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Two-frequency control and suppression of tunneling in the driven double well

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The effect of two-frequency driving of a symmetric double well is investigated classically and quantum mechanically. By computing Husimi distributions it is shown that control and suppression of tunneling may be achieved by driving the system with two fields whose frequencies are in a 1:2 ratio. In particular, a second field of finite duration can be used to selectively trap the wave packet in either well.

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The possibility of controlling the time evolution of a molecular system has long appealed to chemical physicists in their efforts to perform mode selective chemistry, i.e., control the take-up, storage, and disposal of energy in a molecule in order to effect the desired level of product selectivity. Two ways of doing this are currently being investigated and are usually labeled passive and active control [1]. In passive control the system is prepared in a particular way such that its subsequent time evolution will favor the desired product (control of initial conditions). Active control, on the other hand, essentially involves shepherding the wave function using an external field to achieve mode selectivity (direct manipulation of the equations of motion). Some studies have used optimal control theory to try to determine the best field needed to achieve a particular target wave function, although the optimum field may turn out to be unrealizable experimentally [2]. External fields can dramatically change the structure of classical phase space and this, in turn, may have profound effects on the quantum evolution. Recently, Grossman *et al.* [3] demonstrated that an external field can be used to suppress tunneling in a driven double-well system. This seminal finding has stimulated much interest in the use of external fields to suppress tunneling; e.g., Bavli and Metiu [4] found that a semi-infinite laser pulse can be used to localize an electron in one of the wells of a double-well potential. We have studied a similar double-well system, and find that a combination of active and passive control, motivated by a study of classical phase space, can provide remarkable regulation of tunneling in this system. Specifically, a principal driving field is used to enhance the tunneling rate, while a second field of lower field strength is used to switch the tunneling on or off, trapping the particle in either of the wells, essentially at will. Thus, we not only demonstrate *suppression* of tunneling but show that an appropriate combination of the two fields can be used to selectively *control* tunneling in this system.

The double well provides an excellent and realistic paradigm for a variety of important atomic and molecular systems; two of the best known examples being nuclear tunneling in pyramidal molecules like ammonia, and electron tunneling in the hydrogen molecular ion. In addition to microscopic examples, the prediction of tunneling in mesoscopic systems [superconducting quantum interference devices (SQUID's)] promises an especially intriguing manifestation of the phenomenon [5]. It is important to recognize that two related types of tunneling can occur in quantum mechanics. The more well known is tunneling through a physical potential-energy barrier, as exemplified by the undriven symmetric double-well potential. However, tunneling of a different nature may also occur, in which flux moves between two (or more) different regions in *phase space* that are separated classically by dynamical barriers to transport. This is usually referred to as dynamical tunneling and may, for example, connect disjoint regular (nonchaotic) volumes of phase space that are separated by chaotic regions [6]. Because the driven double well combines both dynamical tunneling and classically chaotic dynamics it is an ideal system in which to study the connection between tunneling and chaos [7,8]. From a more practical standpoint the relevance of this problem to devices like the Josephson junction makes it worthy of continued investigation.

The driven double well has been studied from a variety of angles, and, recently, Lin and Ballentine [9] showed that tunneling rates are dramatically enhanced by the presence of the external field. In contrast, Grossmann *et al.* [3] demonstrated that coherent *suppression* of tunneling is also possible by a judicious choice of the frequency and amplitude of the monochromatic driving force. Grossmann *et al.* [3] presented a detailed Floquet analysis to show that suppression of tunneling occurs when the quasienergy states become degenerate. Suppression of tunneling by an external field is clearly of considerable fundamental interest and could conceivably be observed experimentally. In this Rapid Communication the problem of driving a double well at two different frequencies is investigated and it is shown that tunneling can be controlled or suppressed coherently by using two external driving fields whose frequencies are in a 1:2 ratio.

