Relation between decay and delay times

G. GARCÍA-CALDERÓN, J.L. MATEOS AND M. MOSHINSKY*
Instituto de Física
Universidad Nacional Autónoma de México
Apartado postal 20-364, 01000 México, D.F., México

ABSTRACT. The concept of decay time is almost as old as quantum mechanics, while that of delay time is easily formulated in classical mechanics if the energy of the particle is greater than the height of the potential. The purpose of this note is to propose a quantum mechanical definition of delay time for a potential \( V(r) \) using the solution of a time dependent Schrödinger equation with a given initial condition. In particular we consider the 3-dimensional case \( V(r) = b\delta(r - 1) \) and for \( b \gg 1 \) obtain explicitly the delay time as a linear function of \( b^2 \).

1. INTRODUCTION

The concept of decay time is almost as old as quantum mechanics [1], while that of delay time is more recent [2]. During the last few years, work on the properties of tunneling in semiconductor quantum structures has led to controversy regarding the notion of tunneling times [3]. In particular, the well known expression for the delay time, \( \tau_d = \hbar d\phi/dE \), \( \phi \) being the phase of the scattering function and \( E \) the energy, that follows from an argument regarding the scattered time dependent wave function [2], has been subjected to strong criticism [4]. These considerations have motivated us to provide a definition of delay time that is closely related to that of decay time and hence refers to an initial value problem. The results of this paper indicate that the definition of time delay given by Eq. (3.27) is appropriate from a physical point of view, as it has as a particular case the \( \tau_d \) defined above for the single pole case. This will be shown at the end of the paper.

We first consider the standard approach to these concepts. In Fig. 1 we draw a potential \( V(r) \) which, for convenience, we consider radial and limited to the interval between \( a_1 \) and \( a_2 \). A first approach to decay time would be the solution of the Schrödinger equation with this potential for outgoing waves \( \exp(ikr) \) when \( r > a_2 \). This gives [1,2] complex eigenvalues of the energy \( E = E_x - iE_y, E_x, E_y > 0 \) and the lifetimes \( T \) of the resonant

*Member of El Colegio Nacional.
Figure 1. We draw the short range potential $V(r)$ between the points $a_1$ and $a_2$ and the initial wave function $f(r)$ in the interval $0 \leq r \leq a_1$. We also indicate a real energy $E$ at a value larger than the maximum of the potential, which allows to give the classical delay time of Eq. (1.1). Furthermore we indicate by a thick line the complex energy $E_x - iE_y$ associated with outgoing waves at $r \to \infty$, as is appropriate for the decay problem.

states are $(\hbar/E_y)$. Thus for simple potentials, such as a square barrier between $a_1$ and $a_2$, the determination of $T$ is trivial, while for other cases approximate procedures such as WKB can be used.

For the delay time a great deal of controversy arises in relation with its definition [2]. There is no doubt whatever about its existence from a classical standpoint for an energy $E$ above the maximum height of the potential, as illustrated in Fig. 1. We then have to consider the difference $\tau'$ between the time to traverse the potential and the time of going from $a_1$ to $a_2$ as a free particle i.e.

$$\tau' = \int_{a_1}^{a_2} \left\{ \frac{1}{m} [E - V(r)] \right\}^{-1/2} dr - (a_2 - a_1) \left[ \frac{2}{m} E \right]^{-1/2}. \quad (1.1)$$

The point though is to be able to give a quantum mechanical definition of this time, particularly when the energy $E$ is below the maximum height of the potential, in which classically the particle could not arrive at the other side i.e., at $r > a_2$.

To approach this problem we first indicate in Section 2, through a general analysis, how an alternative definition of delay time could be introduced, and in section 3 we discuss a specific example, to finish with some general conclusions about the relations of decay and delay times.

