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Scattering Coefficients for a Trapezoidal Potential

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The trapezoidal potential is the result of the superposition of a rectangular barrier and a linear potential. It has interest in the field of solid-state physics as long as heterostructures are concerned. The determination and discussion of the scattering coefficients for this potential revealed unknown properties of the Airy functions.

KEY WORDS: scattering coefficients; linear potential; trapezoidal potential; Airy functions.

1. INTRODUCTION

The trapezoidal potential is associated with interesting problems found in nanoheterostructure studies. In the field of semiconductors, the tunneling problem is quite important and some mathematical modeling is required. The Schottky potential, for example, can be modeled by a linear potential and plays a central role in the theoretical efforts to describe the phenomenology observed in that field.

The passage of electrons in a semiconductor from the valence band to the transmission one can be achieved, or stimulated, by an applied external electric field. In some situations, the electrons must overcome an internal energy gap that can be modeled by a rectangular potential. The superposition of these two potentials (the Schottky potential, modeled by a linear potential, and the rectangular one) looks like a trapezoidal potential. So there is some interest in considering this situation and exploring some of its characteristics. This is the central content of the paper.

In the next section, we define the trapezoidal barrier and solve the corresponding Schroedinger equation. Some convenient functions that are here defined have been proven to be very useful in the algebraic analysis of the problem. The

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scattering coefficients are found analytically in terms of these functions. Section 3 concerns the limit in which the trapezoidal potential reduces to a linear one. The rectangular potential limit is discussed in Section 4. The scattering coefficients for the linear and rectangular potential, known in the literature, are summarized in the Appendix.

2. THE TRAPEZOIDAL BARRIER

The trapezoidal barrier is the result of the superposition of a rectangular and a linear potential. It is described mathematically by

$$V(x) = \begin{cases} 0, & x < 0 \\ V_0 + \frac{(V_1 - V_0)}{a} x & 0 \leq x \leq a \\ 0, & x > a \end{cases}, \qquad V_0 \geq V_1 \tag{2.1}$$

where V_0 is the maximum height (greater trapeze leg) of the barrier (at $x = 0$) and V_1 is the lower height (smaller leg) at $x = a$.

Let us introduce the dimensionless parameter β defined as

$$\beta = \frac{V_1}{V_0}, \qquad 0 \leq \beta \leq 1 \tag{2.2}$$

Clearly, the case $\beta = 0 (V_1 = 0)$ corresponds to a pure linear potential (modeling the Schottky potential), while when $\beta = 1 (V_1 = V_0)$, we obtain a pure rectangular barrier of height V_0 and width a.

In terms of β, the potential (2.1) can be defined in the region $0 \leq x \leq a$ as

$$V(x) = V_0 + (\beta - 1) V_0 \frac{x}{a}$$

or

$$V(x) = V_0 \left(1 - \eta \frac{x}{a} \right), \quad 0 \leq x \leq a \tag{2.3}$$

where the parameter

$$\eta = 1 - \beta \tag{2.4}$$

has been proven more convenient for the algebraic analysis. In terms of η, we get a pure rectangular potential when $\eta = 0$ and a pure linear potential when $\eta = 1$.

The time-independent Schroedinger equation for a particle of mass m and energy E associated with this problem reads

$$\frac{d^2 \psi(x)}{dx^2} = - \left(\eta \frac{x}{a} + \epsilon^2 - 1 \right) k_0^2 \psi(x) \tag{2.5}$$

where

$$\begin{aligned} \epsilon &= k/k_0 \\ k^2 &= 2mE/\hbar^2 \\ k_0^2 &= 2mV_0/\hbar^2 \\ \rho^2 &= k_0^2 - k^2 \end{aligned} \tag{2.6}$$

where the definition of ρ is anticipated for future usage.

The solution to equation (2.5) is easily found if we introduce the "natural" variable ξ defined as

$$\xi = \xi(x) = q_0 \left(\eta \frac{x}{a} + \epsilon^2 - 1 \right), \quad \eta \neq 0 \tag{2.7}$$

where

$$q_0 = (k_0 a)^{2/3} \eta^{-2/3} \tag{2.8}$$

In terms of ξ, Eq. (2.5) reads

$$\frac{\partial^2 \psi(\xi)}{\partial \xi^2} = -\xi \psi(\xi) \tag{2.9}$$

whose solutions are known to be expressed in terms of the Airy functions $Ai(-\xi)$ and $Bi(-\xi)$ (Abramowitz *et al.*, 1970).

