Complexity, tunneling, and geometrical symmetry

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It is demonstrated in the context of the simple one-dimensional example of a barrier in an infinite well that highly complex behavior of the time evolution of a wave function is associated with the near degeneracy of levels in the process of tunneling. Degenerate conditions are obtained by shifting the position of the barrier. The complexity strength depends on the number of almost degenerate levels which depend on geometrical symmetry. The presence of complex behavior is studied to establish correlation with spectral degeneracy. [S1063-651X(97)09902-9]

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Tunneling processes have become of considerable interest as one of the possible mechanisms for creating highly complex behavior in the structure of the quantum wave function. Tomsovic and Ullmo [1] found that there is an interesting correlation between classical chaotic behavior and the rate of tunneling in the corresponding quantum system. The conclusion of their study is that chaos facilitates tunneling.

On the other hand, Pattanayak and Schieve [2,3] found chaotic behavior in the semiclassical phase space (defined by expectation values) of a one-dimensional time-independent Duffing oscillator where new variables, associated with dispersion of the quantum states, are defined and included in the description of the system. They concluded that quantum tunneling plays a crucial role for the chaotic behavior in the corresponding semiclassical maps. They have argued [3] that the spectrum becomes more complicated in the neighborhood of the separatrix.

In a recent study, we have considered a model in which tunneling leads to highly complex behavior of the quantum wave function and its time dependence. The spectrum, as anticipated by Pattanayak and Schieve [2,3], indeed makes a transition to more complex behavior in the presence of a classical separatrix [4]. It is clear that the near degeneracy of levels is necessary for the existence of significant tunneling. We directly investigate, in this work, the effect of near degeneracy in the presence of tunneling on the complexity and the behavior of the development of the wave function. This criterion is, in fact, closely analogous to the criterion of overlapping resonances for the onset of classical chaos [5].

The model we shall use is related to the one we previously explored [6], i.e., a barrier embedded in an infinite well. By displacing the barrier in the double well system (to the right or to the left), certain positions are passed where the system becomes strongly near-degenerate. These positions occur at almost commensurate intervals. It is exactly for those positions that one may find significant tunneling accompanied by complex behavior. We show, moreover, that in the cases of very high degeneracy, tunneling from left to right has exponential decay, on a significant interval of time, but at other positions, where near degenerate conditions are somewhat weaker, the transition curve develops strong oscillations.

In a study by Nieto *et al.* [7], it was shown that tunneling in an asymmetric double well is a very sensitive function of the potential. The behavior of the development of the wave function under these conditions was not, however, discussed there.

The calculation in this work is done for a square barrier of height $V=5$ and width $w=x_2-x_1=2$ (x_1 is the left boundary of the barrier and x_2 is the right boundary; we take $\hbar\equiv 1, 2m\equiv 1$) embedded in an infinite well of width $2l=110$ [interval $(-l,l)$]. In the calculation, an exact analytic expression is evaluated on the computer; there is no accumulation of error for large times, since there is no integration over time.

We first discuss the energy spectrum according to the location of the barrier. In Fig. 1 one can see the lower energy levels ''almost crossing'' (the levels do not cross, but can become very close to each other) at several locations of the barrier. In the middle [the position c of the center of the barrier is taken at $c=0$; generally, $c=\frac{1}{2}(x_1+x_2)$] every energy level is almost degenerate. In other discrete locations, one finds almost degeneracy for every second level, every third level, and so on.

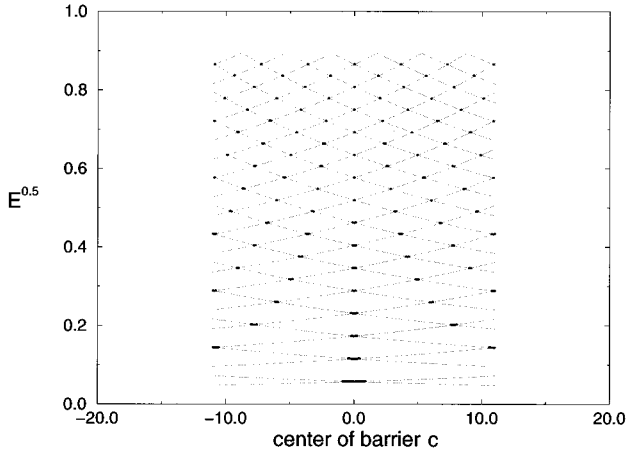

FIG. 1. Square root of energy eigenvalues as a function of the center of the barrier.