2. THE DECAY AMPLITUDE

Let us consider the potential of Fig. 1 with the initial state being an $s$-wave of the type $f(r)$ concentrated in the region $0 \leq r \leq a_1$. 
If we could solve the time dependent equation

$$-\frac{\hbar^2}{2M} \frac{\partial^2 \psi}{\partial r^2} + V(r)\psi = i\hbar \frac{\partial \psi}{\partial t},$$

(2.1)

with the initial condition

$$\psi(r, 0) = f(r), \quad \int_0^{a_1} |f(r)|^2 \, dr = 1,$$

(2.2a, b)

then the amplitude of decay could be defined as

$$A(t) = \int_0^{a_1} f^*(r)\psi(r, t) \, dr,$$

(2.3)

as $|A(t)|^2$ is the probability that the wave function remains in its original form at time $t$.

We could then define a decay time as the value of $t$ at which $|A(t)|^2$ reaches a specified value. Let us denote a value of this type by a real positive constant $c$ and thus the decay time $\tau$ is given by the solution of the equation

$$|A(t)|^2 = c.$$

(2.4)

On the other hand we could also ask about the time required, in the absence of a potential, to reduce the probability amplitude to the same value $c$. In that case we have to solve Eq. (2.1) with $V(r) = 0$, with the same initial condition (2.2), and then take the scalar product of the resulting $\psi_0(r, t)$ with $f(r)$ as in (2.3), thus obtaining $A_0(t)$. We thus are looking for a time $\tau_0$ solution of the equation

$$|A_0(t)|^2 = c.$$

(2.5)

As $1 - |A(t)|^2$, $1 - |A_0(t)|^2$, represent the probability of finding the particle at time $t$, in a state different from the original $f(r)$, respectively in the presence or absence of the potential $V(r)$, it is reasonable to define the delay time as

$$\Delta \tau = \tau - \tau_0.$$

(2.8)

The previous analysis applies to an arbitrary short range potential and initial conditions. To see what it implies it is convenient to analyze a specific example, and we choose one that was discussed recently for other purposes [5] i.e., when $V(r)$ is a $\delta$ function potential at the point $r = a$, as will be described in the next section.

3. DECAY AND DELAY TIME FOR A $\delta$-FUNCTION POTENTIAL

We start by using units in which $\hbar$, the mass $M$ of the particle, and the distance $a$ at which we have the radial potential, are all one i.e.,

$$\hbar = M = a = 1.$$  

(3.1)
The equation corresponding to (2.1) will then be

$$\frac{1}{2} \frac{\partial^2 \psi}{\partial r^2} + b \delta(r - 1) \psi = \frac{i}{\partial t} \psi. \tag{3.2}$$

As for the initial conditions we may assume that originally $b = \infty$ and so

$$f(r) = \sqrt{2} \sin \kappa r, \quad \kappa = m\pi, \ m = 1, 2, 3, \ldots, \tag{3.3}$$

where we use the single letter $\kappa$ instead of $m\pi$ for compactness in the notation. Our problem then is to find $\psi(r, \kappa, t)$ such that

$$\psi(r, \kappa, 0) = \sqrt{2} \sin \kappa r, \tag{3.4}$$

and once we have $\psi(r, \kappa, t)$ we shall be interested in its scalar product with the initial state, i.e.,

$$A(\kappa, t) = \sqrt{2} \int_0^1 \sin \kappa r \psi(r, \kappa, t) \, dr. \tag{3.5}$$

To solve our problem the obvious procedure is to use the Laplace transform

$$\tilde{\psi}(r, \kappa, s) = \int_0^\infty \psi(r, \kappa, t) e^{-st} \, dt, \tag{3.6}$$

and applying it to both sides of Eq. (3.2) we get

$$\left[ \frac{1}{2} \frac{d^2}{dr^2} + b \delta(r - 1) \right] \tilde{\psi}(r, \kappa, k) = \begin{cases} -i\sqrt{2} \sin \kappa r + \frac{1}{2} k^2 \tilde{\psi}(r, \kappa, k), & \text{if } 0 \leq r \leq 1, \\ \frac{1}{2} k^2 \tilde{\psi}(r, \kappa, k), & \text{if } 1 \leq r \leq \infty, \end{cases} \tag{3.7}$$

where we used the notation

$$s = -\frac{i}{2} k^2, \quad k = \sqrt{2i}s, \tag{3.8}$$

and we replaced $\tilde{\psi}(r, \kappa, s)$ by $\tilde{\psi}(r, \kappa, k)$.

