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# Effects of barrier fluctuation on the tunneling dynamics in the presence of classical chaos in a mixed quantum-classical system

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**Abstract.** We present a numerical investigation of the tunneling dynamics of a particle moving in a bistable potential with fluctuating barrier which is coupled to a non-integrable classical system and study the interplay between classical chaos and barrier fluctuation in the tunneling dynamics. We found that the coupling of the quantum system with the classical subsystem decreases the tunneling rate irrespective of whether the classical subsystem is regular or chaotic and also irrespective of the fact that whether the barrier fluctuates or not. Presence of classical chaos always enhances the tunneling rate constant. The effect of barrier fluctuation on the tunneling rate in a mixed quantum-classical system is to suppress the tunneling rate. In contrast to the case of regular subsystem, the suppression arising due to barrier fluctuation is more visible when the subsystem is chaotic.

**Keywords.** Fluctuating barrier; classical chaos; tunneling dynamics.

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## 1. Introduction

Tunneling through fluctuating barrier has received considerable attention because of its potential use for modeling in many branches of physics and chemistry [1–24]. These include long-range electron transfer reactions [1,2], escape of an $O_2$ or CO ligand molecule out of a myoglobin pocket [3], ion channel kinetics in the lipid cell membrane [4] and strongly coupled isomerizations [5], to name a few [6–22]. Indeed, environmental effects on rate processes in complex dynamical systems, such as biomolecules, have been the subject of recent past. The emphasis has been on the dynamics of escape over fluctuating barriers that could arise as a result of stochastic reorientations of a bridge unit or stochastically interrupted electronic pathway as in proteins [6]. So, the fluctuating barrier model can act as a good model for proton or H atom transfer dynamics in biomolecules or proteins where the protonic pathway contains a flipping molecular unit. Iwaniszewski studied the problem of tunneling through a randomly fluctuating barrier in the presence of dissipation in the two-level approximation [17–19]. The most important finding of his research is the appearance of a resonant damping of the tunneling in both possible kinds of evolutions coherent and incoherent relaxations. Li *et al* studied the escape over a fluctuating potential barrier in the presence of both white and multiplicative noises [20,21]. They have shown that the mean first passage time over the fluctuating potential barrier displays a resonant activation. Recently, we explored the tunneling through a fluctuating barrier in the presence of a periodically driving field and studied the interplay between the effects of barrier fluctuation and external electromagnetic field [22]. An interesting situation may appear if a quantum system with fluctuating barrier is coupled to a classical system which is either regular or chaotic as determined by the initial conditions. The systems with mixed quantum-classical description have been the subject of considerable interest in recent years [23–35]. The well-known example is the Maxwell–Bloch equations which describe a model two-state system (quantum) interacting with a strong single mode classical electromagnetic field [25,26]. The other example comprises the models involving nuclear collective motion [27], one-dimensional molecule where the motion of an electron is described by an effective potential provided by the nuclei and other electrons within adiabatic approximation scheme [28]. In the past few years many conjectures have been put forward and tested in various model systems in order to answer the fundamental question: What is the signature of classical chaos in the quantum world? Among these, one of the most intriguing is the idea that classical chaos can induce large scale fluctuations in a genuine quantum phenomenon such as the tunneling process. The tunneling fluctuation is usually interpreted in terms of a process known as chaos assisted tunneling (CAT) [29–36]. From a quantum point of view, the presence of regular and chaotic motion in the classical phase space corresponds to the possibility of having two kinds of states: Regular one localized inside the symmetric tori and chaotic states, being extended through the chaotic region, display a non-negligible overlap with regular regions. The fluctuations in the tunneling rate are thus explained in terms of a three-state tunneling process. The quantum particle first tunnels from the localized state to an extended chaotic one and then from this to the state located in the symmetric torus. The objective of the present paper is to study the effect of classical subsystem or more importantly the effect of classical chaos on the tunneling behaviour of the quantum system when the barrier of the system fluctuates with time. We would like to investigate how the chaos assisted tunneling is further modified due to barrier fluctuation of the quantum system.

