Signature of classical chaos on quantum tunneling

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We examine the signature of classical chaos on a generic quantum phenomenon, namely, quantum tunneling in a nonintegrable, conservative two-degree-of-freedom Hamiltonian system. We show that, as one passes from the regular to chaotic regime, the quantum tunneling probability versus coupling-constant curve exhibits a significant change of slope in the neighborhood of the critical chaotic threshold (beyond which classical chaos sets in). This shows that the presence of Kolmogorov-Arnold-Moser barriers of classical phase space manifests in quantum phenomena such as quantum tunneling.

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I. INTRODUCTION

The problem of quantum chaos [1–6] has been one of the major issues in nonlinear dynamics today. The main question that has been addressed over the years is how a dynamical system that is classically chaotic behaves upon quantization. Although no general correspondence between the classical solutions, i.e., the phase-space trajectories and the quantum solutions (that is, the wave solutions excluding those when the system is integrable), is known, considerable insight has been gained by quantizing the classical system that exhibits complete stochasticity, such as the Sinai billiard system, Arnold's cat map, etc. The related studies are based on some conjectures, including repulsion of energy levels in the stochastic regime, and peaking of energy-level spacing about a finite value rather than having its maximum at zero separation. The situation for near-integrable systems in which the regular and stochastic motions are intermingled on the finest scale poses much more difficult problems, for which one has to look for a "coarse-grained" quantum phase space. A vast body of literature has been devoted to all these studies, formally referred to as quantum chaos.

However, there is a class of problems [7–12] on the related issues that have received relatively less attention. This may be posed in the following way: What is the signature of classical chaos in a generic quantum phenomenon? One early attempt in this direction was made in Ref. [17]. It has been demonstrated that classical Kolomogorov-Arnold-Moser (KAM) barriers still act as barriers even in an intrinsic quantum phenomenon like quantum diffusion. Similarly, in the semiclassical limit, in contrast to regular behavior, the chaotic dynamics may result in an increase in squeezing [11], a generic quantum phenomenon. The object of the present paper is to address a related issue. We know that quantum tunneling is a typical nonclassical effect. We now ask: What is the effect of classical chaos on quantum tunneling? We demonstrate the signature of the presence of KAM barriers in this generic quantum phenomenon.

Before going into further detail, let us first note that quantum tunneling in a one-degree-of-freedom system is an old problem and has been since the birth of quantum mechanics. Since all one-degree-of-freedom systems are integrable, one must consider a tunneling system with more than one degree of freedom in order to analyze the influence of chaotic behavior on this nonclassical effect. Again, from the analytical point of view, the barrier-penetration problem in a system with more than one degree of freedom is a difficult one, since the available perturbation methods are untenable for arbitrary coupling and the higher-dimensional Wentzel-Kramers-Brillouin (WKB) methods [13] are extremely cumbersome to render any useful, tractable result. Very recently, however, a number of numerical methods have been put forward. For example, the tunneling rate has been calculated using the Husimi representation in a driven Hamiltonian system [10]. A complex scaling technique [14] has been extended to calculate the tunneling rate in a two-degree-of-freedom Hamiltonian system describing proton transfer in organic molecules. Our purpose here is twofold. First, to provide an analytical expression for the tunneling rate for a class of two-degree-of-freedom Hamiltonian systems and second, to examine, numerically, the influence of classical chaos on quantum tunneling for a typical nonintegrable system.

Our study is based on a conservative Hamiltonian system consisting of two coupled subsystems, one having a smooth potential-energy function with a metastable minimum, and the other being a simple harmonic oscillator. By virtue of having the finite barrier height associated with the subsystem with a metastable minimum, quantum tunneling is possible. It should be noted that both subsystems are separately integrable. However, the coupled system is classically nonintegrable when the potential of the tunneling subsystem allows an homoclinic orbit to exist. In what follows, we quantitatively relate the quantum tunneling rate to the Fourier spectrum of the classical trajectory in such a nonintegrable system, and show that as we pass from the regular to chaotic regime the quantum tunneling versus coupling-constant curve exhibits a significant change of slope in the neighborhood of the critical classical chaotic threshold. We thus demonstrate the presence of KAM barriers in this nonclassical effect.

