Decay of a quantum discrete state resonantly coupled to a quasi-continuum set of states

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The irreversible exponential decay from a discrete state to the continuum, described by time-dependent perturbation theory, is a difficult task in quantum mechanics learning, because of the complexity of the mathematical tools involved. An easy model which consists in analyzing the decay from a discrete state to a quasi-continuum set of states is developed. The mathematics required to understand the model are easy, allowing for a deep analysis of the model. The physical conditions required to describe the transition produced by a sinusoidal perturbation by an exponential decay are easily deduced.

Keywords: Exponential decay; time-dependent perturbation theory; Zeno quantum effect.

La comprensión del decaimiento exponencial irreversible desde un estado discreto a un continuo de estados, descrito mediante la teoría de perturbaciones dependiente del tiempo, es una tarea difícil dentro del aprendizaje de la teoría cuántica, debido a la complejidad de las matemáticas utilizadas. En este trabajo se desarrolla un modelo sencillo, que consiste en analizar el decaimiento desde un estado discreto a un conjunto cuasi-continuo de estados. Las matemáticas requeridas para comprender el modelo son sencillas, lo que permite un análisis profundo del modelo. Las condiciones físicas que se deben verificar para poder describir una transición producida por una perturbación sinusoidal mediante un decaimiento exponencial, se deducen de forma sencilla.

Descriptores: Decaimiento exponencial; teoría de perturbaciones dependiente del tiempo; efecto Zenón cuántico.

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1. Introduction

Nowadays, there is a pedagogical interest in analyzing the difficulties in understanding the concepts of quantum mechanics [1, 2]. There are a lot of physical processes in which a decay from a discrete quantum state to a continuum, induced by a sinusoidal perturbation, takes place, such as: ionizations induced by an electromagnetic wave, photoelectric effect, etc. [3,4]. The probability of these processes occurring is usually governed, according to the time-dependent perturbation theory, by an irreversible exponential decay [5–7]. In fact, the exponential decay law is quite universal in time dependent quantum systems related to tunneling [8, 10–12], such as in the alpha decay [13, 14]. The understanding and learning of the conditions required to describe this exponential decay at the graduate level is usually a difficult task, since the mathematical tools involved in the demonstrations are complex. In fact, many good textbooks avoid this subject. An easy model which consists in analyzing the decay from a discrete state to a quasi-continuum set of discrete states is developed. Analysis of the model provides a deep understanding of the conditions required to describe a process by using the exponential decay approximation.

2. Hypotheses and equations of the model

Let us consider the following scheme of energy levels: a single state with energy $E = 0$ and $N + 1$ states in an interval of energy ΔE around the value E_f, which constitute the quasi-continuum set of discrete states, their energies being:

$$E_n = E_f - \frac{\Delta E}{2} + \frac{\Delta E}{N}\,(n-1)\,, \qquad n = 1, 2, \cdots N+1. \tag{1}$$

This scheme of energy levels is shown in Fig. 1. We shall consider that $\Delta E \ll E_f$ so that there is no overlapping between the energies of the quasi-continuum and the energy of the ground state.

Let us denote the quantum state corresponding to $E = 0$ as $|0\rangle$ and the corresponding to $E = E_n$ as $|n\rangle$. At the initial time $t = 0$ the system is assumed to be in the state $|\psi(0)\rangle = |0\rangle$, and from this instant a sinusoidal perturbation oscillating at a frequency $\omega = E_f/\hbar$ (so that the initial state

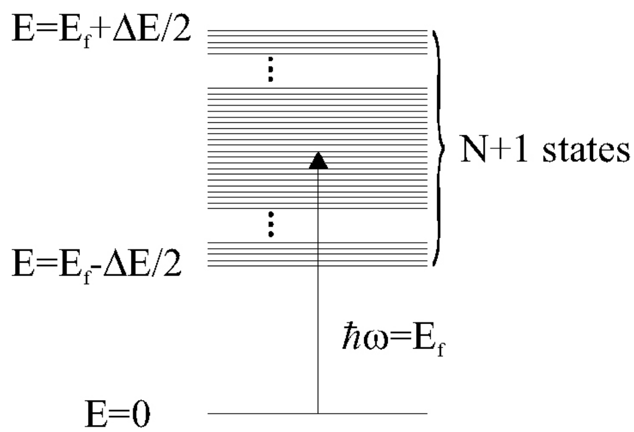

FIGURE 1. Scheme of energy levels.

