The approximate use of the complex gamma function in some wave propagation problems

1973 J. Phys. A: Math. Nucl. Gen. 6 958

(http://iopscience.iop.org/0301-0015/6/7/016)

J. Phys. A: Math., Nucl. Gen., Vol. 6, July 1973. Printed in Great Britain. © 1973

The approximate use of the complex gamma function in some wave propagation problems

J Heading

Department of Applied Mathematics, The University College of Wales, Aberystwyth, Cards, UK

Received 14 February 1973

Abstract. After a historical survey of the problem of the potential barrier, and an examination of the types of approximations introduced and the reason for them, certain fallacious processes are discussed whereby the complex gamma function is given false approximate representations by means of exponential functions.

Two kinds of problems involving complex barriers are then examined; firstly the phenomenon of resonant tunnelling through two complex potential barriers, and secondly reflection phenomena arising from a single complex barrier. The common fallacies are also examined, and the proper treatment of these problems shows when the complex gamma function must be retained and when it can be dispensed with.

1. Introduction

Approximate phase-integral methods have often been applied to the barrier and multibarrier problem governed by the differential equation

$$\frac{d^2w}{dz^2}+k^2q(z)w = 0,$$

in which we shall call the function $q(z)$ the carrier. Historical surveys may be found in the works by Heading (1962), and Berry and Mount (1972). Originally, the method was applied to the problem of one real transition point (a point where $q(z)$ vanishes), the carrier being real along the real axis. Connection formulae linking the approximate WKBJ solutions across the transition point were derived by various methods, though considerable confusion existed about the validity of the reversibility of that particular connection formula that traced an exponentially large solution along a Stokes line across the transition point towards the anti-Stokes line on the other side. Later, this theory for one real transition point was generalized, for example by Furry (1947), to include one complex transition point.

The first applications to quantum mechanics were to potential wells, for which the carrier is real for real z, possessing two real transition points, the carrier being positive between them. The use of the non-disputed connection formula across both transition points easily gave the Bohr–Sommerfeld quantization condition. The second application was to the phenomenon of tunnelling through a potential barrier, the carrier again being real, but negative between the two real transition points. The process of tracing a solution through the two transition points now necessitated the use of one connection formula in the disputed direction. The approximate values of the moduli of the reflection and transmission coefficients are now expressed in terms of a small exponential function, involving the integral of the square root of the carrier between the two transition points.

The propagation of waves in dissipative stratified media also demands the use of this method. Thus ionospheric radio propagation often makes use of the connection formulae in problems involving one and two transition points. The existence of an energy loss mechanism in the underlying physical processes of the problem means that the transition points are now complex points in the complex z plane, the direction of propagation being along the real z axis. It has, however, often been assumed that the formulae derived when the carrier is real are also valid when the carrier is complex, and this has given rise to many erroneous applications of the method. The same interpretative errors are also often made in the approximate analysis of the quantum mechanical phenomenon of resonant tunnelling.

However, the problem with precisely two transition points can be solved exactly, the connection formulae across both transition points being expressed in terms of the complex gamma function. These formulae can also be used in the case where there are two effective transition points (others existing in the complex plane), and the approximate connection formulae are then known as semiclassical parabolic connection formulae. When the carrier is real along the real axis, these gamma functions are of a special form involving the integral of the square root of the carrier between the transition points, expressible as $\Gamma(\mathrm{i}\phi)$ where ϕ is real. In consequence, the moduli of the gamma functions can be expressed in terms of hyperbolic functions.

Three, four or more transition points along the real z axis can be dealt with by these methods, either using the appropriate connection formulae across each transition point separately, or using the semiclassical parabolic formulae across each barrier, suitably connecting the solutions across each well (see Heading 1962, p 119, Connor 1968, Dickinson 1970, Fröman and Dammert 1970, Yngve 1972, Fröman *et al* 1972). The extent to which the traditional formulae relating to the transition points taken separately can be used in such problems has been investigated by Heading (1973), where it is shown that this extent is very limited.

Dangers and analytical errors have arisen when formulae derived relating to several real transition points are then assumed without comment to apply to the same number of complex transition points; several of the above-mentioned authors fall into this trap, though not Fröman and Fröman and their collaborators. It may appear to be very satisfying to use $\sinh \pi\phi$ in the evaluation of $|\Gamma(\mathrm{i}\phi)|$ when ϕ is real, but this usage rests on very insecure foundations when ϕ is complex even when the imaginary part of ϕ is small compared with the real part.

The approximate wave-like solutions of the WKBJ type are always exponential in form, either of the propagating or evanescent variety. Consequently such solutions are always susceptible to physical interpretation, and moreover can easily be calculated numerically from elementary tables. Additionally, when there is one transition point, the reflection coefficient is also expressed in terms of a complex exponential function, and this too is susceptible to interpretation in the sense that the incident wave can be traced through the complex z plane to emerge as a reflected wave (see Budden 1961, p 439). Similarly in the problem of the potential well; exponential functions arise which may be interpreted in terms of standing waves in the well.

When a barrier, however, is considered, there is still the desire to use the complex exponential function (based upon its ease of numerical evaluation, and upon an intuitive feeling for its physical interpretation), and this has led to its use even when analytically it is completely wrong to do so. For two transition points defining a barrier, the appropriate formulae *must* involve the gamma function of a complex argument, but its use has not been widely recognized, partly owing to the lack of accessibility of comprehensive tables, to the fact that the function possesses but few properties expressible in terms of the more elementary functions, and to the fact that a direct physical interpretation of the function is lacking. Lack of experience with the properties of the gamma function has caused a number of investigators in almost mutually exclusive fields to use certain formulae associated with it in domains beyond the validity of the original formulae, or to use certain off-shoot formulae of the gamma function wrongly, not realizing that they were derived from the gamma function under restricted conditions.

In particular, we may mention the work of Hayes (1973), who considers the transition from locked to leaky modes in tropospheric radio propagation. He uses the exponential approximation to the problem which implicitly uses the complex gamma function without it being specifically mentioned, and then extends it beyond its proper domain of validity. The false formula is derived in his paper by an argument that itself contains a vital flaw through not keeping track of the nature and effects of the errors involved in the approximation process.

The same kind of mistake occurs in the work of Connor (1968) and others. They consider resonant phenomena in a system of two potential barriers that requires complex eigenvalues. The formulae derived are based on the assumption that the gamma functions involved are of the form $\Gamma(\mathrm{i}\phi)$ where ϕ is real, but that they may be used without explanation when ϕ is complex. The correct approximate analytical treatment of this problem is considered in the present paper.

The fault in these and similar investigations lies in the failure to state at the beginning the class of admissible functions $q(z)$ and then to be consistent throughout the investigation. To commence with one class of functions, and then to assume that the derived formulae are applicable to an extended class of functions is the ultimate reason for the existence of these prevalent mistakes.

