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Tunneling Through Rectangular Plus Linear Barrier

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Tunneling through the superposition of two potential barriers, one rectangular and other linear, is discussed. Besides its importance in fields like nanostructure, the problem presents some interesting physical and mathematical features.

KEY WORDS: tunneling; reflection time; transmission time; linear barrier; rectangular barrier.

1. INTRODUCTION

Despite being an old subject in theoretical physics, the quantum tunneling phenomenon has many interesting features that lead to yet unsolved problems. If a particle inciding on a potential barrier with unsufficient energy to overcome the barrier emerges in the other side that means the particle someway went through the barrier (the very known tunnel effect). In the literature, good and comprehensive papers on this subject can be found. Among them, we cite the review paper by Hauge and Støvneng (1989), Landauer and Martin (1994), and, more recently, Muga and Leavens (2000). Despite all these and other efforts spent up to now, no consensus was achieved as yet on how to define and evaluate tunneling times. This paper addresses this issue in a special case, namely, that in which a linear and a rectangular potentials superpose.

One legitimatly may ask: What interest the superposition of a rectangular and a linear barrier could have any way? In the first place, the linear barrier has its own importance in the construction of nanoscale electronic devices where this barrier emulates the Schottky potential that emerges because of the presence of an external electric field. In this paper, we consider also the presence of a rectangular barrier as a provision for the situations in which the electrons have to overcome such barrier before reaching the region where the external electric field acts.

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The analysis is robust in the sense that it safely contemplates many sorts of similar potential superposition as, e.g., pure rectangular, pure linear, and square well plus linear potentials.

We will be particularly interested in discussing the reflection and transmission times through the barrier. This problem has many interesting mathematical features associated with some particular combinations of Airy functions, and some limit behavior of them. As it is well known, these functions emerge naturally in the solution of the Schroedinger equation with a linear potential.

To define notations, in the next section we present a summary of the tunneling problem through a rectangular barrier. The superposition analysis is presented in section 3. Results are presented and discussed in section 4.

2. TUNNELING THROUGH A RECTANGULAR BARRIER

A one-dimensional rectangular barrier of height V_0 and width a is defined as

$$V(x) = \begin{cases} 0 & \text{if } x < 0 \quad \text{(region 1, inciding region)} \\ V_0 & \text{if } 0 \le x \le a \quad \text{(region 2, classically forbidden region)} \\ 0 & \text{if } x > a \quad \text{(region 3, transmitted region)} \end{cases} \tag{2.1}$$

The energy eigenstates associated to the solutions to the corresponding Schroedinger equation can be found in most quantum mechanics texts and are given

$$u_E(x) = \begin{cases} u_1(x) = e^{ikx} + A\, e^{-ikx} & \text{if } x < 0 \\ u_2(x) = B\, e^{-\rho x} + C\, e^{\rho x} & \text{if } 0 \le x \le a \\ u_3(x) = D\, e^{ikx} & \text{if } x > a \end{cases} \tag{2.2}$$

where

$$k^2 = \frac{2mE}{\hbar^2}; \quad \rho^2 = k_0^2 - k^2; \quad k_0^2 = \frac{2mV_0}{\hbar^2} \tag{2.3}$$

and the boundary conditions at $x = 0$ and $x = a$ lead to

$$B = -\frac{2\cos\theta}{r}\, e^{-i\theta}\, e^{-i\bar{\alpha}} \tag{2.4}$$

$$C = e^{-2\rho a}\frac{2\cos\theta}{r}\, e^{-i\theta} e^{-i\bar{\alpha}} \tag{2.5}$$

$$D = -e^{-\rho a}\frac{2i\sin 2\theta}{r}\, e^{-ika}\, e^{-i\bar{\alpha}} \tag{2.6}$$

where

$$\cos\theta = k/k_0, \quad \sin\theta = \rho/k_0 \tag{2.7}$$

$$\tan\bar{\alpha} = \coth(\rho a)\, \tan(2\theta) \tag{2.8}$$

and

$$r^2 = 1 + e^{-4\rho a} - 2\,e^{-2\rho a}\cos(4\theta) \tag{2.9}$$

3. THE RECTANGULAR PLUS LINEAR BARRIER

The linear barrier potential of height V_0 and width a is defined as

$$V(x) = \begin{cases} 0 & \text{if } x < 0 \\ V_0(1 - x/a) & \text{if } 0 \le x \le a \\ 0 & \text{if } x > a \end{cases} \tag{3.1}$$