The rest of the paper is organized as follows. In Sec. II we derive the analytical expression for the probability of quantum tunneling in a class of two-degree-of-freedom Hamiltonian systems. In Sec. III we prove the nonintegrability of the model, numerically investigate the classical chaos, and examine its signature on quantum tunneling. Conclusions are presented in Sec. IV.

II. QUANTUM TUNNELING IN A CLASS OF TWO-DEGREE-OF-FREEDOM SYSTEMS

We consider the following Hamiltonian describing a class of two-degree-of-freedom systems:

$$H=\tfrac{1}{2}M\dot{q}^2+V(q)+\tfrac{1}{2}m\dot{x}^2+\tfrac{1}{2}m\Omega^2x^2-kqx \ , \tag{1}$$

where the two subsystems are described by the coordinates $(q,\dot{q})$ and $(x,\dot{x})$. The q subsystem is associated with the potential function $V(q)$. Our first requirement about this subsystem is that it must possess a metastable minimum to qualify it as a tunneling system. The last term denotes the coupling of the two subsystems through the coupling constant k. M, m, and Ω are the mass of the q system, and the mass and frequency of the harmonic oscillator, respectively. We note, in passing, that similar Hamiltonians had been the subject of earlier studies in relation to proton transfer in organic molecules [14] and inhibition of chaos by parametric perturbation [15]. For the present study, we rewrite the Hamiltonian in a more simple form:

$$H=\tfrac{1}{2}\dot{q}^2+V(q)+\tfrac{1}{2}\dot{x}^2+\tfrac{1}{2}\Omega^2x^2-kqx \ , \tag{2}$$

where we have redefined the mass terms as $M=m=1$.

The method of our calculation is the path-integral approach of Feynman, which takes into account of the quantum transition amplitude for the whole system [(q system)$\times$(x system)] to go from coordinates (q_i,x_i) at time zero to (q_f,x_f) at time T, as follows:

$$k(q_i,x_i,0;q_f,x_f,T)=\int_{q(0)=q_i}^{q(T)=q_f}[q(t)]\int_{x(0)=x_i}^{x(T)=x_f}[x(t)]\exp\left[-\frac{1}{\hbar}\int_0^T L(q(t),x(t))dt\right] . \tag{3}$$

Here, L denotes the Euclidean Lagrangian (H). $[q(t)]$ and $[x(t)]$ are the functional measures. One then defines the reduced imaginary-time Green's function for the q system by integrating the x-system or harmonic-oscillator subspace exactly to obtain

$$\bar{k}(q_i,0;q_f,T)=\int dx_i k(q_i,x_i,0;q_f,x_f,T)_{x_i=x_f} \ . \tag{4}$$

Making use of spectral expansion in term of the eigenstates of H, one obtains

$$\bar{k}=\sum_n \int dx \langle q_f|n\rangle\langle n|q_i\rangle\exp(-E_nT/\hbar) \ , \tag{5}$$

where $|q_i\rangle$ and $|q_f\rangle$ are the position eigenstates and T is a positive number.

Leading terms in an expression for large T and small q gives us the energy and wave function of the lowest-lying eigenstates. In particular, the quantum tunneling rate is obtained from a small imaginary part of that energy state after following the analytic continuation procedure. For details, we refer to Refs. [13] and [16]. The quantum tunneling probability P is given by

$$P=(S_{\rm eff}/2\pi\hbar)^{1/2}\omega_0\exp(-S_{\rm eff}/\hbar) \ , \tag{6}$$

where $S_{\rm eff}$ is given by

$$S_{\rm eff}=S_0+S_1 \tag{7}$$

with

$$S_0=\int_0^T[\tfrac{1}{2}\dot{q}^2+V(q)]dt+\text{const}$$

and

$$S_1=-(k^2/4\Omega)\times\int_{-\infty}^{\infty}\int_0^T dt\,dt'\exp(-\Omega|t-t'|)q(t)q(t') \ . \tag{8}$$

Here, ω_0 is the approximate uncoupled bounce frequency of the tunneling system. The effect we consider here is primarily contained in the S_1 part of $S_{\rm eff}$.