Therefore, the general solution for a particle arriving from the left on the trapezoidal barrier potential (2.3) is then given by

$$\psi_k(x) = \begin{cases} \psi_1(x) = e^{ikx} + A\, e^{-ikx} & x < 0 \\ \psi_2(x) = B Ai(-\xi) + C\, Bi(-\xi), & 0 \leq x \leq a. \\ \psi_3(x) = D\, e^{ikx}, & x > a \end{cases} \tag{2.10}$$

The quantities A, B, C, and D can be determined as usual by imposing continuity of the solution and its derivative in the borders of the potential. For this purpose, it is convenient to introduce the functions $F(\xi)$ and $G(\xi)$ defined by

$$F(\xi) = ikAi(-\xi) - \eta \frac{q_0}{a} Ai'(-\xi), \quad \eta \neq 0 \tag{2.11}$$

$$G(\xi) = ikBi(-\xi) - \eta \frac{q_0}{a} Bi'(-\xi), \quad \eta \neq 0 \tag{2.12}$$

where the prime means derivative with respect to the variable $-\xi$. Continuity conditions of ψ_k and its spatial derivative at $x = 0$ and $x = a$ determine the scattering coefficients A, B, C, and D as

$$A = A(k) = -\frac{F^*(\xi_a)G^*(\xi_0) - G^*(\xi_a)F^*(\xi_0)}{\Delta} \tag{2.13}$$

$$B = B(k) = \frac{-2ikG^*(\xi_a)}{\Delta} \tag{2.14}$$

$$C = C(k) = \frac{2ikF^*(\xi_a)}{\Delta} \tag{2.15}$$

and

$$D = D(k) = \frac{F^*(\xi_a)G(\xi_a) - G^*(\xi_a)F(\xi_a)}{\Delta} e^{-ika} = \frac{2ikq_e}{\pi a \Delta} \eta e^{-ika} \tag{2.16}$$

where

$$\xi_0 = \xi(0) = q_0(\epsilon^2 - 1) \tag{2.17}$$

$$\xi_a = \xi(a) = q_0(\epsilon^2 + \eta - 1), \qquad \eta \neq 0 \tag{2.18}$$

$$\Delta = G(\xi_0)F^*(\xi_a) - F(\xi_0)G^*(\xi_a) \tag{2.19}$$

and use was made of the Wronskian $W[Ai(x), Bi(x)] = 1/\pi$ (Abramowitz *et al.*, 1970). The star in (2.13)–(2.19) means complex conjugate.

From now on, we will be particularly interested only in A and D, the reflection and transmission coefficients, respectively. D is already expressed in á suitable form, Eq. (2.16), for our further discussion.

By introducing the auxiliary quantities

$$R_1 = \epsilon^2[A_i(-\xi_0)B_i(-\xi_a) - A_i(-\xi_a)B_i(-\xi_0)] \tag{2.20}$$

$$R_2 = \frac{q_0^2\eta^2}{(k_0a)^2}[A_i'(-\xi_a)B_i'(-\xi_0) - A_i'(-\xi_0)B_i'(-\xi_a)] \tag{2.21}$$

$$I_1 = \frac{\epsilon q_0 \eta}{k_0 a}[A_i(-\xi_a)B_i'(-\xi_0) - A_i'(-\xi_0)B_i(-\xi_a)], \quad \eta \neq 0 \tag{2.22}$$

and

$$I_2 = \frac{\epsilon q_0 \eta}{k_0 a}[A_i'(-\xi_a)B_i(-\xi_0) - A_i(-\xi_0)B_i'(-\xi_a)], \quad \eta \neq 0 \tag{2.23}$$