## 2. The model and the method

Let the microscopic system be described by a one-dimensional bistable potential. Thus, the Hamiltonian of the quantum system $\hat{H}_q$ of our study is

$$\hat{H}_q = \frac{\hat{p}_q^2}{2m} + \frac{1}{2}\hat{x}_q^2 + K_0 \mathrm{e}^{-x^2}, \tag{1}$$

where $\hat{x}_q$ and $\hat{p}_q$ are the position and momentum operators corresponding to position and momentum of the particle respectively. The barrier height of the potential is represented by $K_0$. For the present study we have chosen to work with $K = 9.0$ atomic unit (a.u.). Now the barrier fluctuations are modeled by assuming the parameter $K_0$ in $H_q$ to fluctuate with time according to

$$K_t = K_0[1 + \Delta K R(t)] \tag{2}$$

with $R(t)$ being random numbers of magnitude between $-1$ and $+1$ generated at preselected discrete time steps. The random numbers here correspond to white noise with zero mean. The size of the time steps then determines what we call the barrier fluctuation frequency and $\Delta K$ is the fluctuation strength.

The Hamiltonian which governs the motion of a classical subsystem with mass $M$ and characterised by its position, $x_{\mathrm{cl}}$ and momentum variable $p_{\mathrm{cl}}$ in a double-well potential driven by an external field with frequency $\omega$ is given by

$$H_{\mathrm{cl}} = \frac{p_{\mathrm{cl}}^2}{2M} + Ax_{\mathrm{cl}}^4 - Bx_{\mathrm{cl}}^2 + Gx_{\mathrm{cl}} \cos(\omega t). \tag{3}$$

The values of the parameters of the double-well oscillator $A$ and $B$ are taken as 0.5 and 10.0 respectively. The effect of coupling of the external field to the oscillator is given by the coupling strength $G$ which has the value 10.0 for the present study and the frequency of the driving field $\omega$ has taken the value 6.07. The classical Hamiltonian $H_{\mathrm{cl}}$ is non-integrable and has been widely used by several workers in a variety of situations related to classical and quantum chaos.

The Hamilton's equations corresponding to $H_{\mathrm{cl}}$

$$\frac{\partial H_{\mathrm{cl}}}{\partial p_{\mathrm{cl}}} = \dot{q}_{\mathrm{cl}}$$
$$\frac{\partial H_{\mathrm{cl}}}{\partial q_{\mathrm{cl}}} = -\dot{p}_{\mathrm{cl}} \tag{4}$$

are numerically integrated to obtain the values of $x_{\mathrm{cl}}$ for given initial values of $x_{\mathrm{cl}}$ and $p_{\mathrm{cl}}$.

The total Hamiltonian describing the mixed quantum-classical system is now made complete by considering the coupling of classical and quantum degrees of freedom in terms of the interaction potential $\hat{H}_{q\text{-cl}}(=\lambda x_{\mathrm{cl}}\hat{x}_q)$ so that we have

$$\hat{H} = \hat{H}_q + \hat{H}_{\mathrm{cl}} + \lambda x_{\mathrm{cl}}\hat{x}_q. \tag{5}$$

Here, $\lambda$ is the coupling constant. Since the classical subsystem is coupled to quantum degrees of freedom, it is also necessary to specify the initial conditions for the classical variables. We have chosen the initial conditions for $x_{\mathrm{cl}}$ and $p_{\mathrm{cl}}$, for the regular and chaotic trajectories as $x_{\mathrm{cl}} = -2.0$ for regular and $x_{cl} = -3.5$ for chaotic trajectories, $p_{\mathrm{cl}}$ being chosen to be zero always [31]. The $x_{\mathrm{cl}}$ obtained by solving the corresponding Hamilton's equation are used in the Schrödinger equation. The relevant time-dependent Schrödinger equation is solved by invoking the time-dependent Fourier grid Hamiltonian method [37,38].