The solution of the associated Schroedinger equation is given in terms of Airy functions. To deal with the superposition of such potential with a rectangular one, we introduce the potential

$$V(x) = \begin{cases} 0 & \text{if } x < 0 \\ V_0 + \left(\dfrac{V_1 - V_0}{a}\right)x = V_0\left[1 + (\beta - 1)\dfrac{x}{a}\right] & \text{if } 0 \le x \le a \\ 0 & \text{if } x > a \end{cases} \tag{3.2}$$

where $\beta = V_1/V_0$. The potential (3.2) reduces to the rectangular potential (2.1) when $\beta = 1$, and to the linear potential (3.1) when $\beta = 0$.

For algebraic purpose, it is more convenient to introduce the dimensionless parameter

$$\eta = 1 - \beta \tag{3.3}$$

In terms of η, the superposition potential (3.2) reads

$$V(x) = \begin{cases} 0 & \text{if } x < 0 \\ V_0\left(1 - \eta\dfrac{x}{a}\right) & \text{if } 0 \le x \le a \\ 0 & \text{if } x > a \end{cases} \tag{3.4}$$

When $\eta = 0$, we obtain the rectangular potential, and when $\eta = 1$, we obtain the linear potential (2.1).

The Schroedinger equation associated with the potential (3.4) can be written as

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V_0\left(1 - \frac{\eta}{a}x\right)\psi = E\psi \tag{3.5}$$

which can be rewritten as

$$\frac{d^2\psi(\xi)}{d\xi^2} + \xi\,\psi(\xi) = 0 \tag{3.6}$$

where

$$\xi = \xi(x) = q_0 \left(\frac{\eta}{a} x + \mathcal{E}^2 - 1 \right) \tag{3.7}$$

$$q_0 = (k_0 a/\eta)^{2/3} \tag{3.8}$$

and

$$\mathcal{E} = k/k_0 \tag{3.9}$$

The general solution to the Schroedinger equation (3.6) is given by

$$\psi(x) = \begin{cases} e^{ikx} + A\, e^{-ikx} & x < 0 \\ B\, Ai(-\xi) + C\, Bi(-\xi) & 0 \le x \le a \\ D\, e^{ikx} & x > a \end{cases} \tag{3.10}$$

Continuity conditions at the potential boundary produce the following linear equations for the parameters A, B, C, and D

$$\begin{aligned} 1 + A &= B\, Ai(-\xi_0) + C\, Bi(-\xi_0) \\ D\, e^{ika} &= B\, Ai(-\xi_a) + C\, Bi(-\xi_a) \\ ik(1 - A) &= -\frac{q_0 \eta}{a} [B\, Ai'(-\xi_0) + C\, Bi'(-\xi_0)) \end{aligned} \tag{3.11}$$

where $Ai'(-\xi)$ and $Bi'(-\xi)$ are the derivatives of the Airy functions with respect to $-\xi$. In Eq. (3.11),

$$\xi_0 = \xi(0) = -q_0 \left(\frac{\rho}{k_0} \right)^2 \tag{3.12}$$

and

$$\xi_a = \xi(a) = -\frac{q_0}{k_0^2} (\rho^2 - \eta k_0^2) = \xi_0 + \eta q_0 \tag{3.13}$$