Once the Laplace transform (3.6) is determined we can get $\psi(r, \kappa, t)$ by the inverse Laplace transform over the Bromwich contour but, in terms of the variable $k$, the integral is over the hyperbolic contour $C'$ of Fig. 2 and we obtain [5]

$$\psi(r, \kappa, t) = (2\pi)^{-1} \int_{C'} \tilde{\psi}(r, \kappa, k) \exp(-\frac{1}{2} k^2 t) \, dk. \tag{3.9}$$

As our interest lies in $A(\kappa, t)$ of (3.5) we can invert the order of integration and get

$$A(\kappa, t) = (2\pi)^{-1} \int_{C'} \tilde{A}(k) \exp(-\frac{1}{2} k^2 t) \, dk, \tag{3.10}$$
where
\[ \tilde{A}(\kappa, k) = \sqrt{2} \int_0^1 \sin \kappa r \tilde{\psi}(r, \kappa, k) dr. \]

Clearly then
\[ \tilde{\psi}(r, \kappa, k) = \begin{cases} D \exp(ikr), & r > 1, \\ B \sin kr + G \sin \kappa r, & 0 \leq r \leq 1, \end{cases} \tag{3.12a, b} \]
where there is no \( \exp(-ikr) \) in (3.12a) as in terms of \( s \) of (3.8) it would diverge when \( s \to +\infty \), while
\[ G = \frac{2i\sqrt{2}}{k^2 - \kappa^2}. \tag{3.13} \]

Furthermore \( \tilde{\psi}(r, \kappa, k) \) must be continuous at \( r = 1 \) and, due to the potential \( \delta(\rho - 1) \), when we integrate Eq. (3.7) with respect to \( r \) in the interval around 1 we get
\[ \frac{1}{2} \left[ \frac{d\tilde{\psi}(r, \kappa, k)}{dr} \right]_{1-0}^{1+0} + b\tilde{\psi}(1, \kappa, k) = 0. \tag{3.14} \]

From equations (3.12), (3.13), (3.14) we obtain [5]
\[ B = \frac{(-2i\kappa)\sqrt{2}(-1)^m \exp(ik)}{(k^2 - \kappa^2)(k + ib[1 - \exp(i2k)])}, \tag{3.15} \]
so \( \tilde{\psi}(r, \kappa, k) \) is completely defined in the interval \( 0 \leq r \leq 1 \) and the \( \tilde{A}(\kappa, k) \) of (3.11), is given by
\[ \tilde{A}(\kappa, k) = \frac{2i}{(k^2 - \kappa^2)} + \frac{2\kappa^2}{(k^2 - \kappa^2)^2} \frac{[1 - \exp(i2k)]}{\{k + ib[1 - \exp(i2k)]\}}, \tag{3.16} \]
and we now must calculate \( A(\kappa, t) \) of (3.10).

In Ref. [5] we obtained \( A(\kappa, t) \) exactly using functions \( M(r, k, t) \) defined by Moshinsky [6] and in the notation of Nussenzveig [7]. In the present paper we shall give only an approximate solution using the method of steepest descent, as considered by García-Calderón [8,9], which more clearly brings out the physics of the problem. To begin with we change the contour \( C' \) of Fig. 2 to the contour \( C \) at 45° as indicated in the same figure.
We note though that \( \tilde{A}(k, \kappa) \) has poles given by the zeros of the denominator \( i.e. \), by the equation [5,10]
\[ k + ib[1 - \exp(i2k)] = 0. \tag{3.17} \]
There seems to be also a pole at $k = K$ but this is spurious as it easily checked that the residue there is zero [5].

