

Coherent Destruction of Tunneling

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The phenomenon of tunneling is investigated for a symmetric double-well potential perturbed by a monochromatic driving force. The analysis is based on a numerical treatment of the quantum map that propagates the system over one period of the external force, and of the spectrum of its eigenphases (quasienergies). The variety in the quasienergy spectrum, such as exact and avoided crossings, leads to novel forms of coherent tunneling. In particular, for specific parameter values of the driving force, we find almost complete localization of the wave packet in one of the wells.

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The tunnel effect was recognized long ago during the heyday of quantum mechanics. In 1927, Hund [1] demonstrated that quantum tunneling is of importance for intramolecular rearrangements in pyramidal molecules such as ammonia, as manifested by the *tunnel splitting* of vibrational spectra. Our objective here is to study the influence of periodic driving on such tunnel systems, which may well lead to an enrichment of the dynamics. In the present Letter, we report on analytical and numerical investigations of an archetypical model, a particle moving in a symmetric double well, and driven by a monochromatic (not kick-type) classical force. The Hamiltonian defining this model reads

$$H(x,p) = \frac{p^2}{2} - \frac{1}{4}x^2 + \frac{x^4}{64D} + xS \sin \omega t. \quad (1)$$

Here, we use dimensionless units. In particular, $D = E_B/\hbar\omega_0$ denotes the barrier height E_B in units of $\hbar\omega_0$, with ω_0 denoting the angular frequency of harmonic oscillations on the bottom of each well, and t is measured in units of the corresponding period $2\pi/\omega_0$. This model Hamiltonian is of general interest: It characterizes the physics of a wide class of systems, such as the transfer of hydrogen in atoms and molecules along chemical bonds [2], the transport of hydrogen isotopes or muons between interstitial sites in metals [3,4] and macroscopic quantum coherence phenomena in SQUIDs [5].

In the present work, we attempt to gain insight into the deep quantum regime of this system. That is, we focus on the parameter range of low barriers, such that D is of order unity and, in the corresponding unperturbed problem, there are only a few levels below the barrier. In addition, we do not restrict ourselves to small amplitudes S of the driving force. Consequently, we refrain from the use of semiclassical or perturbative methods. Our approach is based on the Floquet formalism and the concept of quasienergies, as pioneered for the physics of atoms in intense laser fields [6–10]. Moreover, as our results show, a two-level approximation would be insufficient to analyze driven tunneling: In general, the flow of probability between the two wells exhibits an intricate structure both in space and time, and can no longer be described in terms

of the traditional concept of the tunnel splitting Δ . To provide an adequate language, we adopt the concepts of the temporal autocorrelation function (probability to stay) and the local spectrum, well known, e.g., in solid-state physics [11] and quantum chaos [12,13].

Consider the propagator for the operator in (1) over a single period $T=2\pi/\omega$ of the external periodic force. This unitary operator U is the generator of a quantum map, i.e., applied iteratively to some initial state $|\psi_0\rangle$, it provides a stroboscopic, discrete-time evolution of the wave function. In view of the Floquet theorem, the eigenstates of the unitary operator U take the form $|\psi_k(nT)\rangle = \exp(-in\epsilon_k T)|\Phi_k(0)\rangle$, where n denotes the number of time steps, and $|\Phi_k(t+T)\rangle = |\Phi_k(t)\rangle$. The quantities ϵ_k , defined modulo ω , are referred to as quasienergies [6–10]. They are functions both of the driving amplitude S and the driving frequency ω . The generalized parity transformation P , $x \rightarrow -x$, $t \rightarrow t+T/2$, leaves the Hamiltonian (1) invariant. Thus, the Floquet functions can be classified into states of even and odd parity, respectively [14].

