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Total delay time and tunnelling time for non-rectangular potential barriers

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Abstract. The total delay time for a particle tunnelling through a non-rectangular potential barrier is calculated as an explicit function of the potential energy $U(x)$, on a rigorous mathematical basis. The resulting expression is valid for sufficiently smooth potentials. It represents a physically well defined quantity that is measured in the experiment directly. In particular, an explicit expression for the tunnelling time related to the potential $U_0/\cosh^2(x/l)$ is obtained. It is valid if the particle's wavelength, taken far away from the barrier, is small compared with the barrier's effective length l, irrespective of the value of the barrier penetration integral. Exact sufficient conditions for the validity of Connor's parabolic connection formulae are established.

1. Introduction

The problem of tunnelling time, i.e. the time scale associated with the tunnelling of a quantum particle through a potential barrier, is currently a subject under active discussion [1–5]. One of the reasons for an increased interest in the problem is that, due to recent advances in experimental techniques, new high-precision measurements of delay and traversal times have been carried out and reliable experimental data have become available [3, 6–11].

From the theoretical standpoint the problem of the tunnelling time turned out to be a difficult one. Although the problem has been investigated in a number of theoretical works, there is still no generally accepted method available for calculating the tunnelling time, in spite of the importance of this quantity for modern microelectronic tunnelling devices [12, 13]. The need for an appropriate theory becomes especially apparent in view of the very recent, high-precision measurements of single-photon delay time [1], which not only confirm the superluminal photon velocity in the tunnelling process but also report an agreement with Wigner's [14] definition of the delay time.

There seems to be only one non-trivial potential

$$U(x) = \frac{U_0}{\cosh^2(x/l)} \qquad (U_0 > 0) \tag{1}$$

for which the exact solution of the tunnelling problem is known. However, even for this potential, it is not known what the tunnelling time is equal to. For more complicated potentials, the tunnelling problem may be solved only approximately. Taking into account that in tunnelling devices the electron wavelength is small in comparison with typical scales

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associated with the devices [15], we might hope to calculate the tunnelling transmission amplitude using the WKB approximation. However, the resulting WKB expression for the modulus of the transmission amplitude t is valid only if $|t|$ is exponentially small. This requirement is too restrictive to use the result in practice. Moreover, within the WKB approximation it is impossible to obtain the correct phase of the transmission amplitude, which is important for calculating the tunnelling time.

The difficulty of the problem of tunnelling times resides in the fact that, to deal with this problem, we have to extend the semiclassical treatment of the tunnelling problem to energy regions where the phase integral γ (12) is comparable with unity or even less. Several approaches have been developed to manage the latter problem. The first method was proposed by Kemble [16] and then developed in many papers (see [17–19] and references therein). In [16], special attention has been paid to the estimation of the error bounds to the resulting expression for the transmission amplitude. However, the expressions for the error bounds given in this work are difficult to use since they necessitate a search for optimal paths in the complex plane that minimize an integral of a rather complicated function. Besides, by the method of Kemble it is impossible to obtain the phase of the transmission amplitude, or that of the reflection amplitude (see [20, p 112]).

Another approach was first formulated by Miller and Good [21] and then developed by many writers (see [22] and references therein). The idea of Miller and Good [21] (see also [23]) is to obtain the semiclassical connection formulae in the vicinity of the top of the potential barrier by using the exact solutions of Schrödinger's equation in the *parabolic* potential. These solutions are used to bridge the region that contains *two* turning points, where the WKB approximation fails. This is done in much the same way as the exact solutions of Schrödinger's equation in the *linear* potential (the Airy functions) were used by Gans [24] and Jeffreys [25] to bridge the region with just *one* turning point in order to derive the conventional connection formulae. However, while the one-turning-point connection formulae have been put on a rigorous mathematical basis (see [19] and references therein), the parabolic connection formulae (first explicitly written by Connor [26, equations (14) and (15)]) have up to now not been given a mathematical proof. The conditions for the validity of the parabolic connection formulae have not been established. Hence questions about the regions for them to apply, and the error bounds to those formulae, remain open. The accuracy of the results obtained for a given potential may be estimated only numerically (see, for example, [22] and references therein).

That these questions are not of purely mathematical interest has been demonstrated by Dickinson [27]. Indeed, the parabolic potential is not the only one that may be used for establishing the two-turning-points connection formulae. Dickinson [27] pointed out that using three different comparison potentials—the parabolic potential $(-x^2)$ used by Connor [26], the potential $1/\cosh^2(x/l)$ used by Soop [28], and the inverted Morse potential used by Dickinson [27]—results in three groups of connection formulae that are *all different*. By comparing the three types of connection formulae with each other, Dickinson [27] found that in some energy regions (near the top of the barrier) the differences between the three groups become negligible if the barrier is very thick. But in other energy regions (near the base of the barrier) the differences between the three groups of formulae remain significant even for thick barriers. The differences between the connection formulae result, in particular, in different evaluations of the resonance phase shifts in molecular orbiting collisions [26, 27]. The analysis by Dickinson suggests that even for energy paths *just below* the top of the barrier, *finite* portions of the potential barrier are essential for establishing the connection formulae, not just the infinitesimal vicinity of the barrier's top.

The sufficient conditions for the parabolic connection formulae, which are derived below in the present paper, allow us to establish the energy regions where these formulae are valid, and to explain the results obtained in [27]. Our approach consists in using the Weber functions to obtain a uniform (with respect to *all* real x) asymptotic representation for a particle's tunnelling state. The idea of using the Weber functions for uniform asymptotic representations of the solutions of linear differential equations of second order, in problems with two real turning points, is not a new one. This idea has been formulated by Erdélyi *et al* [29], Olver [30] and Langer [31]. Uniform asymptotic expansions for the Weber functions, which cover virtually entire complex planes of their arguments and parameters, have been obtained by Olver [30]. A number of important theorems as well as the very possibility of asymptotic representations in terms of the Weber functions have been proven by Langer [31]. Pike [32] has shown that the formal application of the Weber functions to the bound-state problem and to the tunnelling-state problem reproduces the known results of the WKB approximation. Nonetheless, important as these works are, they should rather be considered as preliminary steps towards the complete solution of the general problem we are interested in. It seems that little or no progress has been made since then, perhaps due to mathematical difficulties related to the problem [32, 33].

In the present paper, the main relations for the tunnelling of a quantum particle through a one-dimensional potential barrier are obtained in section 2. In section 3, the sufficient condition for these relations is investigated. In section 4, the formulae for the transmission and the reflection amplitudes are obtained along with the error bounds to them. The total delay time for a particle's tunnelling is derived and discussed in section 5. An explicit expression for the tunnelling time associated with the potential (1) is obtained in section 6. It is found to be valid if $kl \gg 1$, irrespective of the value of the phase integral; throughout the paper we denote by k the classical momentum of a free particle having total energy $E > 0$, that is,

$$k = \sqrt{2m\,E} \qquad (\hbar = 1) \tag{2}$$

and l is the effective length of the barrier that appears in (1). In section 7, a general discussion and a comparison with the known results are given.

2. Basic relations

Let us consider the tunnelling of a particle having mass m and total energy $E > 0$, through a finite, classically forbidden region on the real x-axis. If the potential energy of the particle is $U(x)$, then the classically inaccessible region is defined by the relation

$$U(x) > E > 0\,.$$

In this paper we assume that (i) $U(x)$ is a real, continuous, and three times differentiable function on the whole of the real axis; (ii) $U(x)$ vanishes as $x \to \pm\infty$; (iii) $U(x)$ is integrable over the real axis, that is

$$\int_{-\infty}^{+\infty} U(x)\,\mathrm{d}x < \infty\,. \tag{3}$$

The relation (3) allows us to define a characteristic length l associated with the potential $U(x)$. If $U_0 > 0$ is the typical value of $U(x)$ on the real axis, then

$$l = \frac{1}{U_0}\left|\int_{-\infty}^{+\infty} U(x)\,\mathrm{d}x\right| < \infty\,.$$

The wavefunction $\psi(x)$ that represents the particle's tunnelling state in the potential $U(x)$ satisfies the Schrödinger equation

$$\frac{d^2\psi}{dx^2} + p^2(x)\psi(x) = 0\,. \tag{4}$$

The function $p^2(x)$ in (4),

$$p^2(x) = 2m\,[E - U(x)] \qquad (\hbar = 1) \tag{5}$$

coincides with the square of the classical momentum of the particle for those values of x that satisfy

$$U(x) \leqslant E\,.$$

The semiclassical treatment of physical problems related to equation (4) is generally based on the theory of uniform asymptotic representations for the solutions of equation (4). As is known, in the domains where $p^2(x)$ may be considered to be a large and slowly varying function, the conventional WKB approximation applies, which makes use of exponential functions for representing the solutions of equation (4).