In deriving expression (8), it has been assumed, as in Ref. [16], that

$$q(t)=q(t+T) \ \text{ for large } T \ , \tag{9}$$

which implies $q(t)$ is quasiperiodic. This quasiperiodicity allows us to make the following Fourier expansion of the classical path:

$$q(t)=\sum_{n=-\infty}^{n=\infty}A(\omega_n)\exp(i\omega_nt) \ , \tag{10}$$

where $A(\omega_n)$ are the complex Fourier coefficients. Using expansion (10) in (8) and performing the integration explicitly for large T (tending to infinity), we obtain

$$S_1=-(k^2/4\Omega)\sum_{n=-\infty}^{n=\infty}\left[\frac{2\Omega A(\omega_n)A(-\omega_n)}{\Omega^2+\omega_n^2}\right] . \tag{11}$$

Inverse Fourier expansion of (10) reveals that $A(-\omega_n)=A^*(\omega_n)$. Therefore, S_1 may be further simplified as follows:

$$S_1=-k^2\int_0^{\infty}\frac{S(\omega)d\omega}{\Omega^2+\omega^2} \ , \tag{12}$$

where we have set $|A(\omega)|^2=S(\omega)$ and transformed the sum into an integral. $S(\omega)$ is simply related to the Fourier spectrum of the classical trajectory $q(t)$.

We have thus related the quantum tunneling probability to the Fourier spectrum of the classical trajectory. Therefore, to examine the effect of classical motion on the quantum tunneling rate, we first have to solve the classical equations of motion for $q(t)$ starting from the Hamiltonian H for a particular $V(q)$, calculate the Fourier spectrum of the trajectory to obtain $S(\omega)$, and then perform the integration in (12) to obtain S_{eff}.

Our first conclusion is the following. Since the integral in Eq. (12) is always positive, the quantum tunneling probability of the q system is increased approximately by a factor $\exp(S_1/h)$ when its coupling to the harmonic oscillator is switched on. Thus the quantum tunneling is enhanced by introduction of another degree of freedom. The detailed nature of this enhancement will be subject to numerical study, as presented in the next section.

III. CLASSICAL CHAOS AND QUANTUM TUNNELING

So far, our treatment of quantum tunneling for a class of two-degree-of-freedom conservative Hamiltonian systems is more or less general, subject to fulfillment of one particular requirement of the q system; that is, $V(q)$ must have a metastable minimum in order to qualify it as a tunneling system. In this section, however, we impose our second requirement on $V(q)$, namely, that a q system must possess a homoclinic orbit. As we show in the next subsection, the presence of this orbit renders the overall Hamiltonian system nonintegrable [17,18,15] for finite nonzero coupling between the two subsystems. Depending on the values of the coupling constant k, one would therefore expect a variety of dynamical features that must be manifested in the Fourier spectrum of classical trajectories obtained from the solutions of Hamilton's equations of motion. Subsequently, quantum tunneling would be affected. With this in mind, we now specifically consider the following potential function $V(q)$ for the q system:

$$V(q)=\alpha q^4-\beta q^2 , \tag{13}$$

where α and β are positive integers.

A. Nonintegrability of the model

The nonintegrability of the present model Hamiltonian,

$$H(q,\dot{q},x,\dot{x})=X(x,\dot{x})+Q(q,\dot{q})+\epsilon H^1(q,\dot{q},x,\dot{x}) , \tag{14}$$