It appears necessary therefore to make some observations on the use of the gamma function in barrier penetration problems, particularly, but not exclusively, when the barrier is not wide with the two transition points defining the barrier lying near the top of the barrier. We also propose to examine the conditions under which explicit reference to the complex gamma function can be dispensed with owing to simpler formulae being available, to note when approximate formulae can be employed, to examine the nature of the analytical mistakes that have plagued work in the past, to recognize the existence of error terms that may be much larger than some small exponential terms otherwise present, and to note when the gamma function cannot be dispensed with.

2. The class of functions under discussion

The function $f(z)$ is given to be an analytic function of z for all z, except at isolated singularities not lying on the real z axis, such points being too far removed from the domain of consideration around the real axis to be of relevance in the approximation theory. Moreover, we shall specify that $f(z)$ is real for real z, though this restriction may be removed in other applications. If A is a complex constant, we define $q(z)$ to equal $f(z)-A$.

We take the differential equation governing wave propagation to be

$$\frac{d^2w}{dz^2}+k^2(f(z)-A)w = 0.$$

We further assume that the number of zeros of the function q lying near the real axis is restricted, and that they lie in a domain near the origin, thereby ensuring that the z plane is free from such transition points in some domain containing the real z axis as $z \to \pm\infty$.

The WKBJ solutions for large $|z|$ along and near the real axis will be of the form

$$q^{-\frac{1}{4}}\exp\left(\pm ik\int^z \sqrt{(f-A)}\,dz\right).$$

It is necessary to decide whether an anti-Stokes line either lies along or is asymptotic to the real axis as $z \to \pm\infty$, namely if $\mathrm{Im}\int^z \sqrt{(f-A)}\,dz \to 0$ or constant as $z \to \pm\infty$. If, for example, $f(z) = z^n, n > 2$, we have

$$\int^z \sqrt{(z^n-A)}\,dz \simeq \int^z z^{\frac{1}{2}n}(1-\tfrac{1}{2}Az^{-n})\,dz = \frac{z^{\frac{1}{2}(n+2)}}{\frac{1}{2}(n+2)}+\frac{A}{2(\frac{1}{2}n-1)z^{\frac{1}{2}n-1}},$$

and the imaginary part of this expression tends to zero since $\frac{1}{2}n-1 > 0$. But this is not true when $0 < n < 2$. For example, if f tends to a constant, c say, the indefinite integral tends to $z\sqrt{(c-A)}$ which certainly is not real for real z when A is complex. In the former case, an anti-Stokes line either lies along, or is asymptotic to the real axis as $z \to \pm\infty$, while in the latter case this is not so. In the former case, a wave propagating along the real z axis in the positive direction is represented by a WKBJ solution that becomes subdominant in a domain where $\mathrm{Im}\, z$ becomes negative from the real axis (see Budden 1961, p 442, Heading 1962, p 74). The resonant condition imposed in this investigation is that waves should be outgoing along both the positive and negative real z axes, implying that the solution must be subdominant in those domains where $\mathrm{Im}\, z$ becomes negative or positive from the positive and negative real z axes respectively. This resonant condition then yields complex values of the parameter A.

But in the latter case where the positive and negative real axes for large $|z|$ lie wholly within domains in which solutions become dominant or subdominant, the boundary conditions to be imposed are that solutions must be subdominant along both the positive and negative real axes for large $|z|$, yielding complex eigenvalues of the parameter A.

Rrestricting ourselves to the case when A has only a small imaginary part, the anti-Stokes lines in the latter case will deviate angularly only slightly from the real axis. The two cases may then be considered as one, provided subdominant domains exist adjacent to the anti-Stokes lines as arg z decreases from the anti-Stokes line, as shown in figure 1. This stipulation yields an equation giving the complex eigenvalues of A.

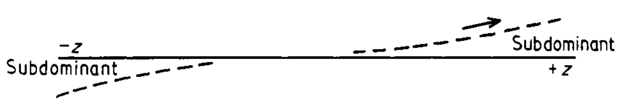

Figure 1. Domains of subdominant solutions with respect to the positive and negative real axes.

3. The double barrier problem

When A is real, we assume that $f(z)$ is such that $q \equiv f(z)-A$ possesses four single transition points on the real axis, namely $z = a, b, c, d$ in order, such that $f-A < 0$ within the two barriers $a < z < b, c < z < d$. When A is slightly complex, the transition points will move off the real axis. Transmission formulae through the double barrier will be derived using transmission formulae through each barrier separately, the solutions being joined together within the well $b < z < c$.

In figure 2, points A, B, C, D lie on the real axis at positions nearest to the complex points a, b, c, d.

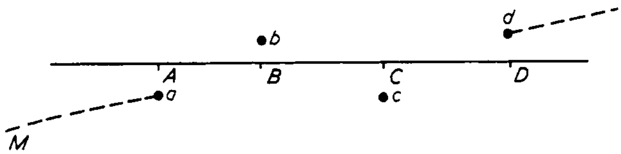

Figure 2. Positions of the complex transition points for a double barrier with energy loss.

One wave along the real axis to the left of A is given by the WKBJ solution

$$(z, a) \equiv^{*} q^{-\frac{1}{4}} \exp\left(-ik \int_a^z q^{\frac{1}{2}}\, dz\right)$$

using the convenient notation introduced by the author to designate WKBJ solutions (Heading 1962). Here, $\arg q = 0$ when A is real, but small when A is slightly complex. This wave propagates to the right, or at least is dominant above the anti-Stokes line aM in the domain containing the negative z axis. The wave that propagates to the left, or that is subdominant above the line aM, is

$$(a, z) \equiv^{*} q^{-\frac{1}{4}} \exp\left(ik \int_a^z q^{\frac{1}{2}}\, dz\right).$$

The star denotes that the right-hand side contains an error term that cannot be explicitly stated. The reason for keeping track of this fact is that serious mistakes can be made as soon as terms on the right-hand side become equal in magnitude to the error terms recognized as being present. In the two WKBJ solutions, the error terms involved tend to zero in the unbounded domain $|z| \to \infty$.

In the well BC, we similarly define two waves represented by (z, b) propagated to the right, and (b, z) to the left. But the approximate waveforms contain errors that cannot be obliterated, since the domain $B < z < C$ is not unbounded. Again, in this well, $\arg q$ is chosen to vanish when A is real, but differs slightly from zero when A is slightly complex.