To simplify the algebraic calculation, it is convenient to introduce the complex quantities

$$F(\xi) = ik\, Ai(-\xi) - \frac{q_0}{a} \eta\, Ai'(-\xi) \tag{3.14}$$

$$G(\xi) = ik\, Bi(-\xi) - \frac{q_0}{a} \eta\, Bi'(-\xi) \tag{3.15}$$

and

$$\Delta = F^*(\xi_a) G(\xi_0) - F(\xi_0) G^*(\xi_a) \tag{3.16}$$

where the star stands for complex conjugate. In terms of these quantities, we get

$$A = \frac{1}{\Delta} [F^*(\xi_0) G^*(\xi_a) - F^*(\xi_a) G^*(\xi_0)] \tag{3.17}$$

$$B = -\frac{1}{\Delta} 2ikG^*(\xi_a) \tag{3.18}$$

$$C = \frac{1}{\Delta} 2ikF^*(\xi_a) \tag{3.19}$$

$$D = \frac{1}{\Delta}[F^*(\xi_a)G(\xi_a) - F(\xi_a)G^*(\xi_a)]\, e^{-ika} = -\frac{2ikq_0\eta}{\pi a \Delta}\, e^{-ika} \tag{3.20}$$

where the use was made of the Wronskian of the Airy functions (Abramowitz and Stegun, 1970)

$$W[A_i(z), Bi(z)] = \frac{1}{\pi}$$

It is also convenient to define the quantities

$$R_1 = \mathcal{E}^2[Ai(-\xi_0)Bi(-\xi_a) - Ai(-\xi_a)Bi(-\xi_0)] \tag{3.21}$$

$$R_2 = \left(\frac{q_0\eta}{k_0 a}\right)^2 [Ai'(-\xi_a)Bi'(-\xi_0) - Ai'(-\xi_0)Bi'(-\xi_a)] \tag{3.22}$$

$$I_1 = \left(\frac{q_0\eta}{k_0 a}\right) \mathcal{E}[Ai(-\xi_a)Bi'(-\xi_0) - Ai'(-\xi_0)Bi(-\xi_a)] \tag{3.23}$$

$$I_2 = \left(\frac{q_0\eta}{k_0 a}\right) \mathcal{E}[Ai'(-\xi_a)Bi(-\xi_0) - Ai(-\xi_0)Bi'(-\xi_a)] \tag{3.24}$$

In terms of these quantities, we have

$$A = -\frac{R_1 + R_2 + i(I_1 + I_2)}{R_2 - R_1 + i(I_1 - I_2)} = -\frac{N_A}{\Delta} \tag{3.25}$$

where

$$N_A = [R_1 + R_2 + i(I_1 + I_2)]\, k_0^2 \tag{3.26}$$

and

$$\Delta = [R_2 - R_1 + i(I_1 - I_2)]\, k_0^2 \tag{3.27}$$

Using the polar representation for the complex numbers N_A and Δ, i.e., $N_A = |N_A|e^{i\alpha}$ and $\Delta = |\Delta|e^{i\lambda}$, it can be shown that

$$\tan\alpha = \frac{I_1 + I_2}{R_1 + R_2} \tag{3.28}$$

and

$$\tan\lambda = \frac{I_1 - I_2}{R_2 - R_1} \tag{3.29}$$

3.1. Reflection and Transmission Times

In terms of the quantities N_A, Δ, α, and λ, defined in (3.26), (3.27), (3.28), and (3.29), the reflected and transmission wave functions read

$$\psi_R(x,t) = -\frac{|N_A|}{|\Delta|} e^{i(\alpha-\lambda)} e^{-ikx} e^{-i\omega t} \tag{3.30}$$

and

$$\psi_T(x,t) = -\frac{2ikq_0\eta}{\pi a|\Delta|} e^{-i\lambda} e^{ikx} e^{-i\omega t} e^{-ika} \tag{3.31}$$

where

$$\omega = \omega(k) = \frac{E}{\hbar} = \frac{\hbar k^2}{2m} \tag{3.32}$$

Imposing stationary phase condition on the wave function (3.30) at the position $x = 0$, we obtain for the reflection time the expression

$$t_R = \left(\frac{d\alpha}{dk} - \frac{d\lambda}{dk}\right)\frac{m}{\hbar k} \tag{3.33}$$

where α and λ are implicitly defined in (3.28) and (3.29).