we can rewrite the reflection coefficient $A(k)$ and Δ as

$$A(k) = \frac{-N_A}{\Delta} \tag{2.24}$$

and

$$\Delta = k_0^2[(R_2 - R_1) + i(I_1 - I_2)] \tag{2.25}$$

with

$$N_A = k_0^2[(R_1 + R_2) + i(I_1 + I_2)] \tag{2.26}$$

By expressing N_A and Δ in polar representation

$$N_A = |N_A|\, e^{i\alpha} \tag{2.27}$$

$$\Delta = |\Delta| \, e^{i\lambda} \tag{2.28}$$

with

$$|N_A| = k_0^2 \sqrt{(R_1 + R_2)^2 + (I_1 + I_2)^2} \tag{2.29}$$

$$\tan\alpha = \frac{I_1 + I_2}{R_1 + R_2} \tag{2.30}$$

and

$$|\Delta| = k_0^2 \sqrt{(R_2 - R_1)^2 + (I_1 - I_2)^2} \tag{2.31}$$

$$\tan\lambda = \frac{I_1 - I_2}{R_2 - R_1} \tag{2.32}$$

the reflection coefficient can be written in a very compact way as

$$A(k) = -\frac{|N_A|}{|\Delta|} \, e^{\imath\alpha} \, e^{-\imath\lambda} \tag{2.33}$$

3. THE LINEAR POTENTIAL LIMIT

By simple inspection of equations (2.11)–(2.32), it can be seen that the limit $\eta = 1$ reproduces exactly all the scattering coefficients associated with the linear potential obtained in Goto *et al*. (2002).

On the other hand, the limit $\eta \to 0$, which is expected to reproduce the results for the rectangular barrier, is not so simple and requires careful analysis. This limit is dealt with in the next section.

4. THE RECTANGULAR POTENTIAL LIMIT

In order to obtain the rectangular potential results from the trapezoidal barrier ones, we start by Taylor expanding the Airy function $Ai(x)$ in some neighborhood $|x - x_0| < R$ of the point x_0 in a series of power of $x - x_0$

$$Ai(x) = \sum_{n=0}^{\infty} \frac{1}{n!} Ai^{(n)}(x_0)(x - x_0)^n. \tag{4.1}$$

The differential equation for the Airy function

$$Ai''(x) = x_0 Ai(x_0) \tag{4.2}$$

allows us to express the derivatives of order 2 and higher in terms of $Ai(x_0)$ and $Ai'(x_0)$. Thus, the expansion (4.1) can be expressed as two infinite sums, one multiplying $Ai(x_0)$ and the other multiplying $Ai'(x_0)$. A careful inspection of these infinite sums identify terms that brought together reproduce the power expansion of the hyperbolic sine and hyperbolic cosine functions and other terms, as it will be shown in the following.

In order to simplify notation, let us define the quantities X and Z as

$$X = x - x_0 \tag{4.3}$$

and

$$Z = X\sqrt{x_0} \tag{4.4}$$

In terms of these quantities, the expansion (4.1), after some rearrangement of the terms, reads

$$\begin{aligned} Ai(x) = Ai(x_0)\Bigg[&\frac{Z^2}{2!} + \frac{Z^4}{4!} + \frac{Z^6}{6!} + \ldots + 1 + \frac{X^3}{6} + \frac{X^6}{180} + \ldots + \frac{x_0 X^5}{30} \\ &+ \frac{x_0 X^8}{1440} + \ldots\Bigg] + Ai'(x_0)\Bigg[X\left(1 + \frac{x_0 X^2}{3!} + \frac{x_0^2 X^4}{5!} + \ldots\right) \\ &+ \frac{X^4}{12} + \frac{X^7}{504} + \ldots + \frac{x_0 X^6}{120} + \frac{13 x_0 X^9}{90720} + \ldots\Bigg] \end{aligned} \tag{4.5}$$