The solution [5] $k_n, n = \pm 1, \pm 2, \ldots$, of (3.17) are all in the lower half of the $k$ plane of Fig. 2 and only those with $n$ positive are in the lower right quadrant between the contour $C$ and $C'$. We surround these poles by circles as indicated in Fig. 2, and in the integral over the contour $C$ we make the replacement

$$k = \exp(-i\pi/4)z. \quad (3.18)$$

As the contribution from the circles is just the residue at the pole we finally get

$$A(\kappa, t) = -i \sum_{n=1}^{\infty} \lim_{k \to k_n} [(k - k_n)k \tilde{A}(\kappa, k)] \exp(-\frac{i}{2}k_n^2 t)$$

$$- \frac{i}{2\pi} \int_{-\infty}^{\infty} z \tilde{A}(\kappa, ze^{-i\pi/4}) \exp(-\frac{1}{2}z^2 t) \, dz. \quad (3.19)$$

The residues at the poles $k = k_n$ in the first term at the right hand side of (3.19) were obtained in Ref. [5]. As to the integral in (3.19), we see that because of the term $\exp(-\frac{1}{2}z^2 t)$, the main contribution comes from $z$ in the vicinity of 0 if $t$ is large. Thus we could consider the development

$$A(\kappa, k) = \sum_{\ell=0}^{\infty} \left[ \frac{d^\ell \tilde{A}(\kappa, k)}{dk^\ell} \right]_{k=0} \exp(-i\ell\pi/4)z^\ell, \quad (3.20)$$
and get integrals of the form
\[
\int_{-\infty}^{\infty} z^{\ell+1} \exp(-\frac{1}{2} z^2 t) \, dz = \frac{1}{2} \left[ 1 - (-1)^\ell \right] \left( \frac{2}{t} \right)^{\frac{\ell}{2}+1} \Gamma\left( \frac{\ell}{2} + 1 \right). \tag{3.21}
\]

The integral (3.21) vanishes for even \( \ell \) and, for large \( t \), the odd \( \ell \) that gives the largest contribution is \( \ell = 1 \). As furthermore from (3.16) we have
\[
\left[ \frac{d\tilde{A}(\kappa, k)}{dk} \right]_{k=0} = \frac{4}{\kappa^2 (1 + 2b)^2},
\tag{3.22}
\]
we see that the steepest descent value for the amplitude of decay is [5]

\[
A_b(\kappa, t) = \sum_{n=1}^{\infty} \frac{4\kappa^2 k_n^2 d_n}{(\kappa^2 - k_n^2)^2} \exp\left( -\frac{i}{2} k_n^2 t \right) + \frac{\exp(i\pi/4)\Gamma\left( \frac{3}{2} \right) 4}{\kappa^2 (1 + 2b)^2} \left( \frac{2}{t} \right)^{3/2} + \cdots \tag{3.23}
\]
where
\[
d_n = \frac{i}{2} \frac{1}{2k_n b + ib(1 + 2b)}.
\tag{3.24}
\]
and the \( k_n \) are given by the roots of equation (3.17). We have added an index \( b \) to the decay amplitude \( A(\kappa, t) \) to indicate explicitly that it depends on the strength \( b \) of the \( \delta \)-function potential. An alternative procedure of deriving the expression (3.23) is by using the resonant state formalism [8].