is resonantly coupled to the quasi-continuum set of states), is applied to the system. Let us consider the perturbation as $\hat{W}(t) = 2\hat{W}\cos\omega t$, $\hat{W}$ being a hermitian operator whose matrix elements are all equal:

$$\langle n|\,\hat{W}\,|m\rangle = W. \tag{2}$$

Therefore, the complete hamiltonian is $\hat{H} = \hat{H}_0 + \hat{W}(t)$, $\hat{H}_0$ being diagonal in the orthonormal basis $\{|n\rangle\}$. The state of the system at time t can be written as follows:

$$|\psi(t)\rangle = b_0(t)\,|0\rangle + \sum_{n=1}^{N+1} e^{-iE_n t/\hbar} f_n(t)\,|n\rangle\,, \tag{3}$$

where $b_0(t) = \langle 0|\psi(t)\rangle$ and $f_n(t) = e^{iE_n t/\hbar}\langle n|\psi(t)\rangle$ The temporal evolution of the coefficients $b_0(t)$ and $f_n(t)$ can be obtained from Schrödinger equation

$$i\hbar\frac{d|\psi(t)\rangle}{dt} = \left[\hat{H}_0 + \hat{W}(t)\right]|\psi(t)\rangle, \tag{4}$$

and yields the following set of equations:

$$\begin{aligned} i\hbar\frac{db_0(t)}{dt} &= b_0(t)W\left(e^{i\omega t} + e^{-i\omega t}\right) \\ &\quad + \sum_{n=1}^{N+1} e^{-iE_n t/\hbar} f_n(t) W\left(e^{i\omega t} + e^{-i\omega t}\right), \end{aligned} \tag{5}$$

$$\begin{aligned} i\hbar\frac{df_n(t)}{dt} &= e^{iE_n t/\hbar} b_0(t)W\left(e^{i\omega t} + e^{-i\omega t}\right) \\ &\quad + \sum_{m=1}^{N+1} e^{i(E_n - E_m)t/\hbar} W\left(e^{i\omega t} + e^{-i\omega t}\right). \end{aligned} \tag{6}$$

If the frequency $\omega = E_f/\hbar$ is large enough (*i.e.* much larger than the inverse of the system evolution time), the secular approximation can be applied and thus we can neglect all the terms containing high frequencies. The low frequencies appearing in the previous equations are $E_n/\hbar - \omega$ and $\omega - E_n/\hbar$, and thus in the secular approximation the set of equations is reduced as:

$$\begin{aligned} i\hbar\frac{db_0(t)}{dt} &= \sum_{n=1}^{N+1} e^{-iE_n t/\hbar} f_n(t) W e^{i\omega t} \\ &= W\sum_{n=1}^{N+1} e^{i(\omega-\omega_n)t} f_n(t), \end{aligned} \tag{7}$$

$$\begin{aligned} i\hbar\frac{df_n(t)}{dt} &= e^{iE_n t/\hbar} b_0(t) W e^{-i\omega t} \\ &= W e^{-i(\omega-\omega_n)t/} b_0(t), \end{aligned} \tag{8}$$

where $\omega_n = E_n/\hbar$. The initial conditions for solving the set of equations are $b_0(0) = 1$ and $f_n(0) = 0$.

Let us obtain an approximate solution to this system of equations. We first integrate the second equation, Eq. (8), including the initial condition:

$$f_n(t) = \frac{1}{i\hbar} W \int_0^t e^{-i(\omega-\omega_n)t'} b_0(t')dt'. \tag{9}$$

Let us introduce this equation into the first equation, Eq. (7):

$$\begin{aligned} \frac{db_0(t)}{dt} &= -\frac{W^2}{\hbar^2}\sum_{n=1}^{N+1} e^{i(\omega-\omega_n)t}\int_0^t e^{-i(\omega-\omega_n)t'} b_0(t')dt' \\ &= -\frac{W^2}{\hbar^2}\sum_{n=1}^{N+1}\int_0^t e^{i(\omega-\omega_n)\left(t-t'\right)} b_0(t')dt'. \end{aligned} \tag{10}$$