Let R_1, T_1 denote the reflection and transmission coefficients for the barrier produced by the transition points a, b when incidence takes place from the left, and let R'_1 and T'_1 denote these coefficients when incidence takes place from the right. We thus have the two connection formulae across the barrier:

$$(z, a)+R_1(a, z) \leftrightarrow T_1(z, b),$$

$$T'_1(a, z) \leftrightarrow (b, z)+R'_1(z, b),$$

or arranged in matrix notation,

$$\begin{pmatrix} 1 & R_1 \\ 0 & T'_1 \end{pmatrix} \begin{pmatrix} (z, a) \\ (a, z) \end{pmatrix} \leftrightarrow \begin{pmatrix} T_1 & 0 \\ R'_1 & 1 \end{pmatrix} \begin{pmatrix} (z, b) \\ (b, z) \end{pmatrix}.$$

Similarly for the second barrier to the right, we have the connection formulae along the real axis

$$\begin{pmatrix} 1 & R_2 \\ 0 & T'_2 \end{pmatrix} \begin{pmatrix} (z, c) \\ (c, z) \end{pmatrix} \leftrightarrow \begin{pmatrix} T_1 & 0 \\ R'_1 & 1 \end{pmatrix} \begin{pmatrix} (z, d) \\ (d, z) \end{pmatrix}.$$

Noting that

$$(b, z) = [b, c](c, z),$$

where $[b, c]$ (in square brackets, denoting that no factor $q^{-\frac{1}{4}}$ is involved), with the same stipulation on arg q as before, is defined by

$$[b, c] \equiv \exp\left(ik \int_b^c q^{\frac{1}{2}} \, \mathrm{d}z \right),$$

we see that

$$\begin{pmatrix} T_2 & 0 \\ R'_2 & 1 \end{pmatrix}^{-1} \begin{pmatrix} 1 & R_2 \\ 0 & T'_2 \end{pmatrix} \begin{pmatrix} [c, b] & 0 \\ 0 & [b, c] \end{pmatrix}^{-1} \begin{pmatrix} T_1 & 0 \\ R'_1 & 1 \end{pmatrix}^{-1} \begin{pmatrix} 1 & R_1 \\ 0 & T'_1 \end{pmatrix} \begin{pmatrix} (z, a) \\ (a, z) \end{pmatrix} \leftrightarrow^* \begin{pmatrix} (z, d) \\ (d, z) \end{pmatrix},$$

where implicit errors are involved in the joining up process within the well.

Expanding this matrix product, we see that a transmitted wave to the right (z, d) is connected to the waves on the left by the relation

$$([b, c] - R_2 R'_1 [c, b])(z, a) + \{[b, c] R_1 + [c, b] R_2 (-R'_1 R_1 + T'_1 T_1)\}(a, z) \leftrightarrow^* T_1 T_2 (z, d).$$

Resonance occurs when the coefficient of (z, a) vanishes, namely when there is no incident wave or when the solution is subdominant as $z \to -\infty$. Hence $[b, c]^2 =^* R'_1 R_2$, or

$$\exp\left(2ik \int_b^c q^{\frac{1}{2}} \, \mathrm{d}z \right) =^* R'_1 R_2.$$

Finally, we conclude that

$$k \int_b^c q^{\frac{1}{2}} \, \mathrm{d}z =^* n\pi - \tfrac{1}{2}\mathrm{i} \ln R'_1 R_2, \tag{1}$$

being a disguised form of a Bohr–Sommerfeld quantization condition.

4. The approximate values of R and T for a complex barrier

One aspect of the values of R and T has been examined by Connor (1968), Dickinson (1970) and Fröman and Dammert (1970), the authors considering the case corresponding to the parameter A being real. Dickinson and Connor derive effectively the same formulae, but tacitly assume that A may be complex. The correct formulae given by Fröman and Dammert are thereby seriously mutilated, and the results of none of these authors provide any complete information as to the proper formulae valid when A is complex. A brief derivation of the approximate formulae for a complex barrier is given here.

The general barrier is compared with the parabolic barrier with exactly two transition points.

Firstly consider the equation

$$\frac{\mathrm{d}^2 W}{\mathrm{d}\xi^2}+k^2(\xi^2-\beta^2)W = 0, \qquad -\tfrac{1}{2}\pi < \arg\beta^2 \leqslant \tfrac{1}{2}\pi. \tag{2}$$

If $n = \frac{1}{2}\mathrm{i}k\beta^2-\frac{1}{2}$, $s = \sqrt{(2k)}\,\mathrm{e}^{\frac{1}{4}\mathrm{i}\pi}\xi$, we obtain the equation of the Weber parabolic cylinder function, with the general solution

$$W = MD_n(s)+ND_n(-s).$$

Using their asymptotic forms (see Whittaker and Watson 1927, p 347) with $\xi = \pm h$, we obtain approximate forms for W containing $h^n\exp(-\frac{1}{2}\mathrm{i}kh^2)$ and $h^{-n-1}\exp(\frac{1}{2}\mathrm{i}kh^2)$. Into these asymptotic expressions we substitute the evaluated forms of the WKBJ solutions for large $\xi = \pm h$:

$$(\beta, \xi) =^* h^{-\frac{1}{2}}(2h/\beta)^{-\frac{1}{2}\mathrm{i}k\beta^2}\exp(-\tfrac{1}{4}\mathrm{i}k\beta^2)\exp(\tfrac{1}{2}\mathrm{i}kh^2), \qquad \xi = h,$$

$$(-\beta, \xi) =^* h^{-\frac{1}{2}}(2h/\beta)^{\frac{1}{2}\mathrm{i}k\beta^2}\exp(\tfrac{1}{4}\mathrm{i}k\beta^2)\exp(-\tfrac{1}{2}\mathrm{i}kh^2), \qquad \xi = -h.$$

We find that

$$\begin{aligned} W =^* {} & M(\xi, \beta)(2/\beta)^{-\frac{1}{2}\mathrm{i}k\beta^2}\exp(-\tfrac{1}{4}\mathrm{i}k\beta^2)\{\sqrt{(2k)}\,\mathrm{e}^{\frac{1}{4}\mathrm{i}\pi}\}^n+N(\xi, \beta)(2/\beta)^{-\frac{1}{2}\mathrm{i}k\beta^2}\exp(-\tfrac{1}{4}\mathrm{i}k\beta^2) \\ & \times\{\sqrt{(2k)}\,\mathrm{e}^{-\frac{3}{4}\mathrm{i}\pi}\}^n-\frac{N\sqrt{(2\pi)}}{\Gamma(-n)}\mathrm{e}^{-n\pi\mathrm{i}}(\beta, \xi)(2/\beta)^{\frac{1}{2}\mathrm{i}k\beta^2}\exp(\tfrac{1}{4}\mathrm{i}k\beta^2) \\ & \times\{\sqrt{(2k)}\,\mathrm{e}^{-\frac{3}{4}\mathrm{i}\pi}\}^{-n-1}, \qquad (\xi = h) \end{aligned}$$

$$\begin{aligned} W =^* {} & M(-\beta, \xi)(2/\beta)^{-\frac{1}{2}\mathrm{i}k\beta^2}\exp(-\tfrac{1}{4}\mathrm{i}k\beta^2)\{\sqrt{(2k)}\,\mathrm{e}^{-\frac{3}{4}\mathrm{i}\pi}\}^n-\frac{M\sqrt{(2\pi)}}{\Gamma(-n)}\mathrm{e}^{-n\pi\mathrm{i}}(\xi, -\beta) \\ & \times(2/\beta)^{\frac{1}{2}\mathrm{i}k\beta^2}\exp(\tfrac{1}{4}\mathrm{i}k\beta^2)\{\sqrt{(2k)}\,\mathrm{e}^{-\frac{3}{4}\mathrm{i}\pi}\}^{-n-1}+N(-\beta, \xi)(2/\beta)^{-\frac{1}{2}\mathrm{i}k\beta^2} \\ & \times\exp(-\tfrac{1}{4}\mathrm{i}k\beta^2)\{\sqrt{(2k)}\,\mathrm{e}^{\frac{1}{4}\mathrm{i}\pi}\}^n \qquad (\xi = -h). \end{aligned}$$

