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Work fluctuations in small quantum spin chains

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We study the work fluctuations of two types of finite quantum spin chains under the application of a time-dependent magnetic field in the context of the fluctuation relation and Jarzynski equality. The two types of quantum chains correspond to the integrable Ising quantum chain and the non-integrable XX quantum chain in a longitudinal magnetic field. For several magnetic field protocols, the quantum Crooks and Jarzynski relations are numerically tested and fulfilled. As a more interesting situation, we consider the forcing regime where a periodic magnetic field is applied. In the Ising case we give an exact solution in terms of double confluent Heun functions. We show that the fluctuations of the work performed by the external periodic drift are maximum at a frequency proportional to the amplitude of the field. In the non-integrable case, we show that depending on the field frequency a sharp transition is observed between a Poisson limit work distribution at high frequencies toward a normal work distribution at low frequencies.

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I. INTRODUCTION

Soon after the derivation of the by now so called Jarzynski equality [21] relating the fluctuation of the non-equilibrium work performed on a system, initially thermalised, to its free energy difference, it was recognized that this relation can be derived from a much more fundamental theorem, namely the fluctuation relation [19]. The fluctuation theorem is a statement on the symmetry of the fluctuations of the entropy production along a non-equilibrium path and it is directly linked to time-reversal symmetry [27]. The first occurrence of such a fluctuation relation was obtained numerically in [15] for steady states systems and was soon after derived for driven thermostated deterministic systems [16], thermostated steady state systems with deterministic [19] and stochastic dynamics [20, 24, 25, 27, 41]. The fluctuation theorem states that the large deviation function $\zeta(p) = \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \ln \pi_\tau(p)$ associated to the distribution $\pi_\tau(p)$ satisfies

$$\zeta(p) = \zeta(-p) + p\sigma \quad (1)$$

for

$$p = \frac{1}{\sigma\tau} \int_0^\tau dt \sigma(\Gamma_t) \quad (2)$$

where $\sigma(\Gamma_t)$ is the entropy production rate along the trajectory Γ_t and $\sigma \geq 0$ the average entropy creation rate. It was shown that in the limit of vanishing entropy pro-

duction, one is able to recover from this theorem the linear (close to equilibrium) fluctuation-dissipation theorem [17, 18, 23].

Whereas this theorem is an asymptotic statement, Crooks derived an interesting identity reading [11, 12]

$$\frac{P_F(S)}{P_B(-S)} = e^S \quad (3)$$

where S is the entropy production for a system driven during time τ within a forward protocol $\lambda_F(t)$, P_F is the distribution of entropy production in the forward process and P_B is the distribution associated to the backward process, that is when the system is driven in a time-reversed manner. One may notice that in general there is no reason that the time-reversed process is identified with the forward one, so that in general $P_F(S) \neq P_B(S)$. From the Crooks relation, utilising for a thermalised system $S = \beta(W - \Delta F)$, with $\Delta F = [F(\lambda_F(\tau)) - F(\lambda(0))]$ and integrating over W we have Jarzynski relation [21]

$$\langle e^{-\beta W} \rangle = e^{-\beta \Delta F}. \quad (4)$$

Fluctuation relations have been extended to the quantum world as well [14, 23, 28, 29, 31, 39] within various setup and prescriptions for the actual measurement of work performed on a quantum system, see Ref. [1] for a discussion. As it is clear from the extensivity of the entropy production, the probability to observe a decrease of entropy in a given non-equilibrium trajectory is exponentially small for a macroscopic system. However, for microscopic or mesoscopic systems, which can be nowadays manufactured quite easily, these untypical trajectories arise with a significant probability and consequently can be observed and measured in actual experimental

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setup. One may mention in particular experimental tests on the stretching of RNA molecules [10, 26], experiments on torsional pendulum [13], on colloidal particles [7, 44], on photochromic defect center in diamonds [43]. See Ref. [38] for an excellent review of the experimental related investigations. It is then interesting to calculate or predict the shape of these fluctuations in some explicit models for small system size [8, 22]. In this contribution we focus our attention to the work fluctuations of two time-dependent quantum spin chains where the time dependence is due to an externally applied magnetic field. The two models considered are the integrable quantum Ising chain in a time-dependent transverse field and the XX -quantum chain with a longitudinal magnetic field that breaks its integrability. We consider these two cases as archetypical of the integrable and non-integrable situations and we expect that the work distributions will reflect somehow these differences. We check Jarzynski and Crooks relations and compute explicitly the non-equilibrium work distributions associated to several magnetic field protocols. In particular, we study the limiting steady distributions in the important case of periodically driven system. The paper is organised as follows: in the next section we derive the quantum version of Crooks relation and show how this equality is linked to time-reversal symmetry. We discuss as well the effect of additional symmetries and the definition of work in the quantal world. The quantum spin models and the results are presented in section 3 and we summarize and discuss our results in the last section.

II. QUANTUM FLUCTUATION RELATIONS

A. Time reversal

As it was emphasized in the introduction, the fluctuation symmetry expressed in the fluctuation theorem is linked to time-reversal symmetry. In quantum mechanics, to time reversal is associated an antiunitary operator K , $K(\alpha\phi + \beta\psi) = \alpha^*K\phi + \beta^*K\psi \ \forall \alpha, \beta \in \mathbf{C}$ and for all vectors ϕ, ψ , together with $K^+K = 1$ whose action is such that the position operator $X \rightarrow KXK^+ = X$, the impulsion $P \rightarrow KPK^+ = -P$ and spin $\mathbf{S} \rightarrow K\mathbf{S}K^+ = -\mathbf{S}$ under time reversal. More generally, we define the time reversed of a linear operator A through

$$(K\phi, \bar{A}K\psi) = (\psi, A\phi) \quad (5)$$

where $K\phi$ and $K\psi$ are the time reversed vectors associated to ϕ and ψ respectively. This leads for the time-reversed operator \bar{A} to the relation

$$\bar{A} = KA^+K^+ . \quad (6)$$

In particular, if U is the unitary evolution operator associated to a given system (which can be explicitly time-dependent), then its associated time-reversed operator

