

## TRANSMISSION THROUGH A REAL POTENTIAL BARRIER TREATED BY MEANS OF CERTAIN PHASE-INTEGRAL APPROXIMATIONS

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**Abstract:** The quantal problem of tunneling and super-barrier transmission through a real potential barrier is treated rigorously by means of certain phase-integral approximations. Given the wave function on one side of a smooth potential barrier, we derive both exact and approximate expressions for the wave function on the other side of the barrier and, under certain conditions, approximate expressions for the wave function inside the barrier. The case when the wave function is a standing wave is especially intricate and is discussed in great detail, since it has important applications in the treatment of scattering and decay problems. The case when the wave function represents an outgoing wave on one side of the barrier is also treated, and expressions for the transmission and reflection coefficients are given.

### 1. Introduction

The treatment by means of the JWKB approximation of the effect of a potential barrier on the wave function has caused much discussion in the literature, see e.g. Jeffreys <sup>1</sup>). The problem so far has not been fully treated, even for a single potential barrier, and for certain physically important cases the available results are not at all sufficient. As concerns earlier treatments of the barrier penetration problem with the aid of the first-order JWKB approximation we refer to the book by Heading <sup>2</sup>), where a historical survey of the method and of its applications is given, and to a review article by Jeffreys <sup>3</sup>). We also refer to a paper by Ford, Hill, Wakano and Wheeler <sup>4</sup>). A critical analysis of the way connection formulae have sometimes been used in earlier treatments of the barrier penetration problem can be found in a previous paper by one of us <sup>5</sup>).

The method for handling the connection problems of the JWKB approximation developed by the present authors a few years ago <sup>6</sup>) allows a complete analysis, within the frame-work of the approximations used in the present paper, of the problem concerning the influence of a single potential barrier on the wave function. The case when the wave function is given as an outgoing wave on one side of the barrier was considered in ref. <sup>6</sup>). In the present paper we shall treat the barrier problem more fully and pay special attention to the intricate case when the wave function is a standing wave outside the barrier. We shall use the higher-order phase-integral approximations derived in a previous paper <sup>7</sup>), since the extension from the JWKB approximation to these higher-order approximations can be made without any essential complication. We refer to refs. <sup>7-9</sup>) for details concerning the properties of the phase-integral

approximations and the adaptation of the methods developed in ref. 6) to these approximations.

Given a solution of the Schrödinger equation on one side of the potential barrier, we shall derive an exact expression for the solution on the other side of the barrier. Using estimates of certain quantities appearing in this exact expression, we obtain an approximate solution which is expressed in terms of the above-mentioned phase-integral approximations of any desired order. Using these exact and approximate solutions, we shall discuss the properties of the wave function in the presence of a potential barrier.

## 2. Exact expressions for the wave function

Let us write the time-independent Schrödinger equation for a particle moving in a one-dimensional potential field as follows

$$\frac{d^2\psi}{dz^2} + Q^2(z)\psi = 0, \quad (1)$$

where, with obvious notations,

$$Q^2(z) = \frac{2m}{\hbar^2} [E - V(z)]. \quad (2)$$

In the present paper we shall consider a single potential barrier for which  $Q^2(z)$  is real on the real axis. Furthermore, we shall assume that  $Q^2(z)$  is an analytic function of  $z$ . The problem will be treated according to the principles outlined in ref. 7). To make the present paper self-contained, to some extent, we quote from ref. 7) the expressions for the basic functions  $f_1(z)$  and  $f_2(z)$ , i.e.

$$f_1(z) = q^{-\frac{1}{2}}(z) \exp \{ +iw(z) \}, \quad (3a)$$

$$f_2(z) = q^{-\frac{1}{2}}(z) \exp \{ -iw(z) \}, \quad (3b)$$

where

$$w(z) = \int^z q(z) dz, \quad (4)$$

$$q(z) = Q(z) \sum_{n=0}^N Y_{2n}(z). \quad (5)$$

The functions  $Y_{2n}(z)$  can be obtained from recursion formulae given in ref. 7), which yield †

$$Y_0(z) = 1, \quad (6a)$$

$$Y_2(z) = \frac{1}{2}\varepsilon_0, \quad (6b)$$

† The expressions (6a, b, c) were given in ref. 7), whereas the expressions (6d, e) have been derived by F. Karlsson and S. Yngve at our institute.

$$Y_4(z) = -\frac{1}{8} \left[ \varepsilon_0^2 + \frac{d^2 \varepsilon_0}{d\zeta^2} \right] = -\frac{1}{8} \varepsilon_0^2 - \frac{1}{8} \frac{d}{d\zeta} \frac{d\varepsilon_0}{d\zeta}, \quad (6c)$$

$$\begin{aligned} Y_6(z) &= \frac{1}{32} \left[ 2\varepsilon_0^3 + 5 \left( \frac{d\varepsilon_0}{d\zeta} \right)^2 + 6\varepsilon_0 \frac{d^2 \varepsilon_0}{d\zeta^2} + \frac{d^4 \varepsilon_0}{d\zeta^4} \right] \\ &= \frac{1}{32} \left[ 2\varepsilon_0^3 - \left( \frac{d\varepsilon_0}{d\zeta} \right)^2 \right] + \frac{1}{32} \frac{d}{d\zeta} \left[ 6\varepsilon_0 \frac{d\varepsilon_0}{d\zeta} + \frac{d^3 \varepsilon_0}{d\zeta^3} \right], \end{aligned} \quad (6d)$$