Introducing the barrier characteristic time

$$t_0 = \frac{\hbar}{2V_0} \tag{3.34}$$

we can express the reflection time as

$$\frac{t_R}{t_0} = \frac{1}{\mathcal{E}}\left(\frac{\partial\alpha}{\partial\mathcal{E}} - \frac{\partial\lambda}{\partial\mathcal{E}}\right) \tag{3.35}$$

where $\mathcal{E}$ is defined in (3.9).

Analogously, imposing stationary phase condition on the wave function (3.31) at the position $x = a$, we obtain for the transmission time the expression

$$\frac{t_T}{t_0} = -\frac{1}{\mathcal{E}}\frac{\partial\lambda}{\partial\mathcal{E}} \tag{3.36}$$

The derivative $\partial\alpha/\partial\varepsilon$ can be readily evaluated by noticing that

$$\frac{\partial}{\partial\alpha}(\tan\alpha)\frac{\partial\alpha}{\partial\varepsilon} = \frac{\partial}{\partial\varepsilon}\left(\frac{I_1 + I_2}{R_1 + R_2}\right) \tag{3.37}$$

to get

$$\frac{\partial\alpha}{\partial\varepsilon} = \cos^2\alpha\,\frac{\partial}{\partial\varepsilon}\left(\frac{I_1 + I_2}{R_1 + R_2}\right) \tag{3.38}$$

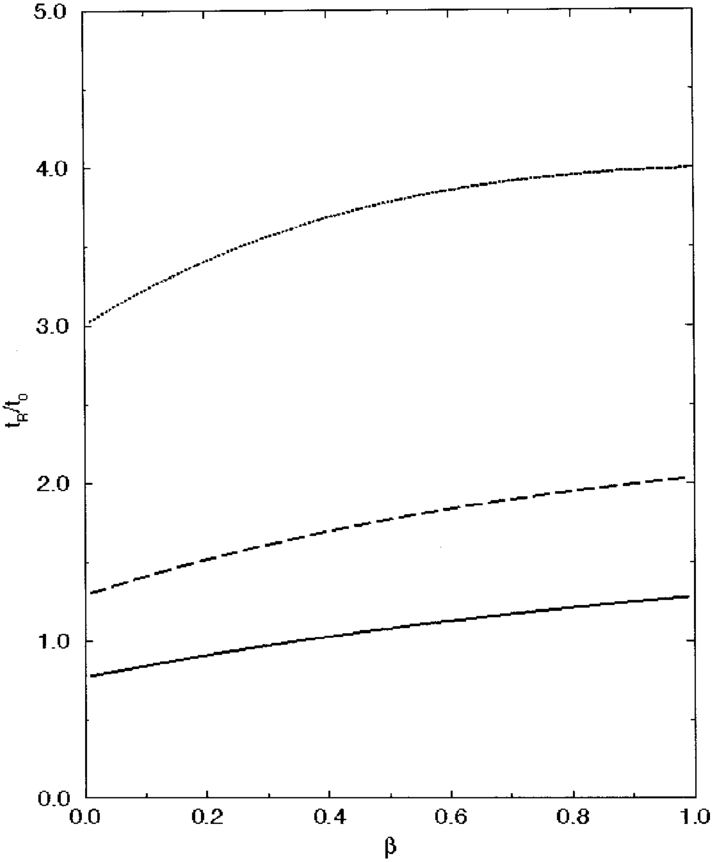

Fig. 1. Reflection time as a function of the barrier parameter β for $k_0 a = 1$, and some values of k. Dotted line: $k/k_0 = 0.5$; dashed line: $k/k_0 = 0.8$; continuous line: $k/k_0 = 1.1$. Notice that $k/k_0 > 1$ means that the particle is inciding above the barrier, and $\beta = 1$ for a pure rectangular potential.