The first terms in the infinite sum multiplying $Ai(x_0)$ are recognized as the Taylor expansion of the function cosh (Z), and the first terms in the infinite sum multiplying $A'(x_0)$ are recognized as the Taylor expansion of X $\sinh(Z)/Z$. Therefore, we can express the expanison (4.1) as

$$Ai(x) = Ai(x_0)\cosh Z + Ai'(x_0)X\frac{\sinh Z}{Z} + O(X^3) \tag{4.6}$$

Proceeding along the same steps, we obtain the Taylor expansions

$$Ai'(x) = Ai'(x_0)\cosh Z + Ai(x_0)x_0 X\frac{\sinh Z}{Z} + O(X^2) \tag{4.7}$$

$$Bi(x) = Bi(x_0)\cosh Z + Bi'(x_0)X\frac{\sinh Z}{Z} + O(X^3) \tag{4.8}$$

$$Bi'(x) = Bi'(x_0)\cosh Z + Bi(x_0)x_0 X\frac{\sinh Z}{Z} + O(X^2) \tag{4.9}$$

Notice that Eqs. (4.7) and (4.9) can be obtained directly from (4.6) and (4.8), respectively.

Coming back to the main problem of this section, let

$$x = -\xi_a = -(\xi_0 + \eta q_0) \tag{4.10}$$

and

$$x_0 = -\xi_0 = q_0\rho^2/k_0^2 = (k_0 a)^{2/3}\frac{\rho^2}{k_0^2}\eta^{-2/3} \tag{4.11}$$

where ρ and q_0 are defined in (2.6) and (2.8), respectively. A straightforward calculation leads to

$$X = -\eta q_0 \tag{4.12}$$

and

$$Z = -\rho a \tag{4.13}$$

where a is the barrier width.

In terms of ξ_a and ξ_0, we have that

$$\begin{aligned} Ai(-\xi_a) &= Ai(-\xi_0)\cosh(\rho a) \\ &\quad -(k_0 a)^{2/3}\eta^{1/3} Ai'(-\xi_0)\frac{\sinh(\rho a)}{\rho a} + O(\eta) \end{aligned} \tag{4.14}$$

$$\begin{aligned} Ai'(-\xi_a) &= Ai'(-\xi_0)\cosh(\rho a) \\ &\quad -\frac{1}{\eta^{1/3}}\frac{\rho^2}{k_0^2}(k_0 a)^{4/3} Ai(-\xi_0)\frac{\sinh(\rho a)}{\rho a} + O(\eta) \end{aligned} \tag{4.15}$$

and analogous expressions for $Bi(-\xi_a)$ and $Bi'(-\xi_a)$.

Substituting these results into equations (2.20)–(2.23), the quantities R_1, R_2, I_1, and I_2 reduce to

$$R_1 = \epsilon^2 \frac{X}{\pi}\frac{\sinh Z}{Z} + O(X^3) = \frac{k^2\left(k_0^2 a\right)^{2/3}}{k_0^2\pi}\frac{\sinh(\rho a)}{\rho a}\eta^{1/3} + O(\eta) \tag{4.16}$$

$$\begin{aligned} R_2 &= \frac{q_0^2\eta^2}{(k_0 a)^2}\frac{x_0 X}{\pi}\frac{\sinh Z}{Z} + O(X^3) \\ &= \frac{\rho^2\left(k_0^2 a\right)^{2/3}}{k_0^2\pi}\frac{\sinh(\rho a)}{\rho a}\eta^{1/3} + O(\eta) \end{aligned} \tag{4.17}$$

$$I_1 = \frac{\epsilon q_0\eta}{\pi k_0 a}\cosh Z + O(X^3) = \frac{k^2\left(k_0^2 a\right)^{2/3}}{\pi k_0^2 a}\eta^{1/3}\cosh(\rho a) Z + O(\eta) \tag{4.18}$$

$$I_2 = -I_1 \tag{4.19}$$

where use was made of the Airy function Wronskian $W[Ai(x), Bi(x)] = 1/\pi$ (Abramowitz *et al.*, 1970) and of Eqs. (2.8), (4.11), (4.12), and (4.13).