In the neighbourhoods of the turning points defined by $p(x) = 0$, the WKB approximation fails. However, if there is just one turning point within a region, but in other respects the function $p^2(x)$ is smooth on the scale associated with the particle's average wavelength, then the wavefunction $\psi(x)$ may be asymptotically represented in terms of the Airy functions uniformly with respect to all x in the region, without exception for the turning point [19]. In a tunnelling state problem, we have to find a uniform asymptotic representation for the wavefunction in a region containing two turning points.

We restrict the ensuing analysis to the energy regions where the equation $p^2(x) = 0$, considered on the real axis $-\infty < x < +\infty$, has two and only two simple, distinct, real roots $x = a$ and $x = b$,

$$p^2(x) = p^2(x) = 0 \qquad a < b$$

such that $p^2(x) < 0$ if $a < x < b$, and $p^2(x) > 0$ if $x < a$ or $x > b$. We assume that $p(x) > 0$ for $x < a$ or $x > b$.

As a basic large parameter in the Schrödinger equation (4) we take

$$k_0 l \gg 1 \tag{6}$$

where k_0 is the characteristic wavenumber associated with the potential $U(x)$

$$k_0 = \sqrt{2m\,U_0}\,. \tag{7}$$

We assume the condition (6) to hold throughout the paper.

Thus, we have to consider the problem of finding an asymptotic representation, which should be valid uniformly with respect to all real x, $-\infty < x < +\infty$, for the wavefunction $\psi(x)$ that describes the particle's tunnelling state in the potential $U(x)$. The appropriate functions to represent $\psi(x)$, which in problems with two real turning points fulfil the role of the Airy functions, are the Weber functions [29–31].

The usual scheme consists in applying Liouville's transformation [19] to equation (4). Here we shall derive the final relations in an equivalent but more straightforward way. Let us define a real, continuous, strictly increasing function, on the real axis $\xi = \xi(x)$, that satisfies the equation

$$\left(\frac{d\xi}{dx}\right)^2 = \frac{p^2(x)}{\xi^2 - \xi_0^2} \tag{8}$$

with a real, positive constant ξ_0. The constant ξ_0 is completely determined by equation (8) if we consider the latter along with the requirement that the derivative $\mathrm{d}\xi/\mathrm{d}x$ be finite, continuous and positive on the real axis including at the two turning points $x = a$ and $x = b$, i.e.

$$\frac{\mathrm{d}\xi}{\mathrm{d}x} > 0 \qquad (-\infty < x < +\infty)\,.$$

Thus we find

$$\xi_0^2 = \frac{2}{\pi}\int_a^b p(x)\,\mathrm{d}x\,. \tag{9}$$

The function $\xi(x)$ is found to be determined by the following relations:

(i) if $x \leqslant a$, then $\xi \leqslant -\xi_0$ and

$$\int_\xi^{-\xi_0} \left(\xi^2 - \xi_0^2\right)^{1/2} \mathrm{d}\xi = \int_x^a p(x)\,\mathrm{d}x \tag{10a}$$

(ii) if $a \leqslant x \leqslant b$, then $-\xi_0 \leqslant \xi \leqslant +\xi_0$ and

$$\int_{-\xi_0}^{\xi} \left(\xi_0^2 - \xi^2\right)^{1/2} \mathrm{d}\xi = \int_a^x |p(x)|\,\mathrm{d}x \tag{10b}$$

(iii) if $x \geqslant b$, then $\xi \geqslant \xi_0$ and

$$\int_{\xi_0}^{\xi} \left(\xi^2 - \xi_0^2\right)^{1/2} \mathrm{d}\xi = \int_b^x p(x)\,\mathrm{d}x\,. \tag{10c}$$

The general properties of the function $\xi(x)$ have been investigated by Langer [31]. He proved that the formulae (10*a*–*c*) determine $\xi(x)$ not only as a continuous and strictly increasing function, but also as a function that is three times continuously differentiable on the whole of the real axis, if the above conditions upon the potential $U(x)$ are fulfilled. Thus the function $\xi(x)$ defines a one-to-one mapping of the x-axis, $-\infty < x < +\infty$, onto the ξ-axis, $-\infty < \xi < +\infty$.

Let us consider the function

$$w(x) = \left[\frac{\xi^2 - \xi_0^2}{p^2(x)}\right]^{1/4} \mathbf{D}_{\mathrm{i}\gamma-1/2}(\sqrt{2}\,\xi\,\mathrm{e}^{\mathrm{i}\pi/4}) \tag{11}$$

where $\mathbf{D}_{\mathrm{i}\gamma-1/2}(\sqrt{2}\,\xi\,\mathrm{e}^{\mathrm{i}\pi/4})$ is Weber's tunnelling function, which is related to the standard Weber functions [34] by the relation

$$\mathbf{D}_\nu(z) = D_{-\nu-1}(-\mathrm{i}z)\,.$$

The functions $D_\nu(z)$ and $\mathbf{D}_\nu(z)$ are linearly independent; their Wronskian never vanishes, whatever the (finite) complex values of z and ν might be [34]. In equation (11), $\xi = \xi(x)$ is the function of x as defined by (10*a*–*c*), and the constant γ is given by

$$\gamma = \frac{1}{2}\xi_0^2 = \frac{1}{\pi}\int_a^b |p(x)|\,\mathrm{d}x\,. \tag{12}$$

By direct differentiation we find that the function (11) satisfies the following differential equation:

$$\frac{\mathrm{d}^2 w}{\mathrm{d}x^2} + \left[p^2(x) + R(x)\right] w = 0 \tag{13}$$

where

$$\begin{aligned} R(x) &= \frac{1}{2}\,\frac{|p(x)|''}{|p(x)|} - \frac{3}{4}\,\frac{|p(x)|'^2}{|p(x)|^2} + \frac{3\xi^2 + 2\xi_0^2}{4\left(\xi^2 - \xi_0^2\right)^2}\,\frac{p^2(x)}{\xi^2 - \xi_0^2} \\ &= -(\xi')^{1/2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}(\xi')^{-1/2} \qquad \xi' \equiv \frac{\mathrm{d}\xi}{\mathrm{d}x} \end{aligned} \tag{14}$$

and the prime denotes differentiation with respect to x. Equation (13) also has another solution

$$u(x) = \left[\frac{\xi^2 - \xi_0^2}{p^2(x)}\right]^{1/4} D_{\mathrm{i}\gamma - 1/2}(\sqrt{2}\,\xi\,\mathrm{e}^{\mathrm{i}\pi/4})\,. \tag{15}$$

The Wronskian

$$w(x)\,u'(x) - u(x)\,w'(x) = -\mathrm{i}\sqrt{2}\,\mathrm{e}^{-\pi\gamma/2} \tag{16}$$

does not vanish for finite γ, so the functions (11) and (15) are linearly independent. They form the fundamental pair of solutions for equation (13).

Let us try an *exact* solution $\psi(x)$ to the Schödinger equation (4), which represents the particle's tunnelling state in the potential $U(x)$, as the sum

$$\psi(x) = w(x) + \varepsilon(x) \tag{17}$$

where $w(x)$ is given by (16), with an additional term $\varepsilon(x)$ that satisfies the boundary conditions

$$\lim_{x\to+\infty} \varepsilon(x) = 0 \qquad \lim_{x\to+\infty} \frac{\mathrm{d}\varepsilon(x)}{\mathrm{d}x} = 0\,. \tag{18}$$

Substituting (17) in (4), we see that $\varepsilon(x)$ satisfies the differential equation

$$\frac{\mathrm{d}^2\varepsilon}{\mathrm{d}x^2} + [p^2(x) + R(x)]\varepsilon(x) = R(x)\,[w(x) + \varepsilon(x)]\,. \tag{19}$$

Taking into account the relations (16) and (18), we rewrite equation (19) in an equivalent integral form

$$\varepsilon(x) = \frac{\mathrm{i}}{\sqrt{2}} \int_x^{+\infty} \mathrm{e}^{\pi\gamma/2}[w(x)\,u(t) - u(x)\,w(t)]\,R(t)\,[w(t) + \varepsilon(t)]\,\mathrm{d}t\,. \tag{20}$$

The solution to the latter integral equation is sought in the form

$$\varepsilon(x) = \left[\frac{\xi^2 - \xi_0^2}{p^2(x)}\right]^{1/4} h_\gamma(x)\,. \tag{21}$$