The Hamiltonian for a particle in a quartic double-well potential subjected to two-frequency forcing is the following:

$$H=\tfrac{1}{2}p^2-\tfrac{1}{2}ax^2+\tfrac{1}{4}bx^4+\lambda_1 x\cos\omega_1 t+\lambda_2 x\cos(\omega_2 t+\phi)\ . \quad (1)$$

Throughout, $a=20$, $b=2$, $\lambda_1=10$, $\omega_1=6.07$, and ω_2, λ_2, and the relative phase ϕ are varied. Atomic units are assumed. The terms in ω_1 and ω_2 will be referred to as the first and second fields, respectively. The frequency ω_1 is quite close to being resonant with the energy difference between the ground and first excited states of the double well, neglecting tunneling splittings. In the absence of the second field, this is the same system as that studied by Lin and Ballentine [9].

Addition of a single driving force to the double well [i.e., $\lambda_1 \neq 0$, $\lambda_2=0$ in Eq. (1)] destroys the integrability of the system and gives rise to chaotic motion. This is evident in Fig. 1, which shows composite Poincaré surfaces of section (SOS) obtained by numerically integrating ten classical trajectories with randomly chosen initial conditions. The SOS were obtained by strobing the classical dynamics at times $t_n^m = 2\pi/\omega_1(n+m/4)$, $n=0,1,\ldots,2500$ for each value of $m=0,1,2,3$. The period of the driving field $\tau=2\pi/\omega_1$. Only SOS for $m=0$ and 2 are shown, corresponding to whole- and half-period strobing, respectively. Note that, while motion in the vicinity of the separatrix is quite strongly chaotic, islands of regular dynamics persist in both wells, indicating the existence of Kolmogorov-Arnold-Moser (KAM) surfaces or tori in an extended phase space [8,9]. The islands are not associated with the elliptic fixed points of the undriven system, but rather correspond to field-induced resonances. The KAM surfaces associated with the fixed points lying at the minima of the undriven potential have disappeared for the value of λ_1 used. At the separatrix an infinite number of resonances converge and, there, the motion is always chaotic for any finite periodic driving force.

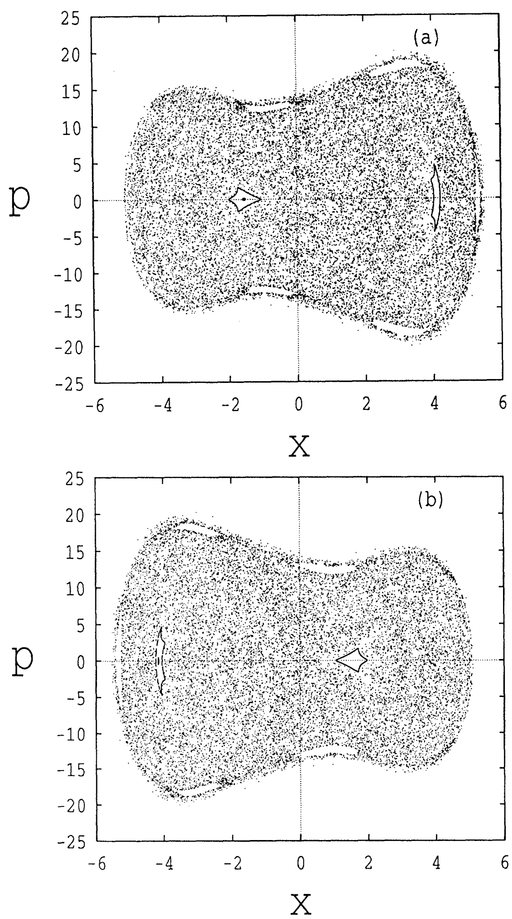

FIG. 1. Poincaré surfaces of section for a single external frequency strobed as described in the text at times t_n^m. In (a), $m=0$; and in (b), $m=2$, i.e., a time π/ω_1 later. Ten classical trajectories were integrated using randomly selected initial conditions.

