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LETTER TO THE EDITOR

Classical–quantum correspondence for barrier crossing in a driven bistable potential

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Abstract. Both quantum and classical analyses are performed to study the barrier crossing dynamics in a driven quartic oscillator. The regions of phase space with regular classical motion are found to be smaller than the size of a quantum state. However, coherent tunnelling is still possible due to the existence of Floquet states localized on two small regular islands. The quantum evolution of localized wavepackets and the classical evolution of the corresponding distributions show similar coherence properties although the degree of coherence is quantally enhanced.

The study of quantum tunnelling for double well potentials in the presence of a periodic time-dependent driving force has been the object of recent theoretical work [1–3]. Among the numerous applications stimulating these studies are: (*a*) macroscopic quantum tunnelling [4], (*b*) the possibility of tunnelling rate enhancement through double quantum wells in semiconductor superlattices [5], (*c*) intramolecular and intermolecular hydrogen transfer processes [6], (*d*) tunnelling processes of hydrogen isotopes and muons between interstitial sites in metals [7], and (*e*) Josephson junctions in the presence of a microwave field [8].

Reichl and Zheng [1] have studied classically the one-dimensional quartic double well potential in the presence of a monochromatic external field and found the appearance of chaotic trajectories with initial energy lower than the barrier height and which are able to increase their energy and cross over the barrier. The phase space chaotic layers increase with the strength of the field, the spreading of chaos being maximum, at a given field strength, for external frequencies close to the harmonic frequency within each well.

This barrier crossing due to energy diffusion is therefore a pure classical effect related to chaos and, therefore, should not be called tunnelling. Here we will use this term to name pure quantum processes that connect phase space regions which are classically separated.

The interplay between chaos and tunnelling is the subject of recent work by Lin and Ballentine [2]. They study the quartic potential in the presence of a sinusoidal driving force. For the parameters chosen in the Hamiltonian, the one-period stroboscopic classical phase space has a small regular island in each well embedded in a dominant chaotic sea. Figure 1 shows these islands and some chaotic trajectories. Lin and Ballentine solved the time-dependent Schrödinger equation in a truncated basis set for different initial wavepackets. If the centre of the initial packet lies within the chaotic sea, then the packet spreads rapidly over the chaotic phase space which extends

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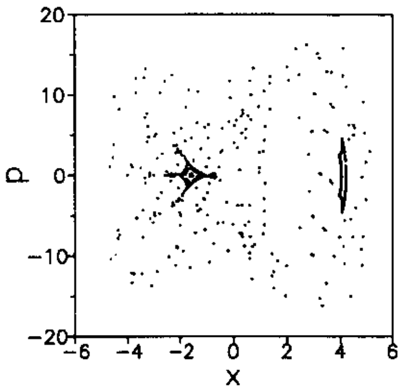


Figure 1. Stroboscopic plots for several trajectories initiated along the $p=0$ axis revealing the two regular islands and the 4:1 periodic orbit near the left island.

across the two wells. On the other hand, if the initial packet is centred at one of the regular islands, coherent tunnelling is observed with a rate several orders of magnitude greater than that corresponding to the undriven system.

The purpose of this work is twofold. First we want to give a formal explanation to Lin and Ballentine's observations using an adequate quantum formalism. Secondly, we intend to establish a connection between the classical and quantum mechanics of this system in order to separate the purely quantum effects from those with a classical analogy.

We begin by presenting the quantum formalism and our quantum analysis. We then perform the classical analysis and its comparison to the quantum results. Finally, we present our conclusions.

(a) The Floquet formalism. The model Hamiltonian has the following form:

$$H = p^2/2m + Bx^4 - Dx^2 + \lambda x\cos(\omega_0 t). \tag{1}$$

The values chosen for the parameters in this equation are from Lin and Ballentine [2], namely $m=1$, $B=0.5$, $D=10$, $\lambda=10$ and $\omega_0=6.07$.