In view of (11) and (15), the substitution of (21) in (20) yields an equation for the correction term $h_\gamma(x)$

$$h_\gamma(x) = \int_z^{+\infty} \mathrm{d}z_1\, K_\gamma(z, z_1)\left(\frac{R(z_1)}{|p(z_1)|}\,\frac{\mathrm{d}t}{\mathrm{d}z_1}\right)\left[\mathbf{D}_{\mathrm{i}\gamma-1/2}(z_1\,\mathrm{e}^{\mathrm{i}\pi/4}) + h_\gamma(z_1)\right] \tag{22}$$

where we have denoted $z_1 = \sqrt{2}\,\xi(t)$. In equation (22), z is a function of x, $z = \sqrt{2}\,\xi(x)$, whereas the kernel is given by

$$K_\gamma(z, z_1) = -\left|\frac{z_1^2}{4} - \gamma\right|^{1/2} \mathrm{i}\,\mathrm{e}^{\pi\gamma/2} \times \left[\mathbf{D}_{\mathrm{i}\gamma-1/2}(z\,\mathrm{e}^{\mathrm{i}\pi/4})\,D_{\mathrm{i}\gamma-1/2}(z_1\,\mathrm{e}^{\mathrm{i}\pi/4}) - D_{\mathrm{i}\gamma-1/2}(z\,\mathrm{e}^{\mathrm{i}\pi/4})\,\mathbf{D}_{\mathrm{i}\gamma-1/2}(z_1\,\mathrm{e}^{\mathrm{i}\pi/4})\right]. \tag{23}$$

A complicated mathematical analysis of the integral equation (22), which is based on the *theorem on singular, integral equations* by Olver (see [19, ch 6, p 217]) results in the following conclusions:

(i) for every $\gamma \geqslant 0$, equation (22) has a unique solution $h_\gamma(x)$, which is continuous on the real axis $-\infty < x < +\infty$;

(ii) the correction term $\varepsilon(x)$ on the right-hand side of (17), which is given by (21), is negligibly small compared with $w(x)$ *for all real* x, and so it may be dropped, if the condition

$$\mathbf{E}(\gamma) \ll 1 \tag{24}$$

is fulfilled.

The function $\mathbf{E}(\gamma)$ in (24) is given by

$$\mathbf{E}(\gamma) = \int_{-\infty}^{+\infty} \frac{\mathrm{d}x}{\left|\xi^2(x) - \xi_0^2\right|^{1/2}} \left|(\xi')^{-1/2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}(\xi')^{-1/2}\right|. \tag{25}$$

It is considered as a function of the phase integral γ (12). This quantity plays a key role in the present analysis. It will be referred to as the *error-control integral*. The properties of the function $\mathbf{E}(\gamma)$ are summarized in the following section.

3. Singularities of the error-control integral

The analysis of the properties of the error-control integral $\mathbf{E}(\gamma)$ (25) is based on the definition (10*a*–*c*) of the function $\xi(x)$. To concentrate on the main features of $\mathbf{E}(\gamma)$, in this section we assume that, in addition to the above hypothesis on the particle's potential energy, the function $U(x)$ is positive and has a single local maximum on the real axis at the point $x = x_0$. Let us denote the maximum value of $U(x)$ by $U_0 = U(x_0)$. Hence the equation $p^2(x) = 0$ has two and only two distinct, simple, real roots $x = a$ and $x = b$ such that $a < b$, for every $E \in (0, U_0)$. With the foregoing conditions upon $U(x)$, we prove the following statements.

(i) The function $\mathbf{E}(\gamma)$ (25) is continuous in the interval $E \in (0, U_0)$. Inside this interval, the magnitude of $\mathbf{E}(\gamma)$ is of the order of $1/(k_0 l)$.

(ii) The points $E = U_0$ and $E = 0$ are the singular points of the function $\mathbf{E}(\gamma)$.

(iii) If the second derivative $U''(x_0) < 0$, then the singularity of the error-control integral at the point $E = U_0$ is a logarithmic one

$$\mathbf{E}(\gamma) \sim \frac{C}{k_0 l}\left|\ln\left(\frac{U_0 - E}{U_0}\right)\right| \qquad (E \to U_0 - 0)\,. \tag{26}$$

The constant factor C in (26) is given by

$$C = \frac{\sqrt{U_0}}{12^2\sqrt{2}} \frac{\left|9\,|U''(x_0)|\,U^{(IV)}(x_0) + 7\,[U'''(x_0)]^2\right|}{|U''(x_0)|^{5/2}}\,. \tag{27}$$

In general, the number C is of the order of unity. However, when $U''(x_0) \to 0$, the factor C increases as $|U''(x_0)|^{-3/2}$ for even functions $U(x)$, or as $|U''(x_0)|^{-5/2}$ otherwise.

(iv) If the second derivative is equal to zero $U''(x_0) = 0$, then the singularity of the error-control integral at the point $E = U_0$ is of the type γ^{-1}, i.e.

$$\mathbf{E}(\nu) \sim \frac{B}{\int_a^b p(x)\,\mathrm{d}x} \qquad (E \to U_0 - 0) \tag{28}$$

where B is a constant factor of the order of unity.

(v) The type of singularity the error-control integral $\mathbf{E}(\gamma)$ has at the point $E = 0$ essentially depends on the rate at which the potential $U(x)$ decreases as $x \to \pm\infty$. The more rapidly $U(x)$ vanishes at infinity, the stronger the singularity is. Thus, for $E \to 0+$ we have

$$\mathbf{E}(\gamma) \sim \begin{cases} \dfrac{1}{k_0 l}\,|\ln(kl)| & \text{if} \quad U(x) \sim |x/l|^{-2} \quad \text{as} \quad x \to \pm\infty \\ \dfrac{1}{\sqrt{(k_0 l)\,kl}} & \text{if} \quad U(x) \sim |x/l|^{-4} \quad \text{as} \quad x \to \pm\infty \\ \dfrac{1}{kl} & \text{if} \quad U(x) \sim \exp(-|x|/l) \quad \text{as} \quad x \to \pm\infty \end{cases} \tag{29}$$

with k given by (2) (in (29) we have omitted constant factors on the right-hand side).

The above relations enable us to derive the asymptotic expressions for the transmission and the reflection amplitudes related to the particle's tunnelling process, along with the proper assessments for their error bounds.

4. Tunnelling transmission amplitude

The *exact* wavefunction $\psi(x)$ (equation (17)), which represents the particle's tunnelling state, may be brought into an equivalent form by substituting the expressions (11) and (21) in (17)

$$\psi(x) = \left[\frac{\xi^2 - \xi_0^2}{p^2(x)}\right]^{1/4} \left[\mathbf{D}_{\mathrm{i}\gamma - 1/2}(\sqrt{2}\xi\,\mathrm{e}^{\mathrm{i}\pi/4}) + h_\gamma(\sqrt{2}\xi)\right] \tag{30}$$

where the correction term $h_\gamma(\sqrt{2}\xi)$ may be neglected if the condition (24) is fulfilled. Let us consider the asymptotic behaviour of the function (30) when $x \to \pm\infty$.

As $x \to +\infty$, the function $\xi = \xi(x)$ tends to positive infinity. From equation (10*c*) we obtain

$$\xi \sim \sqrt{2kx} + \mathrm{O}\big(\gamma \ln(kx)\big) \qquad (k = \sqrt{2m\,E})\,. \tag{31}$$

From equation (21) and the first of the two boundary conditions (18), we see that

$$\lim_{x \to +\infty} \left[\sqrt{\xi}\, h_\gamma(\xi\sqrt{2})\right] = 0\,. \tag{32}$$

Using the asymptotic representation (see [34, p 331]) for Weber's tunnelling function in (30), we obtain the asymptotic form for the wavefunction $\psi(x)$ as $x \to +\infty$

$$\psi(x) \sim \frac{2^{-1/4}\,\mathrm{e}^{-\pi\gamma/4 + \mathrm{i}\pi/8}}{\sqrt{p(x)}}\,\mathrm{e}^{\mathrm{i}\left(\frac{1}{2}\xi^2 - \gamma\ln(\xi\sqrt{2})\right)} + \frac{1}{\sqrt{p(x)}}\sqrt{\xi}\,h_\gamma(\xi\sqrt{2}) \qquad (x \to +\infty)\,. \tag{33}$$

For the expression in the exponent of the first term on the right-hand side in (33) we get from (10*c*)

$$\tfrac{1}{2}\,\xi^2 - \gamma\,\ln(\xi\sqrt{2}) = \int_b^x p(x)\,\mathrm{d}x + \tfrac{1}{2}(\gamma - \gamma\ln\gamma) + \mathrm{O}\left(\frac{\gamma^2}{\xi^2}\right). \tag{34}$$

Thus, finally, as $x \to +\infty$, the wavefunction is given asymptotically by

$$\psi(x) = \frac{2^{-1/4}\,\mathrm{e}^{-\pi\gamma/4+\mathrm{i}\pi/8}}{\sqrt{p(x)}}\,\exp\!\left(\mathrm{i}\int_b^x p(x)\,\mathrm{d}x + \mathrm{i}\,\tfrac{1}{2}\,(\gamma - \gamma\ln\gamma)\right)$$
$$+\frac{1}{\sqrt{p(x)}}\,\sqrt{\xi}\,h_\gamma(\xi\sqrt{2}) + \mathrm{O}\left(\frac{1+\gamma^2}{\xi^2}\right) \qquad (x \to +\infty) \tag{35}$$

and the terms on the second line of (35) vanish in the limit $x \to +\infty$.