$\bar{U} = KU^+K^+$ defines a new evolution operator associated to a conjugated dynamical system. More precisely, using the group decomposition law $U(t_f, t_i) = U(t_N, t_0) = U(t_N, t_{N-1}) \dots U(t_2, t_1)U(t_1, t_0)$ with $t_N > t_{N-1} > \dots > t_1 > t_0$, with the notations $U_k \equiv U(t_k, t_{k-1})$, we have

$$\bar{U} = \bar{U}_1\bar{U}_2 \dots \bar{U}_N \quad (7)$$

If now we have a forward protocol with a step-like time-dependent Hamiltonian $H(t) = H_k$ for $t \in]t_{k-1}, t_k]$ such that $U_k = e^{-iH_k(t_k - t_{k-1})}$, then \bar{U} defines the conjugated backward protocol $H^B(t)$ with a new step-like time-dependent Hamiltonian

$$H_k^B \equiv \bar{H}_{N-k+1} . \quad (8)$$

Note that the backward protocol just defined does not necessarily describe a real physical process but it is merely a mathematical object. In cases where H^B is effectively meaningful in physical terms, the time reversed dynamics \bar{U} is the dynamics associated to the backward physical process. The time-reversible situation $\bar{U} = U$ leads to the condition $\bar{U}_k = U_{N-k+1}$ which in terms of the Hamiltonians translates into

$$H_k^B = \bar{H}_{N-k+1} = H_k \quad (9)$$

so that the backward Hamiltonian is identified with the forward Hamiltonian.

B. Quantum Crooks relation

Consider a forward protocol defined by the time-dependent Hamiltonian $H(t)$ with $t \in [t_i, t_f]$ and its conjugated, as defined in the previous section, backward protocol $H^B(t)$ with $t \in [t_i, t_f]$. The transition probability from an initial state ϕ to a final state χ in the forward process is given by

$$P_F(\phi \rightarrow \chi) = |(\chi, U\phi)|^2 \omega_F^\phi \quad (10)$$

where $\omega_F^\phi = (\phi, \rho_F\phi)$ with ρ_F the density matrix of the initial state. The transition probability of the backward protocol is given by

$$P_B(K\chi \rightarrow K\phi) = |(K\phi, \bar{U}K\chi)|^2 \omega_B^{K\chi} \quad (11)$$

Now since $|(K\phi, \bar{U}K\chi)|^2 = |(\chi, U\phi)|^2$ we have for the ratio

$$\frac{P_F(\phi \rightarrow \chi)}{P_B(K\chi \rightarrow K\phi)} = \frac{\omega_F^\phi}{\omega_B^{K\chi}} \quad (12)$$

and this is basically what is needed to prove a quantum Crooks relation.

Indeed, let the forward process be initially in the canonical state

$$\rho_F = e^{\beta(F^F - H^F(t_i))} \quad (13)$$

where F^F is the corresponding equilibrium free energy. The backward protocol is defined with an initial state given by

$$\rho_B = e^{\beta(F^B - H^B(t_i))} \quad (14)$$

where F^B is its corresponding free energy and $H^F = H(t_i)$ the initial Hamiltonian. In order to avoid ambiguities we consider here only finite Hilbert space systems. Let $\{\phi_n^{F,B}\}$ be the eigenbasis of the initial Hamiltonians $H^{F,B}$ with the corresponding eigenenergies $\{E_n^{F,B}\}$. The ratio P_F/P_B is then expressed as

$$\frac{P_F(\phi_n^F \rightarrow \phi_k^B)}{P_B(\bar{\phi}_k^B \rightarrow \bar{\phi}_n^F)} = e^{-\beta[F^B - F^F]} e^{\beta[E_k^B - E_n^F]} = e^{-\beta[\Delta F - \Delta E_{n,k}]} = e^{\Delta S_{nk}} \quad (15)$$

where we have introduced the suggestive notation $\Delta S = \beta[\Delta E - \Delta F]$ which can be interpreted as the entropy production, with $W = \Delta E$ the externally performed work, along the path $\phi_n^F \rightarrow \phi_k^B$. We define the total probability of having a given variation ΔS in the forward process $\forall n, k$ as

$$P_F(\Delta S) = \sum_{n,k} \delta(\Delta S_{nk} - \Delta S) P_F(\phi_n^F \rightarrow \phi_k^B). \quad (16)$$

Using (15) into this definition, one obtains

$$P_F(\Delta S) = e^{\Delta S} \sum_{n,k} \delta(-\Delta S_{nk} + \Delta S) P_B(\bar{\phi}_k^B \rightarrow \bar{\phi}_n^F). \quad (17)$$

Now assume that the initial Hamiltonians are time-reversible, that is $KH^{F,B} = H^{F,B}K$. It implies that if ϕ_n is an eigenvector associated to E_n then $K\phi_n$ is also an eigenstate associated to the same eigenvalue. This implies then that $-\Delta S_{nk} = \Delta S_{kn}$, where $\Delta S = \beta[\Delta E - \Delta F]$ is interpreted as the entropy production along the conjugated time-reversed protocol. Inserting that into (17) leads finally to the Crooks quantum fluctuation relation:

$$P_F(\Delta S) = e^{\Delta S} P_B(-\Delta S) \quad (18)$$

which can be equivalently rewritten in the form

$$P_F(W) = e^{-\beta\Delta F} e^{\beta W} P_B(-W). \quad (19)$$

From this last form it is very easy to derive a quantum Jarzynski equality integrating over W :

$$\langle e^{-\beta W} \rangle_F \equiv \int dW e^{-\beta W} P_F(W) = e^{-\beta\Delta F}. \quad (20)$$

If, additionally, one assumes a time-reversible process, that is $\bar{U} = U$, then one has to identify P_B with P_F and one obtains a statement that is fulfilled by the probability distribution of a single process, namely the so called transient fluctuation theorem

$$\frac{P(\Delta S)}{P(-\Delta S)} = e^{\Delta S}. \quad (21)$$

C. Additional symmetries

Since we will focus our attention on quantum Ising chain Hamiltonians $H(t)$ with a time-dependence contained in the Zeeman term $-h(t)\sum_j \sigma_j^z$, let us discuss this case in more details. The Zeeman term is not time reversal and since it is proportional to the spin we have

$$\bar{H}(h(t)) = H(-h(t)) = T^+ H(h(t)) T \quad (22)$$

where T is a linear unitary transformation such that the z -component of the spin is spacially reversed: $\sigma_j^z \rightarrow T^+ \sigma_j^z T = -\sigma_j^z$. Such an operator is given by $T = \prod_j T_j$ with $T_j = e^{i\frac{\pi}{2}\sigma_j^x} = i\sigma_j^x$. For a symmetric forward protocol, such that $H(t_f - (t - t_i)) = H(t)$, the time-reversed evolution operator can be written as