$$\begin{aligned} Y_8(z) &= -\frac{1}{128} \left[ 5\varepsilon_0^4 + 50\varepsilon_0 \left( \frac{d\varepsilon_0}{d\zeta} \right)^2 + 30\varepsilon_0^2 \frac{d^2 \varepsilon_0}{d\zeta^2} + 19 \left( \frac{d^2 \varepsilon_0}{d\zeta^2} \right)^2 \right. \\ &\quad \left. + 28 \frac{d\varepsilon_0}{d\zeta} \frac{d^3 \varepsilon_0}{d\zeta^3} + 10\varepsilon_0 \frac{d^4 \varepsilon_0}{d\zeta^4} + \frac{d^6 \varepsilon_0}{d\zeta^6} \right] \\ &= -\frac{1}{128} \left[ 5\varepsilon_0^4 - 10\varepsilon_0 \left( \frac{d\varepsilon_0}{d\zeta} \right)^2 + \left( \frac{d^2 \varepsilon_0}{d\zeta^2} \right)^2 \right] \\ &\quad - \frac{1}{128} \frac{d}{d\zeta} \left[ 30\varepsilon_0^2 \frac{d\varepsilon_0}{d\zeta} + 18 \frac{d\varepsilon_0}{d\zeta} \frac{d^2 \varepsilon_0}{d\zeta^2} + 10\varepsilon_0 \frac{d^3 \varepsilon_0}{d\zeta^3} + \frac{d^5 \varepsilon_0}{d\zeta^5} \right], \end{aligned} \quad (6e)$$

where

$$\varepsilon_0 = Q^{-\frac{3}{2}} \frac{d^2}{dz^2} Q^{-\frac{1}{2}} = \frac{1}{16Q^6} \left\{ 5 \left[ \frac{d(Q^2)}{dz} \right]^2 - 4Q^2 \frac{d^2(Q^2)}{dz^2} \right\}, \quad (7)$$

$$\zeta = \int^z Q(z) dz. \quad (8)$$

In the region of the complex  $z$ -plane of interest to us the function  $Q^2(z)$  has two zeros  $t_1$  and  $t_2$ . We introduce a cut between these two transition points and construct a Riemann surface with two sheets. The phase of  $q^{\pm}(z)$  on the first Riemann sheet is chosen as indicated in figs. 1a and 1b, i.e. analogously as in the treatment of the barrier transmission problem in ref. <sup>6)</sup>, see figs. 6.4, 6.5, and 6.6 in ref. <sup>6)</sup>. Points on the real axis will be denoted by  $x$ , those to the left of the barrier by  $x_1$  and those to the right of the barrier by  $x_2$ . In the case of sub-barrier penetration, points on the real axis inside the barrier are denoted by  $x_0$ .

It is convenient to introduce the following notations

$$w_1(x_1) = \operatorname{Re} \frac{1}{2} \int_{\Gamma_1} q(z) dz, \quad (9a)$$

$$w_2(x_2) = \operatorname{Re} \frac{1}{2} \int_{\Gamma_2} q(z) dz, \quad (9b)$$

where the contours of integration are shown in fig. 1a for the case of sub-barrier penetration and in fig. 1b for the case of super-barrier transmission. When sub-barrier penetration is treated by means of the first-order JWKB approximation  $w_1(x_1)$  and

$w_2(x_2)$  are the well-known quantities  $\int_{t_1}^{x_1} Q(x)dx$  and  $\int_{t_2}^{x_2} Q(x)dx$ , respectively. For phase-integral approximations of any order the integrals  $\int_{\Gamma_1} q(z)dz$  and  $\int_{\Gamma_2} q(z)dz$  are

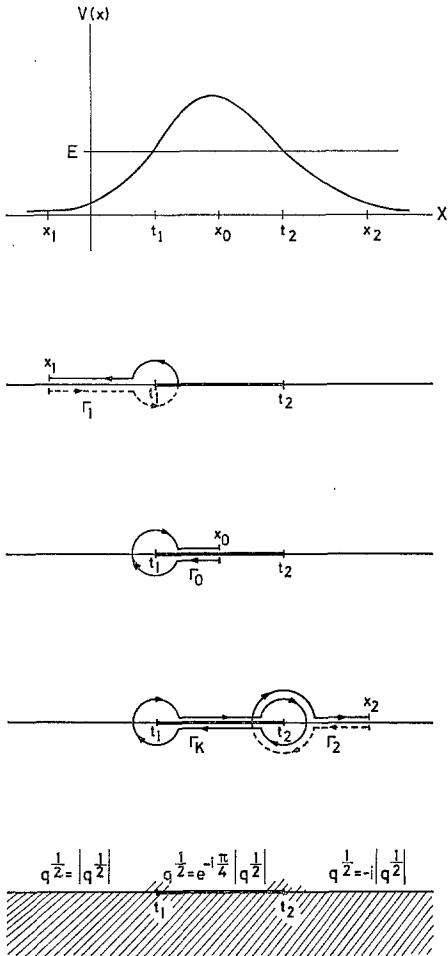


Fig. 1a. This figure refers to the sub-barrier case. It shows the qualitative behaviour of  $V(x)$  and the contours of integration for obtaining  $w(x)$ . The parts of these contours which lie on the second Riemann sheet are indicated by dashed lines. The heavy line indicates a cut. The values of  $q^{1/2}$  given in the figure refer to the first Riemann sheet.