Now we can combine the quantities R_1, R_2, I_1, and I_2 to obtain, in lower order of η

$$R_1 + R_2 = \frac{(k_0 a)^{2/3}}{\pi}\frac{\sinh(\rho a)}{\rho a}\eta^{1/3} \tag{4.20}$$

$$R_2 - R_1 = \frac{\left(k_0^2 a\right)^{2/3}}{k_0^2\pi}\frac{\sinh(\rho a)}{\rho a}\eta^{1/3}(\rho^2 - k^2) \tag{4.21}$$

$$I_1 + I_2 = 0 \tag{4.22}$$

$$I_1 - I_2 = \frac{2k\left(k_0^2 a\right)^{2/3}}{\pi k_0 a}\eta^{1/3}\cosh(\rho a) \tag{4.23}$$

When Eqs. (4.20) through (4.23) are substituted into Eqs. (2.29) through (2.32), we obtain

$$|N_A| = \frac{k_0^2 (k_0 a)^{2/3}}{\rho a \pi}\eta^{1/3}\sinh(\rho a) \tag{4.24}$$

$$\tan\alpha = 0 \tag{4.25}$$

$$|\Delta| = \frac{k_0^2 (k_0 a)^{2/3}}{\rho a \pi}\eta^{1/3}\sqrt{\sinh^2(\rho a) + \frac{4k^2\rho^2}{k_0^4}} \tag{4.26}$$

$$\tan\lambda = \tan(2\theta)\coth(\rho a) \tag{4.27}$$

where the angle θ is defined by the relations

$$k = k_0 \cos\theta \quad \text{and} \quad \rho = k_0 \sin\theta \tag{4.28}$$

4.1. The Reflection Coefficient

Now we are ready to evaluate the reflection coefficient A given in Eq. (2.33), for a trapezoidal potential, in the limit when η goes to zero. When Eqs. (4.24) and (4.26) are substituted into (2.33), we obtain, since $\alpha = 0$ according to Eq. (4.25),

$$A = -\frac{\sinh(\rho a)\, e^{-i\lambda}}{\sqrt{\sinh^2(\rho a) + 4k^2\rho^2/k_0^4}} \tag{4.29}$$

with λ defined in (4.27) and (4.28).

Equation (4.29) is exactly the reflection coefficient for a rectangular potential (Al) given in the Appendix.

4.2. The Transmission Coefficient

Also straightforward is the evaluation of the transmission coefficient D given in Eq. (2.16), for a trapezoidal potential, in the limit when η goes to zero. First, let us rewrite (2.16) as

$$D = \frac{2ikq_0}{\pi a \Delta}\eta\, e^{-ika} = -\frac{2ik\eta^{1/3}(k_0 a)^{2/3} e^{-ika}}{\pi a \Delta} \tag{4.30}$$

where use was made of Eq. (2.8). When Eqs. (2.28) and (4.26) are substituted into equation (4.30), we obtain

$$D = \frac{2i\left(k\rho/k_0^2\right)e^{-ika}\,e^{-i\lambda}}{\sqrt{\sinh^2(\rho a) + 4k^2\rho^2/k_0^4}} \tag{4.31}$$

which is the transmission coefficient for a rectangular barrier (A4) given in the Appendix.

5. DISCUSSION AND CONCLUSION

The trapezoidal potential was analytically treated in detail. Interesting properties of the Airy functions and its first derivative that were unknown, at least to the authors, were revealed in the analysis. The scattering coefficients were determined and it was shown that they have the appropriate limit when the trapezoidal potential is reduced to a linear or a rectangular one.

It is interesting to compare the behavior of the transmission coefficient for a trapezoidal barrier with the known behavior of the transmission coefficient for a rectangular barrier.

In Fig. 1, we show the transmission coefficient (2.16) ($|D|^2$ actually) in function of the width barrier for $k/k_0 = 0.92$ and several values of the barrier parameter β defined in (2.2). Notice that $\beta = 1$ reproduces the rectangular potential. The effect of the external electric field is reflected in the oscillations that appear for lower values of β. This effect can be understood since the smaller values of β imply a greater dominance of the linear potential (read: The external electric field).

These oscillations are much clear in Figs. 2 (where β is fixed at 0.3) and 3 (where k/k_0 is fixed at 0.96). This interesting oscillation feature is very similar to the case of a particle with $E > 0$ inciding on a square-well potential (Bastard, 1988). In the present case, as it is clear from the three figures, the oscillations start appearing for high values of k/k_0 which means particles inciding at the highest part of the trapezoidal barrier, i.e., almost overcoming the potential.