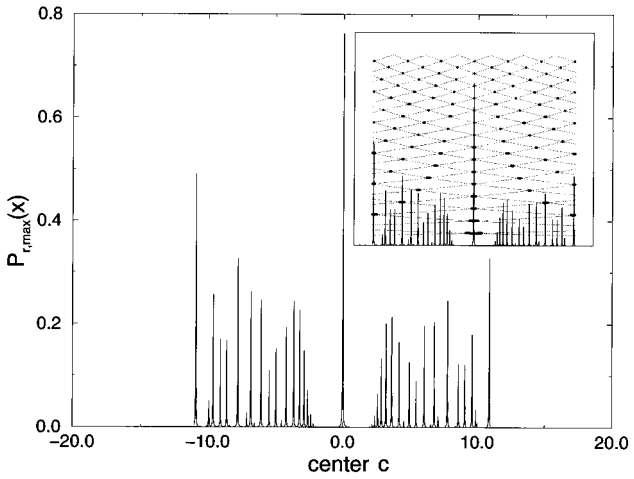

FIG. 2. Maximum probability to be to the right of the barrier. The inset shows partial correspondence between RE (resonance enhancement) and almost degenerate levels.

As an approximation to our model, consider two separate infinite wells with widths $l+x_1$ and $l-x_2$. The energy levels of the two separate wells exhibit very similar behavior to that of the finite barrier, but in this case, exact degeneracy occurs, according to the geometrical configuration of the system. For $x_2=-x_1$, we have complete symmetry and all levels are degenerate. When the width of the left well is twice the width of the right well or vice versa, one obtains degeneracy for every second energy level (of three levels, two are degenerate). If the width of the left well is one-third of that of the right well, every third level is degenerate, and so on. This follows from the relations $E_{n_l}=\hbar^2(\pi n_l)^2/2m(l+x_1)^2$ and $E_{n_r}=\hbar^2(\pi n_r)^2/2m(l-x_2)^2$; if $n_l/n_r=(l+x_1)/(l-x_2)$, then $E_{n_l}=E_{n_r}$ (n_l and n_r are positive integers). The locations for which these degeneracies occur are $c=[(n_r-n_l)/(n_r+n_l)](l-w/2)$. In every n_l+n_r levels we have at least one degeneracy. In our model (barrier in infinite well), the behavior is very similar to the problem of separate wells for the lower energy levels (for the higher energy levels there are, in fact, no crossings); degeneracy locations are, moreover, shifted slightly forwards the center.

In order to study the tunneling process, we constructed a wave packet approximating the form $\psi(x,0)=c\exp[-(x-x_0)^2/(4\sigma^2)+ik_x]$ [where $\sigma=5$, $k_x\sim 0.45$ and $x_0=(x_1-l)/2$], from 28 or less of the first energy levels, located in the middle of the left side of the barrier (the normalization of the wave packet is approximately 0.9999). The average energy is approximately $0.1V$. We then measured the maximum probability to be on the right side of the barrier during a very long time interval ($t_{max}\sim 2\times 5\times 10^5$). The calculation is done for the central region of the well (from $-l/5$ to $l/5$) to avoid a phase space imbalancing effect (if the barrier is located too close to the left side, for example, the probability to be in the left side is much smaller than the probability to be in the right side, just because the available space is much less). It can be seen clearly from Fig. 2, that just several positions (which we call RE, for resonance enhancement) allow tunneling, while in most regions the wave packet is trapped in the left side. The strongest RE is found in the center of the well where we have complete symmetry. Figure 1 and 2 show complete correspondence; the strength of the RE's depend on the number of degenerate energy levels (Fig. 2, inset). The second strongest RE in the picture is found where the system has near degeneracy for every fifth level ($c\sim -54/5$ and $c\sim 54/5$).

An additional factor that one must consider is the projection of the initial state (Gaussian wave packet) on different eigenfunctions, i.e., the coefficients of the representation. It is clear that the strength of a RE depends on the number of almost degenerate states that have a large overlap with the initial state. Thus, in order to get strong RE, there must exist at least one pair of eigenstates, $|j-1>$, $|j>$, which fulfill two conditions: (1) Near degeneracy of levels ($E_{j-1}\sim E_j$), and (2) the scalar product of the eigenstate with the initial state is large enough [i.e., in our case, $(\psi(0),\phi_j)$ appreciable compared to unity]. Condition (1) forms a general underlying symmetry of the system, while condition (2) is a requirement for the symmetry effects to be realized.