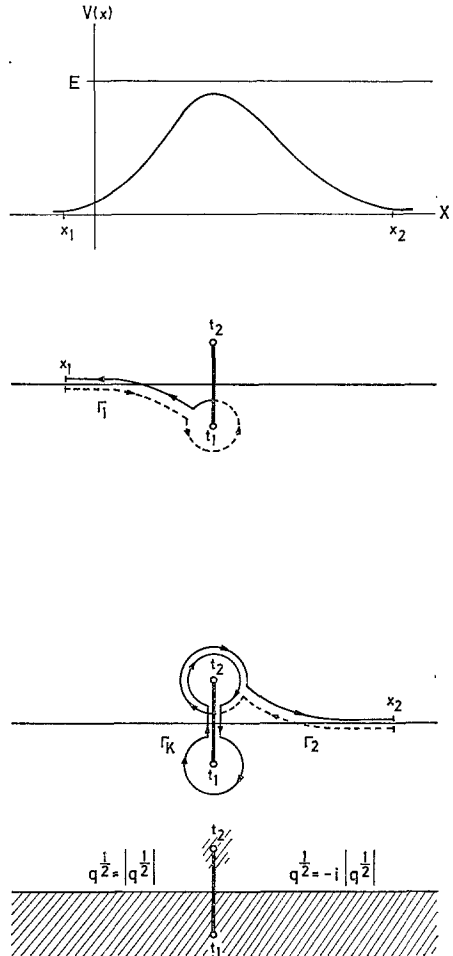


Fig. 1b. This figure refers to the super-barrier case but is for the rest analogous to fig. 1a. The paths of integration depicted in the figure are those appearing in the definitions (9a, b).

real in the sub-barrier case but complex in the super-barrier case. From (9a, b) it follows that  $w_1(x_1)$  and  $w_2(x_2)$  are negative both in the sub-barrier and in the super-

barrier case, i.e. that

$$w_1(x_1) = -|w_1(x_1)|, \quad (10a)$$

$$w_2(x_2) = -|w_2(x_2)|, \quad (10b)$$

in both cases.

The loops of integration depicted in figs. 1a and 1b and used in the definitions (9a, b) have been chosen so as to present a close analogy between the sub-barrier case of fig. 1a and the super-barrier case of fig. 1b. In the latter case one can rewrite the formulae (9a, b) by using other paths of integration. Choosing the cut joining the transition points  $t_1$  and  $t_2$  to coincide with the Stokes' line connecting these two points †, we can in fact write (9a, b) as follows

$$w_1(x_1) = \int_{x_s-0}^{x_1} q(x)dx, \quad (11a)$$

$$w_2(x_2) = \int_{x_s+0}^{x_2} q(x)dx, \quad (11b)$$

where  $x_s$  is the point where the Stokes' line crosses the real axis. The paths of integration in (11a, b) were used in ref. 9).

It is also convenient to introduce the notation

$$K = \frac{1}{2}i \int_{\Gamma_K} q(z)dz, \quad (12)$$

where the contour of integration is shown in fig. 1a for the case of sub-barrier penetration and in fig. 1b for the case of super-barrier transmission. We remark that  $K$  is real in both cases, being positive in the former case and negative in the latter case. In the super-barrier case  $K$  can also be written as follows

$$K = -\operatorname{Im} \int_{r_1} q(z)dz = -\operatorname{Im} \int_{r_2} q(z)dz = -\operatorname{Im} \int_{x_1}^{x_2} q(z)dz, \quad (13)$$

the path of integration in the last integral proceeding in the upper half-plane of the first Riemann sheet and connecting two arbitrary points  $x_1$  and  $x_2$  located on the real axis to the left and to the right, respectively, of the cut joining  $t_1$  and  $t_2$ . When the first-order JWKB approximation is used the definition (12) can be written as follows

$$K = i \int_{t_1}^{t_2} Q(z)dz. \quad (14)$$

In the case of sub-barrier penetration this is precisely the well-known JWKB integral  $\int_{t_1}^{t_2} |Q(x)|dx$ , occurring in the approximate formula for the transmission coefficient.

† If the barrier is symmetric, this Stokes' line coincides with the straight line  $t_1 t_2$  depicted in fig. 1b.

It should be emphasized that those terms in the expressions for  $Y_{2n}(z)$  which are total derivatives with respect to  $\zeta$  do not contribute to the value of  $K$ . This fact greatly simplifies the numerical calculations needed for the practical use of the results of the present paper.

If we choose the fixed lower limit in the integral (4) defining  $w(z)$  conveniently, we have the following formulae [cf. ref. <sup>7</sup>]

$$w(x_1) = w_1(x_1), \quad (15a)$$

$$w(x_2) = w_2(x_2) - iK, \quad (15b)$$

where  $x_1$  and  $x_2$  are points on the real axis lying as indicated in figs. 1a and 1b. For the first-order JWKB approximation we get the formulae (15a, b) by choosing the fixed lower limit of integration in (4) to be  $t_1$  in the sub-barrier case and to be  $x_s - 0$  in the super-barrier case.

Using (3a, b), (15a, b) and (10a, b), and remembering the phases of  $q^{\frac{1}{2}}(x_1)$  and  $q^{\frac{1}{2}}(x_2)$  shown in figs. 1a and 1b, we obtain the formulae

$$f_1(x_1) = |q^{-\frac{1}{2}}(x_1)| \exp \{-i|w_1(x_1)|\}, \quad (16a)$$

$$f_2(x_1) = |q^{-\frac{1}{2}}(x_1)| \exp \{+i|w_1(x_1)|\}, \quad (16b)$$

$$f_1(x_2) = |q^{-\frac{1}{2}}(x_2)| \exp \{K - i[|w_2(x_2)| - \frac{1}{2}\pi]\}, \quad (17a)$$

$$f_2(x_2) = -|q^{-\frac{1}{2}}(x_2)| \exp \{-K + i[|w_2(x_2)| - \frac{1}{2}\pi]\}. \quad (17b)$$

Several results obtained in ref. <sup>6</sup>) can be taken over to our present treatment. For details concerning the general theory we refer to refs. <sup>6-9</sup>).