The time-dependent Schrödinger equation (TDSE) describing our system can be written down as

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}|\Psi(x,t)\rangle &= H(x,t)|\Psi(x,t)\rangle \\ &= \left[\frac{\hat{p}_q^2}{2m}+\frac{1}{2}\hat{x}_q^2+[K_0+\Delta K K_0 R(t)]\mathrm{e}^{-x^2}+\lambda x_{\mathrm{cl}}x_q\right]\Psi(x,t) \\ &= [H_0+V'(x,t)]\,\Psi(x,t), \end{aligned} \tag{6}$$

where $H_0$ is the Hamiltonian representing the double-well oscillator, i.e. in our problem it is $H_q$ (eq. (1)). The perturbation potential $V'(x,t)$ in our problem is $\Delta K K_0 R(t)\mathrm{e}^{-x^2}+\lambda x_{\mathrm{cl}}x_q$. We employ the time-independent Fourier grid Hamiltonian (FGH) method [39] to evaluate the eigenfunctions and eigenvalues of the unperturbed Hamiltonian ($H_0$), giving

$$H_0|\phi_i^0(x)\rangle = E_i^0|\phi_i^0(x)\rangle, \qquad i=1,2,...,N, \tag{7}$$

where $N$ is the number of grid points used for representing $|\phi_i^0\rangle$ in the coordinate space,

$$|\phi_i^0\rangle = \sum_{p=1}^{N}|x_p\rangle\Delta x w_{pi}^0. \tag{8}$$

The quantities $w_{pi}^0$'s in eq. (8) represent the values of the coordinate representative of the state function $|\phi_i^0\rangle$ at the grid points, the values of which are obtained by standard variational recipe. The FGH method as shown by Adhikari *et al* [37,38], can be used to propagate the wave function on the same grid. Thus when the perturbation $V'$ is switched on, the state function $\Psi(x,t)$ is given by

$$|\Psi(x,t)\rangle = \sum_{q=1}^{n} w_q(t)|x_q\rangle\Delta x \tag{9}$$

with $\langle x_p|x_q\rangle\Delta x{=}\delta_{pq}$, $w_q(t) = \Psi(x_q,t)$. The use of the Dirac–Frenkel time-dependent variational principle

$$\delta\left\{\langle\Psi(x,t)|H-i\frac{\partial}{\partial t}|\Psi(x,t)\rangle\right\}=0, \tag{10}$$

then leads directly to the evolution equation for the grid point amplitudes of $|\Psi(x,t)\rangle$:

$$\dot{w}_q(t) = \frac{1}{i\hbar}\left[\sum_{p=1}^{n}\langle x_q|H|x_p\rangle w_p(t)\right] \tag{11}$$

for $q=1,2,...,n$. These equations are numerically integrated by the sixth order Runge–Kutta method after an initial set of amplitudes $w_p(0)$ are provided.

The initial state for propagation is prepared by the linear combination of two lowest degenerate double-well ($H_q$) eigenstates. Let $\phi_1(x)$ and $\phi_2(x)$ be the two lowest eigenstates of $H_q$ having energy $E$. Because $\phi_1(x)$ has even and $\phi_2(x)$ has odd parity, the linear combinations

$$\phi \pm (x) = \frac{1}{\sqrt{2}}[\phi_1(x) \pm \phi_2(x)] \tag{12}$$

are localized in the right or the left well of the oscillator. We have chosen the wave function which is localized in the left well.

The tunneling probability of finding the system for a given realization (random numbers) of barrier fluctuation within the right well of the bistable potential is then calculated by

$$P_{\rm tun}(t) = \sum_{i=m}^{n} |w_i(t)|^2, \tag{13}$$

where $m$ is the leftmost grid point and $n$ the rightmost grid point of the right well. We then average over several realizations of this tunneling probability. The plot of $\log P_{\rm tun}(t)$ as a function of time gives a straight line, the slope of which determines the tunneling rate constant.