In fact, near degeneracy of levels [condition (1)], $E_{j-1}\sim E_j$, implies symmetry properties of a pair of eigenstates, $|j-1\rangle$ and $|j\rangle$. Let us denote the part of the eigenfunction on the left side of the barrier as ϕ_L, and on the right side of the barrier as ϕ_R (we neglect the function under the barrier, since the eigenfunctions are small in this region). Near degeneracy of levels and orthogonality implies that the eigenfunctions are almost the same on one side of the barrier, and opposite in sign on the other side of the barrier, i.e., $\phi_{L,j-1}\sim\phi_{L,j}\equiv\phi_L$ and $\phi_{R,j-1}\sim-\phi_{R,j}\equiv-\phi_R$, or vice versa. Moreover, the eigenvalue condition requires that $\int_L|\phi_L|^2\sim\int_R|\phi_R|^2$, while the normalization condition requires $\int_L|\phi_L|^2+\int_R|\phi_R|^2\sim 1$. Thus, $\int_L|\phi_L|^2\sim\int_R|\phi_R|^2\sim\frac{1}{2}$. These properties imply symmetry and antisymmetry in the central position. We conjecture that this symmetry is the essential property of the central position ($c=0$).

The wave function for the main, central RE exhibits a complex behavior for the evolution. This complexity is due to the large number of almost degenerate levels. When we measure a physical quantity, the difference between levels determines the time dependence (the time-dependent phase is computed according to ΔE_{ij}). The very small frequency due to near degeneracy implies a very large recurrence time. On the other hand, large energy differences are associated with short time scales. The influence of these types of frequencies can be seen in most of the results. However, this behavior does not occur for the total probability in the left side of the well as a function of time, as seen in Fig. 3(a). The curves are smooth and do not reflect the influence of the short time scale. As explained before, at RE locations there exist, at least, one pair of eigenfunctions ϕ_{j-1}, ϕ_j which are approximately the same on the left side and $\int_{-l}^{x_1}\phi_{j-1}\phi_j$ is appreciable (approximately $\frac{1}{2}$). The influence of other (nonneighboring) eigenfunctions on P_{left}, tends to be small. The result is a combination of periodic functions (the number of these functions corresponds to the number of pairs that fulfill the two conditions for RE), with very small frequency differences.

The transition from one side to another, when $c=c_0=0$, exhibits approximate exponential behavior for times not too short or too long [(Fig. 3(a)]. We observe similar behavior, but less clear, in other locations that have very strong RE

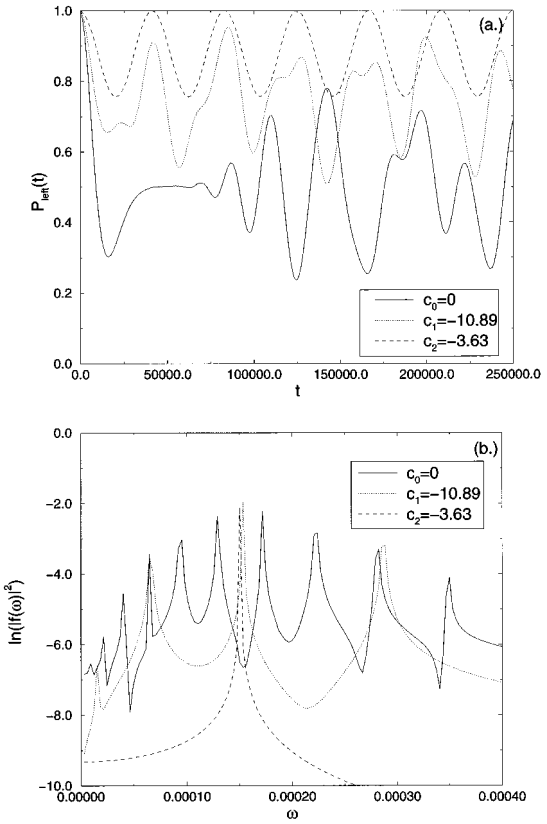

FIG. 3. (a) Probability to be to the left of the barrier as a function of time for three largest RE's [in the interval $(-l/5,l/5)$]. (b) The power spectrum of (a).