This is an integro-differential equation for $b_0(t)$. According to this equation, the temporal evolution of the $b_0(t)$ function at t depends on its whole history, from $t = 0$ to the actual time t. For arbitrary ω values the sum over n will be significant only for $t' \simeq t$. Therefore, a good approximation consists of substituting $b_0(t')$ by $b_0(t)$. By considering this approximation, the last equation yields

$$\frac{db_0(t)}{dt} = -\frac{W^2}{\hbar^2} b_0(t)\sum_{n=1}^{N+1}\int_0^t e^{i(\omega-\omega_n)\left(t-t'\right)}dt'. \tag{11}$$

Let us now consider the change of variable $t - t' = \tau$:

$$\frac{db_0(t)}{dt} = -\frac{W^2}{\hbar^2} b_0(t)\sum_{n=1}^{N+1}\int_0^t e^{i(\omega-\omega_n)\tau}d\tau. \tag{12}$$

We will solve the following sum before integrating:

$$\sum_{n=1}^{N+1} e^{i(\omega-\omega_n)\tau}, \tag{13}$$

where $\hbar\omega_n{=}E_n{=}E_f - \frac{\Delta E}{2} + \frac{\Delta E}{N}\,(n-1)$ and $\hbar\omega{=}E_f$:

$$\begin{aligned} \hbar\left(\omega-\omega_n\right) &= E_f - E_f + \frac{\Delta E}{2} + \frac{\Delta E}{N} - \frac{\Delta E}{N}n \\ &= \frac{\Delta E}{2} + \frac{\Delta E}{N} - \frac{\Delta E}{N}n, \end{aligned}$$

and

$$\begin{aligned} &\sum_{n=1}^{N+1} e^{i(\omega-\omega_n)\tau} \\ &= e^{i\Delta E\tau/2\hbar} e^{i\Delta E\tau/N\hbar}\sum_{n=1}^{N+1} e^{(-i\Delta E\tau/N\hbar)n}. \end{aligned}$$

The last sum is immediate, and yields:

$$\sum_{n=1}^{N+1} e^{i(\omega-\omega_n)\tau} = e^{i\Delta E\tau/2\hbar} e^{i\Delta E\tau/N\hbar} \times \frac{e^{-(N+1)i\Delta E\tau/N\hbar} - 1}{1 - e^{i\Delta E\tau/N\hbar}} = \frac{e^{-i\Delta E\tau/2\hbar} - e^{i\Delta E\tau/2\hbar} e^{i\Delta E\tau/N\hbar}}{1 - e^{i\Delta E\tau/N\hbar}}. \quad (14)$$

Next, we will consider large N values, so that the E_n values constitute something similar to a continuous energy spectrum. In this case we can expand the exponential $e^{i\Delta E\tau/N\hbar}$ in power series and cut the expansion just at the first term:

$$\sum_{n=1}^{N+1} e^{i(\omega-\omega_n)\tau} \simeq \frac{e^{-i\Delta E\tau/2\hbar} - e^{i\Delta E\tau/2\hbar}}{-i\Delta E\tau/N\hbar} = \frac{2N\hbar}{\Delta E\tau}\sin\left(\frac{\Delta E\tau}{2\hbar}\right). \quad (15)$$

Finally, the equation for $b_0(t)$ becomes:

$$\frac{db_0(t)}{dt} = -\frac{W^2}{\hbar^2} b_0(t) \frac{2N\hbar}{\Delta E} \int_0^t \frac{\sin\left(\frac{\Delta E\tau}{2\hbar}\right)}{\tau} d\tau. \quad (16)$$

Let us analyze this equation for short and long periods of time (short-time and long-time approximations). In the short-time approximation, the integral is equal to:

$$\int_0^t \frac{\sin\left(\frac{\Delta E\tau}{2\hbar}\right)}{\tau} d\tau = \frac{\Delta E}{2\hbar} t + \cdots . \quad (17)$$