## 3. Results and discussion

In figure 1 we have shown the tunneling probability as a function of time in the absence of barrier fluctuation when the classical subsystem is (a) regular and (b) chaotic for a fixed value of the coupling strength (0.01). Looking closely into figure 1 we see that the tunneling of the quantum particle is largely enhanced when the classical subsystem is chaotic compared to the regular one. This enhancement may be viewed as a characteristic of the chaos-assisted tunneling. The problem of chaos-assisted tunneling has been a topic of interest for various researchers over many years. Bohigas *et al* [30] studied the two-dimensional autonomous model system and observed that energy splitting in this case can be increased to a great extent with the chaos of the intervening chaotic layer. Using a driven

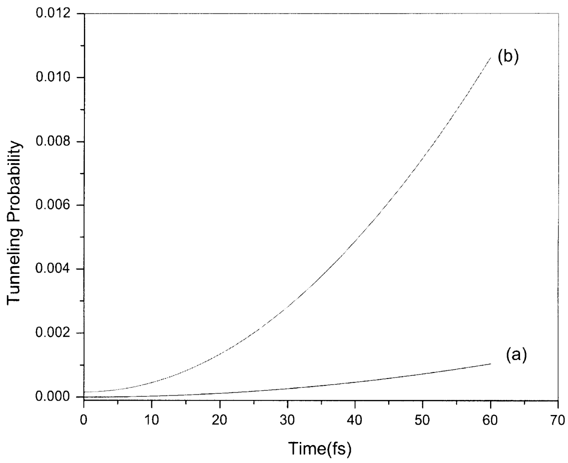


**Figure 1.** The tunneling probability vs. time plot (a) when the classical subsystem is regular and (b) when it is chaotic (coupling strength=0.01).

double-well oscillator model, Lin *et al* [31] showed that the tunneling rate is enhanced by orders of magnitude over that of the undriven system as the separating phase-space layer grows more chaotic with increasing driving strength. Utermann *et al* [32] investigated the same system and pointed out the role of classical chaotic diffusion as a mediator for barrier tunneling. Ashkenazy *et al* [33] investigated the decay process from a time-dependent potential well in the semiclassical regime. The classical dynamics is chaotic and the decay rate shows the irregular behaviour as a function of the system parameters. Chattaraj *et al* [34] studied the quantum domain behaviour of a classical double-well oscillator which exhibits chaos in the presence of an external monochromatic field. They have demonstrated that the classical chaos enhances the quantum fluctuations while quantum nonclassical effects suppress the classical chaos. The enhancement of the tunneling probability by classical chaos in the present model of mixed quantum-classical description can be understood in the light of the classical chaotic diffusion. As the wave packet evolves through the barrier its mean motion, by virtue of the coupling of the bistable potential with classical subsystem, is affected by chaotic diffusion of the subsystem. The chaotic diffusion in turn reduces the decoherence set by classical subsystem thereby increases the tunneling probability.