$$X(x,\dot{x})=\tfrac{1}{2}\dot{x}^2+\tfrac{1}{2}\Omega^2x^2 , \tag{15}$$

$$Q(q,\dot{q})=\tfrac{1}{2}\dot{q}^2-\beta q^2+\alpha q^4 , \tag{16}$$

and

$$H^1(q,\dot{q},x,\dot{x})=-kqx , \tag{17}$$

is amenable to theoretical analysis using Melnikov's method [15,17,18], where one is concerned with the perturbation of the homoclinic manifold in a Hamiltonian system that consists of an integrable part [such as $X(x,\dot{x})+Q(q,\dot{q})$ in the present case] and a small perturbation (H^1). ϵ is a smallness parameter, which may be set equal to 1 at the end of the calculation. As pointed out earlier, the uncoupled system consisting of X and Q systems is integrable. It is well known that if Melnikov's function (which, loosely speaking, measures the leading nontrivial distance between the stable and unstable manifolds) contains simple zeros, then the stable and unstable manifolds (which, for an unperturbed system, coincide as a smooth homoclinic manifold) intersect transversely for small perturbation generating scattered homoclinic points, which asserts nonintegrability and qualitatively explains the onset of stochasticity around the separatrix.

To this end, we note that Q system possesses the homoclinic orbit

$$\begin{aligned} q(t)&=(\beta/\alpha)^{1/2}\text{sech}(2\beta)^{1/2}(t-t_0) , \\ \dot{q}(t)&=-(2/\alpha)^{1/2}\beta\,\text{sech}(2\beta)^{1/2}(t-t_0) \\ &\quad\times\tanh(2\beta)^{1/2}(t-t_0) , \end{aligned} \tag{18}$$

joining the hyperbolic saddle ($q=\dot{q}=0$) to itself. We are then in a position to make direct use of the theorem of Holmes and Marsden [17] to calculate Melnikov's function for the present conservative Hamiltonian system H. The calculation involves the integration of Poisson bracket $\{Q,H^1\}$ around the homoclinic orbit as follows:

$$M(t_0)=\int_{-\alpha}^{\alpha}\{Q,H^1\}dt . \tag{19}$$

Explicit evaluation of the Poisson bracket yields

$$M(t_0)=\pi k(h/\alpha)^{1/2}\cos\Omega t_0\,\text{sech}\left[\frac{\pi\Omega}{2(2\beta)^{1/2}}\right] , \tag{20}$$

where one must take into account that the energy of the homoclinic orbit is zero and $H(x,\dot{x},q,\dot{q})=h$ $(h>0)$.

Since $M(t_0)$ has simple zeros and is independent of ϵ, we conclude that for any $\epsilon>0$ (but sufficiently small), one can have transverse intersection on the energy surface $h>0$, resulting in generation of homoclinic points. This homoclinic chaos is the precursor of the global chaos that is studied numerically in the following subsection.

B. Numerical study of chaos

The equations of motion corresponding to Hamiltonian (2),

$$\begin{aligned} H=&(\dot{q}^2/2)+(q^4/10)-(q^2/2) \\ &+(\dot{x}^2/2)+\Omega^2(x^2/2)-kxq , \end{aligned}$$

have been solved numerically for various values of coupling constant k and for Ω. Figures 1(a)–1(c) display some representative variation of q as function of time for $k=0.0005$, 0.000 66, and 0.0009, and for $\Omega=1.0$. It is immediately apparent that, as k increases, the pattern of complexity in the waveform changes very sharply. The definitive proof of chaotic behavior, however, is obtained by examining the sensitive dependence of initial conditions. In particular, a positive maximal Lyapunov exponent is characteristic of chaos, while its zero and negative values signify a marginally stable orbit and a periodic orbit, respectively. Following the method of Benettin *et al.* [19], which has also been employed by others [20], we have calculated this exponent for the aforementioned parameter ranges. It is also important to note that, for a very low value of coupling constant k, this exponent is found to be negative. But, as the coupling constant increases, the exponent becomes positive beyond a critical threshold ($\approx 0.000\,66$), which determines the onset of stochasticity or irregular behavior. [We have also carried out a calculation based on Toda-Brumer-Duff criteria (a local estimate) in search of a critical energy for the Hamiltonian (2). Unfortunately, the numerical check shows that its magnitude is a large overestimate of the chaotic threshold.]