In order to carry out the quantum analysis of our system we have used the Floquet formalism which is specially adequate for Hamiltonians with periodic time dependence [9]. The time evolution for such systems is completely determined by the one-period propagator. The diagonalization of this operator gives the so called Floquet states χ_i; the eigenvalues can be written in the form $\exp(-\mathrm{i}E_i t)$, where the quasi-energies E_i are real and obtained modulus 2π. Thus for times $t=nT$ (n integer and $T=2\pi/\omega_0$) any solution ϕ of the time-dependent Schrödinger equation can be written as

$$\phi = \sum_i c_i \exp(-\mathrm{i}E_i t)\chi_i. \tag{2}$$

The time-dependent Schrödinger equation for our system is invariant under the two sets of transformations

$$x \to -x \qquad t \to t + T/2$$

and

$$x \to -x \qquad t + T/4 \to -t + T/4 \qquad \text{complex conjugation.}$$

As a consequence of these properties, the one-period time evolution operator is completely determined from the evolution operator for one quarter of a period. This fact can be used to reduce significantly the computational time involved in the calculation of Floquet states and quasi-energies.

In our computations we have used Lin and Ballentine's basis set which consists of the lowest 115 eigenfunctions of a harmonic oscillator with frequency $\omega = 6.25$. We have propagated this basis set for a quarter of a period and from here the one-period evolution matrix was obtained. Further diagonalization of this matrix produced the Floquet states and quasi-energies. The results are stable against changes in ω and in the number of basis functions used.

Some of the Floquet states are presented in figure 2. We have used the Husimi representation which for any state $|\chi\rangle$ is defined as

$$\rho(x, p) \equiv (2\pi\hbar)^{-1}|\langle\alpha(x, p)|\chi\rangle|^2 \qquad (3)$$

where $\langle\alpha(x, p)|$ is a coherent state of the harmonic oscillator chosen for the basis set.

The Floquet states in panels (a), (b) are localized on the regular islands shown in figure 1. This is so in spite of the fact that the size of such islands is not large enough to support a quantum state in a semiclassical sense; the state in panels (c), (d) are also localized although on unstable periodic orbits within the chaotic sea. On the other hand, panel (e) shows a more delocalized state. Localization and delocalization of this kind are frequent features observed in quantum systems with classical chaotic motion [10–12]. For the sake of comparison we give in panel (f) the Husimi representation for the lowest stationary state in the undriven system.