As $x \to -\infty$, we see from (10*a*) that also $\xi \to -\infty$, that is

$$\xi \sim -\sqrt{2k|x|} + \mathrm{O}(\gamma\,\ln(k|x|))\,. \tag{36}$$

We replace Weber's tunnelling function $\mathbf{D}_{\mathrm{i}\gamma-1/2}(\xi\sqrt{2})$ in (30) by its asymptotic form (see p 332 in [34]), and obtain

$$\psi(x) \sim \frac{2^{-1/4}\,\mathrm{e}^{-\pi\gamma/4+\mathrm{i}\pi/8}}{\sqrt{p(x)}}\left[\mathrm{e}^{\pi\gamma-\mathrm{i}\pi/2}\,\mathrm{e}^{\mathrm{i}\,(\frac{1}{2}\xi^2-\gamma\,\ln(|\xi|\sqrt{2}))} + \frac{\sqrt{2\pi}\,\mathrm{e}^{\pi\gamma/2}}{\Gamma(\mathrm{i}\gamma+\frac{1}{2})}\,\mathrm{e}^{-\mathrm{i}\,(\frac{1}{2}\xi^2-\gamma\,\ln(|\xi|\sqrt{2}))}\right]$$
$$+\frac{1}{\sqrt{p(x)}}\,\sqrt{\xi}\,h_\gamma(\xi\sqrt{2}) \qquad (x \to -\infty)\,. \tag{37}$$

For the last term on the right-hand side of (37) we get the assessment ($x < 0$)

$$\left|\sqrt{|\xi|}\,h_\gamma(\xi\sqrt{2})\right| \leqslant 2^{-1/4}\,\mathrm{e}^{3\pi\gamma/4}\big[1+\sqrt{1+\mathrm{e}^{-2\pi\gamma}}\big]\big[\mathrm{e}^{\sigma_\gamma\mathbf{E}(\gamma)} - 1\big] \qquad (x \to -\infty) \tag{38}$$

where the positive parameter σ_γ is a slowly varying function of $\gamma \geqslant 0$ which assumes its maximum value $\sigma_{\max} = 1.096\,718$ at $\gamma = 0.622\,803$. In particular, $\sigma_\gamma = 1$ at $\gamma = 0$, and $\sigma_\gamma = 1.039\,523$ for $\gamma \gg 1$, correct to six decimal places.

From equation (10*a*) we obtain the asymptotic relation

$$\tfrac{1}{2}\,\xi^2 - \gamma\,\ln(|\xi|\sqrt{2}) = \int_x^a p(x)\,\mathrm{d}x + \tfrac{1}{2}(\gamma - \gamma\ln\gamma) + \mathrm{O}\left(\frac{\gamma^2}{\xi^2}\right) \tag{39}$$

for large negative x. Thus, as $x \to -\infty$, the tunnelling wavefunction (30) is asymptotically represented by

$$\psi(x) \sim \frac{2^{-1/4}\,\mathrm{e}^{-\pi\gamma/4+\mathrm{i}\pi/8}}{\sqrt{p(x)}}\left[\mathrm{e}^{\pi\gamma-\mathrm{i}\pi/2}\,\exp\!\left(\mathrm{i}\int_x^a p(x)\,\mathrm{d}x + \mathrm{i}\,\tfrac{1}{2}\,(\gamma - \gamma\ln\gamma)\right)\right.$$
$$\left.+\frac{\sqrt{2\pi}\,\mathrm{e}^{\pi\gamma/2}}{\Gamma(\mathrm{i}\gamma+\frac{1}{2})}\,\exp\!\left(-\mathrm{i}\int_x^a p(x)\,\mathrm{d}x - \mathrm{i}\,\tfrac{1}{2}\,(\gamma - \gamma\ln\gamma)\right)\right]$$
$$+\frac{1}{\sqrt{p(x)}}\,\sqrt{\xi}\,h_\gamma(\xi\sqrt{2}) + \mathrm{O}\left(\frac{1+\gamma^2}{\xi^2}\right) \qquad (x \to -\infty)\,. \tag{40}$$

On the right-hand side in (40), the first exponential in the square brackets asymptotically represents the reflected wave, whereas the second exponential in the brackets stands for the incident wave. From the asymptotic forms (39) and (44) for the tunnelling wavefunction, we obtain the exact expression for the transmission amplitude related to the particle's tunnelling through the potential $U(x)$

$$t = \frac{e^{i\phi}}{\sqrt{1+e^{2\pi\gamma}}} \frac{e^{i\,\Delta\phi}}{1+\theta}\,. \tag{41}$$

In equation (41), γ is the phase integral as defined by (12). The phase ϕ is given by the sum

$$\phi = \int_{-\infty}^{a} [p(x)-k]\,dx + \int_{b}^{+\infty} [p(x)-k]\,dx + [Rg(\gamma) - k(b-a)] \tag{42}$$

of the classical phase ϕ_{clas},

$$\phi_{clas} = \int_{-\infty}^{a} [p(x)-k]\,dx + \int_{b}^{+\infty} [p(x)-k]\,dx \qquad (k = \sqrt{2mE}) \tag{43}$$

which comes from the classically accessible regions $x < a$ and $x > b$, and the *tunnelling phase* ϕ_{tun},

$$\phi_{tun} = Rg(\gamma) - k(b-a) \tag{44}$$

which is associated with the classically forbidden region $a < x < b$. In equation (42) the function $Rg(\gamma)$ is given by

$$Rg(\gamma) = \arg\Gamma\left(i\gamma + \tfrac{1}{2}\right) + \gamma - \gamma\ln\gamma \tag{45}$$

the branch of the argument of the gamma function being continuous and equal to zero at $\gamma = 0$.

The formula (42) for the phase of the transmission amplitude t is a new result. The function (45), which appears as one of the terms in the sum on the right-hand side of

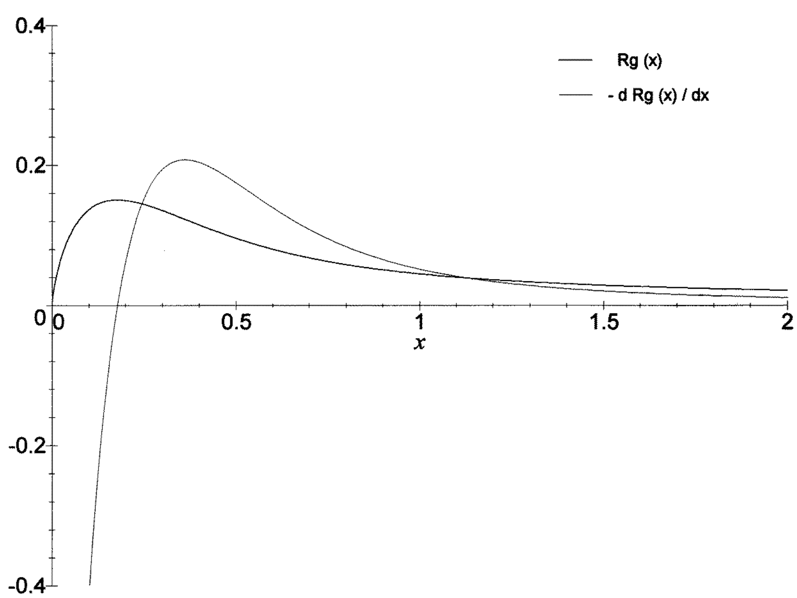

Figure 1. Graphs of the function $Rg(\gamma)$ and its first derivative.

equation (42), was first written explicitly in [26, 35] (in other notation) and then appeared in many papers [27, 33, 36–39, 22] as a correction term in various expressions for the phase of the transmission amplitude. The graph of the function (45), which was first given in [35], is plotted in figure 1 as a bold curve. Thus $Rg(\gamma)$ is a positive function on the positive real axis and it vanishes as $\gamma \to 0+$ or $\gamma \to +\infty$. The corresponding asymptotic forms are [26]

$$Rg(\gamma) \sim -\gamma \ln \gamma + \mathrm{O}(\gamma) \qquad (\gamma \to 0+) \tag{46a}$$

$$Rg(\gamma) \sim \frac{1}{24\,\gamma} + \mathrm{O}\left(\frac{1}{\gamma^3}\right) \qquad (\gamma \to +\infty)\,. \tag{46b}$$

The function $Rg(\gamma)$ attains its maximum value $\max Rg(\gamma) = 0.150\,482$ at $\gamma = 0.178\,127$, correct to six decimal places (cf [26]). The explicit expressions for $Rg(\gamma)$ may be obtained by using Binet's formulae [40] for the logarithm of the gamma function. Thus, making use of the first of Binet's formulae, we get

$$Rg(\gamma) = \frac{1}{2}\,\gamma \ln\left(1 + \frac{1}{4\gamma^2}\right) - \frac{1}{2}\int_0^\infty \frac{\mathrm{d}t}{t}\left[\coth t - \frac{1}{t}\right] \mathrm{e}^{-t} \sin(2\gamma t)\,. \tag{47}$$

The classical phase (43) has a clear physical meaning: it is equal to the excess of the particle's classical action in the potential $U(x)$ over the corresponding action for a free particle. The tunnelling phase (44) will have just the same physical meaning with respect to the classically forbidden region if we look on the function (45) as an analogue to the classical action.

