Study of work on a quantum harmonic oscillator

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Abstract: We define the work probability distribution that is done to a quantum system during some process, from which the average work, its variance and the irreversible work can be obtained. Two limits are introduced according to whether the system evolves adiabatically or it undergoes an instantaneous quench. The time evolution of this system is obtained by solving numerically the time dependent Schrödinger equation through the Crank-Nicolson method.

The two limit situations are explored for the simple case of a quantum harmonic oscillator with a time dependent Hamiltonian, as well as the intermediate regime between both limits. The results for the average work done during the process and its variance agree with the analytical expressions for the two limits. Finally, we study the work probability distribution during a shortcut to adiabacity protocol.

I. INTRODUCTION

The concept of work is not easily translated from classical to quantum systems. In recent years, there has been an effort to define the quantum work done on a quantum system. The idea is to consider a system governed by a Schrödinger equation in which the Hamiltonian is varied with time [1]. For instance, we will consider the work done on a particle confined in a harmonic trap which trapping frequency is varied with time. The main problem with a definition of quantum work is that it cannot be defined from an operator, like for instance energy or position. Instead, it is useful to define the probability distribution of work done on the system during a process [1–3]. The two sources of randomness, which make it appropriate to have a probability distribution, are thermal noise in the preparation of the initial state, and quantum randomness arising from the measurement process at the final time. The aim of this project is to understand the concept of work on quantum systems by studying the simple case of a harmonic oscillator in which the frequency is varied with time.

The following section (Sec. II) provides general definitions of the work probability distribution and its derived quantities (average work, variance of the work and irreversible work). We introduce two limit cases for the process: the adiabatic limit when the Hamiltonian of the system is evolved slowly enough such that the evolved state is always the instantaneous ground state of the time dependent Hamiltonian, and the instantaneous quench for the opposite situation.

In Sec. III we consider a quantum harmonic oscillator with the frequency depending linearly on time. We study how the system evolves for different speeds of variation of the frequency and check if the results for low and high values tend to the adiabatic and instantaneous quench limits, respectively. Besides, the work probability distribution for different final frequencies is analysed.

Finally, Sec. IV is devoted to the study of the shortcut protocol proposed in Ref. [4], which eventually yields the final state of an adiabatic process, i.e. with minimal irreversible work.

II. WORK PROBABILITY DISTRIBUTION OF A QUANTUM SYSTEM

Let's consider a system initially in the ground state $|\psi_0\rangle$ of the Hamiltonian $\hat{\mathcal{H}}(t_i) = \hat{\mathcal{H}}_i$, which evolves with time to the final Hamiltonian $\hat{\mathcal{H}}(t_f) = \hat{\mathcal{H}}_f$. The probability distribution function of the work done on the system [2] is defined by

$$P(W) = \sum_n |\langle\tilde{\psi}_n|\psi(t_f)\rangle|^2 \delta(W - \tilde{E}_n + E_0), \tag{1}$$

where E_0 is the ground state energy of $\hat{\mathcal{H}}_i$, $\{|\tilde{\psi}_n\rangle\}$ are the eigenstates of $\hat{\mathcal{H}}_f$ (with eigenvalues $\{\tilde{E}_n\}$), and $|\psi(t_f)\rangle$ is the final state of the system.

The average work performed during the process $\langle W\rangle = \int W\, P(W)\, \mathrm{d}W$ can be obtained from Eq. (1) as the first moment of $P(W)$

$$\langle W\rangle = \langle\psi(t_f)|\hat{\mathcal{H}}_f|\psi(t_f)\rangle - \langle\psi_0|\hat{\mathcal{H}}_i|\psi_0\rangle. \tag{2}$$