$$\bar{U} = T^+ U T. \quad (23)$$

It is also clear that the unitary transformation T commutes with the time-reversal antilinear operator K : $KT = TK$. From these considerations, if we consider an initial Hamiltonian which is invariant under T , that is $TH(t_i) = H(t_i)T$, which is the case if the external field h is vanishing for the Ising quantum chain then if ϕ_n is an eigenstate of $H(t_i)$ then the transformed vector $T\phi_n$ is also an eigenstate associated to the same eigenvalue. If one chooses for the initial Hamiltonian the eigenbasis $\{\phi_{n,\varepsilon}\}$ which also diagonalises T we have for the backward process

$$\begin{aligned} P_B(\bar{\phi}_{n,\varepsilon} \rightarrow \bar{\phi}_{k,\varepsilon'}) &= |(K\phi_{k,\varepsilon'}, \bar{U}K\phi_{n,\varepsilon})|^2 e^{\beta[F - E_{n,\varepsilon}]} \\ &= |(K\phi_{k,\varepsilon'}, T^+ U T K\phi_{n,\varepsilon})|^2 e^{\beta[F - E_{n,\varepsilon}]} \\ &= |(KT\phi_{k,\varepsilon'}, UKT\phi_{n,\varepsilon})|^2 e^{\beta[F - E_{n,\varepsilon}]} \\ &= |(K\phi_{k,\varepsilon'}, UK\phi_{n,\varepsilon})|^2 e^{\beta[F - E_{n,\varepsilon}]} \\ &= P_F(\bar{\phi}_{n,\varepsilon} \rightarrow \bar{\phi}_{k,\varepsilon'}). \end{aligned} \quad (24)$$

Summing up over all possible transitions, one then recovers the transient fluctuation relation (21).

D. Work operator

In the present study we use as a definition for the work the difference of energies in the final state and initial state, which assumes that we have measurements performed at t_i and t_f . It is clear that this definition differs from the introduction of a work operator defined such that its expectation in the state ρ would give the actual performed work:

$$W = \int_{t_i}^{t_f} ds \text{Tr}\{\rho(s) \frac{dH}{ds}\} \quad (25)$$

which can be shown to be given by

$$W = \text{Tr}\{\rho(t_i) \delta H\} = \text{Tr}\{\rho(t_i) [U^+(t_f, t_i) H(t_f) U(t_f, t_i) - H(t_i)]\} \quad (26)$$

after a short algebra. One is then tempted to define as a work operator $\delta H = \hat{H}(t_f) - H(t_i)$, with \hat{A} the Heisenberg picture of A . However, it is clear that in general the moments $\langle (\delta H)^n \rangle$ would differ from the moments $\langle W^n \rangle = \int dW W^n P(W)$ with $P(W)$ defined in the preceding section and consequently the expectation of the operator $e^{-\beta \delta H}$

$$\langle e^{-\beta \delta H} \rangle = \text{Tr} \{ \rho(t_i) e^{-\beta \delta H} \} \quad (27)$$

will not necessarily give the Jarzynski result $e^{-\beta \Delta F}$. Nevertheless, one can show that the moments so defined will differ only for $n > 2$, so that for the average and average square work one can use the work operator δH since then

$$\begin{aligned} \langle \delta H \rangle &= \text{Tr} \{ \rho(t_i) \delta H \} = \int dW W P(W) \\ \langle (\delta H)^2 \rangle &= \text{Tr} \{ \rho(t_i) (\delta H)^2 \} = \int dW W^2 P(W) \end{aligned} \quad (28)$$

with $P(W) = \sum_{i,f} \delta(\Delta E_{if} - W) |(\phi_f, U \phi_i)|^2 \omega^{\phi_i}$.

III. QUANTUM SPIN CHAINS IN A TIME DEPENDENT FIELD

A. Definition of the model and protocol

In this section we study quantum chains with a time-dependent field, in the context of the fluctuation relation, defined through the following Hamiltonian:

$$H = -\frac{1}{2} \sum_{i=1}^{N-1} \sigma_i^x \sigma_{i+1}^x - \frac{\Delta}{2} \sum_{i=1}^{N-1} \sigma_i^z \sigma_{i+1}^z - \frac{1}{2} h(t) \sum_{i=1}^N \sigma_i^z \quad (29)$$

in particular in the two cases $\Delta = 0$ and $\Delta = 1$. The σ 's are Pauli's matrices and $h(t)$ is a time-dependent magnetic field applied in the z -direction and leading to the Zeeman term $-h(t)M^z$ where M^z is the total z -component of the magnetization.

At $\Delta = 0$, it corresponds to the Ising quantum chain. In a static transverse field the Ising chain can be mapped after a Jordan-Wigner transformation onto a fermionic problem which can be diagonalised after a suitable canonical (Bogoliubov) transformation. In the thermodynamic limit $N \rightarrow \infty$, this model presents a quantum phase transition at $h = h_c = 1$ which is in the 2d classical Ising model universality class. The integrability and non-triviality (in the sense of physical properties) of the model is at the origine of its wide use in many fundamental studies concerning in particular the testing grounds of non-equilibrium quantum statistical mechanics. One may mention for exemple relaxation properties from an inhomogeneous initial state [3, 4, 32, 34, 35, 40], entropy production after a local quench [6, 33], entropy production in the unique NESS (non-equilibrium steady state) generated from a two temperature initial state [2], or even

relaxation properties after a quench through the critical point (basically h is varied from $h_i > h_c$ to $h_f < h_c$) [9, 42].

The case $\Delta = 1$ corresponds to the isotropic XX-quantum chain in a time-dependent magnetic field, which breaks the integrability of the model. With a periodic dependence of the field, this model has to be compared to the quantum kicked Heisenberg chain:

$$H(t) = -\frac{1}{2} \sum_{j=0}^{L-1} (\sigma_j^x \sigma_{j+1}^x + \sigma_j^z \sigma_{j+1}^z + \delta(t) V \sigma_j^y \sigma_{j+1}^y) \quad (30)$$

where the time-dependent perturbation is periodically switched on. This model was studied in the context of the transition from integrability to ergodicity in the thermodynamic limit [30, 36, 37]. Here instead of the two-body interaction (in the fermionic picture) $\sigma_j^y \sigma_{j+1}^y$ we apply a magnetic field in the z -direction which leads to a many-body fermionic term.