Examination of the quarter-period SOS reveals that the islands rotate in each of the two wells as a function of time [9]. An important property of the system also becomes apparent upon examining the SOS; the phase-space structure in Fig. 1(b) is essentially a mirror image of that in Fig. 1(a). This is because the system possesses a discrete symmetry [3,11],

$$H(p,x,t;\lambda_2=0)=H\left[-p,-x,t+\frac{\pi}{\omega_1};\lambda_2=0\right]. \quad (2)$$

Discrete symmetries are closely connected with dynamical tunneling, and in this case the symmetry is responsible for coherent dynamical tunneling between the KAM tori. This was discovered numerically by Lin and Ballentine [9,12], although Peres [11] and Grossmann *et al.* [3] made an explicit connection between the observed tunneling behavior and the symmetry of Eq. (2). The periodicity of the Hamiltonian allows a formulation in terms of *quasienergy* states. For the double well driven at a single frequency the numerical results of Lin and Ballentine seem to indicate that some of the quasienergy states are localized in regular regions of phase space; the fact that they belong to two symmetry classes (odd and even) means that the quasienergies will come as doublets [11]. Grossman *et al.* [3] independently recognized that this could be exploited to completely suppress tunneling by choosing an external field having the appropriate intensity and frequency so as to produce a crossing of the quasienergies and thus suppression of tunneling. (The time scale for tunneling is related to the splitting of the quasienergies and thus a crossing of the quasienergies shuts down the tunneling process completely.) Their calculation achieved this by using frequencies comparable to the bare splitting of the levels in the unperturbed system, and good localization of the packet was observed [3]. (A semiclassical analysis of this problem in terms of a model two-level system has recently been presented by Gomez-Llorente and Plata [10].) These studies demonstrate suppression of tunneling, but it is interesting to speculate as to whether *controlled* suppression and enhancement of tunneling can be achieved. An alternative way of suppressing tunneling might reasonably be to destroy the discrete symmetry itself; for example, by using a second driving field that has the advantage of providing access to additional control parameters.

Addition of a second driving term having a different frequency can have dramatic effects on the classical and quantum dynamics of Hamiltonian as well as non-Hamiltonian systems [13–15]. In principle, a second field can create new resonance zones that serve to connect the original resonances and thus enhance transport in phase space. However, for the double-well potential, motion in the vicinity of the separatrix is not expected to be perturbed strongly by the existence of a second driving term because already an infinite number of classical resonances are starting to overlap in this region. This is borne out by SOS plots for the two-frequency case in Fig. 2, where it is seen that, although new resonances are introduced inside and outside of the separatrix region, the dynamics inside the separatrix layer is very similar to single-frequency driving. One major difference is apparent in the case of a 1:2 ratio of driving frequencies; the symmetry between the two wells is broken quite markedly, indicated by the relative difference in size of the regular regions in the two wells (compare Fig. 1). This effect has significant consequences in the quantum dynamics.

Rather than examining the wave function directly, we follow Lin and Ballentine [9] and compute the Husimi function,

$$\rho=(2\pi\hbar)^{-1}|\langle\phi_{q,p}|\Psi(t)\rangle|^2 , \tag{3}$$

where $\phi_{q,p}$ is a minimum uncertainty function that is Gaussian in position and momentum. In *addition* to examining the Husimi function itself, we also compute its accumulated value by summing the value of ρ at each grid point at each quarter period over the total integration period. The accumulated Husimi plots provide a time history of density movement and reduce the risk of overlooking any fast tunneling that might be occurring in between the times at which the Husimi function is examined. The basic idea is to start out a Gaussian wave packet in one of the regular or chaotic regions and follow its time evolution. First, Lin and Ballentine [9] found that for a wave packet initially localized in one of the regular regions of Fig. 1(a), the tunneling rate between the two wells was significantly enhanced as compared to the undriven system. Second, tunneling between the two wells was coherent over many periods of the field. A wave packet initially located in the chaotic region, by contrast, was found to spread or delocalize significantly on the same time scale.