Similarly, the variance of the work (work fluctuations) $\Delta W^2 = \langle W^2\rangle - \langle W\rangle^2$ is

$$\Delta W^2 = \langle\psi(t_f)|(\hat{\mathcal{H}}_f - E_0)^2|\psi(t_f)\rangle - \langle W\rangle^2, \tag{3}$$

and the irreversible or wasted work is defined as

$$W_{\rm irr} = \langle W\rangle - (\tilde{E}_0 - E_0). \tag{4}$$

Two important limiting scenarios are worth discussing in detail:

a. Adiabatic limit. If the Hamiltonian is varied slowly with time —i.e. slowly enough so at time t the system is on the ground state of the instantaneous Hamiltonian $\hat{\mathcal{H}}(t)$—, the final state will be $|\psi(t_f)\rangle = |\tilde{\psi}_0\rangle$. Therefore, the average work from Eq. (2) for this case becomes simply the difference between the final and initial ground state energies

$$\langle W\rangle = \tilde{E}_0 - E_0, \tag{5}$$

while both the variance of work and the irreversible work are zero.

b. Instantaneous quench. If $\hat{\mathcal{H}}_i$ is instantaneously changed to $\hat{\mathcal{H}}_f$ instead (with t_f insignificantly small), the system will still be on its initial state after a time t_f, so $|\psi(t_f)\rangle = |\psi_0\rangle$, and consequently the average work and its variance from Eqs. (2) and (3) reduce to

$$\langle W\rangle = \langle\psi_0|\hat{\mathcal{H}}_f|\psi_0\rangle - \langle\psi_0|\hat{\mathcal{H}}_i|\psi_0\rangle, \tag{6}$$

and

$$\Delta W^2 = \langle\psi_0|(\hat{\mathcal{H}}_f - E_0)^2|\psi_0\rangle - \langle W\rangle^2, \tag{7}$$

respectively, with the irreversible work given by Eq. (4).

III. HARMONIC OSCILLATOR

In order to study with more detail the work probability distribution and the magnitudes derived on the last section, we will consider the simple yet important case of the one-dimensional quantum harmonic oscillator [5]. The Hamiltonian for such system with a general time dependent frequency $\omega(t)$ can be written as

$$\hat{\mathcal{H}}(t) = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2(t)\hat{x}^2.$$

Its ground state wavefunction and energy at frequency $\omega(0) = \omega_i$ are

$$\psi_0(x) = \left(\frac{1}{a_0^2\pi}\right)^{\frac{1}{4}} \exp\left[-\frac{1}{2}\left(\frac{x}{a_0}\right)^2\right]$$

and $E_0 = \hbar\omega_i/2$, where $a_0^{-2} = m\omega_i/\hbar$. For $\omega(t_f) = \omega_f$, the eigenstates and eigenvalues are given by

$$\tilde{\psi}_n(x) = \left(\frac{1}{\tilde{a}_0^2\pi}\right)^{\frac{1}{4}} \left(\frac{1}{2^n n!}\right)^{\frac{1}{2}} H_n\left(\frac{x}{\tilde{a}_0}\right) \exp\left[-\frac{1}{2}\left(\frac{x}{\tilde{a}_0}\right)^2\right]$$

and $\tilde{E}_n = (n + 1/2)\hbar\omega_f$, respectively, where $\tilde{a}_0^{-2} = m\omega_f/\hbar$ and $H_n(x/\tilde{a}_0)$ are the Hermite polynomials. The variance of x of the ground state of a Hamiltonian with frequency ω is $\Delta x_t^2(\omega) = \hbar/(2m\omega)$.

Generally, the evolution of the system will be described by the time-dependent Schrödinger equation

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = \hat{\mathcal{H}}(t)\psi(x,t), \tag{8}$$

with $\hat{p} = -i\hbar\partial_x$. To simplify notation, we can define a dimensionless variable $\tilde{\omega}(t)$ with which the frequency at time t is defined as $\omega(t) = \tilde{\omega}(t)\cdot\omega_0$, where ω_0 are the units of frequency when $\tilde{\omega} = 1$. Similarly, the energies can be expressed as $E = \tilde{E}\cdot\hbar\omega_0$. From now on both dimensionless variables will be preferably used instead of ω and E.