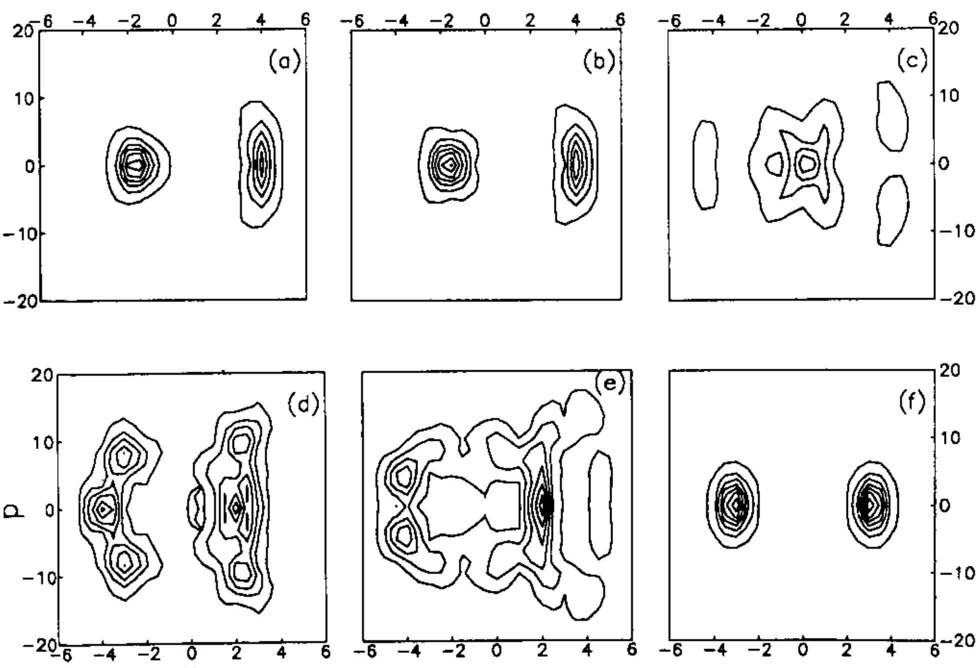


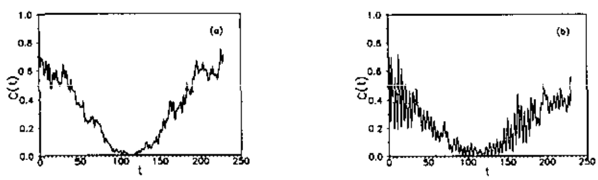
Figure 2. Husimi representations of several Floquet states for driven system (a)–(e). Panel (f) gives the Husimi representation of the lowest stationary state for the undriven system.

(b) The autocorrelation function. Given a solution $|\phi(t)\rangle$ of the time-dependent Schrödinger equation corresponding to an initial state $|\phi(0)\rangle$, then the autocorrelation function or survival probability is defined by

$$C(t)=|\langle\phi(0)|\phi(t)\rangle|^2. \tag{4}$$

The autocorrelation function has proven to be very useful in the extraction of dynamical information from the system time evolution [13]; in particular, we are interested here in information concerning the tunnelling process and its coherence degree. These functions are also specially adequate to study the classical–quantum correspondence which will be carried out later.

For our purposes we have chosen as initial states $|\phi\rangle$ three Gaussian coherent wavepackets located at (a) $x=-1.5, p=0$ (the centre of the left regular island of figure 1); (b) $x=-2, p=0$ (within the island but displaced from its centre), and (c) $x=4.15, p=0$ (within the chaotic sea). Cases (a) and (c) were also studied by Lin and Ballentine [2]. The time evolution $|\phi(t)\rangle$ of these packets was obtained using (2). The correlation functions corresponding to these cases are given in figure 3. Only values for times equal to integer number of periods are presented. Figures 3(a) and 3(b) show one period of a low frequency oscillation which is due to the coming back of the initial packet after tunnelling two times through the barrier. This oscillation persists for longer times with no further decay and is a consequence of the tunnelling coherence already observed by Lin and Ballentine [2]. The lack of coherence reported by these authors in case (c) is also revealed in the correlation function in panel (c) which shows a fast decay to a low amplitude random high frequency oscillation with some revivals reaching 30% of the initial probability. This fast decay takes place in parallel with the spreading of the packet over the two wells giving rise to a fast incoherent barrier crossing. Panel (b) presents an additional coherent oscillation whose period is approximately four times the period of the driving term and which is caused by the fast oscillations of the packet within the well (remember that it was initially displaced from the centre of the regular island).



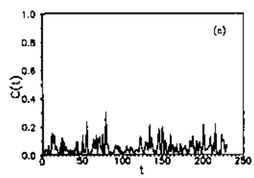


Figure 3. Quantum survival probabilities (equation (4)) for the initial wavepackets corresponding to the cases (a), (b) and (c) discussed in the text. The time unit is a period of the driving force.

Let us now analyse these results in terms of the Floquet states contributing to the initial packet in each case. This contribution is $c_i=\langle\phi(0)|\chi_i\rangle$ in (2) and takes part in the spectrum which is defined as

$$I(E)=\sum_i|\langle\phi(0)|\chi_i\rangle|^2\delta(E-E_i). \tag{5}$$

$I(E)$ is given in figure 4 for the three cases studied.