If \( b = 0 \) Eq. (3.10) still holds but with \( \tilde{A}(k, \kappa) \) having the value (3.16) with \( b = 0 \). Thus there are no poles of the type introduced by Eq. (3.17) and the solution is given just by the last integral in (3.19), with \( b = 0 \) in \( \tilde{A}(\kappa, ze^{-i\pi/4}) \), and thus, as in the analysis leading to (3.23), we obtain

\[
A_0(\kappa, t) = \frac{1}{2\pi} \exp(i\pi/4)\Gamma\left( \frac{3}{2} \right) 4 \left( \frac{2}{t} \right)^{3/2} + \cdots \tag{3.25}
\]

We can now establish for a given constant \( c \) the equations
\[
|A_b(\kappa, t)|^2 = c, \tag{3.26a}
\]
\[
|A_0(\kappa, t)|^2 = c, \tag{3.26b}
\]
to obtain respectively the decay time \( \tau \), and the free escape of the wave packet \( \tau_0 \), so that delay time for a potential of strength \( b \) becomes
\[
\Delta \tau = \tau - \tau_0. \tag{3.27}
\]
In the concluding section we discuss this \( \Delta \tau \) for particular values of \( b \) and \( \kappa = m\pi \).
4. CONCLUSION

We would like now to consider the case when the strength $b$ of the $\delta$ potential is $b \gg 1$. In that case we showed in Ref. [5] that the roots of Eq. (3.17) are given by

$$k_n = [(n\pi) - (n\pi/2b)] - i(n\pi/2b)^2,$$

and so as $\kappa = m\pi$ we get

$$\kappa - k_n = (m - n)\pi + (n\pi/2b) + i(n\pi/2b)^2.$$  

Clearly then we see that the term in the first summation on the right hand side of (3.23) that will prevail, is the one with $m = n$, so restricting ourselves to it we see that when $\kappa = n\pi$,

$$\frac{4\kappa^2 k_n^2 d_n}{(\kappa + k_n)^2(\kappa - k_n)^2} \approx \frac{4\kappa^4 (4b^2)^{-1}}{(2\kappa)^2 (\kappa/2b)^2} = 1,$$

as from (3.24) we observe that for $b^2 \gg 1$ and also $b > m\pi$, $d_n \approx (4b^2)^{-1}$ and $(\kappa - k_n)^2 \approx (\kappa/2b)^2$.

Thus the main term for $b \gg 1$ of $A_b(\kappa, t)$ of (3.23) will be

$$A_b(\kappa, t) \approx \exp(-\frac{i}{2} k_n^2 t),$$

and substituting in (4.1) we see

$$|A_b(\kappa, t)|^2 = \exp(-t/T) = c,$$

where $T$ is the half life of the state given by

$$T \equiv -[\text{Im}(k_n^2)]^{-1} = \frac{2b^2}{n^3 \pi^3}.$$  

From (4.5) we then obtain

$$\tau = T \ln c^{-1}.$$  

Turning now our attention to the escape probability $|A_0(\kappa, t)|^2$ we require that $t$ satisfies the equation

$$|A_0(\kappa, t)|^2 = \left| \frac{1}{\sqrt{\pi}} \left( \frac{2}{t} \right)^{3/2} \frac{1}{(n\pi)^2} \right|^2 = c,$$

which implies that $\tau_0$ becomes

$$\tau_0 = \left( \frac{8}{\pi^5 n^4 c} \right)^{1/3},$$
FIGURE 3. The delay time for the lowest energy state, i.e. \( n = 1 \), as function of the strength of the potential. From eq. (4.11) the curve is a parabola for \( b \gg 1 \), and it no longer holds for \( b \approx 1 \) as shown by the dashed lines in the parabola below the abscissa. In that part we note that by definition, when \( b \to 0 \), \( \Delta \tau \to 0 \) and so we connected the positive part of the arc of the parabola with the origin.

and thus finally the delay time becomes

\[
\Delta \tau_n = \tau - \tau_0 = \frac{2b^2}{n^3 \pi^3} \ln c^{-1} - \left( \frac{8}{\pi^5 n^4 c} \right)^{1/3},
\]

where we added an index \( n \) to \( \Delta \tau \) to indicate the level that is decaying. Note that the delay time \( \Delta \tau_n \) is a linear function of the decay time \( T \) given by (4.6).