In the following, we consider the work distribution, as defined in the previous section, for various magnetic field protocols. The study is numerical, based on the exact diagonalisation of short chains, typically less than $N = 10$ spins. Through the paper we use free boundary conditions. The dynamics is generated by the unitary evolution

$$U(t, t_0) = \prod_{n=0}^{M-1} U(t_{n+1}, t_n) \quad (31)$$

with

$$U(t_n, t_{n-1}) = e^{iH(t_n)\Delta t} \quad (32)$$

where Δt is an elementary time increment. The true dynamics is obtained by taking the limit $\Delta t \rightarrow 0$, and $M \rightarrow \infty$. In the present study we use typically values of Δt of order 10^{-2} . The transition probabilities $w_{\alpha \rightarrow \beta} = |(\psi_\beta, U(t, t_0) \psi_\alpha)|^2$, where ψ_α (ψ_β) are eigenstates of the initial (final) Hamiltonian, are computed numerically using (31) and (32).

B. Jarzynski and Crooks relations

In order to test our numerical procedure we compare first the free energy differences obtained from the Jarzynski equality (20) in a linear varying field protocol with the equilibrium free energy differences calculated directly from the partition function

$$F(h(t)) = -\frac{1}{\beta} \ln \text{Tr} \{ e^{-\beta H(t)} \}. \quad (33)$$

In figure 1 we have plotted the free energy differences obtained from the Jarzynski equality and from a direct equilibrium calculation as a function of the final field value h at inverse temperature $\beta = 1$. The agreement

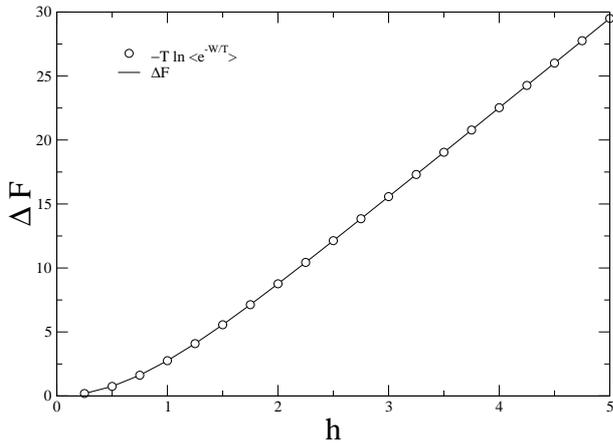


FIG. 1: Free energy difference obtained from the Jarzynski equality compared to the exact value for the Ising chain with $N = 7$ as a function of the terminal field value at $\beta = 1$ and $h(t) = t$.

is excellent with a relative deviation which is less than 10^{-6} .

We have also considered the ratio $P_F(W)/P_B(-W) = P(W)/P(-W)$ for the symmetric protocol $h(t) = h_o \sin(\pi t/\tau)$ for $t \in [0, \tau]$. In figure 2 we see explicitly the exponential dependence $e^{\beta W}$ for $h_o = 1/2$ and 2 for a chain of size $N = 8$. Again, the agreement of the numerics with the analytical Crooks and Jarzynski relations is fulfilled with a relative deviation which is less than 10^{-6} . We have tested also the Crooks relation in the non-symmetrical protocol whose results are presented in figure 3. Again, the exponential dependence $e^{\beta W}$ is clearly seen on the graph.

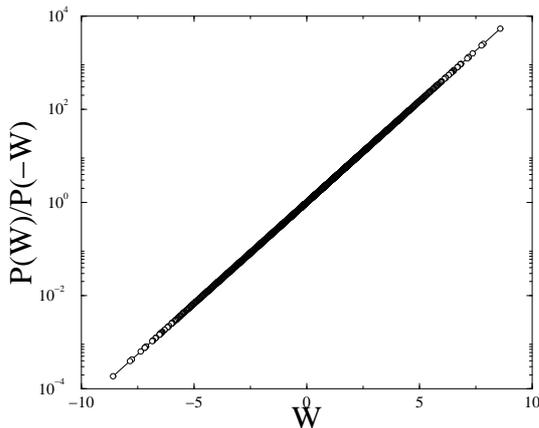


FIG. 2: Crooks fluctuation ratio in the symmetrical case for the XX chain at $\Delta = 1$ with $N = 8$ at $\beta = 1$ and $\tau = 1$.

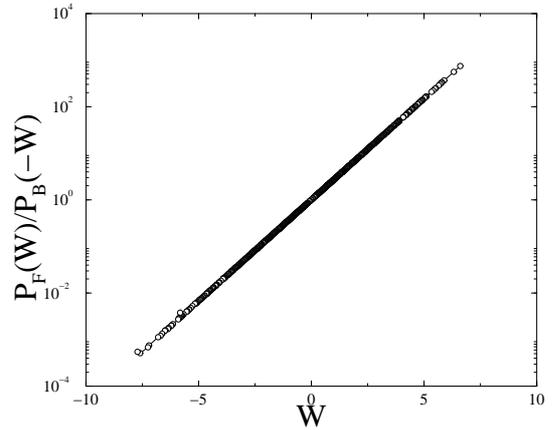


FIG. 3: Crooks fluctuation ratio in the asymmetrical case for the XX chain at $\Delta = 1$ with $N = 8$ at $\beta = 1$.

C. Stationary distributions in the driven regime

1. Ising quantum chain

a. Numerical study We consider now the case where the system is forced with a periodic external field with period τ and maximum value h_o and minimum value 0. We are interested in the limiting stationary work distribution (if any) obtained after many periods of the external driving field.