We can obtain the behavior of the $b_0(t)$ function in the first moments by taking into account that $b_0(t) \simeq 1$, for small t values, and therefore:

$$\frac{db_0(t)}{dt} \simeq -\frac{W^2}{\hbar^2}\frac{2N\hbar}{\Delta E}\frac{\Delta E}{2\hbar} t = -N\frac{W^2}{\hbar^2} t, \quad (18)$$

and

$$b_0(t) \simeq 1 - \frac{N}{2}\frac{W^2}{\hbar^2} t^2. \quad (19)$$

The probability of finding the system in the state $|0\rangle$ in the first moments of the temporal evolution (for small t values) is given by:

$$\mathcal{P}_{00}(t) = |b_0(t)|^2 \simeq \left(1 - \frac{N}{2}\frac{W^2}{\hbar^2} t^2\right)^2 \simeq 1 - N\frac{W^2}{\hbar^2} t^2. \quad (20)$$

Let us see that there is some logic in this result. For a perturbation given by $\hat{W}(t) = 2\hat{W}\cos\omega t$, the transition probability from an initial state i to a final state f is, according to the time-dependent perturbation theory [5]:

$$\mathcal{P}_{if}(t;\omega)_{\omega_{fi}>0} \simeq \frac{4}{\hbar^2}|W_{fi}|^2 \frac{\sin^2[(\omega_{fi}-\omega)t/2]}{(\omega_{fi}-\omega)^2},$$

where W_{fi} is the matrix element of $\hat{W}$ between the two states and ω_{fi} the Bohr frequency. This function (as a function of the frequency) is bell-shaped, with its width equal to $4\pi/t$, and with its center at $\omega = \omega_{fi}$. In the first moments the bell is very wide, and therefore (translating to our case) the system has access to the N states with energies E_n. Therefore, the transition probability for the system to leave the initial state $|0\rangle$ in the first moments (which is equal to $1 - \mathcal{P}_{00}(t)$) is proportional to the number of states to which the system has access. Besides, in the first moments the temporal evolution is very slow since the linear term does not appear in the expansion. This fact is compatible with the Zeno quantum effect [15–17].

Let us see what happens in the long-time approximation. The equation giving us the temporal evolution of $b_0(t)$ is:

$$\frac{db_0(t)}{dt} = -\frac{W^2}{\hbar^2} b_0(t) \frac{2N\hbar}{\Delta E} \int_0^t \frac{\sin\left(\frac{\Delta E\tau}{2\hbar}\right)}{\tau} d\tau. \quad (21)$$

The integral appearing in this equation:

$$\int_0^t \frac{\sin(\Delta E\tau/2\hbar)}{\tau} d\tau,$$

tends to $\pi/2$ for $t \gg 2\hbar/\Delta E$. Therefore, in the long-time approximation we can substitute the integral by $\pi/2$ and the equation for $b_0(t)$ becomes:

$$\frac{db_0(t)}{dt} = -\frac{W^2}{\hbar^2} b_0(t) \pi \frac{N\hbar}{\Delta E} = -\frac{\Gamma}{2} b_0(t),$$

where

$$\Gamma = \frac{2\pi}{\hbar} W^2 \frac{N}{\Delta E}. \quad (22)$$

The solution to this differential equation is:

$$b_0(t) = e^{-\Gamma t/2}, \qquad \text{and} \qquad \mathcal{P}_{00}(\mathrm{t}) = \mathrm{e}^{-\Gamma \mathrm{t}}. \quad (23)$$

Therefore, the probability of finding the system in the initial state $|0\rangle$ shows an exponential decay with time. The typical decay time is:

$$\tau = \frac{1}{\Gamma} = \frac{\hbar}{2\pi}\frac{1}{W^2}\frac{\Delta E}{N} = \frac{\hbar\delta E}{2\pi W^2}, \quad (24)$$

where $\delta E = \Delta E/N$ is the distance in energy between two consecutive states of energy E_n.

Finally, we can evaluate the coefficients $f_n(t)$ for $t \to \infty$, which will give us the distribution of the final states:

$$f_n(t) = \frac{1}{i\hbar} W \int_0^t e^{-i(\omega-\omega_n)t'} b_0(t') dt' = \frac{1}{i\hbar} W \int_0^t e^{-i(\omega-\omega_n)t'} e^{-\Gamma t/2} dt' = \frac{1}{i\hbar} W \frac{e^{-\Gamma t/2} e^{-i(\omega-\omega_n)t'} - 1}{-i(\omega-\omega_n) - \Gamma/2}, \quad (25)$$

and for $t \to \infty$ becomes:

$$f_n(t \to \infty) = -\frac{iW}{\hbar} \frac{1}{\Gamma/2 + i(\omega - \omega_n)}. \tag{26}$$