Given an initial wave packet $|\psi_0\rangle$ and its time evolution under U , the temporal autocorrelation function is defined by

$$P_n = |\langle \psi_n | \psi_0 \rangle|^2. \quad (2)$$

Expanding both $|\psi_0\rangle$ and $|\psi_n\rangle$ in the Floquet basis, and using the role of the Floquet states as eigenfunctions of U , one finds

$$P_n = \xi^{-1} + \sum_{\alpha \neq \beta} \exp[in(\epsilon_\alpha - \epsilon_\beta)T] |\langle \Phi_\alpha | \psi_0 \rangle|^2 |\langle \Phi_\beta | \psi_0 \rangle|^2, \quad (3)$$

where $\xi^{-1} = \lim_{N \rightarrow \infty} N^{-1} \sum_{n=0}^N P_n$ denotes the long-time average of P_n . The spectral counterpart of the autocorrelation function P_n is the two-point correlation function $P_n^{\text{loc}}(\eta)$ of the *local* Floquet spectrum [13]. It is related to P_n by Fourier transformation and thus contains all the frequencies involved in the time evolution of P_n , weighted according to their relative significance for this dynamics.

In the following, we will consider time evolutions starting from one particular type of initial state: A Gaussian

centered, say, in the left well, equivalent to the ground state of the harmonic approximation of that well. This initial state is defined independently of the Floquet basis, and can readily be realized both in numerics and experiments. Moreover, with this initial state, the deviation of P_n from unity provides a first clue of the probability flow into the opposite well. A quantity serving the same purpose, but more specifically tailored to the symmetric double-well problem, is the *occupation probability in the left well*,

$$\rho_n^{\text{left}} = \int_{-\infty}^0 dx |\psi(x, nT)|^2. \quad (4)$$

The concepts introduced in Eqs. (2)–(4) will now be used to discuss the variety in the Floquet spectrum, as shows up in the (S, ω) -parameter space, and the consequences for the tunneling behavior. Only in the opposite limits of very slow (adiabatic) and very fast driving, respectively, are the time scales of the unperturbed double well and of the driving force completely separated, and does the structure of the Floquet spectrum resemble that of the unperturbed energy spectrum. In these two regimes, tunneling can still be described in terms of an effective tunnel splitting $\Delta_{\text{eff}}(S, \omega)$. For finite S and ω , it turns out to be always enhanced, as compared to the unperturbed case, i.e., $\Delta_{\text{eff}} > \Delta$ [15]. The main focus of our work, however, is the range of intermediate frequencies between Δ , the lowest characteristic frequency scale of the unperturbed system, and ω_0 . Here, the Floquet spectrum may lose any similarity to the energy spectrum in the unperturbed case. Features of particular significance are close encounters of levels, as a function of the parameters, since they lead to exceptionally long time scales in the tunneling dynamics. If two quasienergies, approaching each other, belong to different parity classes, they form an exact crossing, whereas in the opposite case, a crossing will be avoided.

A special class of avoided crossings is generated by resonances of the driving force with differences of unperturbed levels. Such resonances occur whenever a μ -fold multiple of the field quantum $\hbar\omega$ coincides with a difference $|E_n - E_m|$ of unperturbed levels, and the parities of μ and of $|n - m|$ agree. These resonances are exact for $S \rightarrow 0$, but evolve into avoided crossings for finite S . As a specific member of this class, we consider the resonance $\hbar\omega_r = E_3 - E_2$, referred to as the fundamental resonance. The other parameter values used are $D = 2$ (this value renders the double well quite similar to the potential that governs nitrogen tunneling in ammonia) and $S = 10^{-4}$. The time evolution of the autocorrelation P_n , Fig. 1(a), shows conspicuous quantum beats, quite different from the familiar picture of tunneling in a double well. Taking the Fourier spectrum of this time evolution to obtain the two-point correlation function of the local spectrum, Fig. 1(b), reveals these beats as the result of the superposition of mainly three frequencies, with some minor contributions from other discrete lines.