According to eq. (3.25a) in ref. <sup>6</sup>) the wave function can be written in exact form as follows

$$\psi(z) = a_1(z)f_1(z) + a_2(z)f_2(z), \quad (18)$$

where  $a_1(z)$  and  $a_2(z)$  change with  $z$  according to eq. (3.26) in ref. <sup>6</sup>), i.e. according to the formula

$$\begin{pmatrix} a_1(z) \\ a_2(z) \end{pmatrix} = \mathbf{F}(z, z_0) \begin{pmatrix} a_1(z_0) \\ a_2(z_0) \end{pmatrix}, \quad (19)$$

where  $\mathbf{F}(z, z_0)$  is a two-by-two matrix which depends on  $z_0$  and  $z$  as well as on the parameters in the function  $Q^2(z)$ . The matrix  $\mathbf{F}(z, z_0)$ , which has been defined in terms of convergent series in ref. <sup>6</sup>), has the property that

$$\det \mathbf{F}(z, z_0) = 1. \quad (20)$$

Using (20), one obtains the inversion formula (3.20) in ref. <sup>6</sup>), i.e.

$$\mathbf{F}(z_0, z) = [\mathbf{F}(z, z_0)]^{-1} = \begin{pmatrix} F_{22}(z, z_0) & -F_{12}(z, z_0) \\ -F_{21}(z, z_0) & F_{11}(z, z_0) \end{pmatrix}. \quad (21)$$

The matrix  $F(x_1, x_2)$ , where  $x_1$  and  $x_2$  are points on the real axis lying as shown in figs. 1a and 1b, fulfills the symmetry relations (6.17a, b) or (6.32a, b) in ref. <sup>6)</sup>, i.e.

$$F_{11}(x_1, x_2) = -F_{22}^*(x_1, x_2) \exp \{2K\}, \quad (22a)$$

$$F_{21}(x_1, x_2) = -F_{12}^*(x_1, x_2) \exp \{2K\}, \quad (22b)$$

as is easily seen from eqs. (5.7a, b) in ref. <sup>6)</sup> and eqs. (15a, b) in the present paper. Substituting (22a, b) into (20), we obtain the relation (6.19) or (6.34) in ref. <sup>6)</sup>, i.e.

$$|F_{12}(x_1, x_2)|^2 - |F_{22}(x_1, x_2)|^2 = \exp \{-2K\}. \quad (23)$$

We recall [cf. p. 92 in ref. <sup>6)</sup>] that in a classically allowed region the functions  $f_1(x)$  and  $f_2(x)$  may be interpreted as waves travelling in opposite directions, if they are approximate solutions of the differential equation good enough for  $a_1(x)$  and  $a_2(x)$  to be considered as constants. To the left of the barrier  $f_1(x)$  represents a wave travelling from left to right, but to the right of the barrier it represents a wave travelling from right to left. The function  $f_2(x)$  behaves in the opposite way.

Assuming that the wave function  $\psi(x)$  is given on one side of the potential barrier, we shall derive an exact expression for the same wave function on the other side of the barrier. The further discussion will be concentrated on two physically very important cases, namely the case when the wave function corresponds to a standing wave and the case when it corresponds to an outgoing wave on one side of the barrier.

## 2.1. WAVE FUNCTION GIVEN TO THE LEFT OF THE BARRIER

2.1.1. *General case.* Let us assume the wave function and its derivative to be given at the point  $x_1$ . This means that in the general expression (18) for the wave function we may consider  $a_1(x_1)$  and  $a_2(x_1)$  as given constants. It is convenient to introduce new constants  $A_1$  and  $B_1$  instead of  $a_1(x_1)$  and  $a_2(x_1)$  by writing

$$a_1(x_1) = A_1 \exp \{-\frac{1}{4}\pi i\}, \quad (24a)$$

$$a_2(x_1) = B_1 \exp \{+\frac{1}{4}\pi i\}. \quad (24b)$$

Using these formulae and (16a, b), we obtain from (18) the formula

$$\begin{aligned} \psi(x_1) = & A_1 |q^{-\frac{1}{2}}(x_1)| \exp \{-i[|w_1(x_1)| + \frac{1}{4}\pi]\} \\ & + B_1 |q^{-\frac{1}{2}}(x_1)| \exp \{+i[|w_1(x_1)| + \frac{1}{4}\pi]\}, \end{aligned} \quad (25a)$$

where the first term represents a wave moving from the left to the right, and the second term represents a wave moving from the right to the left.