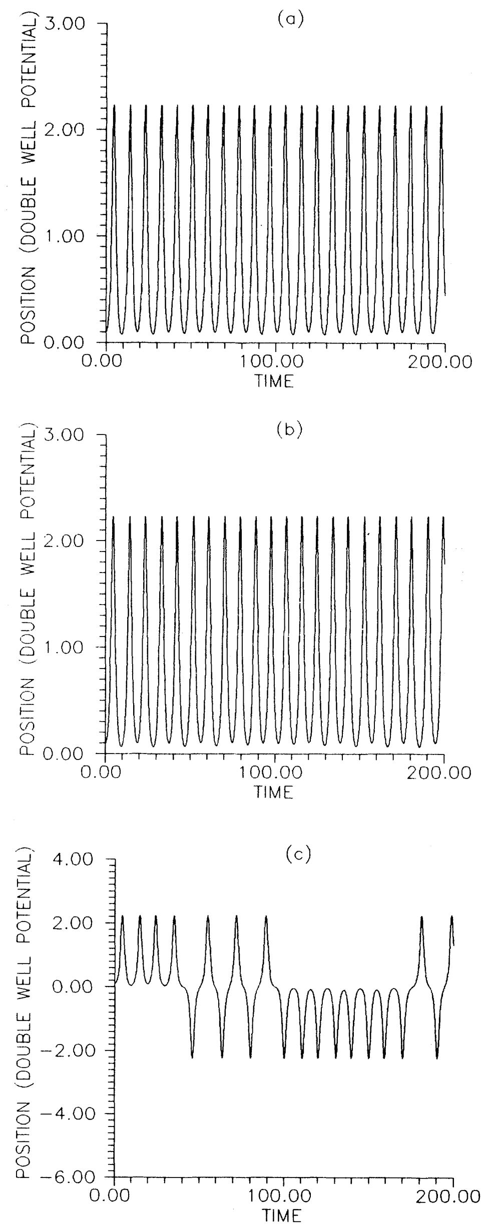

FIG. 1. Some representative variations of position of the double-well oscillator vs time t for (a) $k=0.0005$, (b) $k=0.000\,66$, and (c) $k=0.0009$ (both units are arbitrary).

C. Signature of classical chaos on quantum tunneling

Having solved Hamilton's equation of motion numerically to obtain $q(t)$ as a function of time, we now calculate $|A(\omega)|^2$ as defined in Eq. (10) using a Fourier-transform algorithm for fairly long time series. Explicit evaluation of the sum in Eq. (11) then yields S_1 and hence the quantum tunneling rate according to relation (6).

The results have been plotted in Fig. 2 for a harmonic oscillator having a frequency $\Omega=1.0$. It is evident that the tunneling rate increases slowly at the beginning in the regular region, and then relatively more rapidly as a function of the coupling constant k in the stochastic region. What is immediately apparent is that classical chaos may significantly enhance quantum tunneling. It is important to note that, as one passes from the regular to chaotic region the tunneling probability versus coupling-constant curve exhibits an interesting change of slope in the neighborhood of the classical chaotic threshold, i.e., around 0.000 66. This, we believe, is a clear signature of classical chaos (or of the presence of KAM barriers) on this generic quantum effect. This is also reminiscent of the fact [7] that the classical KAM barrier acts as a barrier in the quantum diffusion process. Our calculations have been done on a conservative Hamiltonian system. The enhancement of tunneling by applying a classical field had been noted earlier [10] numerically (making use of Husimi representation) on a driven system. Our formulation, based on the instanton technique [13], which relates the quantum tunneling rate to the Fourier spectrum of the classical trajectory, is, however, completely analytical.

Next, in Fig. 3, we show how the curve in Fig. 2 depends on Ω. Here the ordinate is plotted on a logarithmic scale for the sake of better comparison. It is immediately apparent that the Ω dependence is manifested in two ways. Curve (a) in Fig. 3 is the same as the curve in Fig. 2, i.e., for $\Omega=1.0$. As Ω is varied on either side of $\Omega=1.0$ by detuning it to 1.25 or to 0.75, the tunneling probability is drastically modified. At a very low value of the coupling constant, where the regular region in phase

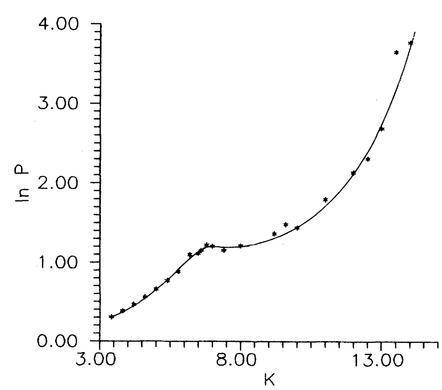

FIG. 2. Variation of ln$P$ (quantum tunneling probability 10^8P) vs k (coupling constant 10^4k) for $\Omega=1.0$. The change of slope at the critical chaotic threshold at $k=0.000\,66$ signifies the presence of KAM barriers (both units are arbitrary).