Although the classical behavior in the separatrix layer is similar for one- and two-frequency driving, the quantum dynamics is quite different. Figure 3 compares the accumulated Husimi distributions for the one- and two-frequency cases after 300τ. For one-frequency driving, peaks appear in both wells, indicating coherent tunneling. However, when two frequencies are present, as shown in Fig. 3(b), tunneling is coherently destroyed and the wave packet remains localized in the left-hand well. Close examination reveals that a relatively small amount of transport into the other well has occurred but is negligible on this time scale. Investigation of time-resolved Husimi distributions and the staying probability of the particle in the well confirmed these conclusions. In essence, the principal field dramatically enhances the tunneling rate, but introduction of a second field of lower maximum amplitude selectively turns off coherent tunneling in the

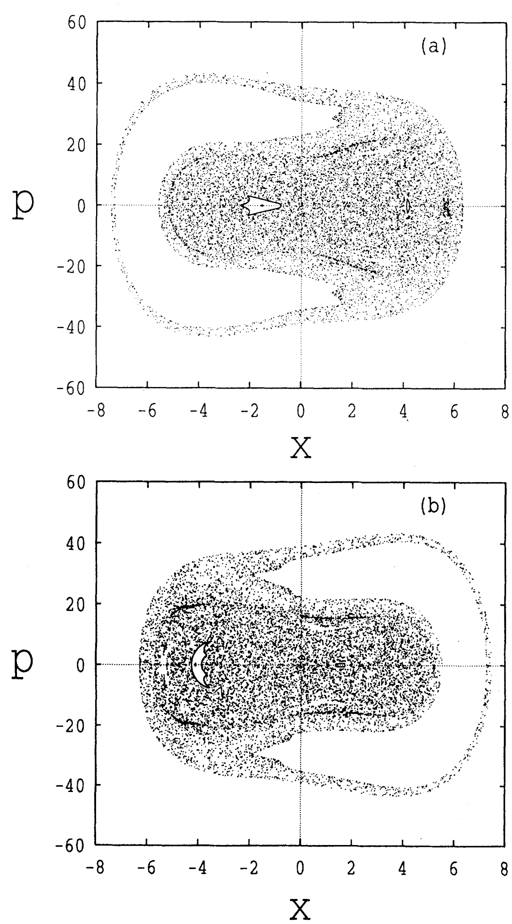

FIG. 2. Poincaré surfaces of section for two-frequency driving. Strobed as in Fig. 1.

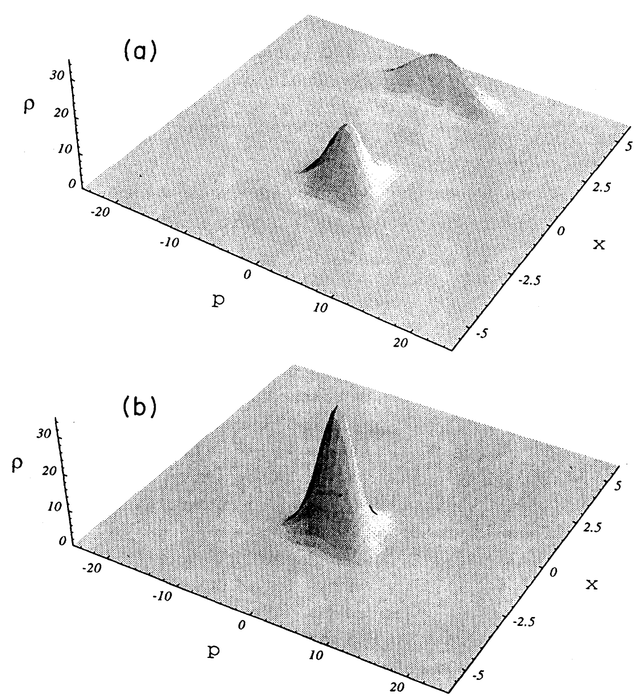

FIG. 3. Accumulated Husimi distributions after 300τ. At each grid point the value of the Husimi function is summed as a function of time. The initial state was the same in both cases, i.e., the initial wave packet had its maximum at $x=-1.5$ and $p=0$. Frame (a) corresponds to single-frequency driving and frame (b) to two frequencies with $\omega_2=2\omega_1$, $\lambda_2=2.5$, and $\phi=0$.