Before going on the driven situation, we concentrate on the fluctuations of the work after one period. In figure 4 we show the distributions obtained on the Ising chain with $N = 7$ spins for $h_o = 1/2$ and for different periods τ of the forcing field for an initial infinite temperature state $\beta = 0$ (equidistribution of the initial eigenstates). In that case, obviously, the average work is vanishing, which is reflected in the symmetry of the work distribution $P(W) = P(-W)$. On figure 4 we see clearly that the evolution of the distribution is not monotonic with the forcing period τ . The width of the distribution first increases with τ , reaching a maximum and then decreases with τ . This behaviour is clearly seen on the second moment $\langle W^2 \rangle$ in figure 5 where we show the variance $\langle W^2 \rangle_{\beta=0}$ as a function of τ for different maximum field values h_o for a $N = 7$ spin chain. We see that the width of the distribution increases with the amplitude of the perturbation, since then the time-dependent perturbation is more effectively coupled with the spin chain. Moreover, the period τ_{max} associated to the maximum width decreases as the amplitude is increased with, as seen from the numerics, a law $\tau_{max} \sim 1/h$ for large fields enough ($h_o > 1$). Moreover we have seen numerically that τ_{max} is almost independent of the system size. As the field is increased, the maximum value of the variance reaches an asymptotic finite value which is linearly depending on the size N of the chain. One has from the numerics $\langle W^2 \rangle_{\beta=0, max} = (N - 1)/2$.

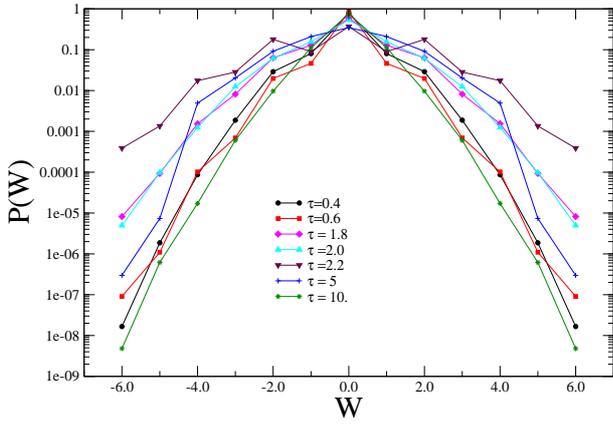


FIG. 4: Work probability distribution for the Ising model at with $N = 7$ spins at $\beta = 0$ for $h_o = 1/2$.

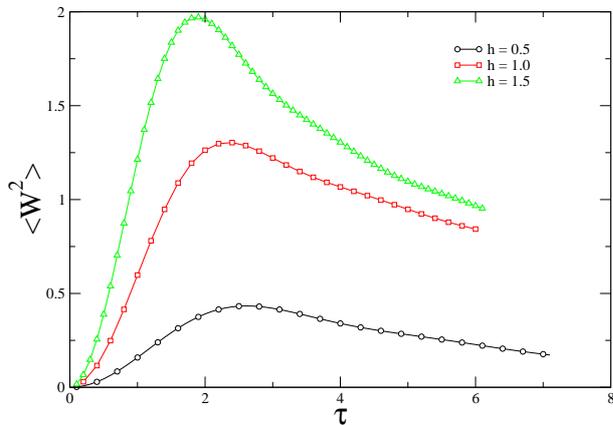


FIG. 5: $\langle W^2 \rangle$ for the Ising model with $N = 7$ spins at $\beta = 0$ as a function of the period τ .

We have also computed the first and second moments of the distribution as a function of τ for different inverse temperatures β . The initial state temperature acts as a scale factor for the moments:

$$\langle W \rangle_\beta = \tanh(\beta/2) \langle \delta W \rangle \quad (34)$$

and as seen on figure 6 one has for the variance

$$\langle W^2 \rangle_\beta - \langle W \rangle_\beta^2 = \langle W^2 \rangle_0. \quad (35)$$

Thus, the width of the distribution is basically independent of the initial state temperature.

We turn now to the driven situation with many periods. In figure 7 we present the time evolution of the average work for different periods τ at a field value $h_o = 1/2$ and inverse temperature $\beta = 1$. As expected, for large periods the system follows almost adiabatically the variation of the associated equilibrium free energy (the reversible work). Moreover, it is seen as expected from the second principle that the actual average work is always greater than the free energy difference (see the inset). As the period of the external transverse field is lowered,

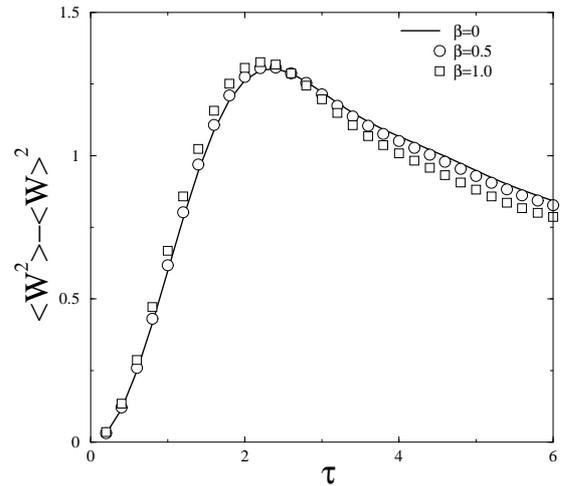


FIG. 6: Variance of the work distribution for the Ising model with $N = 7$ spins at $h_o = 1$ as a function of the period τ for $\beta = 0$, $\beta = 1/2$ and $\beta = 1$.

we see that the deviation from the free energy difference becomes larger and one is no more able to recognize the underlying oscillatory external field. The largest variations and most "chaotic" behaviour is obtained at the value τ_{max} previously identified for one period. At higher frequencies the fluctuations of the average work decrease again.

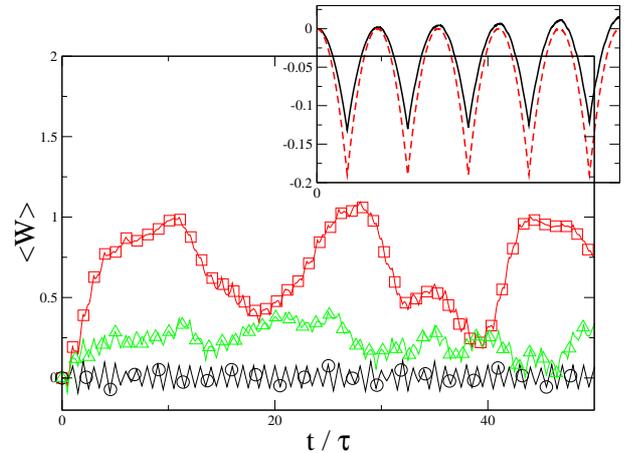


FIG. 7: Time evolution of the average work for the Ising chain with a triangular periodic transverse field at $\beta = 1$ and maximal amplitude $h_o = 1/2$ with periods $\tau = 1$ (circles), $\tau = 3$ (squares) and $\tau = 5$ (triangles). The inset shows the free energy difference (lower curve) and the average work (top curve) for a large period $\tau = 50$ of the field. In this case the transformation is nearly adiabatic.