Using (19), (21) and (22a, b), we get

$$a_1(x_2) = F_{22}(x_1, x_2)a_1(x_1) - F_{12}(x_1, x_2)a_2(x_1), \quad (26a)$$

$$a_2(x_2) = -\exp \{2K\} [F_{22}^*(x_1, x_2)a_2(x_1) - F_{12}^*(x_1, x_2)a_1(x_1)], \quad (26b)$$

where  $K$  is defined by (12). For the sake of simplicity we shall in the following write

$F_{12}$  and  $F_{22}$  for  $F_{12}(x_1, x_2)$  and  $F_{22}(x_1, x_2)$ , respectively. Using (24a, b), we can write (26a, b) as follows

$$a_1(x_2) = [B_1|F_{12}| \exp \{+i(\sigma - \frac{1}{2} \arg F_{22})\} + A_1|F_{22}| \exp \{-i(\sigma - \frac{1}{2} \arg F_{22})\}] \exp \{-i[\frac{1}{4}\pi - (\sigma + \frac{1}{2} \arg F_{22})]\}, \quad (27a)$$

$$a_2(x_2) = -[A_1|F_{12}| \exp \{-i(\sigma - \frac{1}{2} \arg F_{22})\} + B_1|F_{22}| \exp \{+i(\sigma - \frac{1}{2} \arg F_{22})\}] \exp \{2K + i[\frac{1}{4}\pi - (\sigma + \frac{1}{2} \arg F_{22})]\}, \quad (27b)$$

where  $\sigma$  is defined by the formula

$$\sigma = \frac{1}{2}[\arg F_{12}(x_1, x_2) - \frac{1}{2}\pi]. \quad (28)$$

From (18), (27a, b), and (17a, b) we obtain the following expression for the wave function to the right of the barrier

$$\begin{aligned} \psi(x_2) = & [B_1|F_{12}| \exp \{K + i(\sigma - \frac{1}{2} \arg F_{22})\} + A_1|F_{22}| \exp \{K - i(\sigma - \frac{1}{2} \arg F_{22})\}] \\ & \times |q^{-\frac{1}{2}}(x_2)| \exp \{-i[|w_2(x_2)| - \frac{1}{4}\pi - (\sigma + \frac{1}{2} \arg F_{22})]\} \\ & + [A_1|F_{12}| \exp \{K - i(\sigma - \frac{1}{2} \arg F_{22})\} + B_1|F_{22}| \exp \{K + i(\sigma - \frac{1}{2} \arg F_{22})\}] \\ & \times |q^{-\frac{1}{2}}(x_2)| \exp \{+i[|w_2(x_2)| - \frac{1}{4}\pi - (\sigma + \frac{1}{2} \arg F_{22})]\}, \end{aligned} \quad (25b)$$

where the first term represents a wave proceeding from the right to the left, and the second term represents a wave proceeding from the left to the right.

The quantity  $\sigma$  depends only very slightly on  $x_1$  and  $x_2$  provided neither of these points lies close to a transition point. For sufficiently large values of  $|K|$  the quantity  $\sigma$  is at the most of the order of magnitude of the so called  $\mu$ -integral (cf. eq. (44)) along a conveniently chosen path between  $x_1$  and  $x_2$ , as has already been pointed out on p. 89 in ref. <sup>9)</sup> and is shown in detail in sect. 3 of the present paper (cf. eq. (51)). For comparatively small values of  $|K|$ , i.e. for particle energies close to the top of the barrier, the absolute value of  $\sigma$  may be much larger than the  $\mu$ -integral (for the higher-order phase-integral approximations even much larger than unity in a narrow energy interval). For such energies it is therefore in certain physical problems important to know  $\sigma$ . An approximate expression for  $\sigma$ , pertaining to the first-order approximation, is given in ref. <sup>10)</sup>. Expressions for  $\sigma$  pertinent to higher-order phase-integral approximations will be given in a forthcoming paper.

2.1.2. *Standing wave.* If, in particular, we choose

$$A_1 = \frac{1}{2} \exp \{-i(\gamma_1 - \frac{1}{2}\pi)\}, \quad (29a)$$

$$B_1 = \frac{1}{2} \exp \{+i(\gamma_1 - \frac{1}{2}\pi)\}, \quad (29b)$$

where  $\gamma_1$  is any real number, eqs. (25a, b) yield

$$\psi(x_1) = |q^{-\frac{1}{2}}(x_1)| \cos [ |w_1(x_1)| - \frac{1}{4}\pi + \gamma_1 ], \quad (30a)$$

$$\psi(x_2) = \Omega_1 |q^{-\frac{1}{2}}(x_2)| \cos [ |w_2(x_2)| - \frac{1}{4}\pi + \varphi_1 - (\sigma + \frac{1}{2} \arg F_{22}) ], \quad (30b)$$



where  $\Omega_1$  is a positive quantity and  $\varphi_1$  is a real quantity. They are defined by the formula

$$\begin{aligned} \Omega_1 \exp \{i\varphi_1\} = & |F_{12}| \exp \{K + i[\frac{1}{2}\pi - \gamma_1 - (\sigma - \frac{1}{2} \arg F_{22})]\} \\ & + |F_{22}| \exp \{K - i[\frac{1}{2}\pi - \gamma_1 - (\sigma - \frac{1}{2} \arg F_{22})]\}. \end{aligned} \quad (31)$$

Separating this equality into real and imaginary parts, we get

$$\Omega_1 \cos \varphi_1 = \exp \{K\} (|F_{12}| + |F_{22}|) \cos [\frac{1}{2}\pi - \gamma_1 - (\sigma - \frac{1}{2} \arg F_{22})], \quad (32a)$$

$$\Omega_1 \sin \varphi_1 = \exp \{K\} (|F_{12}| - |F_{22}|) \sin [\frac{1}{2}\pi - \gamma_1 - (\sigma - \frac{1}{2} \arg F_{22})]. \quad (32b)$$