In the basic formula (42), the second factor on the right-hand side represents the corrections to the modulus and the phase of the main first factor. The correction $\Delta\phi$ to the phase ϕ has the assessment

$$|\Delta\phi| \leqslant \arcsin \rho \tag{48}$$

where ρ is obtained from (38)

$$\rho = \left(1 + \frac{1}{\sqrt{1 + \mathrm{e}^{-2\pi\gamma}}}\right)\left[\mathrm{e}^{\sigma_\gamma \mathbf{E}(\gamma)} - 1\right] \tag{49}$$

while for the real parameter θ in (41) we get

$$|\theta| \leqslant \rho\,. \tag{50}$$

The relations (48)–(50) are suitable for numerical evaluations of the corrections to the modulus and the phase of the transmission amplitude (41). An example is given below in figure 2.

Suppose that the condition (24) is fulfilled and the error-control integral $\mathbf{E}(\gamma)$ is small compared with unity. Then from (48) and (50) we find

$$|\Delta\phi| \leqslant C_\gamma \mathbf{E}(\gamma) + \mathrm{O}(\mathbf{E}^2(\gamma)) \tag{51a}$$

$$|\theta| \leqslant C_\gamma \mathbf{E}(\gamma) + \mathrm{O}(\mathbf{E}^2(\gamma))\,. \tag{51b}$$

The number C_γ in (51*a*),

$$C_\gamma = \left(1 + \frac{1}{\sqrt{1 + \mathrm{e}^{-2\pi\gamma}}}\right)\sigma_\gamma \tag{52}$$

is of the order of unity for all $\gamma \geqslant 0$. In particular, for $\gamma = 0$ we have $C_0 = 1.707\,107$, whereas $C_\gamma = 2.079\,046$ for $\gamma \gg 1$, correct to six decimal places. In other words, the

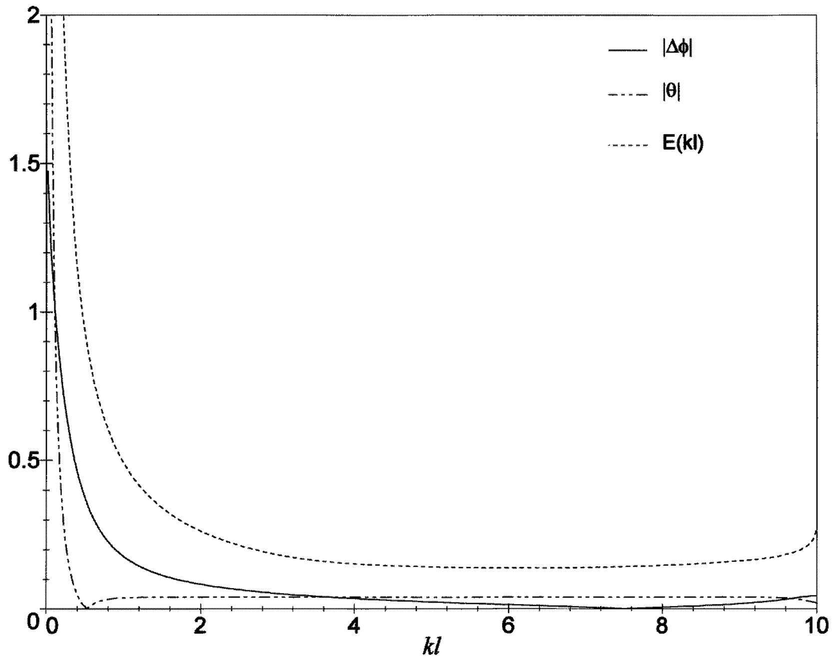

Figure 2. Exact absolute values of the correction terms $|\Delta\phi|$ (full curve) and $|\theta|$ (chain curve), which appear in the exact formula (41) for the transmission amplitude t of a particle tunnelling through the the potential barrier $U_0/\cosh^2(x/l)$. The broken curve represents the graph of the error-control integral $\mathbf{E}(\gamma)$ (equation (25)) for the same potential. The graphs have been calculated numerically for $k_0 l = 10$.

asymptotic condition (24) allows us to write an asymptotic formula for the transmission amplitude (41)

$$t = \frac{e^{i\phi}}{\sqrt{1+e^{2\pi\gamma}}}\,[1 + O\,(\mathbf{E}(\gamma))\ . \tag{53}$$

In the main approximation, we obtain from (53) the transmission coefficient

$$T = \frac{1}{1+\exp\left[2\int_a^b |p(x)|\,dx\right]}\ . \tag{54}$$

This result was first obtained by Kemble [16] and then confirmed in many papers (for references see [17, 22]). As we see, Kemble's formula (54) is true if the condition (24) is fulfilled. On the other hand, as was noted in [20, p 112], it is not possible to obtain the expression (42) for the phase ϕ in (53) by using the phase-integral method.

The corresponding asymptotic expression for the reflection amplitude r is found to be

$$r = \frac{e^{i\phi_r}}{\sqrt{1+e^{-2\pi\gamma}}}\ \left[1 + O\,(\mathbf{E}(\gamma))\right] \tag{55}$$

where the phase ϕ_r is given by

$$\phi_r = -\frac{\pi}{2} + 2\int_{-\infty}^{a} [p(x) - k]\,dx + 2ka + Rg(\gamma)\,. \tag{56}$$

In the main approximation, the reflection coefficient R is found from (55)

$$R = \frac{1}{1 + \exp\left[-2\int_a^b |p(x)|\,\mathrm{d}x\right]}\,. \tag{57}$$

The results of section 3 show that the condition (24) is essentially different from the conventional condition $\gamma \gg 1$, i.e.

$$\int_a^b |p(x)|\,\mathrm{d}x \gg 1 \tag{58}$$

which determines the validity of the WKB approximation. The fact of principal importance is that the condition (24) may be fulfilled even if the phase integral on the left-hand side of (58) is of the order of unity, provided the semiclassical parameter $k_0 l$ (6) is sufficiently large. In order to differentiate the relation (24) from the WKB condition (58), we shall refer to (24) as the condition for the *post-classical approximation*. To make the difference clear we notice that the WKB approximation is a physically self-consistent approach which is based on the assumption that phase integrals are large compared with unity†. This assumption makes it possible to regard Planck's constant $\hbar$ as a formal small parameter (compared with typical values of the classical action of the system), and to develop a regular procedure of treating quantum systems by means of expansions in powers of $\hbar$. As a result, within the WKB approximation wavefunctions are represented as linear forms of exponential functions that contain large phase integrals in their exponents. In the post-classical approximation, we also make use of classical phase integrals so this approximation is semiclassical in nature. But in contrast to the WKB approximation, phase integrals are now allowed to be comparable with unity or even less, which excludes the possibility of considering $\hbar$ as a small parameter. As a consequence, wavefunctions and related quantities are found to be expressed in terms of more complicated (non-exponential) functions of phase integrals. Kemble's formulae (54) and (57) just reflect this feature. Further examples are furnished by the expression (11) for the wavefunction and equation (42) for the tunnelling phase.

5. Delay and tunnelling times

For the motion of a particle over a potential barrier, the semiclassical expression for the phase α of the transmission amplitude is well known

$$\alpha = \int_{-\infty}^{+\infty} [p(x) - k]\,\mathrm{d}x \qquad (k = \sqrt{2mE})\,. \tag{59}$$

Obviously, differentiating this phase α with respect to the particle's energy E yields the total delay time

$$\tau = \frac{\mathrm{d}\alpha}{\mathrm{d}E} = \int_{-\infty}^{+\infty} \left[\frac{\mathrm{d}x}{v(x)} - \frac{\mathrm{d}x}{v_0}\right]. \tag{60}$$

† Note that in the tunnelling problem there are two different types of phase integrals: (i) the barrier penetration integral γ (equation (12)), and (ii) the integral $\int_b^x p(x)\,\mathrm{d}x$ related to the current position x of the particle. Both of them should be large in the WKB approximation.