When incidence takes place from the left, we choose $N = 0$ so that the coefficient of (β, ξ) vanishes, giving

$$\begin{aligned} R & = \frac{\text{coefficient of }(-\beta, \xi)}{\text{coefficient of }(\xi, -\beta)} \\ & = \mathrm{i}(2\pi)^{-\frac{1}{2}}(\tfrac{1}{2}k\beta^2)^{\frac{1}{2}\mathrm{i}k\beta^2}\exp(\tfrac{1}{4}\pi k\beta^2)\exp(-\tfrac{1}{2}\mathrm{i}k\beta^2)\Gamma(\tfrac{1}{2}-\tfrac{1}{2}\mathrm{i}k\beta^2), \end{aligned} \tag{3}$$

$$T = \frac{\text{coefficient of }(\xi, \beta)}{\text{coefficient of }(\xi, -\beta)} = R\,\mathrm{e}^{n\mathrm{i}\pi}. \tag{4}$$

When incidence takes place from the right, we choose $M = 0$, yielding $R' = R$, $T' = T$.

Suppose now that we have a more general barrier governed by the equation

$$\frac{\mathrm{d}^2 w}{\mathrm{d}z^2}+k^2(z^2-a^2)g(z)w = 0,$$

where $q(z) \equiv (z^2-a^2)g(z)$. The change of variables $z = z(\xi)$, $w(z) = X(\xi)(\mathrm{d}z/\mathrm{d}\xi)^{\frac{1}{2}}$ yields

$$\frac{\mathrm{d}^2 X}{\mathrm{d}\xi^2}+k^2\left(\frac{\mathrm{d}z}{\mathrm{d}\xi}\right)^2(z^2-a^2)gX = \text{residual terms in } X. \tag{5}$$

We now choose $z(\xi)$ so that

$$\left(\frac{\mathrm{d}z}{\mathrm{d}\xi}\right)^2(z^2-a^2)g(z) = (\xi^2-\beta^2),$$

or

$$q^{\frac{1}{2}}\,\mathrm{d}z = (\xi^2-\beta^2)^{\frac{1}{2}}\mathrm{d}\xi,$$

branches being chosen to correspond in both planes in the neighbourhood of the barriers. The integrals

$$\int_{-a}^{z} q^{\frac{1}{2}}\,\mathrm{d}z = \int_{-\beta}^{\xi}(\xi^2-\beta^2)^{\frac{1}{2}}\,\mathrm{d}\xi$$

ensure that $z = -a$ and $\xi = -\beta$ are corresponding transition points. Moreover, we assert that

$$\int_{-a}^{a}(-q)^{\frac{1}{2}}\,\mathrm{d}z = \int_{-\beta}^{\beta}(\beta^2-\xi^2)^{\frac{1}{2}}\mathrm{d}\xi = \tfrac{1}{2}\pi\beta^2,$$

ensuring that the transition points $z = a$, $\xi = \beta$ correspond, at the same time determining β.

The approximate solution of equation (5) is found by neglecting its right-hand side, which has no singularities at these two transition points by this choice of β. The comparison equation (2) is thereby attained. Hence the approximate solution for X is the solution already found for W, the phase integral $\int_{-\beta}^{\xi}(\xi^2-\beta^2)^{1/2}\,\mathrm{d}\xi$ occurring in W in forms such as $(-\beta, \xi)$ now being replaced by $\int_{-a}^{z} q^{\frac{1}{2}}\,\mathrm{d}z$.

It follows that approximate values of R, R', T, T' are given by results (3) and (4), with β^2 replaced by

$$\beta^2 = \frac{2}{\pi}\int_{-a}^{a}(-q)^{\frac{1}{2}}\,\mathrm{d}z,$$

where $\arg(-q) = 0$ along the axis between the transition points when q is real, slightly deviating from zero when complex transition points are necessary.

We conclude that

$$R_1 =^{*} \mathrm{i}(2\pi)^{-\frac{1}{2}}\alpha_1^{\mathrm{i}\alpha_1}\exp(\tfrac{1}{2}\pi\alpha_1)\exp(-\mathrm{i}\alpha_1)\Gamma(\tfrac{1}{2}-\mathrm{i}\alpha_1) \tag{6}$$

where

$$\alpha_1 = \tfrac{1}{2}k\beta_1^2 = \frac{k}{\pi}\int_a^b(-q)^{\frac{1}{2}}\,\mathrm{d}z = \frac{k}{\pi}\int_a^b(A-f)^{\frac{1}{2}}\,\mathrm{d}z,$$

and

$$R_2 =^{*} \mathrm{i}(2\pi)^{-\frac{1}{2}}\alpha_2^{\mathrm{i}\alpha_2}\exp(\tfrac{1}{2}\pi\alpha_2)\exp(-\mathrm{i}\alpha_2)\Gamma(\tfrac{1}{2}-\mathrm{i}\alpha_2) \tag{7}$$

where

$$\alpha_2 = \tfrac{1}{2}k\beta_2^2 = \frac{k}{\pi}\int_c^d(-q)^{\frac{1}{2}}\,\mathrm{d}z = \frac{k}{\pi}\int_c^d(A-f)^{\frac{1}{2}}\,\mathrm{d}z,$$

with the stated convention for the interpretation of $\arg(-q)^{\frac{1}{2}}$.

Note that when α_1 and α_2 are large, $R_1 = R_2 \sim \mathrm{i}$ asymptotically by Stirling's formula.

If in either case α is real (and this is not to be expected in an eigenvalue problem), R may be expressed in the form

$$R =^* \mathrm{i}(2\pi)^{-\frac{1}{2}}\alpha^{\mathrm{i}\alpha}\,\mathrm{e}^{-\mathrm{i}\alpha}\,\mathrm{e}^{\frac{1}{2}\pi\alpha}\bigg/\sqrt{\left(\frac{\pi}{\cosh\pi\alpha}\right)}\exp\{\mathrm{i}\arg\Gamma(\tfrac{1}{2}-\mathrm{i}\alpha)\}$$

$$=^* \frac{\exp[\mathrm{i}\{\frac{1}{2}\pi-\alpha+\alpha\ln\alpha+\arg\Gamma(\frac{1}{2}-\mathrm{i}\alpha)\}]}{\sqrt{(1+\mathrm{e}^{-2\pi\alpha})}},$$

where we have used the exact formula

$$|\Gamma(\tfrac{1}{2}-\mathrm{i}\alpha)| = \sqrt{(\pi/\cosh\pi\alpha)}$$

valid *only* when α is real. If α is large,

$$\arg\Gamma(\tfrac{1}{2}-\mathrm{i}\alpha) =^* \alpha-\alpha\ln\alpha,$$

giving

$$R =^* \frac{\mathrm{i}}{\sqrt{(1+\mathrm{e}^{-2\pi\alpha})}}, \tag{8}$$

expressible also in the further approximate forms

$$R =^* \frac{\mathrm{i}}{1+\frac{1}{2}\mathrm{e}^{-2\pi\alpha}} =^* \mathrm{i}(1-\tfrac{1}{2}\mathrm{e}^{-2\pi\alpha}) \tag{9}$$

by the binomial. This formula must be used with extreme caution, since

$$\arg\Gamma(\tfrac{1}{2}-\mathrm{i}\alpha) = \alpha-\alpha\ln\alpha+\mathrm{O}(\alpha^{-1}),$$

yielding

$$R =^* \frac{\mathrm{i}\exp\{\mathrm{O}(\alpha^{-1})\}}{\sqrt{(1+\mathrm{e}^{-2\pi\alpha})}} = \mathrm{i}\{1+\mathrm{O}(\alpha^{-1})+\mathrm{O}(\mathrm{e}^{-2\pi\alpha})\}.$$