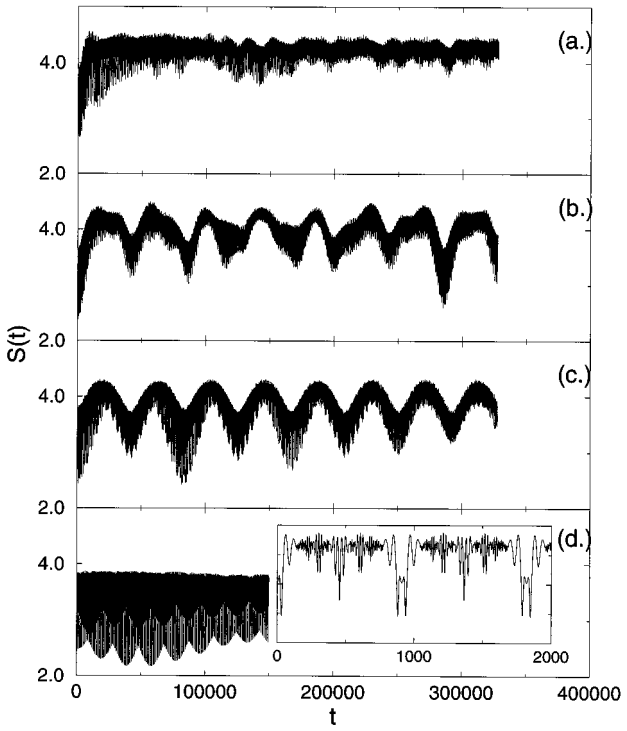

FIG. 4. The entropy function as a function of time for different locations. (a) $c=c_0=0$ (b) $c=c_1=-10.89$, (c) $c=c_2=-3.63$, (d) $c=c_3=-1$; the inset shows an enlargement of typical periodic oscillations.

(locations such as $c\sim-54/3$ and $c\sim-54/2$). It appears that this exponential decay is due to the behavior of a sum of periodic functions with very small different frequencies, as can be seen in Fig. 3(a). After this interval of decay, P_{left} enters a domain of large oscillations.

In Fig. 3(a), we show also the results of the same calculation for some other RE locations. As expected, we find a periodic (or almost periodic) behavior. The Fourier transform [Fig. 3(b)] shows very strong frequency peaks that fit the most dominant near degenerate energy levels, and show clearly that very small frequencies dominate the motion.

The near degeneracy of levels that produces a high level of complexity, i.e., chaoticlike behavior, occurs in the presence of strong tunneling. We have observed this effect in Ref. [6]. We study here one of the most clear ways to display this connection. We compare, in Fig. 3(a), results of four positions. For $c_1=-10.89$, there is a large RE with three pairs of dominant, near degenerate, eigenstates, and for $c_2=-3.63$ there is a smaller RE with one pair of dominant almost degenerate eigenstates. The choice of $c_3=-1$ results in no RE, no degeneracy, and no tunneling at all. The main RE, at $c=c_0=0$, reflects a very complex behavior, as we have shown in Ref. [6].

In Fig. 4 the entropy defined by $S(t)=-\int|\psi(x,t)|^2\ln|\psi(x,t)|^2dx$ is computed. For c_0, shown in Fig. 4(a), the entropy rises sharply accompanied by high-frequency oscillations and then remains a long time in a ''quasiequilibrium state.'' The second RE, c_1, shown in Fig. 4(b), shows a tendency to recurrence after 280 000 time units, while c_2, shown in Fig. 4(c), returns to almost the initial condition after approximately 80 000 time units. The entropy for non-RE locations shows almost periodic behavior [Fig. 4(d); the inset shows the structure at increased scale]. A similar behavior can be seen for $\rho(t)=\langle\langle x^2\rangle-\langle x\rangle^2\rangle$.

Comparison between different locations shows that one can characterize the behavior by two time scales. The first is the time of approach to equilibrium (Δt_{eq}), and the second is the recurrence time (Δt_{rc}). The approach to equilibrium time corresponds to averaging small frequencies (i.e., $\langle\Delta E\rangle$ over all energies that satisfy near degeneracy). One can easily identify Δt_{eq} from Fig. 3(a) (for c_0) and from Fig. 4(a), while Δt_{rc} can be calculated analytically from the known eigenvalues. It appears that $\Delta t_{eq}/\Delta t_{rc}$ can give a measure for the complexity of the behavior of the system, as seen in these results. In all cases Δt_{eq} is approximately the same, while Δt_{rc} is changed drastically from c_0 to c_3 (one cannot recognize recurrence in the c_0 location, while c_1 and c_2 exhibit near recurrence as mentioned in the previous paragraph). Thus, the ratio of these two time scales is largest for c_3 (largest RE and maximum complexity), and decreases when the RE's become stronger (or when the complexity becomes stronger).