Since  $|F_{12}/F_{22}| > 1$  according to (23), it follows from (32a, b) that the angle  $\varphi_1$  lies in the same quadrant as the angle  $\frac{1}{2}\pi - \gamma_1 - (\sigma - \frac{1}{2} \arg F_{22})$ . From (32a, b) we get

$$\Omega_1 = \exp \{K\} \{(|F_{12}| - |F_{22}|)^2 + 4|F_{12} F_{22}| \sin^2 [\gamma_1 + (\sigma - \frac{1}{2} \arg F_{22})]\}^{\frac{1}{2}}, \quad (33a)$$

$$\varphi_1 = \arctg \left\{ \frac{|F_{12}| - |F_{22}|}{|F_{12}| + |F_{22}|} \operatorname{tg} [\frac{1}{2}\pi - \gamma_1 - (\sigma - \frac{1}{2} \arg F_{22})] \right\}, \quad (33b)$$

with the requirement that the angle  $\varphi_1$  shall lie in the same quadrant as the angle  $\frac{1}{2}\pi - \gamma_1 - (\sigma - \frac{1}{2} \arg F_{22})$ , which makes  $\varphi_1$  uniquely determined (except for the addition of an arbitrary multiple of  $2\pi$ ).

2.1.3. *Outgoing wave to the left of the barrier.* Choosing  $A_1 = 0$  and  $B_1 = 1$  in (25a, b) we get

$$\psi(x_1) = |q^{-\frac{1}{2}}(x_1)| \exp \{+i[|w_1(x_1)| + \frac{1}{4}\pi]\}, \quad (34a)$$

$$\begin{aligned} \psi(x_2) = & |F_{12}| |q^{-\frac{1}{2}}(x_2)| \exp \{K - i[|w_2(x_2)| - \frac{1}{4}\pi - 2\sigma]\} \\ & + |F_{22}| |q^{-\frac{1}{2}}(x_2)| \exp \{K + i[|w_2(x_2)| - \frac{1}{4}\pi - \arg F_{22}]\}. \end{aligned} \quad (34b)$$

The function (34a) represents a transmitted wave. The first term on the r.h.s. of (34b) corresponds to an incident wave, whereas the second term corresponds to a reflected wave.

## 2.2. WAVE FUNCTION GIVEN TO THE RIGHT OF THE BARRIER

2.2.1. *General case.* Let us next assume that the wave function is given at a point  $x_2$  to the right of the barrier, and let us write the coefficients  $a_1(x_2)$  and  $a_2(x_2)$  as follows

$$a_1(x_2) = A_2 \exp \{-K - \frac{3}{4}\pi i\}, \quad (35a)$$

$$a_2(x_2) = -B_2 \exp \{K + \frac{3}{4}\pi i\}, \quad (35b)$$

where  $A_2$  and  $B_2$  are arbitrary constants. Using (18), (35a, b) and (17a, b), we obtain the following expression for the wave function at the point  $x_2$

$$\begin{aligned} \psi(x_2) = & A_2 |q^{-\frac{1}{2}}(x_2)| \exp \{-i[|w_2(x_2)| + \frac{1}{4}\pi]\} \\ & + B_2 |q^{-\frac{1}{2}}(x_2)| \exp \{+i[|w_2(x_2)| + \frac{1}{4}\pi]\}, \end{aligned} \quad (36a)$$

where the first term represents a wave moving from the right to the left, and the second term represents a wave moving from the left to the right. Proceeding analogously as in the derivation of (25b), we obtain the following exact expression for the wave function at the point  $x_1$  to the left of the barrier

$$\begin{aligned} \psi(x_1) = & [B_2|F_{12}| \exp \{K + i(\sigma + \frac{1}{2} \arg F_{22})\} + A_2|F_{22}| \exp \{K - i(\sigma + \frac{1}{2} \arg F_{22})\}] \\ & \times |q^{-\frac{1}{2}}(x_1)| \exp \{-i[|w_1(x_1)| - \frac{1}{4}\pi - (\sigma - \frac{1}{2} \arg F_{22})]\} \\ & + [A_2|F_{12}| \exp \{K - i(\sigma + \frac{1}{2} \arg F_{22})\} + B_2|F_{22}| \exp \{K + i(\sigma + \frac{1}{2} \arg F_{22})\}] \\ & \times |q^{-\frac{1}{2}}(x_1)| \exp \{+i[|w_1(x_1)| - \frac{1}{4}\pi - (\sigma - \frac{1}{2} \arg F_{22})]\}, \end{aligned} \quad (36b)$$

where, as always in this paper,  $F_{12}$  and  $F_{22}$  stand for  $F_{12}(x_1, x_2)$  and  $F_{22}(x_1, x_2)$ , respectively. On the r.h.s. of (36b) the first term represents a wave travelling from the left to the right, and the second term represents a wave travelling from the right to the left.

2.2.2. *Standing wave.* If, in particular, we choose

$$A_2 = \frac{1}{2} \exp \{-i(\gamma_2 - \frac{1}{2}\pi)\}, \quad (37a)$$

$$B_2 = \frac{1}{2} \exp \{+i(\gamma_2 - \frac{1}{2}\pi)\}, \quad (37b)$$

where  $\gamma_2$  is any real number, eqs. (36a, b) become

$$\psi(x_2) = |q^{-\frac{1}{2}}(x_2)| \cos [ |w_2(x_2)| - \frac{1}{4}\pi + \gamma_2 ], \quad (38a)$$

$$\psi(x_1) = \Omega_2 |q^{-\frac{1}{2}}(x_1)| \cos [ |w_1(x_1)| - \frac{1}{4}\pi + \varphi_2 - (\sigma - \frac{1}{2} \arg F_{22}) ], \quad (38b)$$

where the quantities  $\Omega_2$  (positive) and  $\varphi_2$  (real) are defined by the formula

$$\begin{aligned} \Omega_2 \exp \{i\varphi_2\} = & |F_{12}| \exp \{K + i[\frac{1}{2}\pi - \gamma_2 - (\sigma + \frac{1}{2} \arg F_{22})]\} \\ & + |F_{22}| \exp \{K - i[\frac{1}{2}\pi - \gamma_2 - (\sigma + \frac{1}{2} \arg F_{22})]\}. \end{aligned} \quad (39)$$