It can be seen that the exponentially small term is irrelevant compared with the term $\mathrm{O}(\alpha^{-1})$. Yet investigators frequently use formulae (8) or (9) without a clear understanding of the approximations implied or the relevance of the small exponential term. Work that pays no attention whatsoever to the existence of error terms is very misguided indeed. The origin of the term $\mathrm{e}^{-2\pi\alpha}$ as a series correction term in the modulus of R has been investigated by Heading (1972).

Another common fallacy is to use formulae (8) or (9) even when α is complex, taking

$$R =^* \frac{\mathrm{i}}{1+\frac{1}{2}\mathrm{e}^{-2\pi\alpha}}$$

when α is complex (provided $|\mathrm{e}^{-2\pi\alpha}|$ is small), though perhaps omitting the factor i and sometimes the factor $\frac{1}{2}$ (see Hayes 1973). Some numerical consequences of this are examined in § 6.

5. The complex double barrier

Using the approximate values (6) and (7) found for R_1 and R_2 containing the complex gamma functions, the eigenvalue condition (1) now becomes

$$k\int_b^c (f-A)^{\frac{1}{2}}\,\mathrm{d}z =^* \pi n-\tfrac{1}{2}\mathrm{i}\ln R_1R_2$$
$$=^* \pi n-\tfrac{1}{2}\mathrm{i}\{\mathrm{i}\pi-\ln 2\pi+\mathrm{i}\alpha_1\ln\alpha_1+\mathrm{i}\alpha_2\ln\alpha_2+\tfrac{1}{2}\pi(\alpha_1+\alpha_2)-\mathrm{i}(\alpha_1+\alpha_2)$$
$$+\ln\Gamma(\tfrac{1}{2}-\mathrm{i}\alpha_1)+\ln\Gamma(\tfrac{1}{2}-\mathrm{i}\alpha_2)\}, \tag{10}$$

this equation determining the eigenvalue A, and hence the transition points a, b, c, d.

We now write explicitly $A = R+\mathrm{i}\delta I$, with $|\delta I| \ll |R|$, and we consider the three integrals involved in condition (10). When $A = R$, let b and c be the two real transition points defining the well. But when A is altered to $R+\mathrm{i}\delta I$, let b and c become $b+\delta b$, $c+\delta c$ respectively, where $f(b+\delta b) = R+i\delta I$, so to the first order $f'(b)\delta b = \mathrm{i}\delta I$, or

$$\delta b = \frac{\mathrm{i}\delta I}{f'(b)}, \qquad \delta c = \frac{\mathrm{i}\delta I}{f'(c)}.$$

In the calculation of α_1, we write

$$\alpha_1 = \frac{k}{\pi}\int_{a+\delta a}^{b+\delta b}(R+\mathrm{i}\delta I-f)^{\frac{1}{2}}\,\mathrm{d}z$$
$$= \frac{k}{\pi}\int_{a+\delta a}^{a}(-q)^{\frac{1}{2}}\,\mathrm{d}z+\frac{k}{\pi}\int_a^b(-q)^{\frac{1}{2}}\,\mathrm{d}z+\frac{k}{\pi}\int_b^{b+\delta b}(-q)^{\frac{1}{2}}\,\mathrm{d}z.$$

The first and third integrals vanish to the first order, since the integrands vanish at $z = a$ and b respectively, while the second integral gives:

$$\alpha_1 =^* \frac{k}{\pi}\int_a^b (R-f)^{\frac{1}{2}}\left(1+\frac{\mathrm{i}\delta I}{2(R-f)^{\frac{1}{2}}}\right)\mathrm{d}z$$
$$=^* \frac{k}{\pi}\int_a^b (R-f)^{\frac{1}{2}}\,\mathrm{d}z+\frac{k\mathrm{i}\delta I}{2\pi}\int_a^b\frac{\mathrm{d}z}{(R-f)^{\frac{1}{2}}} \equiv J_1+\mathrm{i}\delta IK_1,$$

say. Similarly,

$$\alpha_2 =^* \frac{k}{\pi}\int_c^d (R-f)^{\frac{1}{2}}\,\mathrm{d}z+\frac{k\mathrm{i}\delta I}{2\pi}\int_c^d\frac{\mathrm{d}z}{(R-f)^{\frac{1}{2}}} \equiv J_2+\mathrm{i}\delta IK_2,$$

while the left-hand side of (8) is written in the form

$$k\int_b^c (f-R)^{\frac{1}{2}}\,\mathrm{d}z-\frac{k\mathrm{i}\delta I}{2}\int_b^c\frac{\mathrm{d}z}{(f-R)^{\frac{1}{2}}} \equiv \pi J_{\mathrm{W}}-\mathrm{i}\delta I\pi K_{\mathrm{W}},$$

say, the suffix W referring to the well, where a, b, c, d are the real zeros of $f-R$.

The eigenvalue condition (10) becomes

$$\pi J_{\mathrm{W}}-\mathrm{i}\delta I\pi K_{\mathrm{W}} =^* \pi n-\tfrac{1}{2}\mathrm{i}\{\mathrm{i}\pi-\ln 2\pi+\mathrm{i}(J_1+\mathrm{i}\delta IK_1)\ln(J_1+\mathrm{i}\delta IK_1)$$
$$+\mathrm{i}(J_2+\mathrm{i}\delta IK_2)\ln(J_2+\mathrm{i}\delta IK_2)+\tfrac{1}{2}\pi(J_1+\mathrm{i}\delta IK_1+J_2+\mathrm{i}\delta IK_2)$$
$$-\mathrm{i}(J_1+\mathrm{i}\delta IK_1+J_2+\mathrm{i}\delta IK_2)+\ln\Gamma(\tfrac{1}{2}-\mathrm{i}\alpha_1)+\ln\Gamma(\tfrac{1}{2}-\mathrm{i}\alpha_2)\}.$$