A little more algebra produces the results

$$\frac{\partial\alpha}{\partial\varepsilon} = \frac{(R_1 + R_2)\frac{\partial}{\partial\varepsilon}(I_1 + I_2) - (I_1 + I_2)\frac{\partial}{\partial\varepsilon}(R_1 + R_2)}{|\Delta|^2} k_0^4 \tag{3.39}$$

Analogously, we obtain

$$\frac{\partial\lambda}{\partial\varepsilon} = \frac{(R_2 - R_1)\frac{\partial}{\partial\varepsilon}(I_1 - I_2) - (I_1 - I_2)\frac{\partial}{\partial\varepsilon}(R_2 - R_1)}{|\Delta|^2} k_0^4 \tag{3.40}$$

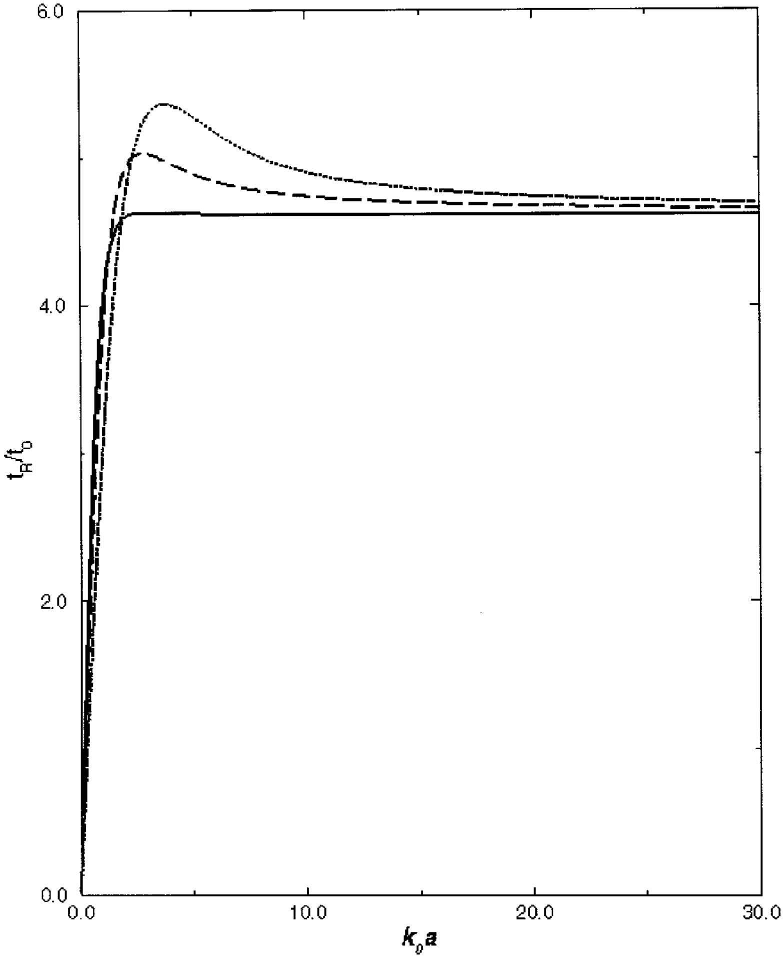

Fig. 2. Reflection time as a function of the barrier width a, for $k/k_0 = 0.5$, and several values of the barrier parameter β. Dotted line: $\beta = 0.01$; dashed line: $\beta = 0.5$; continuous line: $\beta = 0.99$.

The derivatives of the quantities R_1, R_2, I_1, and I_2 can be obtained from known relations between the Airy functions and its derivatives (Abramowitz and Stegum, 1970). The results are

$$\frac{\partial R_1}{\partial \varepsilon} = \frac{2R_1}{\varepsilon} + 2\varepsilon^2 \frac{k_0 a}{\eta}(I_1 + I_2) \tag{3.41}$$

$$\frac{\partial R_2}{\partial \varepsilon} = \frac{2k_0 a}{q_0 \eta}(\xi_a I_1 + \xi_0 I_2) \tag{3.42}$$