From (39) we obtain

$$\Omega_2 = \exp \{K\} \{ (|F_{12}| - |F_{22}|)^2 + 4|F_{12}F_{22}| \sin^2 [\gamma_2 + (\sigma + \frac{1}{2} \arg F_{22})] \}^{\frac{1}{2}}, \quad (40a)$$

$$\varphi_2 = \arctg \left\{ \frac{|F_{12}| - |F_{22}|}{|F_{12}| + |F_{22}|} \operatorname{tg} [\frac{1}{2}\pi - \gamma_2 - (\sigma + \frac{1}{2} \arg F_{22})] \right\}, \quad (40b)$$

where  $\varphi_2$  shall lie in the same quadrant as the angle  $\frac{1}{2}\pi - \gamma_2 - (\sigma + \frac{1}{2} \arg F_{22})$ .

2.2.3. *Outgoing wave to the right of the barrier.* To obtain a wave function representing an outgoing wave to the right of the barrier we put  $A_2 = 0$  and  $B_2 = 1$  in (36a, b), getting

$$\psi(x_2) = |q^{-\frac{1}{2}}(x_2)| \exp \{+i[|w_2(x_2)| + \frac{1}{4}\pi]\}, \quad (41a)$$

$$\begin{aligned} \psi(x_1) = & |F_{12}| |q^{-\frac{1}{2}}(x_1)| \exp \{K - i[|w_1(x_1)| - \frac{1}{4}\pi - 2\sigma]\} \\ & + |F_{22}| |q^{-\frac{1}{2}}(x_1)| \exp \{K + i[|w_1(x_1)| - \frac{1}{4}\pi + \arg F_{22}]\}. \end{aligned} \quad (41b)$$

On the r.h.s. of (41b) the first term represents an incoming wave and the second term represents a reflected wave to the same degree of approximation as  $f_1(x)$  and  $f_2(x)$  satisfy the Schrödinger equation. Provided  $f_1(x)$  and  $f_2(x)$  tend to exact solutions as  $x \rightarrow \pm \infty$ , we obtain from (41a, b) the exact formulae for the reflection and transmission coefficient given by (9.9a, b) in ref. <sup>6</sup>). The exact formulae (9.10a, b) and (9.11) in ref. <sup>6</sup>) also remain valid in the present treatment.

The formulae (34a, b) and (41a, b) are quite analogous except that the phase of the reflected wave contains the term  $-\arg F_{22}$  in (34b) but the term  $+\arg F_{22}$  in (41b). The transmission coefficient as given by (9.9b) or (9.10b) in ref. <sup>6</sup>) is exactly the same when the incident wave comes from the r.h.s. of the barrier as when it comes from the l.h.s.. In this connection we also remark that the phase of the incident wave depends on  $\sigma$ , whereas the transmission coefficient is independent of  $\sigma$ .

For a symmetric barrier we have  $Q^2(-z) = Q^2(z)$ , and from (7) it follows that  $\varepsilon_0(-z) = \varepsilon_0(z)$ . Using these facts and formula (8) in the present paper together with eq. (8a) in ref. <sup>7</sup>), we realize that  $Y_{2n}(-z) = Y_{2n}(z)$  for  $n = 0, 1, 2, \dots$ . From (5) it then follows that  $q^2(-z) = q^2(z)$ . Thus the assumptions made in the derivation of eq. (46) in ref. <sup>9</sup>) are fulfilled, and we have the formula

$$\arg F_{22}(x_1, x_2) = 0 \quad \text{if } x_1 = -x_2. \quad (42)$$

### 3. Estimates of $F_{12}(x_1, x_2)$ and $F_{22}(x_1, x_2)$

In subsect. 6.4 of ref. <sup>6</sup>) the elements of the matrix  $F(x_1, x_2)$  are estimated for an overdense potential barrier both when the energy lies well below the top of the barrier and when the energy lies only slightly below the top of the barrier. The estimates obtained are given by (6.23) for the case referred to in fig. 6.4, and by (6.29) and (6.30) for the case referred to in fig. 6.5.

In the first part of subsect. 6.5 in ref. <sup>6</sup>) an underdense barrier is treated by cutting the  $z$ -plane and choosing the phase of  $q^{\frac{1}{2}}(z)$  and the paths of integration similarly as in fig. 6.5. Fig. 6.6 refers to this treatment. As has been pointed out on p. 53 in ref. <sup>6</sup>) one can give a unified treatment of the two cases corresponding to figs. 6.5 and 6.6, since all relations for the elements of the matrix  $F(x_1, x_2)$  are formally identical in both cases, and the paths between  $x_1$  and  $x_2$  in fig. 6.5 and fig. 6.6 are analogous as concerns the monotonic properties of  $|\exp \{i w(z)\}|$ . The estimates obtained for the case in fig. 6.6 are again the formulae (6.29) and (6.30) in ref. <sup>6</sup>) with the modifications described in ref. <sup>6</sup>)<sup>†</sup>.