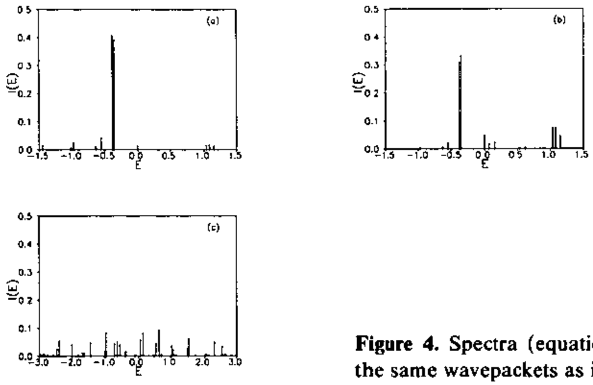


Figure 4. Spectra (equation (5)) corresponding to the same wavepackets as in figure 3.

The spectra corresponding to cases (a) and (b) show as a similar feature a dominant contribution coming from the same two Floquet states with very close quasi-energies; the Husimi representations of these states are given in panels (a) and (b) of figure 2. They look alike but, in the coordinate representation, one of the states is positive for all x values whereas the other changes sign from left to right wells. Therefore, symmetric and antisymmetric superposition of these two states produces wavepackets respectively located in each well, whose time evolution will give rise to completely coherent tunnelling with a rate determined by the quasi-energy splitting. This splitting is 0.0281 from which a tunnelling time of 112 periods is readily found. All this explains the dominant coherent component of the tunnelling process for the wave packets of cases (a) and (b). In particular, since approximately 80% of the initial packet (a) is made up of these two localized states, the survival probability reaches 80% of the initial value after the first tunnelling period. In case (b) the value is 60%. The incoherent component is due to the participation of other pairs of Floquet states with different splittings on one hand and individual delocalized states on the other. The tunnelling rate obtained here is in total agreement with Lin and Ballentine's result [2]. They estimated the rate for the undriven system to be several orders of magnitude slower. If the packet is made up of the superposition of the two lowest states for the undriven system the rate will be determined by the energy splitting between these two states. We have found this splitting to be of the order of 10^{-11} confirming the drastic effect of the driving term. This considerable increase in the tunnelling rate can be understood as a reduction of the effective barrier in the driven system, which is consistent with the fact that the Floquet states represented in figures 2(a), (b) have the two regions of maximum probability closer than in the case of the two lowest states for the undriven system (cf figure 2(f)).

In case (c) the spectrum (figure 4(c)) shows similar contributions from many Floquet states such as those in figure 2(d), (e). They are poorly localized like the one in figure 2(e) or show localization on unstable periodic orbits as the one in figure 2(d). All of them have almost zero probability values within the regular phase space regions. The fast decay in $C(t)$ is related to the obvious lack of correlation in $I(E)$, and the revivals of the wavepacket a consequence of the discrete nature of the spectrum.

The classical correlation function which is a classical analogue to (4) may be written [13] as

$$C(t) = \mathrm{Tr}\,\rho(0)\rho(t) \tag{6}$$

where Tr stands for the classical trace (integral over the phase space coordinates),

$\rho(0)$ is the Wigner phase space distribution corresponding to the initial wavepacket and $\rho(t)$ is the classical Liouville evolution of $\rho(0)$.

The integral in (6) was evaluated by Monte Carlo sampling of initial conditions with a Gaussian random number generator corresponding to the distribution $\rho(0)$. The same cases (*a*), (*b*) and (*c*) have been studied classically. A total of 500 trajectories were used in each case and the Hamilton equations were numerically integrated to get the values of $\rho(t)$. The results are stable against changes in the number of trajectories and in the accuracy of the integrator. The correlation functions calculated in this way are presented in figure 5. For cases (*a*) and (*b*) they decay relatively slowly to a non-zero average value which is larger for case (*a*). The high frequency oscillation appearing in case (*b*) has a periodicity equal to that observed in the corresponding quantum case (cf figure 3) meaning that its origin is a classical one: the regular trajectories in the island need four periods to come back closer to their initial point. This is due to a 4:1 resonance periodic orbit which appears near the boundary of the island within the chaotic sea [1]. Some of the chaotic trajectories in the neighbourhood of this periodic orbit mimic for shorrt times its motion as can be seen in figure 1. The regular trajectories within the island and close to its boundary also feel the resonance region. The non-zero long time value of the autocorrelation function and the fact that the above oscillation persists for long times indicates that part of the initial distribution of trajectories remains coherently localized in one well. This is confirmed by following the evolution of the initial distribution in phase space. Since the initial distribution in case (*a*) was located closer to the centre of the island the 4:1 oscillations almost disappear; on the other hand the portion of the packet which remains coherently localized in one well case increases in this case giving rise to a higher long time average in the autocorrelation function.