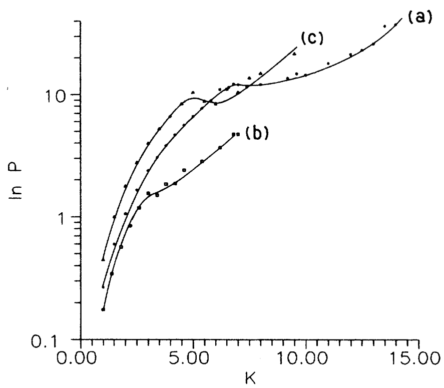

FIG. 3. Variation of ln$P$ (quantum tunneling probability 10^9P) on a logarithmic scale vs k (coupling constant 10^4k) for three different values of the harmonic-oscillator frequency Ω: (a) $\Omega=1.00$, (b) $\Omega=1.25$, and (c) $\Omega=0.75$. Critical chaotic thresholds appear at (a) $k=0.000\,66$, (b) $K=0.0003$, and (c) $K=0.0005$ (units are arbitrary).

space prevails, the tunneling probability decreases with an increase in the frequency of the oscillator. Beyond the critical threshold, however, the situation is much more complicated. Also, an examination of the change of slope reveals that the chaotic threshold at $\Omega=1.0$ goes downward as one switches the harmonic-oscillator frequency Ω to 0.75, or to 1.25. It is important to note that in all our calculations we have considered the barrier penetration of the particle whose starting point is one of the classical turning points of the double-well potential at $q=0.1$ and $p=0.0$.

IV. CONCLUSION

To summarize, we have demonstrated the signature of classical chaos (or the presence of KAM barriers) in a generic quantum phenomenon such as tunneling in a nonintegrable conservative two-degree-of-freedom Hamiltonian system. Our study reveals that for a coupled system such as Eq. (2), the tunneling rate can be quantitatively related to the Fourier spectrum of the classical trajectories. Although the spectrum has been studied analytically and numerically on several occasions [21] in the case of maps for forward and reverse bifurcations (largely in the context of dissipative dynamics), and some universal scaling laws have been proposed, such scaling behavior of the spectrum for conservative systems is yet to be discovered.

So far, we have concentrated on the barrier-penetration problem of a double-well oscillator coupled to a harmonic oscillator. A pertinent question in this context is: Does the effect we have discussed survive in the classical case, where barrier tunneling is replaced by a thermally activated barrier crossing? This is important in relation to the study of the influence of deterministic coupling between the reaction coordinate and a transverse normal mode on the activated barrier crossing (which has been investigated in the context of classical dynamics [22,23]). From studying the variation of reaction rate with coupling constant, it has been observed that the reaction rate attains a plateau that is maintained until the coupling parameter k approaches a threshold value (not chaotic threshold) similar to that shown by the curve in Fig. 2; there is a very marked increase in reaction rate around this value. Based on perturbation theory, this has been explained as a noise-induced transition. Since classical KAM barriers, which have a direct bearing on the rate of a chemical reaction, make their presence felt in a number of different phenomena—such as classical and quantum diffusion, and in barrier tunneling (as shown in the present case)—it is quite plausible that such a signature of classical chaos in activated barrier crossing is present. For this, one must go beyond perturbation theory to deal with the reactive mode. We hope to address this problem as a separate issue. We also note, in passing, that enhancement of tunneling by addition of a single degree of freedom is exactly the opposite of what happens in the case of macroscopic quantum tunneling.

ACKNOWLEDGMENTS

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