COMMENTS

Comments are short papers which criticize or correct papers of other authors previously published in the **Physical Review**. *Each Comment should state clearly to which paper it refers and must be accompanied by a brief abstract. The same publication schedule as for regular articles is followed, and page proofs are sent to authors.*

Comment on "Signature of classical chaos on quantum tunneling"

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In a recent article, Chaudhuri and Ray [Phys. Rev. E **47**, 80 (1993)] examined tunneling in a two-dimensional, nonintegrable Hamiltonian and apparently found a correlation between the onset of chaos and a dramatic change in the tunneling rate. Examination of the classical dynamics using the technique of Poincaré surfaces of section reveals that the motion is, in fact, extremely regular *throughout* the regime considered by Chaudhuri and Ray. Implications are considered.

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The general question of the effects of Kolmogorov-Arnold-Moser barriers and classical chaos on quantum tunneling rates is a problem of some current interest [1–3]. Lin and Ballentine [2], e.g., have shown that tunneling rates between disjoint regular regions of phase space can be enhanced significantly by an external driving field. They also noted an extreme sensitivity of tunneling rates as external parameters were varied. In a related computation for the same system Farrelly and Milligan [3] demonstrated that selective suppression of tunneling could be achieved by using a second external driving field. In a recent paper, Chaudhuri and Ray [1] studied tunneling in a two degree of freedom double well potential. They apparently discovered a clear correlation between the onset of classical chaos and a qualitative change in the tunneling rate as a function of a coupling parameter. Previous studies have failed to uncover a clear signature of classical chaos on tunneling behavior, and, consequently, the findings of Chaudhuri and Ray [1] are worthy of further investigation.

Chaudhuri and Ray [1] studied the two degree of freedom Hamiltonian,

$$H=\frac{(p_q^2+p_x^2)}{2}+V_q(q)+V_x(x)+V_c(x,q)\ , \tag{1}$$

where V_q is a quartic double well potential

$$V_q=q^4/10-q^2/2\ , \tag{2}$$

V_x is a harmonic oscillator,

$$V_x=\Omega^2x^2/2\ , \tag{3}$$

and the coupling potential $V_c=-kqx$. We consider only $\Omega=1$ which is the principal case studied in Ref. [1]. The minima for the potential in this case occur at

$$q=\pm\left[\frac{5(1+k^2)}{2}\right]^{1/2},\quad x=\pm k\left[\frac{5(1+k^2)}{2}\right]^{1/2}$$

while the barrier maximum is at $q=0$, $x=0$ for all k. This type of Hamiltonian has been studied extensively in chemical physics; Makri and Miller [4] employed a similar Hamiltonian in their study of energy splittings in hydrogen atom transfer processes and subsequently, Rom, Moiseyev, and Lefebvre [5] used a time independent complex coordinate method (similar to that developed by Moiseyev *et al.* [6]) to study tunneling rates as a function of the coupling strength. Importantly, all of these studies revealed that tunneling probabilities (as evidenced by level splittings) *decreased* as the coupling increased. In the present example this is due, in part, to the increase in the distance between the two potential minima for nonzero values of k. Using Melnikov's method, Chaudhuri and Ray established that H is nonintegrable and, further, claimed that the onset of global chaos occurs at $k=0.000\,66$ for $\Omega=1$. Their conclusion was based on a computation of Lyapunov exponents, which is certainly an acceptable means of establishing when and if a transition to chaos occurs. However, a simpler alternative, at least in two degree of freedom systems, is to compute Poincaré surfaces of section (SOS) which provide a more pictorial view of the global structure of phase space. The results presented in Ref. [1] are sufficiently intriguing to warrant examination of Poincaré SOS in the regime where the change in tunneling rate is reported. In their paper Chaudhuri and Ray [1] do not provide the energy range in which they computed Lyapunov exponents, but they do state that their initial conditions were such that