b. Exact solution for the driven Ising model With a sinusoidal forcing field $h(t) \propto \sin(\omega t)$ it is in fact possible to solve exactly the dynamics of the Ising quantum chain. Indeed, following the lines of Ref.[5], we can put the periodic boundary conditions Hamiltonian (29), after

a Jordan Wigner transformation followed by a Bogoliubov one, into a sum of commuting operators:

$$H = \sum_{p=1}^{N/2} \tilde{H}_p \quad (36)$$

with

$$\begin{aligned} \tilde{H}_p &= (\cos \phi_p - h(t)) [a_p^+ a_p + a_{-p}^+ a_{-p}] \\ &\quad - i \frac{1}{2} \sin \phi_p [a_p^+ a_{-p}^+ + a_p a_{-p}] + h(t) \end{aligned} \quad (37)$$

where $[\tilde{H}_p, \tilde{H}_q] = 0$ and where $\phi_p = 2\pi p/N$. The a^+, a are Fermi operators in momentum space. Using the following basis ($|0\rangle, a_p^+ a_{-p}^+ |0\rangle, a_p^+ |0\rangle, a_{-p}^+ |0\rangle$), where $|0\rangle$ is the vacuum of the a fermions, we have the 4×4 representation

$$\tilde{H}_p = \begin{pmatrix} h(t) & -i \sin \phi_p & 0 & 0 \\ i \sin \phi_p & 2 \cos \phi_p - h(t) & 0 & 0 \\ 0 & 0 & \cos \phi_p & 0 \\ 0 & 0 & 0 & \cos \phi_p \end{pmatrix} \quad (38)$$

In the Heisenberg picture, the time evolution matrix $U_p(t)$ in the subset p is governed by the equation ($\hbar = 1$)

$$i \frac{d}{dt} U_p(t) = U_p(t) \tilde{H}_p(t) \quad (39)$$

with the boundary condition $U_p(0) = I$. Using (38) and (39), it is easy to obtain for the non vanishing elements of the 4×4 matrix $U_p(t)$ the differential equation

$$\begin{aligned} i \frac{d}{dt} \begin{pmatrix} U_p^{11}(t) & U_p^{12}(t) \\ U_p^{21}(t) & U_p^{22}(t) \end{pmatrix} &= \begin{pmatrix} U_p^{11}(t) & U_p^{12}(t) \\ U_p^{21}(t) & U_p^{22}(t) \end{pmatrix} \times \\ \begin{pmatrix} h(t) & -i \sin \phi_p \\ i \sin \phi_p & 2 \cos \phi_p - h(t) \end{pmatrix} \end{aligned} \quad (40)$$

and $U_p^{33}(t) = U_p^{44}(t) = e^{-it \cos \phi_p}$. From the two-coupled first order differential equations, it is easy to obtain the decoupled second order ones. For exemple, one has for the 11-component

$$iu'' - 2 \cos \phi u' - (h' - i \sin^2 \phi + ih[2 \cos \phi - h])u = 0 \quad (41)$$

with $u(0) = 1$, $u'(0) = -ih(0)$ and similar equations for the other components. Taking for the field the form $h(t) = h_1 + h_2 \cos(\omega t)$ and putting it in the differential equation (41) one gets solutions in terms of double confluent Heun function H_D , namely for $U_p^{11}(t)$ and U_p^{12} one has

$$\begin{aligned} U_p^{11}(t) &= \frac{1}{2h_2} [(\cos \phi_p - h_1) e^{iA_t} H_D(\alpha, \beta, \gamma, \delta, -iz) \\ &\quad - (\cos \phi_p - 2h_2 - h_1) e^{-iA_t} H_D(-\alpha, \beta, \gamma, \delta, iz)] \quad , (42) \end{aligned}$$

$$\begin{aligned} U_p^{12}(t) &= \frac{i \sin \phi_p}{2h_2} [e^{iA_t} H_D(\alpha, \beta, -\gamma, \delta, -iz) \\ &\quad - e^{-iA_t} H_D(-\alpha, \beta, -\gamma, \delta, iz)] \quad , (43) \end{aligned}$$

with $z = \tan(\omega t/2)$, $A_t = \frac{h_2}{\omega} \sin(\omega t) - t \cos \phi_p$, $\alpha = \gamma/2 = 4h_2/\omega$, $\beta = \frac{4}{\omega^2} [h_2^2 - |h_2 - h_1 + e^{i\phi_p}|^2]$ and $\delta = -\frac{4}{\omega^2} [h_2^2 - |h_2 + h_1 + e^{i\phi_p}|^2]$, and similar expressions for the other components.

The equilibrium initial state is factorized as $\rho(0) \propto \prod_{p=1}^{N/2} e^{-\beta \tilde{H}_p(0)}$ and its time-evolution is given by the tensor product

$$\rho(t) = \rho_1(t) \rho_2(t) \dots \rho_{N/2}(t) \quad (44)$$

with

$$\rho_p(t) = U_p(t) \rho_p(0) U_p^\dagger(t) \quad (45)$$

The average work performed on the system during the time t with the periodic forcing is given by the integral of the magnetisation:

$$\langle W \rangle(t) = - \int_0^t ds h'(s) Tr \{ \rho(s) M^z \} \quad (46)$$

where $M^z = \sum_{p=1}^{N/2} M_p^z$, with $M_p^z = a_p^+ a_p + a_{-p}^+ a_{-p} - 1$, is the total magnetisation operator in the z -direction. Using the factorised form of $\rho(t)$ and the additive structure of M^z , it is easy to compute $\langle M^z \rangle(t)$ and one obtains

$$\begin{aligned} \langle M^z \rangle(t) &= \sum_{p=1}^{N/2} \frac{\tanh\left(\frac{\beta \Lambda_p}{2}\right)}{\Lambda_p} [(h(0) - \cos \phi_p) (2|U_p^{11}|^2 - 1) \\ &\quad - 2 \sin \phi_p Im \{ U_p^{12} U_p^{11*} \}] \end{aligned} \quad (47)$$

with $\Lambda_p = \sqrt{\sin^2 \phi_p + (h(0) - \cos \phi_p)^2}$. Together with the solutions of the U_p components in terms of Heun functions, this formally solves the problem for the average work. One may notice that the factor $\tanh(\frac{\beta \Lambda_p}{2})$ in this expression leads to the previously observed $\tanh(\beta/2)$ in (34) since in that case $h(0) = 0$ and then $\Lambda_p(0) = 1 \forall p$ and one has for the average magnetization

$$\begin{aligned} \langle M^z \rangle(t) &= - \tanh\left(\frac{\beta}{2}\right) [1 + 2 \sum_p \cos \phi_p |U_p^{11}|^2 \\ &\quad + \sin \phi_p Im \{ U_p^{12} U_p^{11*} \}] \quad . (48) \end{aligned}$$