The probability of obtaining the value E_n when measuring the energy is:

$$\begin{aligned}\mathcal{P}_E(E_n, t \to \infty) &= |f_n(t \to \infty)|^2 \\ &= W^2 \frac{1}{\hbar^2\Gamma^2/4 + (E_n - E_f)^2}.\end{aligned} \tag{27}$$

This probability distribution is a Lorentzian centered at E_f with width $\hbar\Gamma = \hbar/\tau$. This fact is compatible with the energy-time uncertainty principle.

To finish the treatment let us enumerate the validity conditions for the exponential decay to the continuum to be valid.

For the secular approximation to be valid, the frequency $\omega = E_f/\hbar$ must be much greater than the inverse of the typical evolution time, τ

$$E_f = \hbar\omega \gg \Gamma\hbar. \tag{28}$$

In order to expand the exponential $e^{i\Delta E\tau/N\hbar}$ for times of the order of $\tau = 1/\Gamma$ and to cut the expansion at the first term, the following condition must be fulfilled:

$$N \gg \Delta E/\Gamma\hbar. \tag{29}$$

Finally, for times of the order of $\tau = 1/\Gamma$ the integral in Eq. (21) should be approximately equal to $\pi/2$ and this happens to occur if

$$\Delta E \gg \Gamma\hbar. \tag{30}$$

This last condition can be understood as a requirement for the Lorentzian distribution to fit in the interval ΔE.

As a summary, we have seen that under certain conditions, if the initial state is resonantly coupled to a quasi-continuum set of states, an exponential decay with a typical time $\tau = 1/\Gamma$ takes place. In the final situation, the distribution of states consists of a Lorentzian centered at $E_f = \hbar\omega$, with a width of the order of $\hbar\Gamma$. If the definition of δE is taken into account, the conditions (28) and (29) for the exponential decay to be valid can be written as

$$\delta E \ll \Gamma\hbar \ll E_f = \hbar\omega. \tag{31}$$

The first inequality can be understood as a condition for the set of final states to be a quasi-continuum, so that the distance in energy between two consecutive states must be much less than the width of the final distribution of states. The second inequality is the condition for the secular approximation to be valid. Finally, the condition given by Eq. (30), for the final distribution of states to fit in the interval ΔE, must also be fulfilled.

Let us test the results obtained with a particular example. Consider a system with the following scheme of energy levels: the energy of the ground state is null and there are 81 states equally spaced in energy and with energies between $E_1 = 96\hbar/\delta t$ and $E_{81} = 104\hbar/\delta t$, so that $\Delta E = 8\hbar/\delta t$, δt being a parameter with dimensions of time. Therefore $E_f = 100\hbar/\delta t$ and $N = 80$. Let us introduce the following perturbation:

$$\begin{aligned}&\hat{W}(t) = 2W\cos\omega t, \qquad \text{with} \\ &\omega = 100/\delta t, \qquad \text{and} \qquad \mathrm{W} = 0.1\hbar/\delta\mathrm{t}.\end{aligned} \tag{32}$$

According to the previous exposition the Γ value is:

$$\Gamma = \frac{2\pi}{\hbar} W^2 \frac{N}{\Delta E} = \frac{2\pi}{\hbar} \frac{0.01\hbar^2}{\delta t^2} \frac{80\delta t}{8\hbar} = 0.6283/\delta t. \tag{33}$$

We can see that all the conditions are fulfilled:

$$\begin{aligned}&E_f \gg \Gamma\hbar, \qquad \text{since} \\ &E_f = 100\hbar/\delta t, \quad \text{and} \quad \Gamma\hbar = 0.6283\hbar/\delta\mathrm{t}, \\ &N \gg \Delta E/\Gamma\hbar, \qquad \text{since} \\ &N = 80, \quad \text{and} \quad \Delta\mathrm{E}/\Gamma\hbar = 12.7, \\ &\Delta E \gg \Gamma\hbar, \qquad \text{since} \\ &\Delta E = \frac{8\hbar}{\delta t}, \quad \text{and} \quad \Gamma\hbar = 0.6283\hbar/\delta\mathrm{t}.\end{aligned} \tag{34}$$

