FRACTAL DIMENSIONS IN TUNNELING PROCESSES AND EFFECTS OF ENVIRONMENTAL FLUCTUATIONS

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Abstract

We study electron tunneling between two infinite potential square wells connected via an opaque barrier and find that time evolution of the probability of the presence of a Gaussian wave packet, localized initially in one of the wells, shares the fractal behavior of tunneling in a quartic potential, discovered by Dekker (H. Dekker, Phys. Rev. A35, 1825 (1987). However, the fractal dimensions are found to be closer to those of a conventional Weierstrass function than those appropriate to the quasi-Weierstrass behavior of Dekker. It is argued that the usual exponential decay predicted by conventional relaxation processes can be recovered only as an effect of thermal fluctuations.

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1. INTRODUCTION

In the last few years there has been an increasing interest in what is now called chaos assisted tunneling. The subject of chaos assisted tunneling, pioneered by Davis and Heller\textsuperscript{1} is now becoming so popular that it has been widely discussed in some of the most recent review papers on the subject of semiclassical quantization. We refer the reader especially to Ref. 2, a review paper which also explains the reasons for the increasing interest in the field of chaos assisted tunneling. It is expected that the technology in the field of condensed matter might soon offer a unique opportunity to observe non-conventional tunneling properties experimentally. The rapid developments in the field of heterostructures,\textsuperscript{3} for instance, in addition to the attraction of the new technological perspectives, might also offer such an opportunity.

The attention of the researchers is mainly concentrated on the tunneling processes of those dynamical systems which, in the classical limit, would be characterized by deterministic chaos. Thus, the related calculations mainly concern the so called tunneling doublet.\textsuperscript{4} However, from both an experimental and a technological viewpoint the problem to solve is that of the transmission of a wavepacket, and this is equivalent to studying the joint motion of infinitely many independent doublets. Let us consider a double-well potential, with no external perturbation producing chaos in the classical limit. Let us place in the left well a Gaussian wavepacket. This will split into infinitely many tunneling doublets and, as originally observed by Dekker,\textsuperscript{5} the resulting time evolution of the population of the left well is expected to result in a Mandelbrot-Weierstrass process. More recently, without realizing the connections with the original findings of Dekker, similar results have been found by Pattanyak and Schieve\textsuperscript{6} and Ashkenazy et al.\textsuperscript{7}

Since the transmission of a wavepacket, as earlier noticed, always involves the joint motion of infinitely many tunneling doublets, this kind of chaos, with no classical counterpart is certainly a property of technological, as well as theoretical, interest. However, if an experimental perspective is adopted, a further effect has to be considered to get a physical picture which can be considered to be a fair representation of reality. As repeatedly stated by Zurek,\textsuperscript{8} no isolated systems exist in nature, and, even in the case of an extremely weak interaction with the environment, the quantum mechanical coherence of a given quantum mechanical system can be quickly destroyed by the dephasing process associated with these weak interactions. Thus, in this paper, in addition to developing a theoretical picture, which is slightly different from the original work of Dekker and leads to fractal dimensions closer to those of a conventional Weierstrass function\textsuperscript{9} than to the quasi-Wieierstrass behavior of Dekker, we address the crucial issue of the role that the environmental fluctuations have on processes of this kind. In particular, we describe our findings on some aspects of electron tunneling which might have considerable relevance to some issues in the current literature.\textsuperscript{10-18} We believe that these neglected properties might be of importance to recent experiments on the time development of wave packets in real space in atoms, molecules\textsuperscript{19} and solids, as well as to some recent model calculations.\textsuperscript{20}

2. FRACTAL TUNNELING

We adopt the model illustrated in Fig. 1 and assume that the initial condition on the electron is given by a Gaussian wave packet of width $\sigma$ located in the middle the left-hand side well of the double-well potential, i.e., that the initial wave function is given by

$$\Psi(x, 0) = \frac{1}{(\pi \sigma^2)^{1/4}} \exp \left[ - \frac{(x - x_0)^2}{2 \sigma^2} \right]$$  \hspace{1cm} (1)

We get the probability of the electron in the left-hand well to be given by

$$P_L(t) = \frac{1}{2} \sum_{m=1}^{N} |\alpha_m|^2 \left[ 1 - \cos \left( \frac{2 \Delta E_m t}{\hbar} \right) \right],$$  \hspace{1cm} (2.1)

where

$$P_L(t) = \int_0^L |\Psi(x, t)|^2 dx,$$

$$\alpha_m = \sqrt{\frac{2}{L}} \int_0^L \Psi(x, 0) \sin \left( \frac{m \pi x}{L} \right) dx,$$  \hspace{1cm} (2.2)