Finally, taking $h_1 = -h_2 = h_o/2$, such that $h(t) = h_o \sin^2(\frac{\omega t}{2})$, we have an exact solution for a situation which closely resembles to the triangular drift treated above numerically. We show the behaviour of the average work on figure 8 for different periods $\tau = 2\pi/\omega$. As previously observed, the average work fluctuations are maximum around $\tau = 3$.

2. XX chain in a longitudinal magnetic field

Finally we present the results obtained in the forced regime for the XX chain. In figure 9 we show the stationary work probability distributions for short and long period τ on a chain of $N = 8$ spins obtained from an

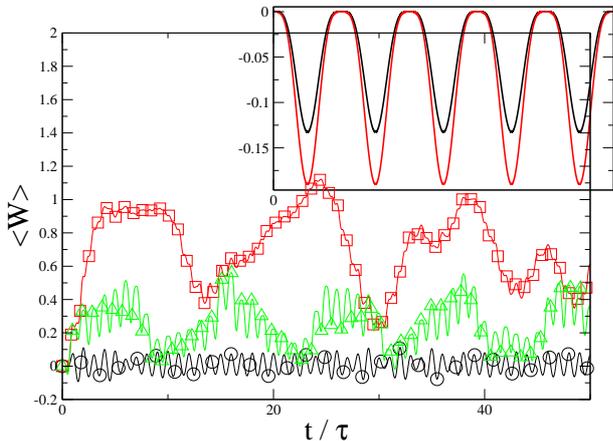


FIG. 8: Time evolution of the average work for the Ising chain with a sine square periodic transverse field at $\beta = 1$ and maximal amplitude $h_o = 1/2$ with periods $\tau = 1$ (circles), $\tau = 3$ (squares) and $\tau = 4$ (triangles). The inset shows the free energy difference (lower curve) and the average work (top curve) for a large period $\tau = 50$ of the field. In this case the transformation is nearly adiabatic.

initial infinite temperature state after applying the field over typically several tens of periods (after about 30 periods the work distributions are collapsing nicely on the same curve). We see clearly the appearance of two different regimes depending on the time scale τ . For very short periods $\tau \ll 1$, the distribution is very well approximated by an exponential law $e^{-|W|/\alpha}/(2\alpha)$ while for long enough time scale τ the distribution is close to a normal law. One may notice on figure 9 the very good collapse of the distributions for different values of the period τ in both short and long periods regimes. To give evidences

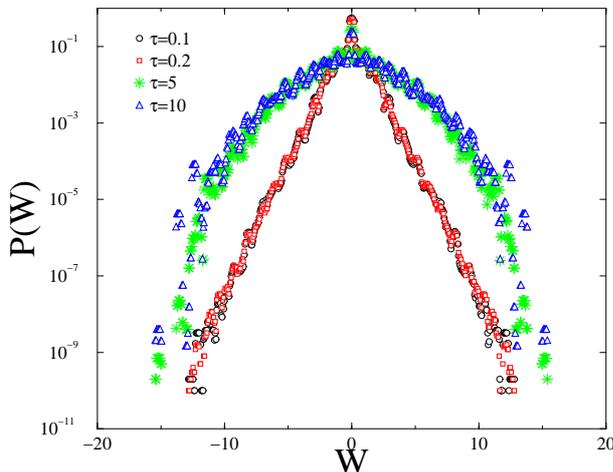


FIG. 9: Work probability distribution for the XX quantum chain with $N = 8$ spins at $\beta = 0$ for $h_o = 1/2$.

of this transition, we have plotted on figure 10 the variance $\langle W^2 \rangle_0$ (the average work is vanishing since $\beta = 0$) of

the distribution $P(W)$ as a function of the time scale τ . For a system of size $N = 8$, we observe a sharp increase of the variance from values around 0.25 at time scales smaller than for $\tau_c \simeq 1$ to values around 2.5 at larger periods τ where the shape is gaussian-like. Note that the threshold value τ_c is depending on the system size, decreasing as the size is increased. On figure 11 we show

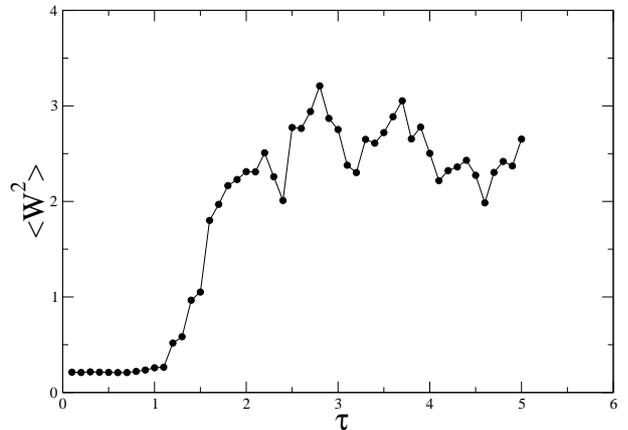


FIG. 10: Second moment of the work distribution for the XX quantum chain with $N = 8$ spins at $\beta = 0$ for $h_o = 1/2$ as a function of the field period τ .

the field amplitude dependence of the variance $\langle W^2 \rangle_0$ of the work distribution for short and long periods of the external drift. One may notice that at long periods, the increase of the variance with the field amplitude is almost linear, while it is more curved at short periods. On