Therefore, if the system begins at $t = 0$ in the ground state, the probability of its remaining in this state in the long-time approximation is given by:

$$\mathcal{P}_{00}(t) = e^{-\Gamma t} = e^{-0.6283t/\delta t}. \tag{35}$$

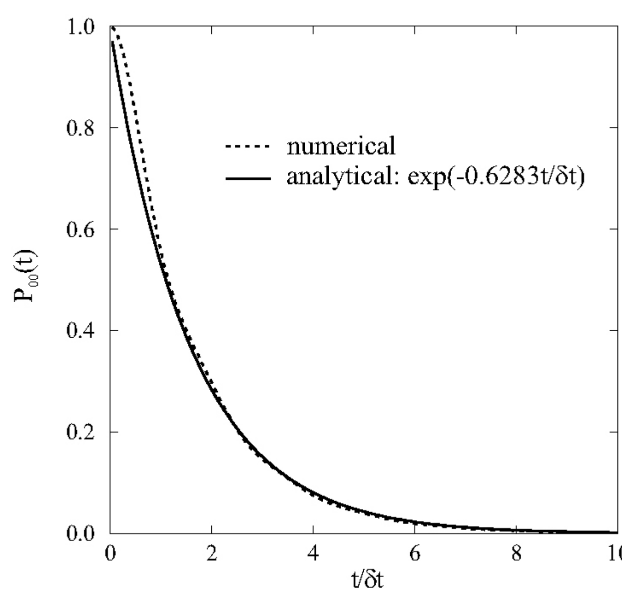

FIGURE 2. Temporal evolution of the probability of remaining in the ground state for long times.

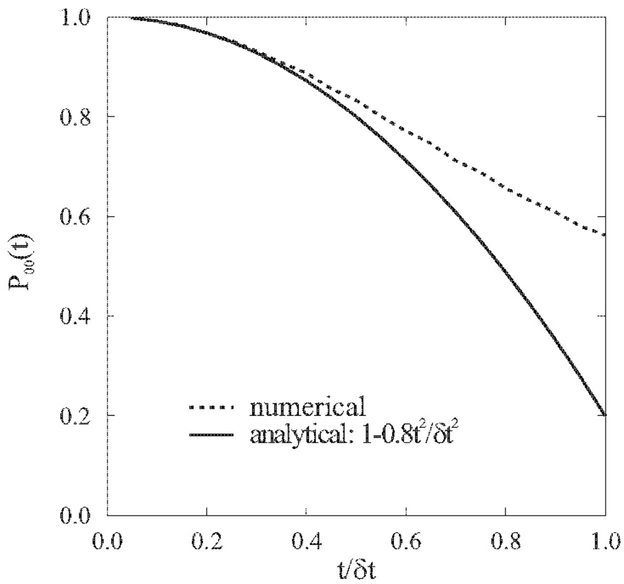

FIGURE 3. Temporal evolution of the probability of remaining in the ground state for short times.

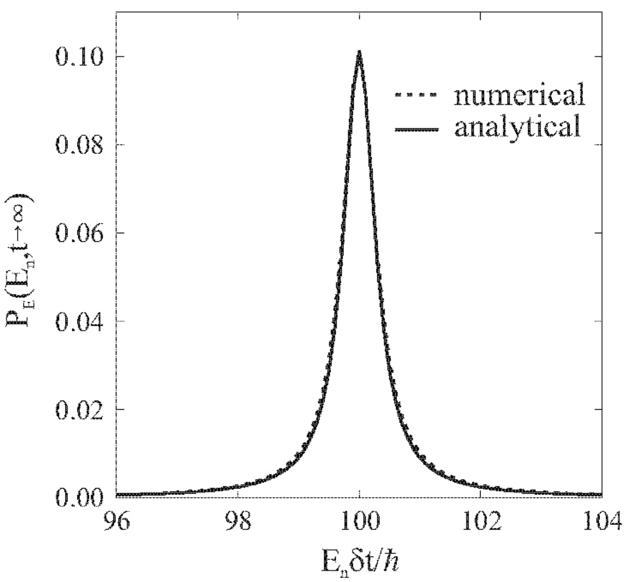

FIGURE 4. Final distribution of states.