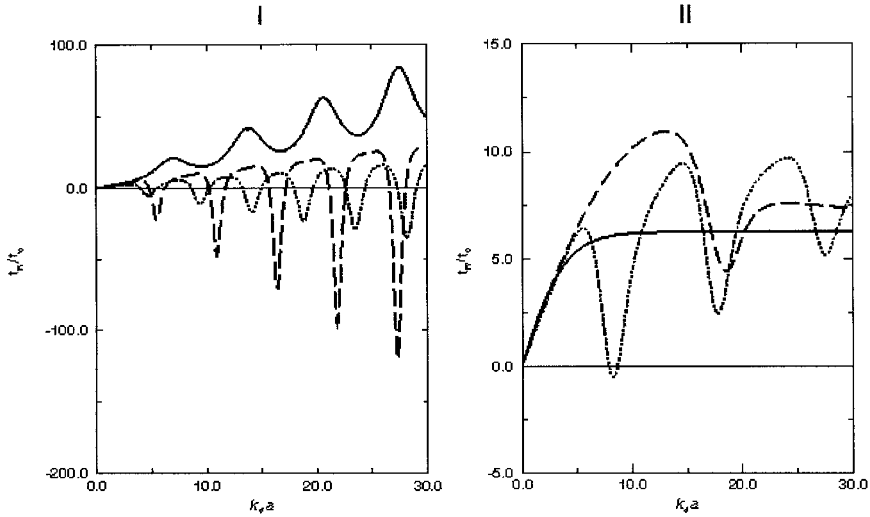

Fig. 3. Reflection time as a function of the barrier width, and several values of the barrier parameter β. (I) $k/k_0 = 1.1$ (particle inciding above the barrier); (II) $k/k_0 = 0.94$. Dotted line: $\beta = 0.5$; dashed line: $\beta = 0.75$; continuous line: $\beta \approx 1$.

$$\frac{\partial I_1}{\partial \varepsilon} = \frac{I_1}{\varepsilon} - 2\frac{\varepsilon^2 k_0 a}{\eta} R_2 - 2\frac{k_0 a}{q_0 \eta} \xi_0 R_1 \tag{3.43}$$

$$\frac{\partial I_2}{\partial \varepsilon} = \frac{I_2}{\varepsilon} - 2\frac{\varepsilon^2 k_0 a}{\eta} R_2 - 2\frac{k_0 a}{q_0 \eta} \xi_a R_1 \tag{3.44}$$

4. RESULTS AND DISCUSSION

In the previous few figures, we show the behavior of the reflection and transmission times for particular situations.

Figure 1 displays the reflection time, in units of t_0, Eq. (3.34), as a function of the barrier parameter β, for a barrier of width $a = 1$ (in units of k_0^{-1}), and several values of k. When $k/k_0 > 1$, the particle is inciding above the barrier.

Figure 2 displays the reflection time, in units of t_0, as a function of the barrier width a, for $k/k_0 = 0.5$, and several particular values of the barrier parameter β. Notice that $\beta = 0$ implies a pure linear potential and $\beta = 1$ implies a pure rectangular potential. For very thick barrier ($k_0 a \gg 1$), the top of the trapezoidal potential is nearly flat as felt by the inciding particle. In this case, the reflection time shows very little dependence on the potential parameter β.

Figure 3 displays the reflection time, in units of t_0, as a function of the barrier width a, for $k/k_0 = 1.1$ (particle inciding above the barrier), and $k/k_0 = 0.94$ for