Accepting quantities to the first order only, and resolving into real and imaginary parts, we have

$$\pi J_{\mathrm{W}} =^* \pi n+\tfrac{1}{2}\pi+\frac{1}{2}\bigg\{J_1 \ln J_1+J_2 \ln J_2+\tfrac{1}{2}\pi(K_1+K_2)\delta I-(J_1+J_2)+\arg\Gamma(\tfrac{1}{2}-\mathrm{i}J_1)$$

$$+\arg\Gamma(\tfrac{1}{2}-\mathrm{i}J_2)+\left(K_1 \operatorname{Im}\frac{\Gamma'(\frac{1}{2}-\mathrm{i}J_1)}{\Gamma(\frac{1}{2}-\mathrm{i}J_1)}+K_2 \operatorname{Im}\frac{\Gamma'(\frac{1}{2}-\mathrm{i}J_2)}{\Gamma(\frac{1}{2}-\mathrm{i}J_2)}\right)\delta I\bigg\},$$

$$-\pi K_{\mathrm{W}}\delta I =^* \frac{1}{2}\bigg\{\ln 2\pi+(K_1 \ln J_1+K_2 \ln J_2)\delta I-\tfrac{1}{2}\pi(J_1+J_2)-\ln|\Gamma(\tfrac{1}{2}-\mathrm{i}J_1)|$$

$$-\ln|\Gamma(\tfrac{1}{2}-\mathrm{i}J_2)|-\left(K_1 \operatorname{Re}\frac{\Gamma'(\frac{1}{2}-\mathrm{i}J_1)}{\Gamma(\frac{1}{2}-\mathrm{i}J_1)}+K_2 \operatorname{Re}\frac{\Gamma'(\frac{1}{2}-\mathrm{i}J_2)}{\Gamma(\frac{1}{2}-\mathrm{i}J_2)}\right)\delta I\bigg\}.$$

The first equation contains zero-order terms, first-order terms and many error terms. To the zeroth order

$$J_{\mathrm{W}} = n+\tfrac{1}{2}+\tfrac{1}{2}\pi^{-1}\{J_1 \ln J_1+J_2 \ln J_2-J_1-J_2+\arg\Gamma(\tfrac{1}{2}-\mathrm{i}J_1)+\arg\Gamma(\tfrac{1}{2}-\mathrm{i}J_2)\},$$

corresponding in effect to Connor's and Dickinson's formula, explaining why the numerical results are so accurate in spite of their misguided analysis.

Moreover,

$$\begin{aligned}\ln|\Gamma(\tfrac{1}{2}-\mathrm{i}J_1)| &= \ln\surd\{\pi/(\cosh \pi J_1)\}\\ &= \tfrac{1}{2}\ln 2\pi-\tfrac{1}{2}\ln\{\exp(\pi J_1)+\exp(-\pi J_1)\}\\ &=^* \tfrac{1}{2}\ln 2\pi-\tfrac{1}{2}\pi J_1-\tfrac{1}{2}\exp(-2\pi J_1),\end{aligned}$$

yielding

$$-K_{\mathrm{W}}\delta I =^* \frac{1}{2\pi}\bigg\{(K_1 \ln J_1+K_2 \ln J_2)\delta I+\tfrac{1}{2}\{\exp(-2\pi J_1)+\exp(-2\pi J_2)\}$$

$$-\left(K_1 \operatorname{Re}\frac{\Gamma'(\frac{1}{2}-\mathrm{i}J_1)}{\Gamma(\frac{1}{2}-\mathrm{i}J_1)}+K_2 \operatorname{Re}\frac{\Gamma'(\frac{1}{2}-\mathrm{i}J_2)}{\Gamma(\frac{1}{2}-\mathrm{i}J_2)}\right)\delta I\bigg\}. \tag{11}$$

What terms can be sorted out from equation (11) with any degree of certainty? Unfortunately none, since the terms $\exp(-2\pi J_1)$ and $\exp(-2\pi J_2)$ are exponentially small compared with the increment δI and with the error terms existing implicitly in the equation. Consequently no conclusions can be drawn; certainly on analytical grounds it does not follow immediately that

$$\delta I = -\tfrac{1}{4}K_{\mathrm{W}}^{-1}\{\exp(-2\pi J_1)+\exp(-2\pi J_2)\}, \tag{12}$$

where terms of the form $\mathrm{O}(\delta I)$ are neglected on the right-hand side. If in a particular model, numerical investigation suggests that (12) does after all yield numerically good results, then this fact must be regarded as a coincidence and not analytically validated for all models, until it is conclusively proved that the error terms and the terms involving δI on the right-hand side of (11) are in fact negligible *in toto* compared with the term $\tfrac{1}{2}\{\exp(-2\pi J_1)+\exp(-2\pi J_2)\}$. If authors refuse to recognize the existence of implicit error terms, then equation (12) has no meaning, and it cannot properly be used in any application of the theory. Even solving equation (11) directly as it stands for δI cannot be done with any certainty, owing to the inherent errors involved in the $=^*$ sign arising from the WKBJ method. The methods presented in this paper provide no way out of this difficulty, and only by a deeper analysis of the problem based, for example, on the higher-order approximations of Fröman and Fröman and their collaborators, can the nature of the implicit error terms be sorted out.

6. The single complex barrier examined

The exact reflection coefficient for a parabolic barrier with two complex transition points $\pm\beta$ has been found in equation (3) to be

$$R = \mathrm{i}(2\pi)^{-1/2}\alpha^{\mathrm{i}\alpha}\,\mathrm{e}^{\frac{1}{2}\pi\alpha}\,\mathrm{e}^{-\mathrm{i}\alpha}\Gamma(\tfrac{1}{2}-\mathrm{i}\alpha),$$

with $\frac{1}{2}k\beta^2 = \alpha$ and $-\pi < \arg\alpha \leqslant \pi$. Asymptotically, $R \sim \mathrm{i}$ provided $\arg\alpha \neq -\frac{1}{2}\pi$, in which case $\Gamma(\frac{1}{2}-\mathrm{i}\alpha)$ would have a series of poles for appropriate values of $|\alpha|$. In this formula for R, it must be appreciated that $-\beta$ is taken to be the 'phase-reference level' for the incident and reflected waves. Any adjustment to a real phase-reference level is trivial and not of direct relevance here, though it would considerably alter the value of $|R|$, and the curves given in figure 3 must be interpreted in the light of this fact.

When α is real, two cases arise.

(i) When $\arg\alpha = 0$,

$$|R| = \frac{1}{\sqrt{(1+\mathrm{e}^{-2\pi\alpha})}} =^* \frac{1}{1+\frac{1}{2}\,\mathrm{e}^{-2\pi\alpha}}.$$

It has been suggested that the formula

$$R =^* \frac{\mathrm{i}}{1+\frac{1}{2}\mathrm{e}^{-2\pi\alpha}} \tag{13}$$

might be used for all $\arg\alpha$ for which $|\mathrm{e}^{-2\pi\alpha}| < 1$, namely $-\frac{1}{2}\pi < \arg\alpha < \frac{1}{2}\pi$. Hayes (1973) even omits the factor $\frac{1}{2}$, and seeks to provide a physical argument based on physically reflected evanescent and growing waves in a barrier to support his proposition. But this physical argument is without foundation, since there is not taken into account the error terms existing implicitly in the WKBJ solutions. The realization of the existence of these error terms would prevent the use within the barrier of any linear combination of evanescent and growing WKBJ solutions. Hayes also produces numerous numerically computed curves showing a comparison between the use of (13) and exact calculations. M S Smith (1973, private communication) has recalculated these curves using the factor $\frac{1}{2}$.