A. Adiabatic limit

If the frequency is varied adiabatically from ω_i to ω_f, the average work for the harmonic oscillator results

$$\langle W\rangle = \left(\frac{\omega_f}{\omega_i} - 1\right)\frac{\hbar\omega_i}{2}, \tag{9}$$

with $\Delta W^2 = 0$ and $W_{\text{irr}} = 0$.

B. Instantaneous quench and probability distribution of work

If the frequency is instantaneously varied from ω_i to ω_f, the average work is

$$\langle W\rangle = \frac{1}{2}\left[\left(\frac{\omega_f}{\omega_i}\right)^2 - 1\right]\frac{\hbar\omega_i}{2}, \tag{10}$$

the variance of work results

$$\Delta W^2 = \frac{1}{2}\left[\left(\frac{\omega_f}{\omega_i}\right)^2 - 1\right]^2\left(\frac{\hbar\omega_i}{2}\right)^2, \tag{11}$$

and the irreversible work is

$$W_{\text{irr}} = \frac{1}{2}\left(\frac{\omega_f}{\omega_i} - 1\right)^2\frac{\hbar\omega_i}{2}. \tag{12}$$

For this particular case, the Hamiltonian becomes time-independent after t_f, and thus we can study how the system evolves once it has undergone the quench. Since the evolution of the system is described by Eq. (8), and considering that now the Hamiltonian remains constant with time, the state it reaches after a certain time $t > t_f$ will be given by $\exp(-i\hat{\mathcal{H}}_f t/\hbar)|\psi_0\rangle$ as

$$|\psi(t)\rangle = \sum_n \langle\tilde{\psi}_n|\psi_0\rangle \exp\left(-i\tilde{E}_n t/\hbar\right)|\tilde{\psi}_n\rangle. \tag{13}$$

Considering a system with an initial frequency $\tilde{\omega}_i = 3.0$ that is changed instantaneously to ω_f, the probability distribution of work $P(W)$ from Eq. (1) has been plotted on Fig. 1 as a function of the work for different cases of ω_f (first panel), as well as a function of the final frequency for the different modes of the distribution (second panel). In order to evaluate $P(W)$, the series have been truncated up to order 20 (for a larger n the value of $|\langle\tilde{\psi}_n|\psi_0\rangle|$ becomes virtually zero), with $\tilde{\omega}_f$ ranging from 1 to 20.

On the first panel of Fig. 1 we can see that for the cases where the final frequency is almost equal to the initial frequency ($r_\omega \approx 1$), the mode which contributes most is $n = 0$, while the other contributions are approximately zero. As the final frequency moves away from the initial frequency, the probablity of the zeroth mode decreases, and the other modes begin to contribute. Similarly, on