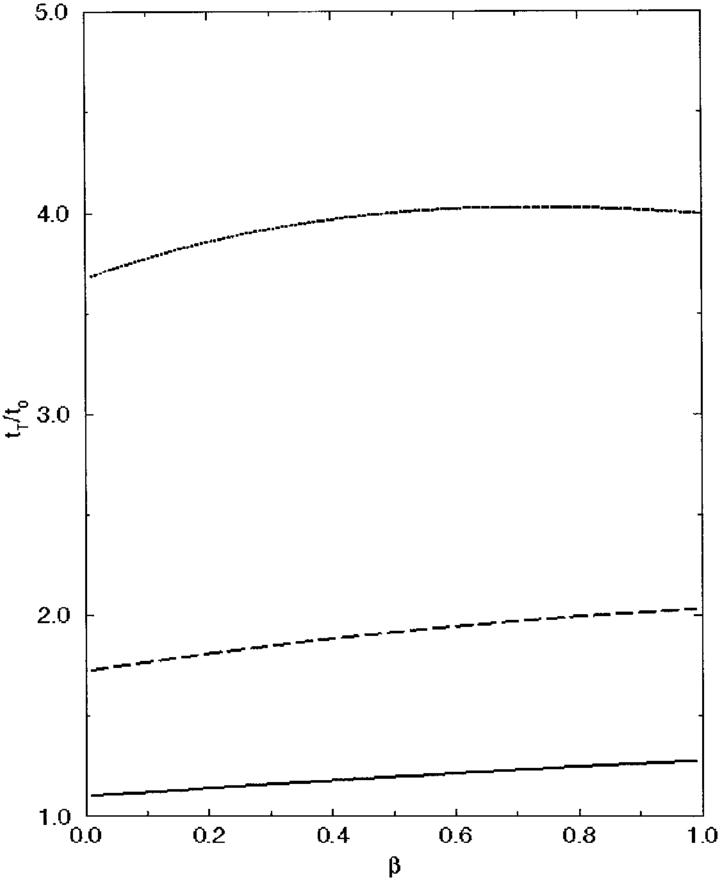

Fig. 4. Transmission time as a function of the barrier width, for $k/k_0 = 0.5$, and several values of the barrier parameter β. Dotted line: $\beta = 0.1$; dashed line: $\beta = 0.5$; continuous line: $\beta = 0.9$.

several values of the barrier parameter β. The oscillations in the reflection time are indication of occurrence of resonances, which produce negative reflection times for some values of β when $k/k_0 \approx 1$. These resonances are present in a rectangular barrier but the negative times are not. This known result is illustrated by the continuous curve ($\beta \approx 1$).

Figure 4 displays the transmission time, in units of t_0, Eq. (3.34), as a function of the barrier parameter β, for a barrier of width $a = 1$ (in units of k_0^{-1}), and several values of k. When $k/k_0 > 1$, the particle is inciding above the barrier.

Figure 5 displays the transmission time, in units of t_0, as a function of the barrier width a, for $k/k_0 = 0.8$ and several values of the barrier parameter β. The

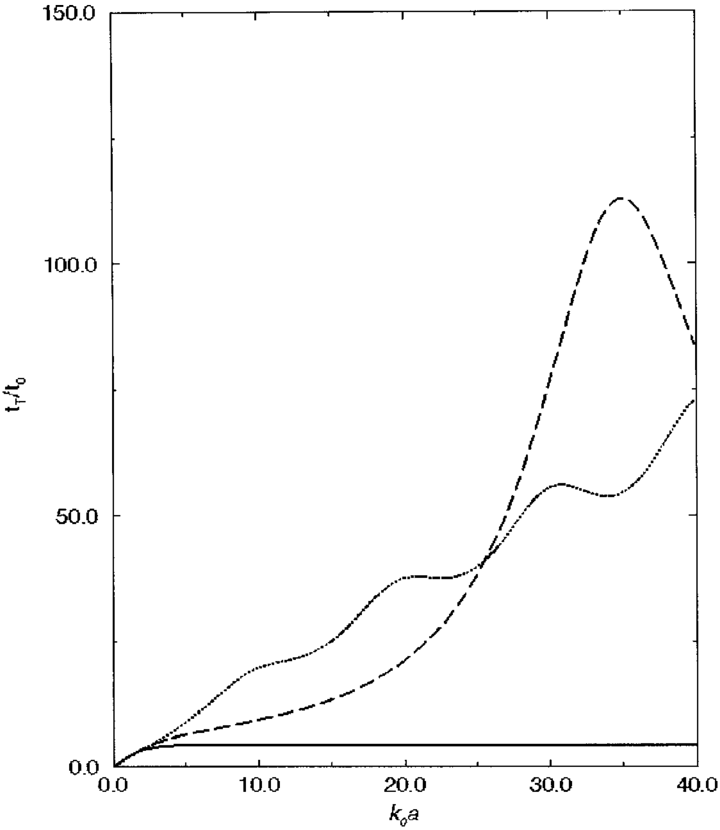

Fig. 5. Transmission time as a function of the barrier width a, for $k/k_0 = 0.8$, and several values of the barrier parameter β. Dotted line: $\beta = 0.1$; dashed line: $\beta = 0.5$; continuous line: $\beta = 0.9$.

oscillations in the transmission time disappear for a nearly rectangular potential, unless the particle reaches the potential with higher energy than the barrier height (see next figure).