(ii) When $\arg\alpha = \pi$, we find that

$$|R| = \frac{1}{\sqrt{(1+\mathrm{e}^{2\pi\alpha})}} =^* \frac{1}{1+\frac{1}{2}\mathrm{e}^{2\pi\alpha}}.$$

Again it has been suggested that we may take

$$R =^* \frac{\mathrm{i}}{1+\frac{1}{2}\mathrm{e}^{2\pi\alpha}}$$

whenever $|\mathrm{e}^{2\pi\alpha}| < 1$, namely $-\pi < \arg\alpha < -\frac{1}{2}\pi$, $\frac{1}{2}\pi < \arg\alpha \leqslant \pi$.

Of course, when $|\alpha|$ is large, the modulus of these suggested false formulae is nearly unity, in keeping with its correct value. The deviation of $|R|_f$ from $|R|_c$ (where f and c stand for false and correct) is then very small, but this observation cannot give any justification for using analytically false formulae. The falseness of the assumptions can be seen by presenting some curves calculated when $|\alpha|$ is not large. We compare

$$|R(\alpha)|_c = (2\pi)^{-1/2}|\alpha^{i\alpha}\, e^{\frac{1}{2}\pi\alpha}\, e^{-i\alpha}\Gamma(\tfrac{1}{2}-i\alpha)|$$

with

$$|R(\alpha)|_f = \begin{cases} \left|\dfrac{1}{\sqrt{(1+e^{-2\pi\alpha})}}\right| & -\frac{1}{2}\pi < \arg\alpha < \frac{1}{2}\pi, \\ \left|\dfrac{1}{\sqrt{(1+e^{2\pi\alpha})}}\right| & -\pi < \arg\alpha < -\frac{1}{2}\pi,\ \ \frac{1}{2}\pi < \arg\alpha \leqslant \pi, \end{cases}$$

with no suggested false formula possible when $\arg\alpha = \pm\frac{1}{2}\pi$.

Writing $\alpha = r\,e^{i\theta} = r\cos\theta + ir\sin\theta = x+iy$, we have

$$|R|_c = \exp\{-\tfrac{1}{2}\ln 2\pi + x(\tfrac{1}{2}\pi-\theta) + y(1-\ln r) + \operatorname{Re}\ln\Gamma(\tfrac{1}{2}+y-ix)\}.$$

This is to be compared with

$$|R|_f = \frac{1}{\sqrt[4]{(1+2e^{-2\pi x}\cos 2\pi y + e^{-4\pi x})}} \qquad -\tfrac{1}{2}\pi < \arg\alpha < \tfrac{1}{2}\pi,$$

$$|R|_f = \frac{1}{\sqrt[4]{(1+2e^{2\pi x}\cos 2\pi y + e^{4\pi x})}} \qquad -\pi < \arg\alpha < -\tfrac{1}{2}\pi,\ \ \tfrac{1}{2}\pi < \arg\alpha \leqslant \pi.$$

A complete comparison of $|R|_c$ with $|R|_f$ for all x and y would require the computation of the surfaces $|R|_c$ and $|R|_f$ above the x, y plane. Instead, we have computed these moduli within the range $-1 \leqslant x \leqslant 1$ for $y = 0$, 0·2, 0·4, 0·6, 0·8, 1·0, and these results are presented in figure 3. The computation was carried out to 9 significant figures using the Tables of the Gamma Function for Complex Arguments (1954) which give $\ln\Gamma(z) = U+iV$ for $\operatorname{Re} z = 0{\cdot}0(0{\cdot}1)10{\cdot}0$ and $\operatorname{Im} z = 0{\cdot}0(0{\cdot}1)10{\cdot}0$ correct to 12 significant figures, and using a Sumlock Compucorp 322G programmable electronic desk computer displaying results to 10 figures, a model that possesses the facility of instant computation of the special functions involved.

The graphs display a wide deviation of $|R|_c$ from $|R|_f$, showing beyond doubt the impossibility of conceiving that the false formula may be useful in analytical work. Whereas the $|R|_c$ curves are uniform in their properties—all have a minimum when $x = 0$, yet the $|R|_f$ curves are more erratic, sometimes possessing a minimum and sometimes a maximum at $x = 0$. We have not illustrated the case when $|R|_f$ has a pole at $x = 0$; such occurs when $y = \operatorname{Im}\alpha = 0{\cdot}5$. Neither have we illustrated how the $|R|_f$ curve with a minimum changes to a curve with a maximum; such occurs near where $\cos 2\pi y = -\frac{1}{2}$, namely, $y = \frac{1}{3}$, for which

$$|R|_f = (1-e^{2\pi x}+e^{4\pi x})^{-1/4}, \qquad x < 0.$$

The discontinuity in gradient of the $|R|_f$ curves at $x = 0$ arises from the fact that distinct formulae are used to the right and to the left. Only when $y = 0$ does the $|R|_c$ curve also have a discontinuity in gradient at $x = 0$, arising from the term $x(\frac{1}{2}\pi-\theta)$ occurring in $|R|_c$; in any case $|R|_f = |R|_c$ when $y = 0$ (that is, when $\arg\alpha = 0, \pi$).

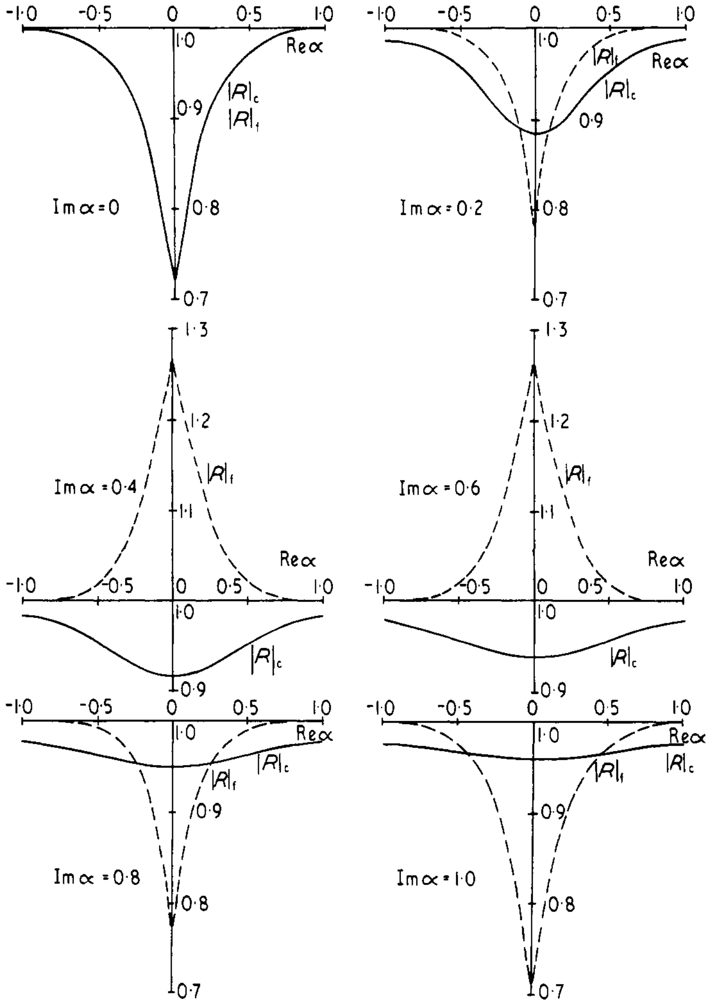

Figure 3. Comparison of the moduli of the reflection coefficients calculated from exact and false formulae for a single potential barrier with energy loss.