The role of barrier fluctuation is quite intriguing since one is concerned here with three interplaying aspects of the evolution, namely, tunneling, classical chaos and barrier fluctuation. In figure 2 we have shown the tunneling rate constant as a function of the coupling strength when the classical subsystem is regular. The curve (a) gives variation of the rate constant in the presence of barrier fluctuation while the curve (b) represents the variation of the same in the absence of barrier fluctuation. Similar results are shown in figure 3, when the classical subsystem is chaotic. From the curves in figures 2 and 3 it is clear that the tunneling rate constant decreases with the increase of coupling strength and this behaviour of tunneling rate constant is independent of whether the classical subsystem is regular or chaotic. The decrease in tunneling rate constant with increasing coupling strength arises due to decoherence induced by the classical subsystem. Decoherence is a process enforced by the interaction between a quantum system and its environment. From both figures 2 and 3 it is seen that the tunneling rate constant in the presence of barrier fluctuation has lower values compared to static barrier case. So the presence of barrier fluctuation suppresses the tunneling. The mechanism of suppression of tunneling rate by barrier fluctuation can be understood in the following way. Tunneling is extremely sensitive to any disruption of coherence as it occurs due to the unavoidable coupling to the environment. The presence of barrier fluctuation therefore further reduces the quantum coherence and this is just one example of the general rule that decoherence tends to restore classical behaviour and also quantum suppression of classical chaos. As a consequence, in the presence of barrier fluctuation, decoherence becomes far more effective and accordingly suppresses the tunneling. From figures 2 and 3 we see that the effect of barrier fluctuation becomes more dominant when the classical subsystem is chaotic. In the chaotic case, the presence of barrier fluctuation results in quantum suppression of classical chaos and so reduces the chaotic diffusion which is basically the reason for enhanced tunneling in the presence of classical chaos and hence decreases the tunneling rate constant to a greater extent compared to classical regular case.

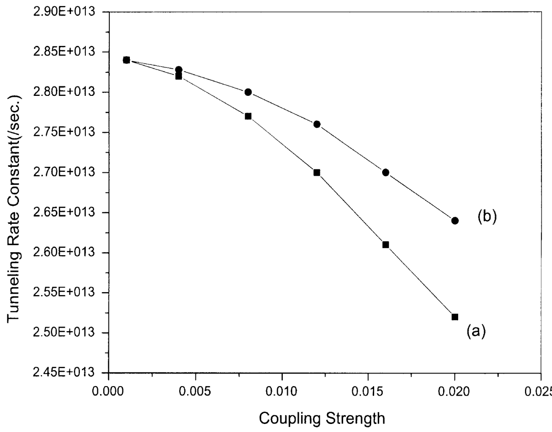


**Figure 2.** The tunneling rate constant as a function of coupling strength when the classical sub-system is regular (a) for fluctuating barrier (fluctuation strength = 0.4 and fluctuation frequency = 5.0E16 cycles/s) and (b) for static barrier.

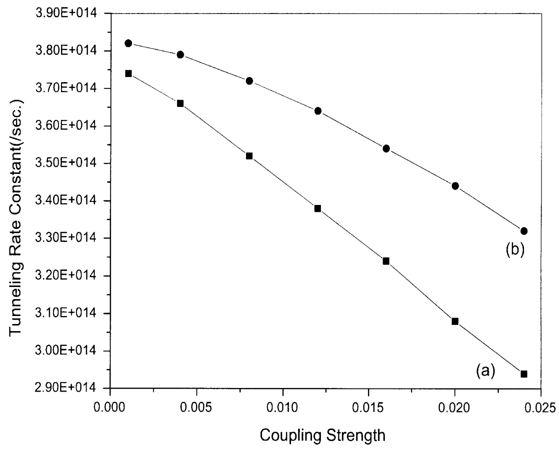


**Figure 3.** The tunneling rate constant as a function of coupling strength when the classical subsystem is chaotic (a) for fluctuating barrier (fluctuation strength = 0.4 and fluctuation frequency = 5.0E16 cycles/s) and (b) for static barrier.

In figure 4 we have plotted the tunneling rate constant as a function of frequency of barrier fluctuation when the classical subsystem is regular. We have plotted the same in figure 5 when the subsystem is chaotic. In drawing these curves, the values of the coupling strength and barrier fluctuation strength were kept constant (parameters are in the figure captions). These figures clearly show that the tunneling rate constant first increases with the frequency of barrier fluctuation, reaches a maximum and then decreases. Both the figures exhibit similar behaviour although the magnitudes of the rate constant are relatively higher for the chaotic case. The other interesting observation is that the maxima appear at the same

