Tr}(\Pi_I)+1}. \tag{D3}$$

Since the operator for which the spectral variance has to be determined contains only projectors and unitaries, i.e., has only eigenvalues with absolute values between zero and one, an upper bound on the spectral variance is readily found:

$$\sigma^2(\Pi_I U^\dagger \Pi_F U \Pi_I) < 1. \tag{D4}$$

(This bound may easily be tightened, but this is of no further relevance here.) This yields an upper bound for the Hilbert-space variance

$$\mathrm{HV}[P_E(W)] < \frac{1}{\mathrm{Tr}(\Pi_I)+1}. \tag{D5}$$

The crucial quantity here is obviously $\mathrm{Tr}(\Pi_I)$, which is just the number of eigenstates of the initial Hamiltonian $H(0)$ within the energy interval of size δ around E. For any given δ it is to be expected that this number of eigenstates increases quickly (exponentially) with increasing bath size. Hence, for large baths $\mathrm{HV}[P_E(W)]$ becomes very small, thus rendering the outcome for $P_E(W)$ for the overwhelming majority of individual $|\psi_E\rangle$ indeed very close to the outcome one obtains from the microcanonical initial state ρ^I_{mc}. In other words, all the above findings on microcanonical initial states ρ^I_{mc} transfer to pure initial states $|\psi_E\rangle$ for all practical purposes. In this sense the JR also applies to many pure states.

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