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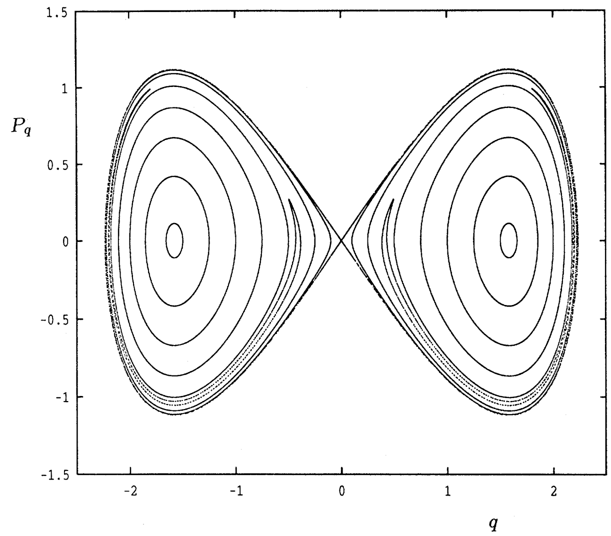

FIG. 1. Composite Poincaré surface of section obtained by integration of several different trajectories for the Hamiltonian (1). The SOS is defined by $x = 0$, $P_x > 0$ and the parameters used were $k = 0.000\,66$ and $E = 0$.

at time $t = 0$, $q = 0.1$, $p_q = 0.0$. Assuming $x = p_x = 0$ this gives an energy, $E = -0.004\,99$, which is rather close to the top of the barrier, and this is precisely the energy range where a chaotic separatrix layer is expected to form. We considered energies in the range $-0.005 < E < 0$ and a typical SOS is shown in Fig. 1. In no case could we locate chaotic motion for the relatively small k values used in Ref. [1]. Chaudhuri and Ray [7] later stated that they chose initial conditions corresponding to an energy $E = 1.119\,91$ which is well above the saddle in the potential. The particular initial condition they cite is completely regular. However, the level of chaos at this energy for $k = 0.000\,66$ is minimal. It is unclear what the relevance is, of chaos at this high energy, to tunneling through the barrier: the lowest lying state in the potential lies *below* the saddle. Further, it is possible to find an equivalent level of chaos for smaller values of k simply by increasing the energy further. This implies that the correlation between the onset of chaos and a change in the tunneling rate is at best ambiguous. The chaotic threshold for $E = 0$ appears to be at $k \approx 0.027$ although widespread chaos does not set in until $k \approx 0.1$ as evidenced by Fig. 2.

Also puzzling are Figs. 1(a)–1(c) in Ref. [1]. These figures supposedly show that "as k increases, the pattern of complexity in the wave form changes very sharply." In fact, Figs. 1(a) and 1(b) of Ref. [1] appear to be identical despite the fact that Fig. 1(b) corresponds to

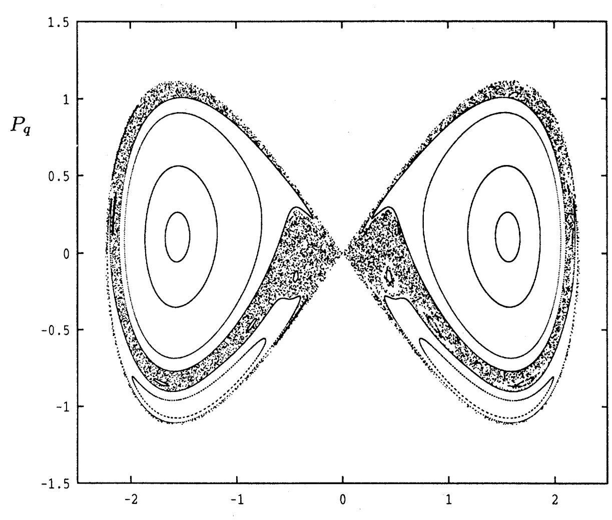

FIG. 2. Same as Fig. 1 but for $k = 0.1$.