Figure 6 displays the transmission time, in units of t_0, as a function of the barrier width a, for $k/k_0 = 1.1$ (particle inciding above the barrier), and several values of the barrier parameter β.

Finally, by taking the Taylor expansion of the Airy functions, $Ai(-\xi_a)$, $Bi(-\xi_a)$ and is derivative $Ai'(-\xi_a)$, $Bi'(-\xi_a)$ around ξ_0, it can be shown that the scattering coefficients associated with the trapezoidal potential reproduce those associated with the rectangular potential (limit of $\beta \to 1$) (Iwamoto *et al.*, in press). Some cumbersome but straighforward calculations show that in this limit, and

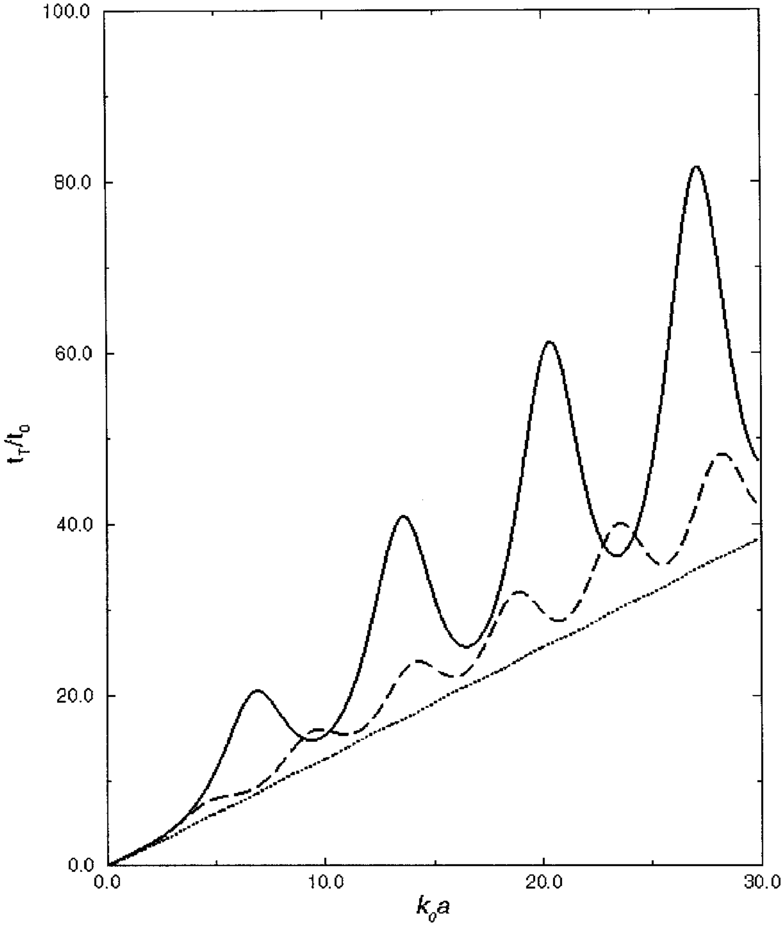

Fig. 6. Transmission time as a function of the barrier width a, for $k/k_0 = 1.1$, and several values of the barrier parameter β. Dotted line: $\beta = 0.01$; dashed line: $\beta = 0.5$; and continuous line: $\beta = 0.99$.

when the particle is inciding above the barrier, the reflection and transmission times coincide with the phase time. This result is seen in Fig. 3 and 6, continuous line.

When $\beta \ll 1$, the behavior of transmission time is the same as for a linear potential discussed in Goto *et al.* (2002).

5. ACKNOWLEDGMENT

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