In equation (60), $v(x)$ is the classical velocity of the particle calculated at the point x in the potential $U(x)$,

$$v(x) = \sqrt{\frac{2}{m}[E - U(x)]} \qquad v_0 = \sqrt{\frac{2E}{m}}\,. \tag{61}$$

By definition, the delay time τ associated with a given distance L is equal to the actual time required to cover the distance L when the particle moves in the potential $U(x)$, minus the time the particle would have needed to cover the same distance L if it had been free, i.e. in the absence of the potential $U(x)$. For a classical motion over a barrier, there is no ambiguity in the definition (60) for the delay time τ.

From the formal standpoint, the difference between the phase α (equation (59)) for an overbarrier motion, on the one hand, and the phase ϕ (equation (42)) for an underbarrier motion, on the other hand, consists in replacing the portion of the integral (59),

$$\int_a^b [p(x) - k]\,\mathrm{d}x \tag{62}$$

which comes from the segment $[a, b]$ delimited by the two turning points, by the tunnelling phase (44). Hence, according to the physical contents of the explicit expression (42), differentiating the phase ϕ of the transmission amplitude (42) with respect to the total energy E yields the total delay time τ for a particle moving through the potential barrier $U(x)$ from $x = -\infty$ to $x = +\infty$. This statement was first formulated by Wigner [14] and then proven as a general physical principle by Goldberger and Watson [41, ch 8]. As a result, on differentiating (42), we get the *total delay time*

$$\tau = \int_{-\infty}^{a} \left[\frac{\mathrm{d}x}{v(x)} - \frac{\mathrm{d}x}{v_0}\right] + \int_{b}^{+\infty} \left[\frac{\mathrm{d}x}{v(x)} - \frac{\mathrm{d}x}{v_0}\right] + \left[\tau_{\text{tun}} - \frac{b-a}{v_0}\right]. \tag{63}$$

The last term on the right-hand side of (63) fulfils the role of the *tunnelling delay* time associated with the classically forbidden region. It is equal to the *'tunnelling time'*

$$\tau_{\text{tun}} = \frac{1}{\pi}\left(-Rg'(\gamma)\right) \int_a^b \frac{\mathrm{d}x}{|v(x)|} \tag{64}$$

minus the corresponding free flight time $(b - a)/v_0$ for a free particle with the same total energy E (the prime in (64) denotes differentiation with respect to the function's argument). Note that the formula (63) has been derived for a single particle with a *definite* total energy E. The derivation was based on the mechanical sense of the phase (42) and made no appeal to wavepackets. Hence the expression (63) for the total delay time is free from the known difficulties that are implicated by representing a quantum particle by means of wavepackets [5].

Regarding the quantity τ_{tun} (equation (64)), we have to emphasize that its physical contents are defined by the combined relations (63) and (64), and consist of

(i) τ_{tun} has the physical dimension of time,
(ii) τ_{tun} is associated with the classically forbidden region precisely, and
(iii) in the structure of the physically well determined expression (63) for the total delay time, τ_{tun} occupies just the place a classical traversal time would have occupied if the particle had been a classical one (as does, for instance, the classical traversal time $\int_a^b \mathrm{d}x/v(x)$ in expression (60) for a particle moving over a potential barrier).

There are no other physical concepts associated with the above (and subsequent) use of the term 'tunnelling time'. Therefore it would be improper to think of the quantity $\tau_{\rm tun}$ as the time required for a quantum particle to move under the potential barrier from the point $x = a$ to the point $x = b$. In particular, the quantity defined by (64) does not necessarily have to be positive, as would be expected from a classical viewpoint.

The graph of the function $-Rg'(\gamma)$, which appears as a factor in (64), is plotted in figure 1 as a thin curve. We see that $-Rg'(\gamma)$ attains its maximum value 0.207 639 at $\gamma = 0.361\,050$, and it vanishes at $\gamma = 0.178\,127$, correct to six decimal places. The explicit expression for $-Rg'(\gamma)$ may be obtained from (47) by direct differentiation

$$-\frac{\mathrm{d}Rg(\gamma)}{\mathrm{d}\gamma} = \frac{1}{1+4\gamma^2} - \frac{1}{2}\ln\left(1+\frac{1}{4\gamma^2}\right) + \int_0^\infty \mathrm{d}t\left[\coth t - \frac{1}{t}\right]\mathrm{e}^{-t}\cos(2\gamma t)\,. \tag{65}$$

In particular, the asymptotic forms for the function (65) are

$$-Rg'(\gamma) \sim \ln\gamma + 1.963\,510\,027 + \mathrm{O}(\gamma^2) \qquad (\gamma \to 0+) \tag{66a}$$

$$-Rg'(\gamma) \sim \frac{1}{24\,\gamma^2} + \mathrm{O}\left(\frac{1}{\gamma^4}\right) \qquad (\gamma \to +\infty). \tag{66b}$$

While deriving the formula (63), we have dropped the derivative $\mathrm{d}(\Delta\phi)/\mathrm{d}k$ of the correction term $\Delta\phi$, which appears in the exact expression (41) for the phase of the transmission amplitude. However, although the asymptotic relation (51*a*) for the term $\Delta\phi$ has been given a rigorous proof, we have no general proof for the analogous relation

$$\frac{\mathrm{d}\Delta\phi}{\mathrm{d}k} = \mathrm{O}\left(\mathbf{E}(\gamma)\right) \tag{67}$$

regarding the derivative of $\Delta\phi$. In section 6 we will prove the relation (67) for the potential $U_0/\cosh^2(x/l)$. Namely, we prove that for this potential the differentiation of the correction term $\Delta\phi$ with respect to k is legitimate and that the derivative $\mathrm{d}(\Delta\phi)/\mathrm{d}k$ is negligibly small if the condition $kl \gg 1$ is fulfilled, irrespective of the value of the phase integral γ. From the physical standpoint, this statement is likely to hold true with respect to other smooth potentials as well, provided the above hypotheses upon the latter are fulfilled.

6. Tunnelling times for the potential $U_0/\cosh^2(x/l)$

Let us consider the tunnelling of a quantum particle with a total energy $E > 0$ through a potential barrier described by the potential (1). The particle's wavefunction $\psi(x)$ satisfies the Schrödinger equation (4), where

$$p^2(x) = k_0^2\left[\frac{(kl)^2}{(k_0 l)^2} - \frac{1}{\cosh^2(x/l)}\right]. \tag{68}$$

In equation (68), the parameters k_0 and k are defined by

$$k_0 = \sqrt{2m\,U_0} \qquad k = \sqrt{2m\,E} \qquad (\hbar = 1) \tag{69}$$

where k is the momentum of a free particle. As long as we are considering a tunnelling problem, we have $0 \leqslant E \leqslant U_0$, so $k_0 \geqslant k \geqslant 0$.

The potential (1) provides a rare example when the exact expressions for the transmission and the reflection amplitudes are known [42]. Hence the results obtained within the semiclassical approximation may be compared with the exact ones.

The turning points $x = a$ and $x = b$, as determined from the equation $p^2(x) = 0$, are found to be

$$b = l\ \ln\left(\frac{k_0 l + \sqrt{(k_0 l)^2 - (kl)^2}}{kl}\right) \qquad a = -b\,. \tag{70}$$

For the phase integral (12) we obtain an exact expression

$$\gamma = \frac{1}{\pi}\int_a^b |p(x)|\,\mathrm{d}x = k_0 l - kl\,. \tag{71}$$

Let us consider the general condition (24) under which the semiclassical treatment is legitimate. As long as the relation (6) is fulfilled, the condition (24) puts limits to the validity of the semiclassical treatment near the singular points of the error-control integral (25), i.e. near the top of the barrier as well as near its base. The function $U(x)$ in (1) decreases exponentially as $|x| \to \infty$. Hence, taking into account the third of the relations (29), we see that the condition (24) requires that $kl \gg 1$. Then, on substituting (26) in (24), we get from the latter the second condition

$$|\ln(k_0 l - kl)| \ll k_0 l\,. \tag{72}$$

For the potential (1), the error-control integral $\mathbf{E}(\gamma)$ has been calculated as a function of kl, for $k_0 l = 10$, by performing direct numerical integration in (25). The graph of $\mathbf{E}(kl)$ is plotted in figure 2 as a broken curve.