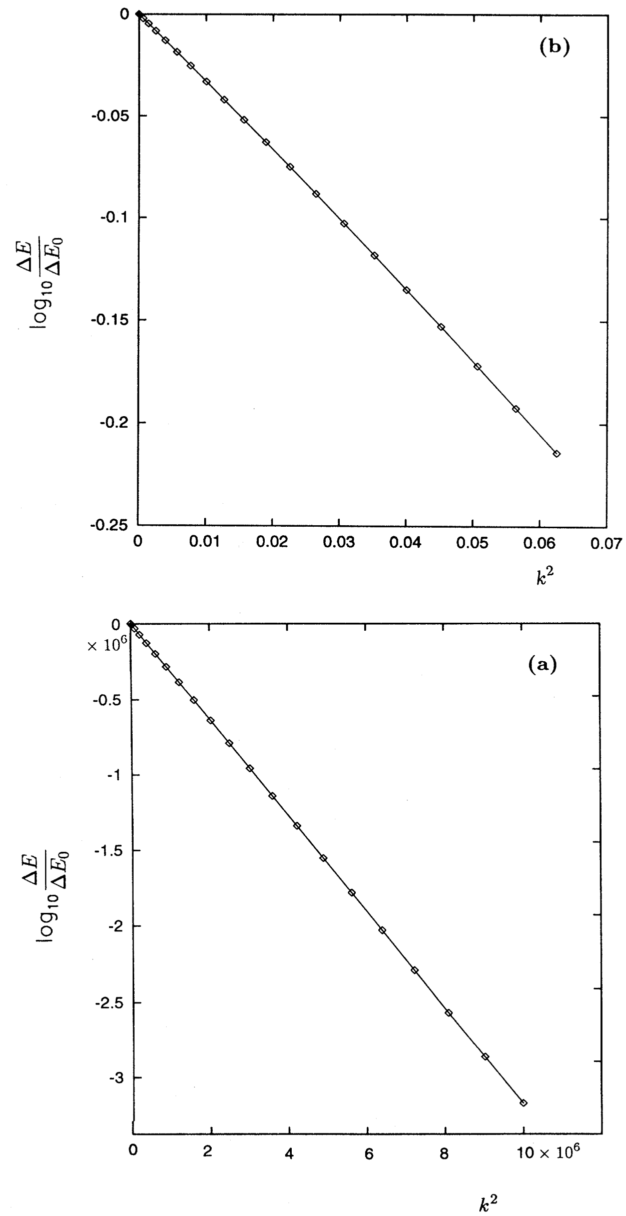

FIG. 3. Tunneling splitting of the ground state (ΔE) versus k^2 over two different ranges of k (see Ref. [4]); (a) contains $k = 0.000\,66$ and (b) contains k values for which widespread chaos occurs. E_0 is the splitting when $k = 0$.

$k = 0.000\,66$, the value at which global chaos is claimed to occur. The wave form in Fig. 1(c) is certainly different from 1(a) and 1(b) but all three figures seem to be quasiperiodic.

The reader might legitimately ask why a significant change in the tunneling rate should occur at $k = 0.000\,66$. To study this issue further, we calculated the ground state splitting of the quantum eigenvalues of H using a basis of 400 harmonic oscillator functions. This basis is adequate to converge the eigenvalues and eigensplittings [4]. The double well potential V_q supports only one pair of states below the barrier top. Tunneling splittings for the lowest energy doublet are shown in Fig. 3 over two ranges of k values; one spanning the value $k = 0.000\,66$ and the other the actual k value for which significant chaos is visible in the SOS. In both cases the splitting decreases sharply as the coupling parameter is increased. This can be explained simply by noting that as k increases the distance between the two minima also increases. Our findings are in excellent qualitative agreement with the results of Makri and Miller [4] and conflict with the statements in Ref. [1] that, (i) the tunneling probability increases with coupling, (ii) the rate of change of the *ground state* tunneling probability changes dramatically in the vicinity of $k = 0.000\,66$, and, (iii) the *ground state* tunneling rate changes significantly as the transition to global classical chaos occurs.

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[1] S. Chaudhuri and D. S. Ray, Phys. Rev. E **47**, 80 (1993).
[2] W. A. Lin and W. E. Ballentine, Phys. Rev. Lett. **65**, 2927 (1990).
[3] D. Farrelly and J. A. Milligan, Phys. Rev. E **47**, R2225 (1993).
[4] N. Makri and W. H. Miller, J. Chem. Phys. **87**, 5781 (1987); **86**, 1451 (1987).
[5] N. Rom, N. Moiseyev, and R. Lefebvre, J. Chem. Phys. **95**, 3562 (1991).
[6] N. Moiseyev, N. Lipkin, D. Farrelly, O. Atabek, and R. Lefebvre, J. Chem. Phys. **91**, 6246 (1990).
[7] S. Chaudhuri and D. S. Ray (private communication).