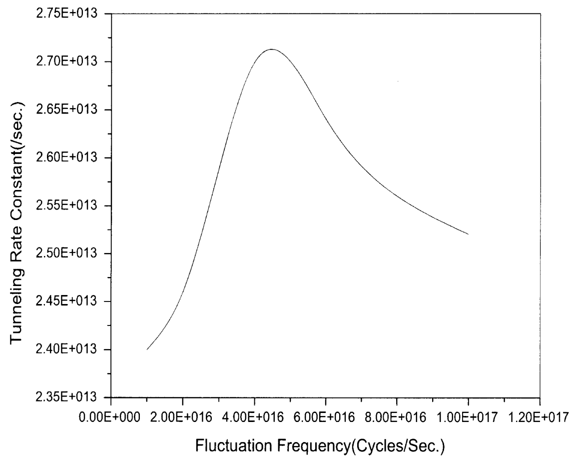


**Figure 4.** The tunneling rate constant as a function of fluctuation frequency for fixed values of barrier fluctuation strength (0.4) and coupling strength (0.01) for a classical regular subsystem.

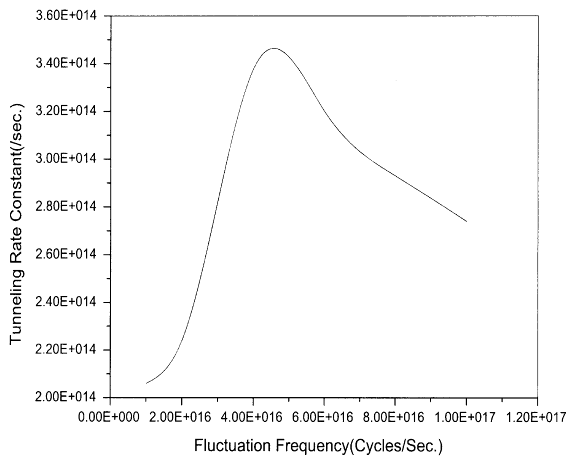


**Figure 5.** The tunneling rate constant as a function of fluctuation frequency for a fixed value of barrier fluctuation strength (0.4) and fixed coupling strength (0.01) for a classical chaotic subsystem.

value of fluctuation frequency independently of whether the classical subsystem is regular or chaotic. This observation is in contrast with our earlier observation on the tunneling of a quantum particle through a fluctuating barrier in the presence of deterministic periodic driving [22]. In the presence of periodic driving the tunneling rate constant when regarded as a function of barrier fluctuation frequency passes through a well-defined minimum. The appearance of the maximum in the present mixed quantum-classical system can be explained qualitatively in the following way. When the fluctuation frequency is small, the tunneling rate constant has low value corresponding to that for bare quantum system. As the fluctuation frequency

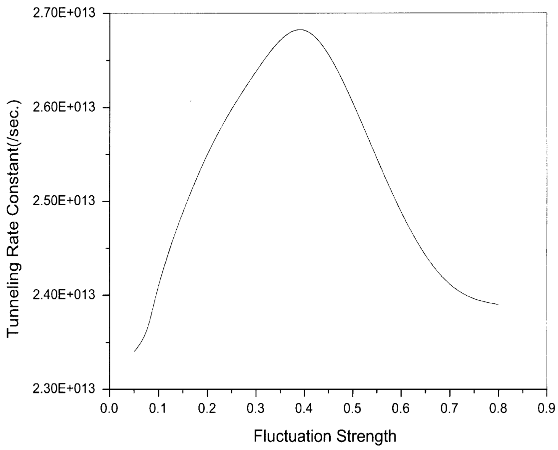


**Figure 6.** The tunneling rate constant as a function of fluctuation strength for fixed values of barrier fluctuation frequency (5.0E16 cycles/s) and coupling strength (0.01) for a classical regular subsystem.