$L$ being the width of either well and $X_o = 0.5L$. The upper limit $N$ of the summation in Eq. (2.1) denotes the number of states lying below the barrier in either well. It is given by the integer part of $\xi$ defined as,

$$\xi = \frac{L}{\pi} \sqrt{\frac{2MV_0}{\hbar^2}},$$  \hspace{1cm} (2.3)
where $V_0$ is the height of the barrier (see Fig. 1). It is helpful to notice that, if we define $E_0 = \frac{\hbar^2 \pi^2}{2M^2}$ as the ground state energy of a particle of mass $M$ moving in a single infinite potential square well of width $L$, Eq. (2.3) can be rewritten simply as

$$\xi = \sqrt{\frac{V_0}{E_0}}.$$  \hspace{1cm} (2.4)

To facilitate further calculations, we now make two simplifying assumptions: we take the width of the initial wave packet to be much smaller than the width of the well i.e., $\sigma/L \ll 1$, and we assume that the energy of the packet is small with respect to the height of the separating barrier, i.e. $N_{\max}^2 \ll \xi^2 - (L/\pi b)^2$. Equation (2.1) shows that the motion of the electron consists of a superposition of well-defined oscillations between the two wells. In light of the above two assumptions, the frequencies of oscillation are $2\Delta E_m/h$ where $\Delta E_m$ is given by

$$\Delta E_m \cong \frac{8}{\pi} E_0 \frac{m^2}{\sqrt{\xi^2 - m^2}} \exp \left(-\pi \frac{b}{L} \sqrt{\xi^2 - m^2} \right),$$

(3)

$b$ being the width of the barrier separating the two wells. The oscillation amplitudes $|a_m|^2$ in (2.1) are

$$|a_m^2| \cong \left(2\pi \sigma^2 \sqrt{\frac{\sigma^2}{L}} \sin^2 \left(\frac{m\pi}{2}\right) \right) \times \exp \left(-\frac{1}{2} \left(\frac{\pi \sigma}{L}\right)^2 m^2 \right)$$

where $\sigma$ is the width of the initial wave packet. The structure of Eq. (2.1) is the same as that of conventional relaxation processes, as for instance, in the well-known model of Friedrichs for the decay of excited quantum states via spontaneous emission of radiation. According to conventional wisdom, one would expect that Eq. (2) results in an irreversible process characterized by a predominant exponential decay plus weak corrections to it, and that the deviations from exponential behavior can be made arbitrarily weak by increasing the time-scale separation between the decay process and the underlying microscopic dynamics. Advances have been made recently to derive a rigorous expression for the rate of the exponential relaxation process in the continuum limit as $N$ tends to infinity.

The result [Eq. (2.1)] for the probability of finding the electron in the initially occupied well is plotted in Fig. 2. We see that the actual behavior of $P_L(t)$ is remarkably different from the conventional expectation discussed above. An exponential relaxation still exists. However, the fast exponential-like relaxation is followed by strong and highly erratic fluctuations around the supposed equilibrium value of $P_L(t) = 1/2$. We "prove" below that this erratic behavior is a Weierstrass process, which can be thought of as the square well counterpart of the fractal discovered by Dekker in the case of a quartic potential.

Actually, the chaos-like behavior of Fig. 2 is related to a conventional Weierstrass-Mandelbrot (WM) function rather than the quasi-WM function of Dekker. Indeed, focusing our attention on the low-m levels, which dominate the time evolution of $P_L(t)$, and adopting an approximation at the first order in $(m/\xi)^2$ and $\xi \gg m$, $\xi \geq m^2$ we get

$$P_L(t) \cong \left(\pi \sigma^2 \sqrt{\frac{\sigma^2}{L}} \right) \sum_{m=1}^{N} \sin^2 \left(\frac{m\pi}{2}\right) \times \frac{1}{\delta m^2} \left[1 + \cos(\gamma m^2 \Omega t)\right],$$

(5)
where

\[ \gamma \equiv \exp \left( \frac{b}{L \xi} \right) , \]

\[ \delta \equiv \exp \left\{ \frac{1}{2} \left( \frac{\delta}{L} \right)^2 \right\} , \tag{6} \]

\[ \Omega \equiv \frac{16}{\pi} \frac{E_0}{\hbar} \exp \left( -\pi \frac{b}{L \xi} \right) , \]

By contrast, the quartic potential\(^2\) would lead to [Eq. (2.1)] with

\[ |\alpha_m|^2 = \frac{(2m)! (\tanh R)^{2m}}{(m!)^2 \cosh(R)} , \quad m = 0, 1, 2, \ldots \tag{7} \]

\[ \Delta E_m = \frac{\beta^{2m}}{(2m)!} , \quad \beta = V_0/\hbar \omega_0 , \tag{8} \]

where \( R = \log(\sigma) , V_0 \) is the height of the potential and \( \omega_0 \) is the level spacing of the simple harmonic oscillator.