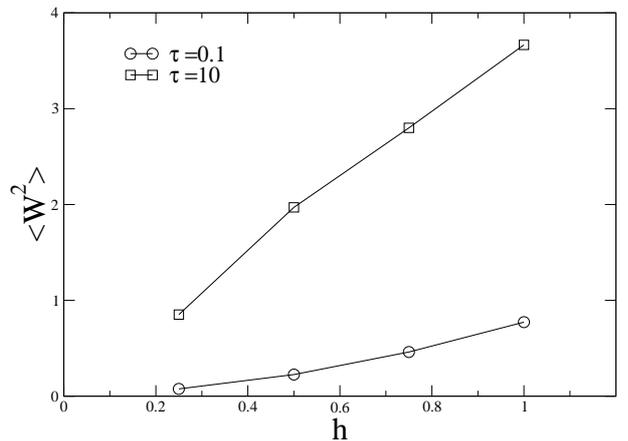


FIG. 11: Second moment of the work distribution for the XX quantum chain with $N = 8$ spins at $\beta = 0$ as a function of the field maximal amplitude h_o .

figure 12 we see that as the size is increased the variance at large time scales strongly grows with N , while there

is almost no dependence on the size at high frequencies. It means that when the period of the external field is too short, the system has no time to follow the perturbation and only transitions between nearby levels are significantly induced. On the contrary, and as the system size is increased, at long periods enough, meaning that the external field drives efficiently the system from its initial level to a new state, transitions between far apart levels are becoming significant.

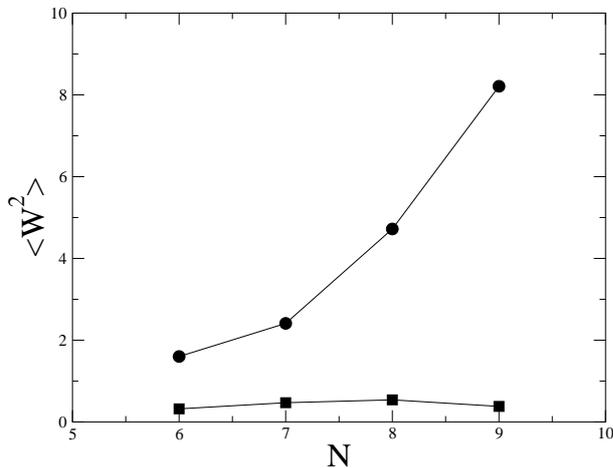


FIG. 12: Second moment of the work distribution for the XX quantum chain with $h_o = 1/2$, at $\beta = 0$ as a function of the system size N for $\tau = 0.1$ (squares) and $\tau = 10$ (circles).

Finally, we have analysed the temperature dependence of the work distribution $P(W)$ in the large τ regime. As seen on figure 13, the average work after a first increase with β seems to finally saturate at a value close to 0.44. We have checked that this shape is compatible with a $\tanh(\mu\beta)$ behaviour. Contrary to the temperature independent variance of the Ising case distributions, we see here that the variance of the distribution is decreasing (increasing) with β (temperature), which is what one would normally expect.

IV. SUMMARY AND DISCUSSION

In this study we have presented the numerical and analytical results we have obtained for the work distribution of small quantum systems driven by an external field. We have considered two different models, namely the integrable Ising quantum chain in a time-dependent transverse field and the XX quantum chain in a time-dependent longitudinal magnetic field. In this last model, the presence of the longitudinal field breaks the free fermionic structure of the chain, while the transverse field in the Ising case preserves the free particles structure which obviously leads to integrability. In a first stage, we have checked the validity of both quan-

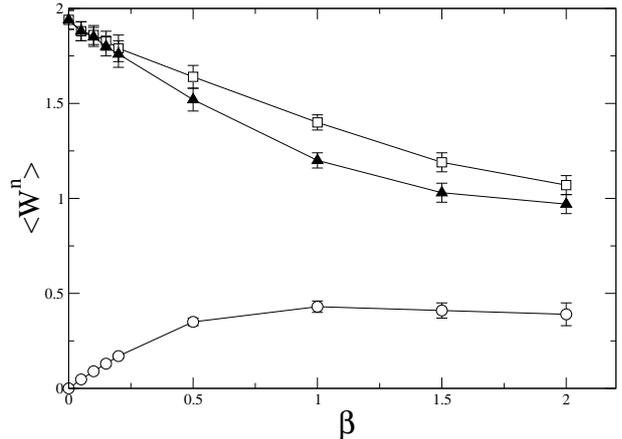


FIG. 13: First moment (circles), second moment (squares) and variance (triangles) of the work distribution for the XX quantum chain with $N = 8$ spins at $\tau = 10$ at $h_o = 1/2$ as a function of the inverse temperature β .

tum Jarzynski and quantum Crooks relations that were largely discussed in section 2. After this initial check, validating our numerical approach, we focused our attention to the periodic driven situation. In the Ising chain, exploiting its free fermionic structure, we solved exactly the unitary dynamics of the system in terms of somehow complicated double confluent Heun functions. The main features observed are, as expected, that for a slow enough process, that is large period of the oscillations of the field compared to the coupling constant, we recover the adiabatic situation where the work slightly differs, from above, from the equilibrium free energy difference. This is a statement of the second principle. As the process is fastened, the average work starts to deviate significantly from the free energy difference with fluctuations in time that are growing as the frequency of the field is increased. Nevertheless, at very high frequencies, the work fluctuations decrease again to zero. In this case, the variation of the field is so fast that the system is not able to follow it anymore. The maximum amplitude of the work fluctuations is obtained at an intermediate period which is of order of the inverse field amplitude, at least for large field enough. This threshold is understood as a dynamical resonance. In the Ising chain, one is not able to observe a steady work distribution. The behaviour of the XX chain in a longitudinal periodic field is quite different. We observe numerically, that the long-time work distribution reaches a steady shape which is strongly dependent on the frequency of the field. Indeed, at high frequencies the distribution is well fitted by an exponential curve, $e^{-|W|/\alpha}/(2\alpha)$, where α is almost size-independent. Lowering the frequency, there is a sharp transition toward a Gaussian like behaviour for the work distribution. The width of the normal distribution strongly increases as the size of the system is

increased, probably leading asymptotically to a flat distribution. The change of shape from exponential-like to Gaussian-like could be linked to the integrability of the model. Indeed, at very short periods, the system is not able to follow the external perturbation and its behaviour is governed by the initial integrable Hamiltonian

(XX -chain without field) while at larger periods the system feels effectively its non-integrability, possibly leading to a Gaussian distribution of level spacing (which is our work). To confirm eventually this scenario one needs to push further this investigation.

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