On the other hand, in the short-time approximation, the temporal evolution is given by:

$$\mathcal{P}_{00}(t) = 1 - N\frac{W^2}{\hbar^2}t^2 = 1 - 0.8\frac{t^2}{\delta t^2}. \tag{36}$$

Figure 2 shows a comparison between the long-time approximation of the probability $\mathcal{P}_{00}(t)$ given by Eq. (35) and the numerical result obtained by solving the equations of the model, Eqs. (5) and (6), with the fourth order Runge-Kutta method.

Figure 3 shows a comparison between the short-time approximation of the probability $\mathcal{P}_{00}(t)$ given by Eq. (36) and the numerical result.

Finally, the distribution of the final states is given (by using the long-time approximation) by:

$$\begin{aligned}\mathcal{P}_E(E_n, t\to\infty) &= ^2/4 + (E_n - E_0)^2 \\ &= \frac{0.01}{9.8696\cdot 10^{-2} + (E_n\delta t/\hbar - 100)^2}.\end{aligned} \tag{37}$$

Figure 4 shows a comparison between this distribution and the one obtained by numerically solving the equations of the model. We can see in Figs. 2-4 that the analytical formulas found are quite a good approximation to the numerical results. If any of the conditions given by Eqs. (28)-(30) is not fulfilled, the exponential approach given by Eq. (23) may not be valid.

To end this section, we can compare the result obtained from the coupling to a quasi-continuum set of states to that of a continuum set of states. In this last case, if certain conditions are fulfilled, an exponential decay is again obtained for the probability of finding the system in the initial state, with

$$\begin{aligned}\Gamma = \frac{2\pi}{\hbar}\int d\beta\left|\left\langle\beta, E = E_i + \hbar\omega|\hat{W}|\varphi_i\right\rangle\right|^2 \\ \times\rho(\beta, E = E_i + \hbar\omega),\end{aligned} \tag{38}$$

where $|\varphi_i >$ is the initial state, and the final states are labelled with the energy E and a set of parameters β (which are necessary if the unperturbed hamiltonian does not constitute a Complete Set of Commuting Observables itself); the time dependent is supposed to be $\hat{W}(t) = 2\hat{W}\cos\omega t$ and finally ρ is the density of states. If we compare Eq. (38) with Eq. (22), the factor $N/\Delta E = 1/\delta E$ in the definition of Γ plays the role of the density of states. Let us define the following function:

$$K(E) = \frac{2\pi}{\hbar}\int d\beta\left|\left\langle\beta, E|\hat{W}|\varphi_i\right\rangle\right|^2\rho(\beta, E), \tag{39}$$

and then $\Gamma = K(E_i + \hbar\omega)$.

For the exponential approach to be valid in the case of a coupling to a continuum, similar conditions to those of Eqs. (28)-(30) must be fulfilled. The condition given by Eq. (28) must be fulfilled with $E_f = E_i + \hbar\omega$, and the condition given by Eq. (29) is obviously fulfilled in the case of a coupling to a continuum. Finally, the function $K(E)$ must have a plateau with a width larger than $\Gamma\hbar$ around the value $E = E_i + \hbar\omega$, or in other words, if $K(E)$ has a plateau around the value $E = E_i + \hbar\omega$ of width ΔE, then the condition given by Eq. (30) must be fulfilled.

3. Conclusions

A simple model has been developed, for the decay of a quantum discrete state which is resonantly coupled to a quasi-continuum set of states, to obtain an analytical approximate solution that is accurate and requires elementary mathematical knowledge. The cases of short-time approximation and long-time approximation have been treated separately. In the short-time approximation the probability of finding the system in the initial state evolves proportionally to the time squared, a fact which is compatible with the Zeno quantum effect. In the long-time approximation this probability has an exponential decay if certain conditions are fulfilled. This exponential decay appears in many physical situations such as ionization induced by an electromagnetic wave or the photoelectric effect and is the origin of the exponential decay, characteristic of many important dynamical processes in atomic, molecular, nuclear and particle physics. The conditions for the exponential decay approximation to be valid have been analyzed. The distribution of the final states is given by the characteristic Lorentzian distribution function whose width is related to the decay time by the energy-time uncertainty principle. Finally, a comparison with the case of a coupling to a continuum set of final states, rather than a quasi-continuum, has been analyzed.

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