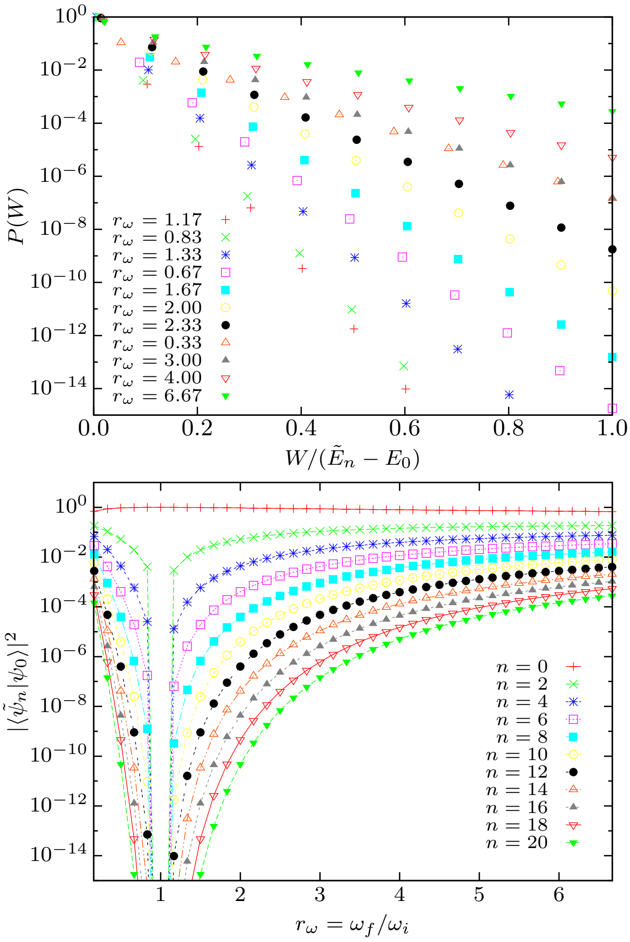

Figure 1: Probability distribution of work as a function of the normalized work $W/(\tilde{E}_n - E_0)$ for different final frequencies (first panel) and as a function of the frequencies ratio $r_\omega = \omega_f/\omega_i$ for several modes of order n (second panel). In both plots $\tilde{\omega}_i = 3.0$ is fixed for all cases. $\tilde{E}_n$ is the energy of the maximum order mode (i.e. $n = 20$) and E_0 is the initial ground state energy.

the second panel we observe that the zeroth order mode has probability 1 when $\omega_f = \omega_i$, while for larger or lower ω_f the probability of this mode decreases.

Finally, the average work, variance of work and irreversible work at a certain time $t > t_f$ after the quench have been calculated, with the final state from Eq. (13). Though the obtained values did coincide with the analytical ones, for large final frequencies ($\omega_f > 8\omega_i$) the numerical results show a significant discrepancy with the expected values. This deviation of the numerical points arises from the fact that the harmonic trap is too narrow for final frequencies large enough, so the spatial discretisation (the number of x points) becomes insufficient for the eigenstates of the final hamiltonian to be well described.

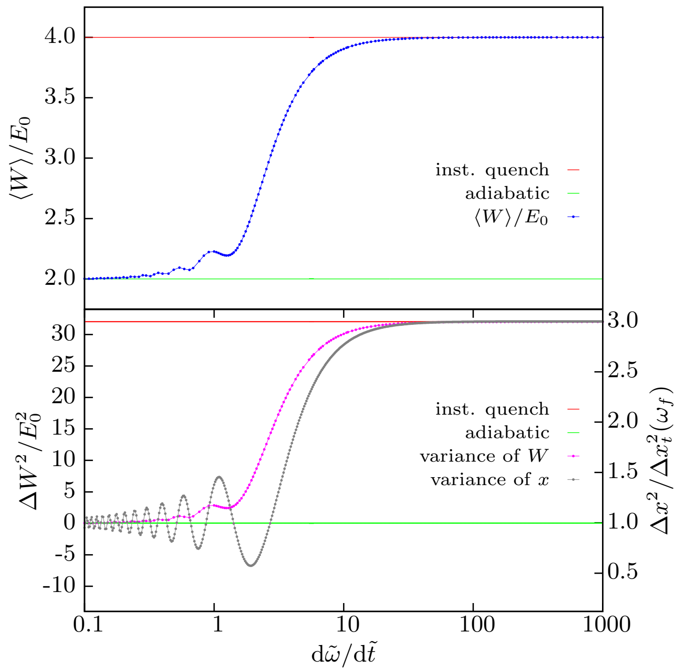

Figure 2: Average work (first panel; the irreversible work shows the same behaviour but shifted two units towards the x-axis), variance of the work and variance of x (second panel) as a function of $\dot{\omega}(t)$ for a harmonic oscillator with initial frequency $\tilde{\omega}_i = 1.0$ and final frequency $\tilde{\omega}_f = 3.0$, where $\Delta x_t^2(\omega)$ is the theoretical value of the variance of x for the ground state of a Hamiltonian with frequency ω. The analytic values for the three magnitudes corresponding to the instantaneous quench (red solid lines) and adiabatic limits (green solid lines) are plotted on both panels.