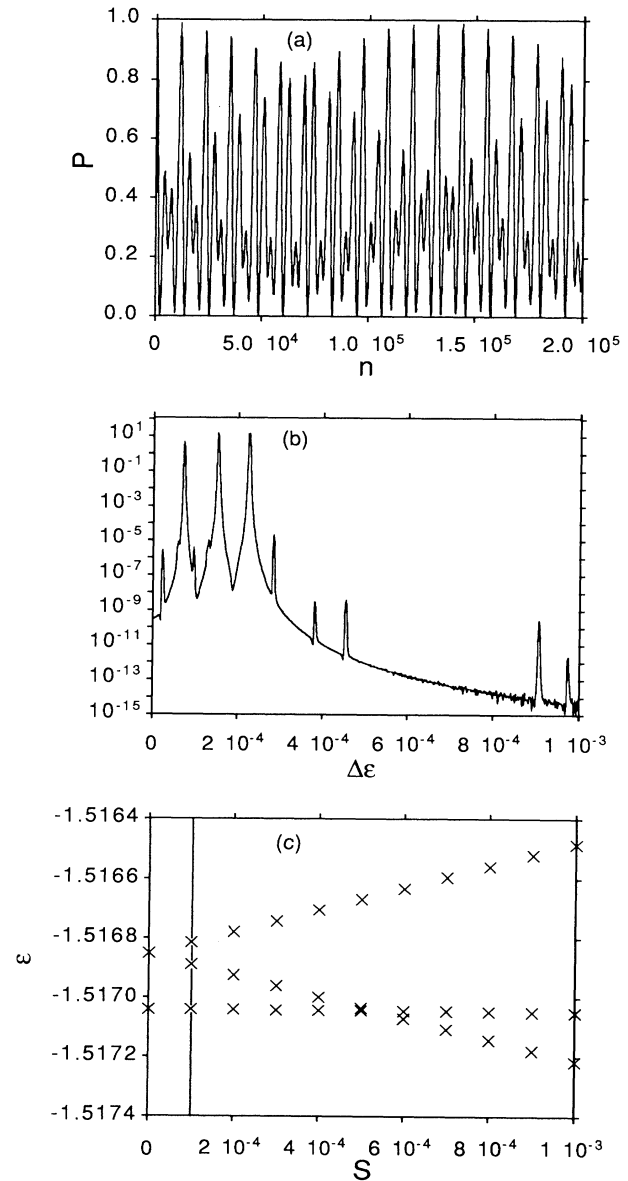


FIG. 1. Driven tunneling at an avoided crossing: (a) time evolution, over the first 2×10^5 time steps, of the autocorrelation function P_n ; (b) corresponding local quasienergy correlation function (abscissa in arbitrary units); and (c) quasienergies involved in the dynamics shown in (a) and (b), as a function of the driving amplitude S , at the driving frequency ω used in (a) and (b). The parameter values are $\omega = \omega_r \approx 0.876$, the fundamental resonance (see text), and $S = 10^{-4}$, as indicated by the vertical line in (c).

These three frequencies, in turn, can be identified by analyzing the Floquet spectrum at the parameter values chosen. Figure 1(c) represents a section, at $\omega = \omega_r$, through the $\epsilon(S, \omega)$ space. It shows how an avoided crossing evolves out of the fundamental resonance, and suggests associating the three frequencies dominating the

local spectrum with the separations of the quasienergies emerging from E_1 , E_2 , and $E_3 - \hbar\omega_r$, respectively.

Exact crossings of quasienergies can have even more surprising consequences, as we will discuss now. Consider the two lowest eigenstates of the unperturbed case: They form the well-known doublet of a symmetric and an antisymmetric state which is responsible for the familiar tunneling phenomenon. With the driving force S switched on (but still small), they evolve into two Floquet eigenstates Φ_e , Φ_o , respectively, with similar shape and, in particular, with the same parity as their unperturbed counterparts. These two "lowest" Floquet states, therefore, allow for *exact* crossings of their respective quasienergies, as functions of S and ω . In fact, we find a *one-dimensional manifold* in the (S, ω) plane where they cross. The consequences of such crossings are intriguing: The time scale for a wave packet prepared as a superposition $(\Phi_e \pm \Phi_o)/\sqrt{2}$ to cross the barrier diverges, and so it will remain localized in the initially populated well.

The results of a numerical investigation of this unexpected phenomenon are presented in Fig. 2. The parameter values chosen here are $S = 3.17 \times 10^{-3}$, $\omega = 0.01$, and again, $D = 2$. Figure 2(a) shows the time evolution of P_n over the first 10^3 time steps. This time span corresponds to about 20 times the period of the tunneling process in the unperturbed system, i.e., $\Delta = 1.9 \times 10^{-4}$. The fact that P_n remains near unity, within 10%, is a first indication of a coherent suppression of tunneling. A more reliable measure of the transfer of probability to the opposite well is ρ_n^{left} , plotted, in Fig. 2(b), over the same time window. Its deviation from unity does not even exceed 2.5%. In Fig. 2(c), we compare the initial state with the state at $n = 458$, where P_n reaches one of its minima. Even here, both states approximately coincide. Finally, we also generated a finely resolved time evolution, over one period of the driving force, of the two diagnostic quantities mentioned (not shown). It clearly excludes the possibility of fast tunneling with the frequency of the driving force, which could have escaped the stroboscopic description used in all the other simulations.