The exact expression for the transmission coefficient T, for the potential (1), written in the present notation, is [42]

$$T = \frac{\sinh^2(\pi kl)}{\sinh^2(\pi kl) + \cosh^2\left(\pi\sqrt{(k_0 l)^2 - \frac{1}{4}}\right)}\,. \tag{73}$$

Under the conditions $k_0 l \geqslant kl \gg 1$, the expression (73) reduces to

$$T = \frac{1}{1 + \mathrm{e}^{2\pi(k_0 l - kl)}} \tag{74}$$

which, in view of (71), coincides with Kemble's formula (54) exactly. Thus we see that, in fact, the semiclassical expression (74) is valid for *all* non-negative values of the phase integral $\gamma = k_0 l - kl$, *including* $kl = k_0 l$, provided the condition $kl \gg 1$ is fulfilled.

Let us now consider the phase ϕ of the transmission amplitude t. The exact expression for Φ is also known

$$\Phi = \frac{\pi}{2} + \arg\Gamma\left(\tfrac{1}{2} + \mathrm{i}\sqrt{(k_0 l)^2 - \tfrac{1}{4}} - \mathrm{i}kl\right) + \arg\Gamma\left(\tfrac{1}{2} - \mathrm{i}\sqrt{(k_0 l)^2 - \tfrac{1}{4}} - \mathrm{i}kl\right) + 2\arg\Gamma(\mathrm{i}kl) \tag{75}$$

where $\Gamma(z)$ is the gamma function. We have to write the expression (75) in the semiclassical approximation, i.e. taking into account that $k_0 l \geqslant kl \gg 1$. To do this, we notice that the expressions that appear in the arguments of the second and third gamma functions on the right-hand side in (75) are large, so we may replace the last two terms in the latter formula by their asymptotic forms. These asymptotic forms are easily obtainable if one takes into account the relation

$$\arg\Gamma(z) = \mathrm{Im}\,[\ln\Gamma(z)]\,. \tag{76}$$

When writing the required asymptotic expressions, accurate assessments for the remainder terms are needed for our purposes. To obtain such assessments, we take advantage of the known relations for the logarithm of the gamma function [19]

$$\ln\Gamma(z) = \left(z - \tfrac{1}{2}\right)\ln z - z + \tfrac{1}{2}\ln(2\pi) + R_1(z) \tag{77a}$$

$$|R_1(z)| \leqslant \frac{\pi - \delta}{6\sin\delta}\,\frac{1}{|z|} \qquad (|\arg z| \leqslant \pi - \delta,\ \delta > 0) \tag{77b}$$

and its derivative [19]

$$\psi(z) \equiv \frac{\mathrm{d}\ln\Gamma(z)}{\mathrm{d}z} = \ln z - \frac{1}{2z} + U_1(z) \tag{78a}$$

$$|U_1(z)| \leqslant \frac{1}{12}\sec^3\left(\frac{1}{2}\arg z\right)\frac{1}{|z|^2} \qquad (|\arg z| \leqslant \pi - \delta,\ \delta > 0)\,. \tag{78b}$$

As $|z| \to \infty$, the known asymptotic relations follow from (77*a*) and (78*a*):

$$\ln\Gamma(z) = \left(z - \tfrac{1}{2}\right)\ln z - z + \tfrac{1}{2}\ln(2\pi) + \mathrm{O}\left(\frac{1}{|z|}\right) \qquad (|\arg z| < \pi) \tag{79a}$$

$$\frac{\mathrm{d}\ln\Gamma(z)}{\mathrm{d}z} = \ln z - \frac{1}{2z} + \mathrm{O}\left(\frac{1}{|z|^2}\right) \qquad (|\arg z| < \pi)\,. \tag{79b}$$

Comparison of (79*b*) with (79*a*) shows that the relation (79*b*) for the derivative is obtainable from the asymptotic relation (79*a*) for the logarithm of the gamma function itself through a formal differentiation of the latter, *including* the formal differentiation of the O term in (79*a*) (the meaning of the latter procedure is clear from comparison of the last two formulae).

Using equations (76) and (79*a*), we find, for $k_0 l \geqslant kl \gg 1$,

$$\arg\Gamma\left(\tfrac{1}{2} - \mathrm{i}\sqrt{(k_0 l)^2 - \tfrac{1}{4}} - \mathrm{i}kl\right) = (k_0 l + kl) - (k_0 l + kl)\ln(k_0 l + kl) + \mathrm{O}\left(\frac{1}{kl}\right) \tag{80a}$$

$$\arg\Gamma(\mathrm{i}kl) = -kl + kl\ln(kl) - \frac{\pi}{4} + \mathrm{O}\left(\frac{1}{kl}\right) \tag{80b}$$

and that each one of the two asymptotic relations (80*a*) may be formally differentiated with respect to k, including the O terms in (80*a*).

Let us now substitute (80*a*) into the exact expression (75) for the phase Φ. We get

$$\Phi = \phi + \Delta\phi \tag{81}$$

where

$$\phi = \arg\Gamma\left(\tfrac{1}{2} + \mathrm{i}k_0 l - \mathrm{i}kl\right) + (k_0 l - kl) - (k_0 l + kl)\ln(k_0 l + kl) + 2kl\ln(kl) \tag{82}$$

and

$$\Delta\phi = \mathrm{O}\left(\frac{1}{kl}\right) \qquad \frac{\mathrm{d}\,\Delta\phi}{\mathrm{d}k} = l\mathrm{O}\left(\frac{1}{(kl)^2}\right). \tag{83}$$

First, we analyse the main term ϕ given by (82). Our purpose is to compare the expression (82) with the semiclassical formula (42) for the phase of the transmission amplitude, and, as a result of the comparison, to extract from (82) the expression for the tunnelling time τ_{tun}. As a first step, we have to subtract from (82) the first two terms on the right-hand side of (42), which come from the classical regions $x < a$ and $x > b$. The calculation yields

$$\int_{-\infty}^{a} [p(x) - k]\,\mathrm{d}x + \int_{b}^{+\infty} [p(x) - k]\,\mathrm{d}x$$
$$= 2(kl)\ln\left(\frac{k_0 l + \sqrt{(k_0 l)^2 - (kl)^2}}{\sqrt{(k_0 l)^2 - (kl)^2}}\right) - 2(k_0 l)\ln\left(\frac{k_0 l + kl}{\sqrt{(k_0 l)^2 - (kl)^2}}\right). \tag{84}$$

Subtracting equation (84) from equation (82) yields the tunnelling phase ϕ_{tun} (44),

$$\phi_{\mathrm{tun}} = \left[\arg\Gamma\left(\tfrac{1}{2} + \mathrm{i}k_0 l - \mathrm{i}kl\right) + (k_0 l - kl) - (k_0 l - kl)\ln(k_0 l - kl)\right]$$
$$- 2(kl)\ln\left(\frac{k_0 l + \sqrt{(k_0 l)^2 - (kl)^2}}{kl}\right). \tag{85}$$

Taking into account the expression (70) for the turning point b, we see that the last term on the right-hand side of (85) is equal to $[-k(b - a)]$ exactly, while the expression that appears in the square brackets in (85) is just the function $Rg(\gamma)$ (45), with $\gamma = k_0 l - kl$ as its argument, in accordance with (71).

Hence, we have found the expression (85) to match the general formula (44) exactly. We also have found that the expression (85) for the tunnelling phase ϕ_{tun} related to the potential (1) is valid, if $kl \gg 1$, uniformly with respect to the difference $(k_0 l - kl) \in [0, k_0 l)$, i.e. up to and including the top of the barrier. In view of the relations (83), differentiating the expression (82) for the phase ϕ with respect to k is legitimate. Performing it, we obtain the tunnelling time for the potential (1)

$$\tau_{\mathrm{tun}} = [-Rg'(k_0 l - kl)]\frac{l}{v_0} \tag{86}$$

where v_0 is the velocity of a free particle having total energy E. We see that the expression (86) is valid for *all* non-negative values of the phase integral $\gamma = k_0 l - kl$, *including* $\gamma = 0$ $(k_0 l = kl)$, provided the condition $kl \gg 1$ is fulfilled. Moreover, the relations (83) show that the difference $\Delta\tau_{\mathrm{tun}}$ between the exact tunnelling time (which we do not know) and its semiclassical expression (86) satisfies the relation

$$\Delta\tau_{\mathrm{tun}} = \mathrm{O}\left(\frac{1}{(kl)^2}\right) \tag{87}$$

uniformly with respect to the difference $(k_0 l - kl) \in [0, k_0 l)$.