APPENDIX

In this appendix we present some known results for the rectangular (Kobe *et al.*, 2001) and linear (Goto *et al.*, 2002) potentials.

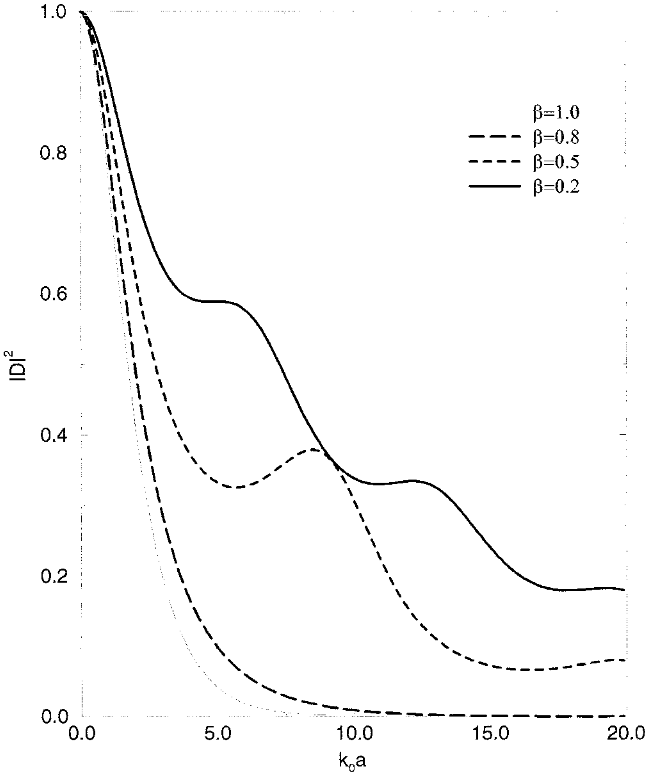

Fig. 1. Transmission coefficient $|D|^2$ for a trapezoidal barrier as function of the barrier width for several values of β and fixed inciding energy ($k/k_0 = 0.92$).

A. 1. Rectangular Barrier Reflection Coefficient

$$A = -\frac{\sinh(\rho a)\, e^{-i\lambda}}{\sqrt{\sinh^2(\rho a) + 4k^2\rho^2/k_0^4}} \tag{A1}$$

where

$$\tan\lambda = \tan(2\theta)\coth(\rho a) \tag{A2}$$

and the angle θ is defined by the relations

$$k = k_0\, \cos\theta \quad \text{and} \quad \rho = k_0\, \sin\theta \tag{A3}$$

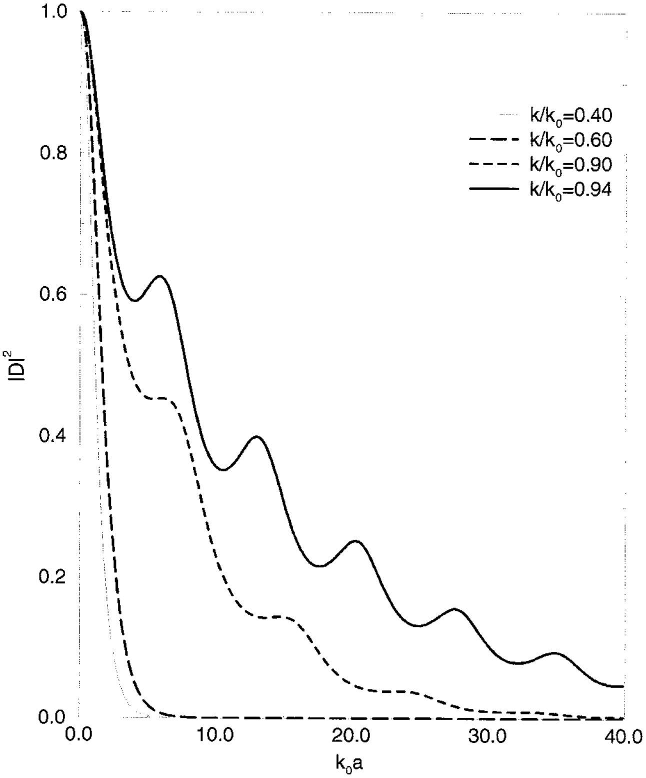

Fig. 2. Transmission coefficient $|D|^2$ for a trapezoidal barrier as function of the barrier width for several values of the inciding energy and β fixed at 0.3.