C. Intermediate regime with a linear ramping for the frequency

Now we can consider a more general situation where the frequency varies linearly over time such that $\omega(t) = \omega_i + (\omega_f - \omega_i)\,t/t_f$ when $t \leq t_f$, while $\omega(t > t_f) = \omega_f$. For $t \leq t_f$, its derivative $\dot{\omega} = \mathrm{d}\omega/\mathrm{d}t = (\omega_f - \omega_i)/t_f$ is constant and depends inversely on the final time t_f.

The evolution of the system's initial state was determined by solving Eq. (8) with the Crank-Nicolson method [6] for a Hamiltonian $\hat{\mathcal{H}}(t)$, with a total time $T_{\max} \geq t_f$ generally different from t_f (time at which the frequency reaches ω_f). Other parameters used on the program are the temporal and spatial steps Δt and Δx, and the grid half-width L.

Given a system with initial frequency $\tilde{\omega}_i = 1.0$ and final frequency $\tilde{\omega}_f = 3.0$, the average work, variance of the work and variance of x have been obtained for different values of $\dot{\omega}$ and are represented in Fig. 2, where the total time is $T_{\max} = t_f$ with time step $\Delta\tilde{t} = 0.001$ (20000 steps), grid width $2\tilde{L} = 20.0$ with 400 x points, and $\tilde{t}_f$ is varied from 0.002 to 20.0.

From Fig. 2 we can see that all magnitudes verify both the instantaneous quench limit for large values of $\dot{\omega}$ and the adiabatic limit for rather small values of $\dot{\omega}$, as was expected. If instead of stopping the evolution right at t_f we considered a larger total time $T_{\max}$ fixed for all the data points, we would obtain that the average work, variance of the work and irreversible work coincided with the data plotted on Fig. 2. This occurs because all the expected values remain constant once the Hamiltonian becomes time independent (after time t_f). However, the variance of x would show a clear discrepancy with the current plot, specially for large $\dot{\omega}$, because the wavefunction of the state does not maintain its shape after reaching t_f.

The average work, variance of the work and irreversible work have been recalculated for three more situations: reducing the time step to $\Delta\tilde{t} = 0.0001$, defining a fixed $\tilde{T}_{\max} = 20.0$, and with a smaller grid $2\tilde{L} = 8$ (800 x points). In either case, the results coincided with the original points from Fig. 2. Similarly, the stability of the points for the variance of x have been studied by increasing and decreasing the number of time steps, and again the values obtained coincided with the original points. Therefore, we can conclude that Fig. 2 is stable with respect to Δt and Δx.

IV. SHORTCUT TO ADIABACITY

Assuming we are interested in minimising the irreversible work, we can use the protocol provided by Ref. [4]. This article is focused on finding a functional form for the frequency $\omega(t)$ of a harmonic oscillator that leads the system to the final state of an adiabatic process in the shortest time possible. Such function $\omega(t)$ must satisfy that

$$\omega^2(t) = \frac{\omega_i^2}{b^4(t)} - \frac{\ddot{b}(t)}{b(t)}, \tag{14}$$

along with the following conditions: $b(0) = 1$, $\dot{b}(0) = 0$ and $\ddot{b}(0) = 0$ at $t = 0$, and $b(t_f) = \gamma$, $\dot{b}(t_f) = 0$ and $\ddot{b}(t_f) = 0$ at $t = t_f$, where $\omega_i = \omega(0)$, and $\gamma = \sqrt{\omega_i/\omega_f}$.