For the potential (1), the exact values of the correction terms $\Delta\phi$ and θ, which appear in (41), have been calculated numerically. Namely, $\Delta\phi$ is the difference between the exact phase Φ (equation (75)), and its approximate value ϕ as given by (42). The parameter θ represents the deviation of the semiclassical transmission coefficient (74) from the exact transmission coefficient T (equation (73)), according to (41). The graphs of $|\Delta\phi|$ and $|\theta|$ are plotted in figure 2 for $k_0 l = 10$. For comparison, the graph of the error-control integral $\mathbf{E}(kl)$ is also plotted in figure 2 as a broken curve. This figure illustrates the meaning of the condition $kl \gg 1$ as well as the quality of the estimates (51*a*) and (51*b*) for the corrections $\Delta\phi$ and θ.

7. Discussion and conclusions

(i) The importance of deriving quantum corrections to the WKB expressions has been emphasized by Breit and Kramers (see [23]). Jeffreys [43] pointed out the difficulty of the choice of a large parameter in order to treat the problem (4), with two real turning points, by means of asymptotic methods. As a large parameter, he took the phase integral γ (equation (12)). The same choice of a large parameter was made by Langer [31], Moriguchi [44], and Pike [32]. In the present paper, the large parameter (6) has been chosen in accordance with [45], which allows the phase integral (12) to be comparable with unity or even less. The parameter $k_0 l$ (6) defines the effective thickness of the potential barrier.

(ii) The sufficient condition for the semiclassical treatment to be valid in tunnelling problems is given by the relation (24). In this respect, the critical points on the energy axis coincide with the singular points of the error-control integral (25). For simple potential barriers, these critical points are the base of the barrier $E = 0$ and the barrier's top $E = U_0$ (cf section 3). This fact indicates that the quantum features of a particle's motion become important both near the top of the barrier and near its base. The importance of quantum effects in the vicinity of a barrier's top was first emphasized by Ford *et al* [23]. As has been shown above, the quantum effects are even more important near the barrier's base since the singularity of the error-control integral near the barrier's base is stronger than that near its top (cf equations (26) and (29)). For this reason, the semiclassical treatment of the tunnelling cannot be applied to the region of very low energies, in spite of the fact that in this region the phase integral (12) may be very large.

(iii) Comparing the formulae (35) and (40) of the present paper with the expressions (14) and (15) in [26] we see that the former reduce to the latter if we neglect the terms on the last line of (35) and of (40). The sufficient condition for the term $\sqrt{\xi}\, h_\gamma(\xi\sqrt{2})$ to be dropped is given by (24). If this condition is fulfilled, then the formulae (35) and (40) reduce *asymptotically* (as $|x| \to \infty$) to the expressions (14) and (15) in [26], respectively. The problem of determining how far to the right from the right turning point b, and to the left from the left turning point a, one must go in order to make the terms $O(\xi^{-2})$ in (35) and (40) negligible, requires a special mathematical investigation that is beyond the scope of the present paper.

(iv) Let us consider the vicinity of a barrier's top in more detail. Suppose the function $U(x)$ is given such that the conditions $U''(x_0) < 0$ and $k_0 l \gg 1$ are fulfilled. The conditions (24) and (26) show that, for a fixed value of the parameter $k_0 l$, the parabolic connection formulae are, in general, not valid if the particle's energy E is too close to the barrier's top U_0, i.e. in the energy region defined by

$$\frac{1}{k_0 l}\left|\ln\left(\frac{U_0 - E}{U_0}\right)\right| > 1\,. \tag{88}$$

However, for any fixed energy $E < U_0$, which is arbitrarily close to the barrier's top, the validity of the parabolic connection formulae may be ensured by taking the parameter $k_0 l$ sufficiently large to make the left-hand side of (88) small compared with unity. Taking into account that the parameter denoted by t in [27] is identical to the barrier's effective thickness $k_0 l$, we thus obtain an explanation for the fact that the three groups of connection formulae examined in [27] become identical near the barrier's top, in the limit $k_0 l \gg 1$. In contrast to that, the third of the relations (29) explains why the difference between the parabolic connection formulae obtained in [26], on the one hand, and those obtained in [28] by using (1) as a comparison potential, on the other hand, cannot be made small near the base of the barrier even for very thick barriers, when $k_0 l \gg 1$.

(v) From figure 1 we see that the tunnelling time (64) may become negative if the phase integral (12) is sufficiently small, i.e. on energy ways near the top of the barrier. For such energy ways, the tunnelling time (64) is negative whereas its absolute value tends to infinity following the logarithmic law $|\ln(U_0 - E)|$. If interpreted from the classical viewpoint,

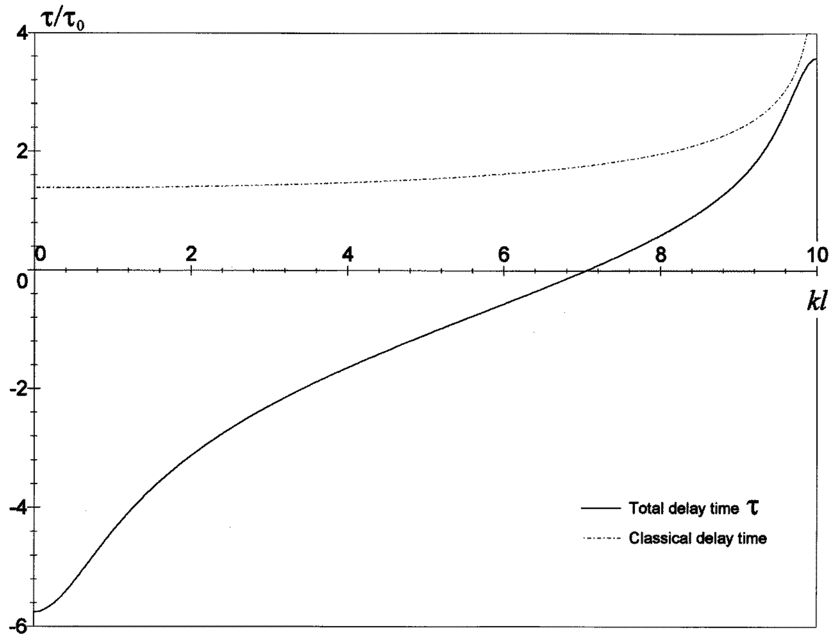

Figure 3. Total delay time for the potential barrier $U_0/\cosh^2(x/l)$ (full curve) calculated for $k_0l = 10$ ($\tau = l/v_0$). The chain curve represents the classical delay time, which has a logarithmic singularity at the top of the barrier (as $kl \to k_0l - 0$).

negative tunnelling times correspond to negative group velocities related to the classically forbidden region. Negative or even infinite group velocities have been predicted in [46] and detected experimentally for photons in [47]. As discussed in [46, 47, 7], this effect is due to a pulse reshaping and does not necessarily violate special relativity or causality. Further discussion is given in [1, 2].

(vi) The problem of excessively small or negative values does not arise with respect to the total delay time τ (equation (63)). This time remains finite, and of reasonable value, even in the vicinity of the barrier's top. Indeed, as $E \to U_0 - 0$, the classical delay time

$$\int_{-\infty}^{a} \left[\frac{dx}{v(x)} - \frac{dx}{v_0}\right] + \int_{b}^{+\infty} \left[\frac{dx}{v(x)} - \frac{dx}{v_0}\right] \tag{89}$$

which is due to the classically accessible regions, is positive and tends to infinity as $|\ln(U_0 - E)|$. A *classical* particle with $E = U_0$ would never reach even the top of the barrier at $x = x_0$. In contrast to that, as a result of cancellation of the two logarithmic terms in the sum (63), the *total* delay time (63) for a *quantum* particle remains finite even in the limit $E = U_0$. This result should be compared with Miller's [35] conclusion about the finite value of the escape time for a particle escaping from a potential well through a finite potential barrier. The effect is illustrated in figure 3 for the potential (1). The full curve in this figure represents the total delay time (63) plotted for $k_0l = 10$ as a function of the parameter kl ($\tau_0 = l/v_0$ and v_0 is given by (61)). The chain curve in figure 3 represents the classical delay time (89), which is positive for all energies and has a logarithmic singularity as $kl \to k_0l - 0$ (that is, near the top of the barrier). We see that the *tunnelling delay* time, which is given by the last term on the right-hand side of (63), is negative for all energies

$E \in (0, U_0)$. In other words, the potential barrier as a whole may either slow the particle down ($\tau > 0$ on energy ways sufficiently close to the barrier's top) or speed it up ($\tau < 0$ on energy ways sufficiently far below the top of the barrier).

(vii) The cancellation of the two logarithmic terms in the sum (63) indicates that the separation of individual terms on the right-hand side of (63) is to a certain extent artificial, especially in the vicinity of the barrier's top. This is due to the uncertainty in the actual positions of the turning points $x = a$ and $x = b$, the uncertainty becoming appreciable as one approaches the top of the barrier, where the quantum effects are important. Only the expression (63) taken as a whole is physically well defined and represents a quantity measured in the experiment directly.

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