We noticed that a replacement of \( m^2 \) by \( m \) in our square well formula [Eq. (5)] results in the conventional WM function\(^9,24\) This led us to carry out computer simulations to explore numerically the fractal dimension of our process. We found that they are at least close to those of a conventional WM function. This computational “proof” proceeds as follows. The result [Eq. (2.1)] plotted in Fig. 2 is replotted in Fig. 3 by zooming into the figure by four orders of magnitude. The fractal character of the function is clarified by this procedure. To evaluate the fractal dimension, we apply the standard techniques of Ref. 24. The result of this calculation is illustrated in Fig. 4, in the case where \( \gamma = 3.2 , \delta = 1.2 \) with an upper bound \( m = 3 \). In this case we find the fractal dimension is \( D = 1 + \alpha = 1.3 \). This is extremely close to the conventional WM dimension, \( \alpha \) being the slope of the log-log plot, calculated by the least squares method.
3. ENVIRONMENTAL FLUCTUATIONS

According to the relaxation theory of Ref. 21, deviations from the exponential behavior are admitted, and they turn out to be fast but regular oscillations with amplitude proportional to the inverse of time. Furthermore, this amplitude can be made arbitrarily small by increasing the time-scale separation between system and bath. In the present case, on the contrary, the deviations from the exponential decay are characterized by a chaos-like behavior and are not damped. Nevertheless, we
Fig. 4  Comparison of the fractal dimensions (a) of the conventional WM function, (b) Dekkers quasi-WM function and (c) our present result.

Fig. 5  Temperature effects produced by fluctuations of the barrier width. The dotted line shows the prediction of Eq. (6) with $\Gamma = 0.1$ and $\langle \sigma^2 \rangle = 0.1$. The solid line is the zero-temperature behavior of Eq. (2).
believe that the predictions of the traditional relaxation theories can be recovered and a collapse into the exponential regime can be triggered by the interactions with the environment (thermal fluctuations). The study of the effects of thermal fluctuations can be easily carried out by remarking that the model we adopt corresponds to studying the dynamics of a collection of N two-level systems not interacting with one another. Then the problem becomes equivalent to that of the fluctuating density matrix studied in Ref. 25. The theoretical approach of Ref. 25 is strongly simplified by making the assumption that the thermal fluctuations are independent of the state of the system. We represent the case where thermal fluctuations influence the width b of the barrier of Fig. 1 by assuming that

\[ b(t) = b_0 + \varepsilon(t), \]  

where \( \varepsilon(t) \) is a Gaussian noise with vanishing mean value. We obtain

\[ P_L(t) = \frac{1}{2} \sum_{m=1}^{N} |\alpha_m|^2 \times \left[ 1 + \exp(-\Gamma_m t) \cos \left( \frac{2\Delta E_m t}{\hbar} \right) \right] \]  

where

\[ \Gamma_m = 16 \frac{E_0^2}{r^2} \frac{\langle \varepsilon^2 \rangle}{\Gamma} \frac{m^4}{\pi} \exp \left[ -2\pi \frac{b_0}{r} \sqrt{\langle \varepsilon^2 \rangle - m^2} \right] \]  

where \( \langle \varepsilon^2 \rangle \) is proportional to the temperature \( T \) and \( 1/\Gamma \) is the correlation of the noise. The result of Eq. (10) is plotted in Fig. 5. In the special case where the interaction with the environment makes the bottom of the two wells undergo independent fluctuations, it can be shown easily that a formula like that of Eq. (10) can be derived with the further simple feature that the damping factor is independent of \( m \). It is evident that, even in this case, the increase of temperature fluctuations leads to the same behavior as that illustrated in Fig. 5, viz., the cancellation of the chaos-like deviations from the exponential behavior.

4. CONCLUSIONS

We thus find that, the tunneling of Gaussian wave packets exhibits significant deviations from the predictions of standard relaxation theories. The explanation for this interesting occurrence may be given basically using the findings of Dekker. The physics of tunneling through a square well barrier, analyzed by us here, does not differ substantially from that within the quartic potential investigated by Dekker. In other words, the “fractal” deviation from an exponential relaxation seems to be a general property of tunneling processes, regardless of the detailed nature of the potential used. The additional and remarkable component of our findings is that the square well produces fractal dimensions closer to the fractal dimension of the conventional WM function. The special relation between amplitude of oscillation and frequency of oscillation necessary to produce the Weiherstrass behavior is lost when the interaction with the environment makes the oscillation frequencies become random functions of time (an effect of thermal fluctuations). The theory of Ref. 25 shows that, as an effect of such interaction, the single harmonic oscillations are damped and this, in turn, upon increase of temperature, destroys the Weiherstrass behavior completely, making valid again the predictions of standard relaxation theories. The key mechanisms responsible for the exponential nature of the experimental signals (or, equivalently, for the collapse into the so-called subdynamics\textsuperscript{12} state) are not yet understood clearly.\textsuperscript{21} From the results of this note we are led to believe that thermal fluctuations seem to play a predominant role on this crucial “exponentialization” process. This might be of importance to an experimental investigation on the Weiherstrass nature of tunneling processes, as a warning to keep under control the effects of thermal fluctuations.

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