It is now a question of selecting the parameter \( c \) so that the assumptions made in deriving \( A_b(\kappa, t) \) of (3.23) and \( A_0(\kappa, t) \) of (3.25) are valid. For the latter we require that \( \tau_0 \gg 1 \) so that the method of steepest descent applies, and this means that \( c \ll 1 \) in (4.9), which in turn implies from (4.9) that \( \tau \gg T \), i.e., the time at which we measure the decay corresponds to a large number of lifetimes of the state, which is a desired situation if we want the exponential law (4.4) to hold. If, for example \( \tau = \ell T \), where \( \ell \) is an integer larger than 1, then from (4.5) we see that \( c = e^{-\ell} \) and so it is smaller than 1 but larger than zero.

Thus equation (4.10) is valid if \( b \gg 1 \), \( c \ll 1 \), and as a function of \( b \) and \( n \) it can be written as

\[
\Delta \tau_n = A \frac{b^2}{n^3} - \frac{B}{n^{4/3}},
\]

with \( A, B \) being some constants that can be obtained from (4.10).

In Fig. 3 we graph \( \Delta \tau_1 \) as function of \( b \) which gives a parabola where negative values of \( \Delta \tau_1 \) appear when \( b \) is comparable with 1, where the approximation is not valid, and so we mark the curve with a dashed line in that region. As for \( b = 0 \), \( \Delta \tau_n = 0 \), we substitute the dashed part by a full line that connects the origin with the parabola but going above the abscissa.
The delay time for the states $n = 1, 2, 3$ as function of the strength $b$ of the potential. From Eq. (4.11) we see that the parabolas widen as $n$ increases.

In Fig. 4 we draw the corresponding curves for $n = 1, 2, 3$ showing that for $b \gg 1$ the parabolas open up, as is to be expected from (4.11) due to the term $n^3$ in the denominator.

Thus the delay time increases with the height of the potential $b$ and decreases with the energy of the initial state $(n^2 \pi^2)/2$, as is to be expected.

We note that in this paper we use Eq. (3.26) of the decay probability with and without potential to define the delay time. It would have been more correct to replace $1 - |A(t)|^2$ by the probability of finding the particle outside the potential $1 - P(t)$ where, in the present problem

$$P(t) = \int_0^1 \psi^*(r, \kappa, t) \psi(r, \kappa, t) \, dr.$$  \hspace{1cm} (4.12)

We have shown though [11] that if the strength $b$ of the $\delta$ potential is large $b \gg 1$ and our initial state is close to a resonance then $B(t) \simeq |A(t)|^2$ and all the discussions of this section continues to be valid.

As a final point we compare our result (4.10) for $\Delta \tau_n$ with the notion of the delay time which, in our units, is $\tau_d = d\phi/dE$ as mentioned in the introduction. Using the well-known one-pole approximation for the $S$ matrix,

$$S = e^{2i\phi} = \frac{E - \mathcal{E} - i\Gamma/2}{E - \mathcal{E} + i\Gamma/2},$$  \hspace{1cm} (4.13)

where

$$\mathcal{E} = \frac{k_n^2}{2}.$$  \hspace{1cm} (4.14)
with $k_n$ given by (4.1). This implies that $\Gamma = T^{-1}$, where the latter is defined in (4.6). We note that

$$\frac{d\phi}{dE} = \frac{\Gamma/2}{(E - \varepsilon)^2 + \Gamma^2/4}$$

(4.15)

and thus at resonance, i.e., $E = \varepsilon$ we have that

$$\left( \frac{d\phi}{dE} \right)_{E=\varepsilon} = \frac{2}{\Gamma} = 2T.$$  

(4.16)

This result coincides with our formula (4.10) if we select our constant $c$ appropriately, as for $b \gg 1$ the last term in the right-hand side of (4.10) can be disregarded.

Acknowledgments

The authors would like to thank K.W. McVoy and H.M. Nussenzveig for helpful discussions.

References

1. G. Gamow, Z. Phys. 51 (1928) 204.