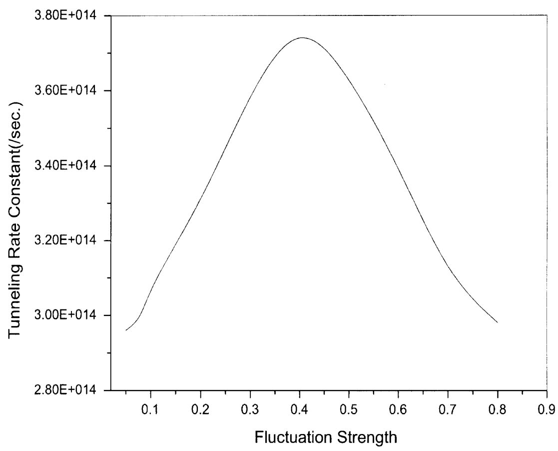


**Figure 7.** The tunneling rate constant as a function of fluctuation strength for fixed values of barrier fluctuation frequency (5.0E16 cycles/s) and coupling strength (0.01) for a classical chaotic subsystem.

increases the population starts oscillating with time such that tunneling could also takes place from the excited states. This increases the tunneling rate constant. But after a certain value of fluctuation frequency, dephasing of population transfer sets in. The dephasing reduces the coherent population transfer from one well to the other and the tunneling rate constant decreases.

In our earlier studies on the tunneling dynamics through a fluctuating barrier in the presence of periodic driving we observed a decrease in the tunneling rate constant with the increase in the fluctuation strength [22]. The decrease in the tunneling rate was attributed to the phenomenon of dephasing of coherent population transfer. Figures 6 and 7 display the tunneling rate constant as a function of barrier fluctuation strength for fixed values of barrier fluctuation frequency and coupling strength for regular and chaotic subsystems respectively. Here we see that as in figure 4, the tunneling rate constant first increases, passes through a maximum and then decreases. As the fluctuation strength increases at a fixed value of fluctuation frequency, the population get excited and tunneling from the excited state causes the increase in tunneling rate constant. But at still higher values of fluctuation strength the intra-doublet transition (i.e. the population transfer among the several doublets within the same well; in our case this is the left well) increases through population oscillation. The superposed state is such that the system remains confined within the well for a considerable amount of time. Consequently, one can expect a decrease in the tunneling rate constant after a certain value of fluctuation strength. In this context we may compare our results with that of Lin and Ballentine [31]. They have computed the Husimi distribution for a particle in a double-well potential and an oscillatory driving force. The extended phase space of the classical system contains two disjoint stable tubes of regular orbits embedded in a chaotic sea. For the corresponding quantum system they have observed coherent oscillatory tunneling between these stable tubes and the tunneling rate is many orders of magnitude higher than the rate of ordinary undriven tunneling. We have also observed enhancement of tunneling rate in our mixed quantum-classical model when the classical subsystem is chaotic compared to classical regular subsystem. In the present model we have also considered the fluctuation of the barrier height in the double-well potential. The tunneling rate here also orders of magnitude greater for the classical chaotic subsystem than regular classical subsystem.

## 4. Conclusion

In the present study we have considered the tunneling of a quantum particle in a bistable potential which in turn is coupled to a non-integrable classical system. Because of non-integrability, the classical subsystem admits chaotic behaviour. By introducing time-dependent barrier height, one realizes a mechanism of barrier fluctuation in the quantum dynamics. We studied the interplay of classical chaos, barrier fluctuation in the tunneling of a quantum particle and found that when a quantum system is coupled to a classical subsystem, the tunneling rate is always lower than that of the coupling-free case. The lowering observed does not depend on whether the classical subsystem is regular or chaotic. This lowering in tunneling rate constant is due to the decoherence induced because of the interaction of the quantum system with the classical subsystem. The presence of chaos always enhances the tunneling rate constant. The effects of barrier fluctuation on the tunneling in our mixed quantum-classical system result in the suppression of the tunneling rate and the suppression is more pronounced when the classical subsystem is chaotic rather than regular. Barrier fluctuation thus plays a significant role in the evolution of a tunneling process in the presence of classical chaos.

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