We conclude this discussion of the coherent destruction of tunneling at exact quasienergy crossings with some remarks on the role of the preparation of the initial state. It is obvious, from Figs. 2(a)–2(c), that the localization of the wave packet is not perfect. This is due to the fact that we did *not* prepare the initial state as an exact superposition $(\Phi_e \pm \Phi_o)/\sqrt{2}$ of the two Floquet "ground states," but rather, as emphasized above, as a Gaussian wave packet defined independently from the Floquet basis. In the particular case studied here, it so happens that the difference between these two states is not significant: The true initial state is almost, but not completely, exhausted by the two Floquet states forming the exact crossing, i.e., there is a very small but finite contribution from "higher" Floquet states to the dynamics. However, it is to be expected that this situation will be

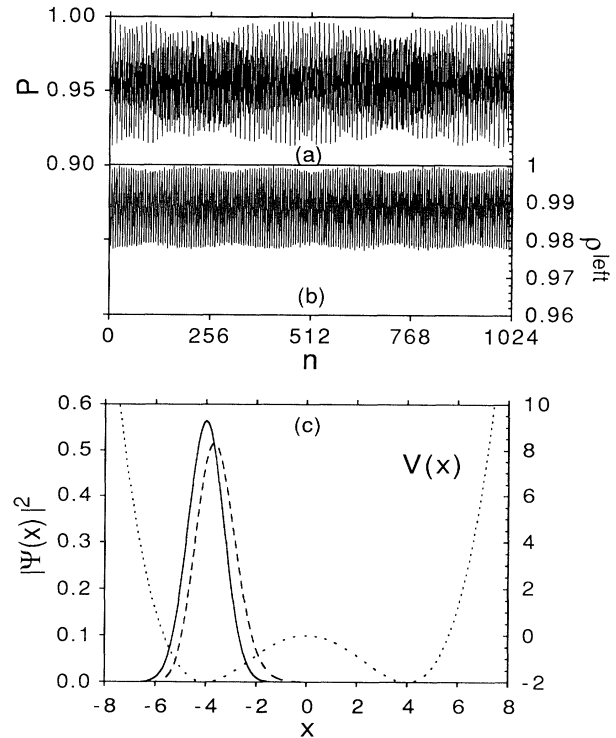


FIG. 2. Driven tunneling at an exact crossing of the two "lowest" quasienergies (see text): time evolution, over the first 10^3 time steps, of (a) the autocorrelation function P_n and (b) the occupation probability ρ_n^{left} in the initially populated well; (c) comparison of the initial state with the state at $n = 458$, where P_n reaches one of its minima. Even here, both states approximately coincide. Finally, we also generated a finely resolved time evolution, over one period of the driving force, of the two diagnostic quantities mentioned (not shown). It clearly excludes the possibility of fast tunneling with the frequency of the driving force, which could have escaped the stroboscopic description used in all the other simulations. The parameter values are $\omega = 0.01$ and $S = 3.171 \times 10^{-3}$.

much less favorable at exact crossings formed by Floquet states other than the two lowest ones.

The results reported in this Letter show that external driving of a bistable quantum system gives rise to quite complex and partially unexpected modifications of the familiar notion of tunneling. In particular, *periodic driving may slow down tunneling by any desired degree or even suppress it altogether, in a perfectly coherent way*. This surprising effect is achieved by tuning the driving force to a suitably chosen frequency in the vicinity of an exact crossing of those two Floquet states that correspond to the ground-state doublet of the unperturbed double well. It enables localization of an otherwise bistable quantum system in one of its metastable states. Since it occurs along a one-dimensional manifold in the parameter space spanned by frequency and amplitude of the driving force, it should be readily observable in a variety of experimental situations: Possible applications range from quantum chemistry (proton transfer, inversion motion of atoms in pyramidal molecules such as NH_3) to mesoscopic systems

(ac-driven SQUIDS) [16].

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