In Fig. 5, we compare the $\langle p\rangle$:$\langle x\rangle$ maps, sampled at peak times (times at which the wave function forms peaks). For each location of the barrier $(c_0,c_1,\ldots)$, we measure the time between peaks of $|\psi(x_1,t)|^2$. At c_0 (a) the map moves toward the center and then accumulates in the central region. The map of c_1 (b) shows some ordered lines, and it is easy to see that the wave packet stays most of the time in the left side. More ordered behavior appears in the map of c_2 (c), where the lines appear as semiperiodic paths. (The mapping

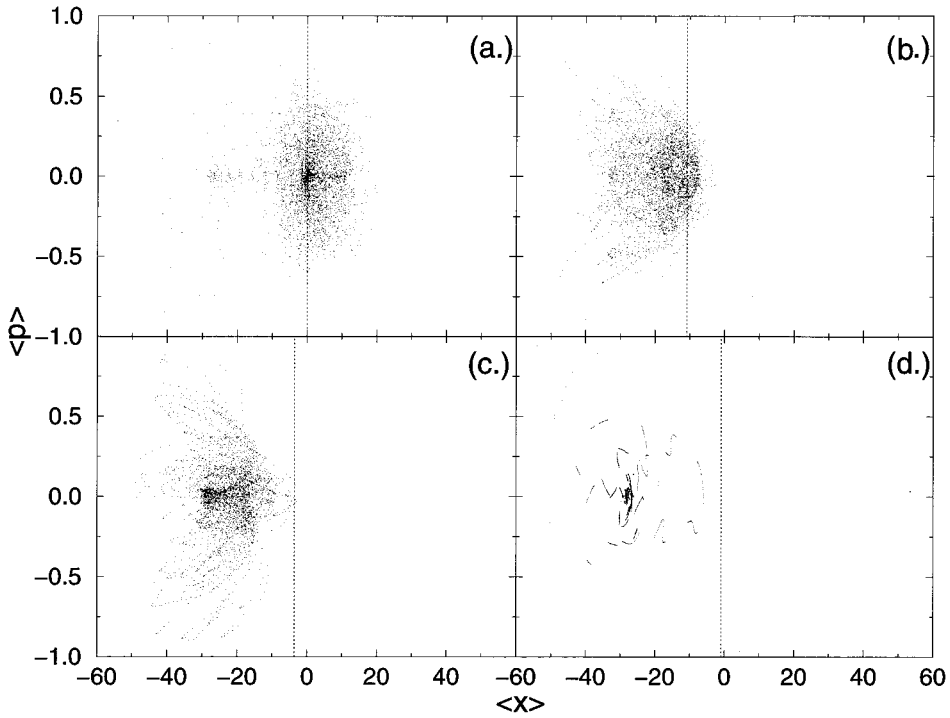

FIG. 5. The accumulation of points in the $\langle x\rangle$:$\langle p\rangle$ plane according to peak times for different locations. (a) $c=c_0=0$, (b) $c=c_1=-10.89$, (c) $c=c_2=-3.63$, (d) $c=c_3=-1$. The dotted line indicates the position of the center of the barrier.

oscillates back and forth, each time adding points to paths.) Finally, c_3 (d) provides ordered maps, as expected. The same pattern can be seen also in $\langle\pi\rangle$:$\langle\rho\rangle$ ($\pi=d\rho/dt$), at peak times, and from the Poincaré maps $\langle p\rangle$:$\langle x\rangle$ sampled when $\rho(t)$ is minimum [i.e., $\pi(t)=0$ and $d\pi/dt>0$] [2]. A period doubling behavior (small circles within large circles) can be seen in the $\langle p\rangle$:$\langle x\rangle$ plane, and in the $\langle\pi\rangle$:$\langle\rho\rangle$ plane, as shown in Ref. [6]. The behavior becomes more ordered as the RE height decreases, while for c_3 there are just large circles.

We have shown in this study that tunneling in the presence of near degeneracy of levels provides necessary and sufficient conditions for the development of complex behavior of the wave functions of a quantum system. A large number of near degenerate levels induces a high level of complexity. In general, a pair of near degenerate levels has a pair of equivalent eigenfunctions for which one is nonalternating and the other alternating. Moreover, in this case, the probability to be to the left side is approximately equal to the probability to be to the right side, without connection to the barrier position. These conditions suggest an underlying symmetry property which depends strongly on the geometry of the system.

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