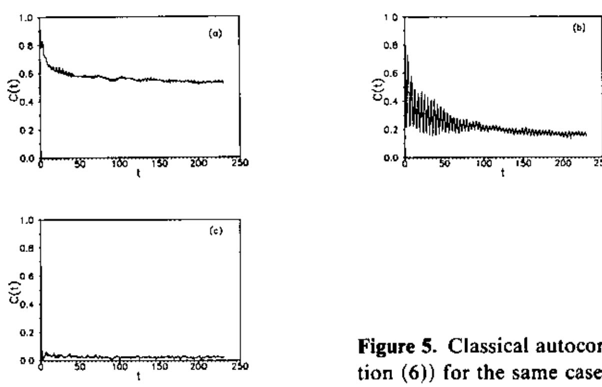


Figure 5. Classical autocorrelation functions (equation (6)) for the same cases as in figure 3.

Case (*c*) which corresponds to a distribution located within the chaotic sea gives an autocorrelation function with a fast decay to almost zero due to the exponential divergence of the chaotic trajectories which dominate the initial distribution in this case. Most of these trajectories are able to gain enough energy to cross over the barrier producing a long time distribution completely delocalized over the two wells.

In summary, there are features in the autocorrelation functions which are common in both classical and quantum cases. For example, the coherence in the evolution of the wavepacket could have been anticipated from a classical study. The 4:1 additional frequency has also a classical origin. Finally, in case (*c*) both classical and quantum correlation functions show the same fast decay and incoherence and the barrier crossing has its main origin in the energy diffusion of the chaotic trajectories. There are, on the other hand, typically quantum features like the low frequency tunnelling oscillation in cases (a) and (b). There is also a quantum enhancement of the classical coherence in these two cases; namely the quantum survival probability after a tunnelling period is approximately 50% greater than the classical long time value in case (a) and 300% greater in case (b). Finally, some quantum revivals appear in the autocorrelation function for case (c) with no classical analogues.

From the results of the present work we can extract the following conclusions. The coherence properties of the time evolution of localized wavepackets in the driven quartic oscillator is determined by the localization properties of the Floquet states contributing to the wavepacket. In particular, the coherent tunnelling has been associated with the participation of a pair of Floquet states localized on two islands of regular motion which exist in the classical phase space. Symmetric and antisymmetric superposition of these states produce packets initially localized in each well which later oscillate between wells with a tunnelling rate determined by their energy splitting. This splitting is much higher than the corresponding to the lowest pair of states in the undriven system, and can be interpreted as a reduction of the effective barrier caused by the driving force. Packets localized on classically chaotic regions of phase space are superposition of several delocalized and periodic orbit localized Floquet states. These packets spread rapidly over the whole chaotic region which extends over the two wells.

The coherence in the quantum evolution of the packets initially located on the stable islands has a classical analogue, namely the coherence of the trajectories trapped in the stable islands which do not dephase in a similar way as the trajectories for a harmonic oscillator. Since the island localization for the pair of Floquet states responsible for such coherence also covers part of the near chaotic regions, the coherence observed in the quantum evolution of these packets is greater than that of the classical analogues. Tunnelling is a pure quantum effect superimposed to this coherence. Classical distributions of trajectories initially located within the chaotic sea show the same fast decay observed in their quantum analogues. In this case some apparently quantum beats corresponding to partial revivals of the wavepacket appear as quantum features without classical counterparts.

Finally, the obvious differences in the classical phase space structure for both driven and undriven systems is the main cause of the drastically different behaviours observed in their classical and quantum dynamics.

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