We may finally mention other approximations that have been suggested. Ford and Hill (1959) and Miller (1968) give

$$\arg\Gamma(\tfrac{1}{2}+\mathrm{i}\alpha) \simeq \tfrac{1}{2}\alpha\ln\{(\alpha/\mathrm{e})^2+(1/4\gamma)^2\},$$

$$\Gamma(\tfrac{1}{2}+\mathrm{i}\alpha) \simeq \surd(\pi/\cosh\pi\alpha)\{(\alpha/\mathrm{e})^2+(1/4\gamma)^2\}^{\frac{1}{2}\mathrm{i}\alpha}, \tag{14}$$

$$\arg\Gamma(\tfrac{1}{2}+\mathrm{i}\alpha) \simeq \frac{\alpha}{2}\ln\left(1+\frac{1}{4\alpha^2}\right)-\frac{2\alpha\{1+(\alpha^2-\frac{3}{4})/60(\alpha^2+\frac{1}{4})^2\}}{24(\alpha^2+\frac{1}{4})},$$

$$\Gamma(\tfrac{1}{2}+\mathrm{i}\alpha) \simeq \left(\frac{\pi}{\cosh\pi\alpha}\right)^{1/2}\left(1+\frac{1}{4\alpha^2}\right)^{\frac{1}{2}\mathrm{i}\alpha}\exp\left(\frac{-2\mathrm{i}\alpha\{1+(\alpha^2-\frac{3}{4})/60(\alpha^2+\frac{1}{4})^2\}}{24(\alpha^2+\frac{1}{4})}\right), \tag{15}$$

when α is real and positive. If, when α is real and positive, we write exactly,

$$\Gamma(\tfrac{1}{2}+\mathrm{i}\alpha) = \surd(\pi/\cosh\pi\alpha)\exp\{\mathrm{i}\arg\Gamma(\tfrac{1}{2}+\mathrm{i}\alpha)\} \equiv r(\alpha)\,\mathrm{e}^{\mathrm{i}\theta(\alpha)}, \tag{16}$$

say, where $r(\alpha)$ and $\theta(\alpha)$ are real functions of real α, then when α is complex formula (16) still persists, thereby making r and θ complex functions not in any sense now related to modulus and argument. Such a form as (16) tends to be very misleading, suggesting that the hyperbolic functions enter the form of the complex gamma function, whereas this is not really so; only when α is real can this rightly be asserted. But when approximate forms for $\theta(\alpha)$ are used as in (14) and (15), then the use of these expressions when α is complex is a much more delicate question. Miller gives various curves showing how good the approximations are for the argument when α is real. The approximations are uniform for all real α, but when α is complex this cannot be asserted. In fact, if α is placed equal to $-\frac{1}{2}\mathrm{i}$ in (14), a pole appears on the right-hand side, which is quite absent from $\Gamma(1)$. This could not occur in the exact form (16), since the offending denominator $\cosh \pi\alpha$ would in effect be cancelled by a corresponding factor in $\theta(\alpha)$. It is, in fact, this nonuniformity that causes the breakdown in the suggested formula (13) when α is complex. The factor i in its numerator represents an approximate phase factor when α is real, and cannot be extended uniformly into the complex domain when α is complex.

In any case, approximations as (14) and (15) are only immediately useful when the gamma functions enter the *exact* solutions of a barrier problem—in particular for the parabolic barrier and for the other barriers investigated by Heading (1972). As soon as semiclassical analysis of the barrier problem is employed, the question of the balance of differing error terms must be carefully weighed. The magnitude of the correction terms in the approximate versions of the gamma function (14) and (15) must be taken into account together with the inherent errors in the WKBJ solutions, and the errors involved in using barrier formulae derived from the parabolic barrier for the non-parabolic case. The paper by Miller does not seem to recognize this question of the balance of errors, which, it is appreciated, is a very awkward one. The object of our present paper has been to pursue the analysis as far as possible *without* knowing the nature of the inherent errors in the WKBJ solutions, and if this knowledge is not forthcoming, then further correction terms introduced in other parts of the analysis must be viewed with extreme suspicion and caution.

7. Conclusions

We have examined exact and approximate solutions of the potential barrier problem, showing how the complex gamma function must arise, and also how small correction terms cannot be relied upon when they stand in conflict with many small error terms allowed to exist in the phase-integral method. Moreover, we have discussed under what conditions it is legitimate to simplify the gamma function, either accurately or approximately. We have also examined certain recent work, and have compared numerically certain correct and false formulae which have often been used by some authors. It is hoped that the paper may terminate the manipulation of the complex gamma function under nonlegitimate conditions.

References

Berry M V and Mount K E 1972 *Rep. Prog. Phys.* **35** 315–97
Budden K G 1961 *Radio Waves in the Ionosphere* (Cambridge: Cambridge University Press)
Connor J N L 1968 *Molec. Phys.* **15** 37–46

Dickinson A S 1970 *Molec. Phys.* **18** 441–9
Ford K W and Hill D L 1959 *Ann. Phys., NY* 7 239–58
Fröman N and Dammert O 1970 *Nucl. Phys.* A **147** 627–49
Fröman N, Fröman P O, Myhrman U and Paulsson R 1972 *Ann. Phys., Lpz* **74** 314–23
Furry W H 1947 *Phys. Rev.* **71** 360–71
Hayes M G W 1973 *J. Phys.* A: *Math., Nucl. Gen.* **6** 177–91
Heading J 1962 *An Introduction to Phase-Integral Methods* (London: Methuen)
—— 1972 *Proc. Camb. Phil. Soc.* **71** 353–67
—— 1973 *Proc. Camb. Phil. Soc.* **74** in the press
Miller W H 1968 *J. chem. Phys.* **48** 1651–8
Tables of the Gamma Function for Complex Arguments 1954 *Natn. Bur. Stand. appl. Maths. Ser. No* 34 (Washington: US Government Printing Office)
Whittaker E T and Watson G N 1927 *A Course of Modern Analysis* (Cambridge: Cambridge University Press)
Yngve S 1972 *J. math. Phys.* **13** 324–30