problem. After 600τ the packet in the two-frequency case remains localized as in Fig. 3(b). Varying the phase ϕ also affects the propensity of tunneling. For the field amplitudes used, suppression of tunneling was most efficient when $\phi=0$ and did not occur at all for $\phi=\pi/2$. This is related to the symmetry of the total field about the time axis; the combined driving field is most asymmetric about the time axis when $\phi=0$ and is symmetric when $\phi=\pi/2$. Correspondingly the discrete symmetry is most strongly broken when $\phi=0$. This level of control requires a careful search for the appropriate initial conditions, including particular frequencies and parameters, and is in accord with the conclusions of Bavli and Metiu [4], who also noted a similar level of sensitivity. Thus, use of two fields represents a combination of active and passive control, in that both careful initial-state preparation and subsequent manipulation of the time evolution are involved.

In Fig. 4 the Husimi function itself is shown after 175 periods. In this case a single driving term was applied for 110.5 periods, at which point the second field was turned on (using a trapezoidal rule) over 10τ. The second field then remained on for a further 54.5τ. The parameters used were $\lambda_2=2.5$ and $\phi=\pi$. Phase-space density, initially localized in the left-hand well, has tunneled coherently to the right-hand well, where it remains trapped until the second field is turned off. In general, the more rapid the turn-on of the second field, the more effectively is the packet localized. Increasing the field strength of the second field also improves the trapping. In practice, by turning the second field on and off, control of tunneling can be achieved over long times and the wave packet may be shuttled back and forth between the two wells many times, essentially at will. These results reveal the possibility of using a second driving term of lower maximum amplitude to selectively manipulate tunneling in this system.

This work extends previous studies in which localization was achieved by use of a single field of infinite or semi-infinite duration. By using two external driving fields tunneling in a double-well system could be suppressed over hundreds of periods of the driving fields. The main driving field had the effect of dramatically enhancing the tunneling rate, while addition of a second perturbing term was used to suppress tunneling coherently. By turning the second field on and off in a realistic fashion, control of coherent tunneling between the two wells was achieved. In this, the second field acts like a switch. There clearly remains considerable scope for future work, particularly analysis of the quasienergy states in the more general case of two (or more) arbitrary frequencies. Floquet analysis of multimode systems is difficult, or impossible, if the driving-field frequencies are incommensurate (quasiperiodic). However, we emphasize that multimode Floquet analysis is possible in the present special situation in which the frequency ratios are commensurate (1:2) and, more generally, when the frequencies are either exactly commensurate or when their ratio can be approximated by a ratio of (preferably small) integers. A relevant and related example is provided by double-frequency ionization experiments and calculations for Rydberg atoms [16–18].

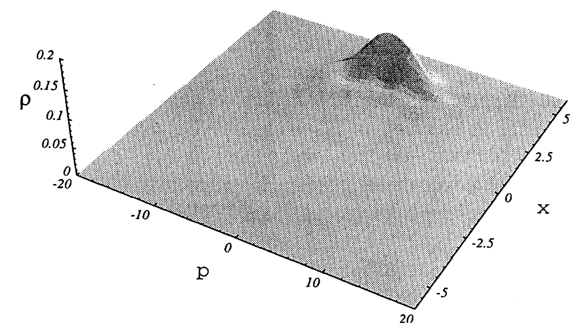

FIG. 4. Husimi distribution after 175τ. The initial state was the same as in Fig. 3. After 110.5 periods the second field was turned on, as described in the text, trapping the packet in the right-hand well.

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