A. 2. Rectangular Barrier Transmission Coefficient

$$D = -\frac{2i\left(k\rho/k_0^2\right)e^{-ika}\,e^{-i\lambda}}{\sqrt{\sinh^2(\rho a) + 4k^2\rho^2/k_0^4}} \tag{A4}$$

It can be seen easily that

$$|A|^2 + |D|^2 = 1 \tag{A5}$$

as it should be.

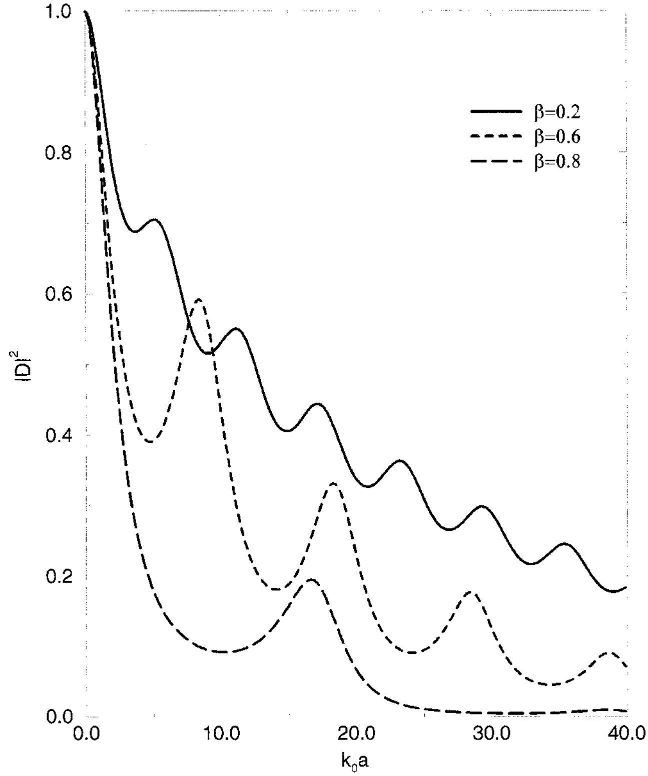

Fig. 3. Transmission coefficient $|D|^2$ for a trapezoidal barrier as function of the barrier width for several values of β and fixed inciding energy ($k/k_0 = 0.96$).

A. 3. Linear Barrier Reflection Coefficient (Goto *et al.*, 2002)

$$A = \frac{G^*(\xi_a)F^*(\xi_0) - F^*(\xi_a)G^*(\xi_0)}{\Delta} \tag{A6}$$

where

$$\Delta = G(\xi_0)F^*(\xi_a) - F(\xi_0)G^*(\xi_a) \tag{A7}$$

The quantities F, G, ξ_0, and ξ_a are defined in (2.11), (2.12), (2.17), and (2.18), respectively, with $\eta = 1$. Linear barrier transmission coefficient

$$D = \frac{F^*(\xi_a)G(\xi_a) - F(\xi_a)G^*(\xi_a)}{\Delta} \tag{A8}$$

the other coefficients being

$$B = -\frac{2ikG^*(\xi_a)}{\Delta} \tag{A9}$$

$$C = \frac{2ikF^*(\xi_a)}{\Delta} \tag{A10}$$

REFERENCES

Abramowitz, M. and Stegun, I. (1970). *Handbook of mathematical functions,* Dover, New York.

Bastard, Gerard (1988). *Wave mechanics applied to semi-conductor heterostructure.* Hasted Press, John Wiley, New York.

Goto, M., Iwamoto, H., Aquino, V. M., and Aguilera-Navarro, V. C. (2002). *International Journal of Theoretical Physics* **41**, 877.

Kobe, Donald H., Iwamoto, H., Goto, M., and Aguilera-Navarro, V. C. (2001). *Physical Review A*, 022104.