If both requirements are fulfilled, the state reached by the system at t_f will be that of an adiabatic process, with minimum irreversible work and both the energy and the wave function an eigenvalue and eigenstate of the final Hamiltonian.

A simple choice for $b(t)$ is the 5th-order polynomial [4]

$$b(t) = 6(\gamma-1)s^5 - 15(\gamma-1)s^4 + 10(\gamma-1)s^3 + 1,$$

with $s = t/t_f$, and where its first and second time derivatives are $\dot{b}(t)$ and $\ddot{b}(t)$.

Returning to the case considered on the last subsection (system with initial and final frequencies $\tilde{\omega}_i = 1.0$ and $\tilde{\omega}_f = 3.0$) with time step $\Delta\tilde{t} = 0.0001$, grid half-length $\tilde{L} = 4.0$ (400 x points), and $\tilde{T}_{\max} = \tilde{t}_f = 1.0$, we can now calculate the average work, variance of the work, irreversible work and variance of x using the shortcut to define $\omega(t)$. The values obtained for the average and

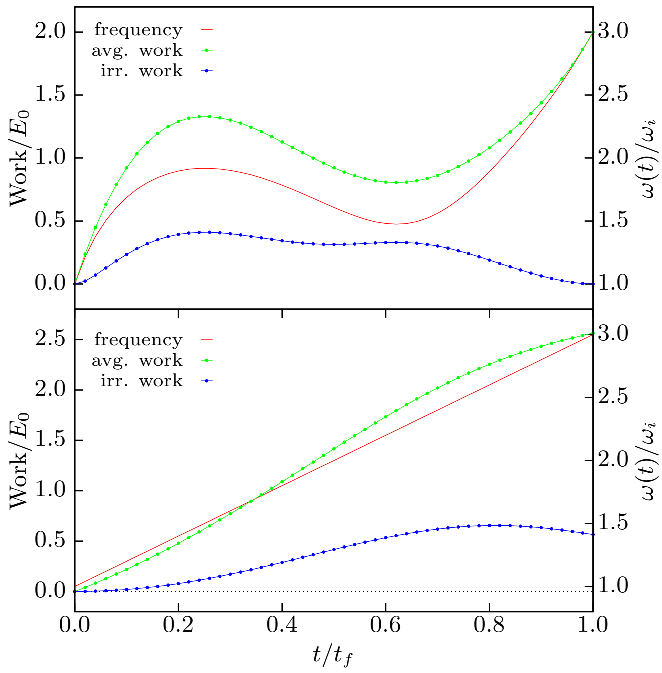

Figure 3: Frequency, average work and irreversible work as a function of time for the shortcut protocol (first panel) and the linear ramping (second panel), with initial frequency $\tilde{\omega}_i = 1.0$, final frequency $\tilde{\omega}_f = 3.0$ and final time $\tilde{t}_f = \tilde{T}_{\max} = 1.0$.

irreversible work (Fig. 3, first panel) are compared with the results found when the frequency is varied linearly with time (Fig. 3, second panel), with the corresponding frequency $\omega(t)$ plotted in both cases.

From Fig. 3 we can see on both plots that the average work behaves similarly to the frequency, since an increase on the frequency (the harmonic trap narrows) implies that the energy of the states raises too and thus the work required grows. We can also see that with the shortcut both the average work and the irreversible work at $t = t_f$ coincide with the adiabatic limit, while with the linear ramping a much larger time will be required to reach the adiabatic limit. In particular, the irreversible work obtained with the shortcut is approximately zero while for the linear ramping it falls far from the adiabatic limit. Thus, with the linear ramping more states than the ground state have been excited at $t = t_f$, resulting on a non-zero irreversible work, while with the shortcut the system evolves into the ground state of the final Hamiltonian, and thus the irreversible work is zero.

Finally, the evolution of the variance of x (Fig. 4) and the probability density (Fig. 5) are represented for both the shortcut and the linear case, choosing $T_{\max} = 4t_f$ in order to see the state of the system some time after it reaches ω_f at t_f.

From Figs. 4 and 5 we can see that with the shortcut the variance remains constant after $t = t_f$, while when $\omega(t)$ is changed linearly with time the variance of x oscillates for $t > t_f$. This means that the shape of the

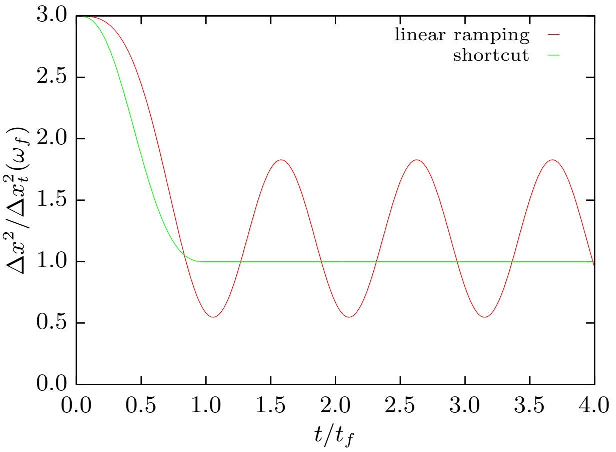

Figure 4: Evolution of the variance of x with $\tilde{t}_f = 1.0$ and total time $T_{\max} = 4t_f$, where $\Delta x_t^2(\omega_f)$ is the variance of x at the final state.

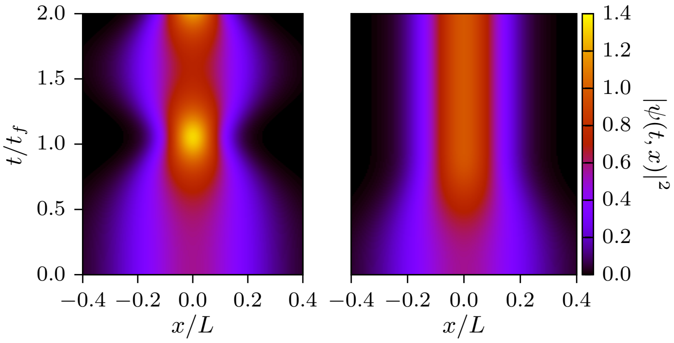

Figure 5: Evolution of the probability density obtained with the linear ramping (left) and the shortcut (right), where again $\tilde{t}_f = 1.0$ and L is the grid half-width ($\tilde{L} = 4.0$).

probability distribution $|\psi(x,t)|^2$ for the shortcut does not vary after t_f, while it does on the linear case. This shows again that with the shortcut the system reaches an eigenstate of the final Hamiltonian while with the linear ramping, in general, it does not.

V. CONCLUSIONS & SUMMARY

In this work we have defined the work probability distribution of a general quantum system and introduced two limit situations: the instantaneous quench and the adiabatic limit.

We have considered the particular case of a harmonic oscillator undergoing a process in which the frequency is varied linearly with time. Exploring different speeds for the variation of the frequency, we have calculated the average work and its variance for each process. Then we have shown that the numerical results agree with the analytical values expected for both limits.

Finally, we have studied a shortcut protocol which minimises the irreversible work within a short time. Comparing the results obtained with the shortcut and the linear ramping, we have seen that the adiabatic limit is successfully reached using the shortcut protocol for a small final time. The linear case results for the same final time, however, are far from the adiabatic limit, since an adiabatic process with the linear ramping would require a much longer time. Moreover, we have shown that if the system is let to evolve after the final time, the variance of x remains constant with the shortcut protocol as expected, whereas it oscillates for the linear ramping.

Therefore, we can conclude that the protocols derived to shortcut the adiabatic following provide an efficient way to minimise the irreversible work after the time evolution. In particular they are clearly better than a linear ramping.

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