Here we would like to point out that the case referred to in fig. 6.4 in ref. <sup>6</sup>) can also be included in the above mentioned unified treatment. On the path between  $x_1$  and  $x_2$  depicted in fig. 6.4 we have the same qualitative behaviour of  $|\exp \{i w(z)\}|$  as in figs. 6.5 and 6.6, which means that the treatment on pp. 48 and 49 in ref. <sup>6</sup>),

<sup>†</sup> See ref. <sup>6</sup>) p. 53 lines 3-6 from the bottom, where we should, however, have written  $\exp \{K\}O(\mu) + O(\mu^2)$  instead of only  $\exp \{K\}O(\mu)$ , as has been pointed out by Ö. Dammert.

and hence the results (6.29) and (6.30), apply directly also to the case when the path of integration for obtaining  $\mu$  proceeds as depicted in fig. 6.4.

The estimates obtained in the unified treatment discussed above can be written

$$F_{22}(x_1, x_2) = 1 + \exp \left\{ \frac{1}{2}(|K| - K) \right\} O(\mu), \quad (43a)$$

$$F_{12}(x_1, x_2) = i \exp \{ 2i\sigma \} [1 + \exp \{-2K\}]^{\frac{1}{2}} [1 + \exp \left\{ -\frac{1}{2}(|K| - K) \right\} O(\mu) + O(\mu^2)], \quad (43b)$$

where  $\sigma$  is defined by (28), and  $\mu$  denotes the integral

$$\mu(x_1, x_2) = \int_{x_1}^{x_2} \left| \left\{ \frac{Q^2 - q^2}{q} + q^{-\frac{1}{2}} \frac{d^2}{dz^2} q^{-\frac{1}{2}} \right\} dz \right| \quad (44)$$

along the appropriate one of the paths of integration depicted in figs. 6.4, 6.5 and 6.6 in ref. <sup>6)</sup>.

As has been explained above the estimates (43a, b) are also valid when  $K$  is positive and so large that the path between  $x_1$  and  $x_2$  can be chosen as in fig. 6.4 of ref. <sup>6)</sup>. In this case one obtains, however, estimates containing information about the phase of  $F_{12}(x_1, x_2)$  by proceeding as in the first part of subsect. 6.4 in ref. <sup>6)</sup>. The result is the estimates (6.23) in ref. <sup>6)</sup> according to which

$$F_{22}(x_1, x_2) = 1 + O(\mu), \quad (45a)$$

$$F_{12}(x_1, x_2) = i[1 + O(\mu)]. \quad (45b)$$

Substituting (45a, b) into (23), we obtain

$$\exp \{-2K\} = O(\mu). \quad (46)$$

Thus, when  $K$  is positive and so large that the path between  $x_1$  and  $x_2$  can be chosen as in fig. 6.4 in ref. <sup>6)</sup>, the  $\mu$ -integral for this path cannot be much smaller than  $\exp \{-2K\}$ . However, even when  $K$  is positive and rather large it seems possible that the  $\mu$ -integral for a path such as that in fig. 6.5 of ref. <sup>6)</sup> may be much smaller than  $\exp \{-2K\}$  provided one uses phase-integral approximations of higher order. Thus, in the estimates (45a, b) the  $\mu$ -integral, which shall be performed along a path such as that shown in fig. 6.4 of ref. <sup>6)</sup>, cannot be much smaller than  $\exp \{-2K\}$ , but in the estimates (43a, b), where the  $\mu$ -integral shall be calculated along a path proceeding as shown in fig. 6.5 in ref. <sup>6)</sup>, it might be possible to achieve that  $\mu$  is much smaller than  $\exp \{-2K\}$  even when  $K$  is large by using phase-integral approximations of higher order.

When  $K$  is negative and sufficiently large in absolute value it is convenient to estimate the matrix  $F(x_1, x_2)$  in terms of the  $\mu$ -integral along the real axis between  $x_1$  and  $x_2$ . To this purpose we first note that for an arbitrary choice of the lower limit in the integral (4) defining  $w(z)$  [cf. p. 21 in ref. <sup>6)</sup>] we obtain instead of formula

(7.6b) in ref. <sup>6)</sup> with  $n = 1$  the formula

$$F(z', z) = \begin{pmatrix} 0 & i \exp \left\{ -2i \left[ w(z) - \frac{1}{2} \int_{z'}^z q(z) dz \right] \right\} \\ i \exp \left\{ 2i \left[ w(z) - \frac{1}{2} \int_{z'}^z q(z) dz \right] \right\} & 0 \end{pmatrix}, \quad (47)$$

where  $z'$ , which is the point corresponding to  $z$  on the next Riemann sheet, is obtained by starting from  $z$  and going in the positive sense one turn around a simple zero of  $Q^2(z)$ . Let this zero be the transition point  $t_2$  in fig. 1b, and let  $x'_2$  and  $x_2$  correspond to  $z'$  and  $z$ , respectively, which means that the integral from  $z'$  to  $z$  occurring in (47) corresponds to the integral along the contour  $\Gamma_2$  in fig. 1b. Using (15b), (9b), and (13), we then obtain from (47) the exact formula

$$F(x'_2, x_2) = \begin{pmatrix} 0 & i \exp \{-K\} \\ i \exp \{K\} & 0 \end{pmatrix}. \quad (48)$$

Using this formula and the estimates (6.3a, b) in ref. <sup>6)</sup> in the identity  $F(x_1, x_2) = F(x_1, x'_2)F(x'_2, x_2)$ , we get the estimates

$$F_{22}(x_1, x_2) = \exp \{-K\} O(\mu) = \exp \{|K|\} O(\mu), \quad (49a)$$

$$F_{12}(x_1, x_2) = i \exp \{-K\} [1 + O(\mu)] = i \exp \{|K|\} [1 + O(\mu)], \quad (49b)$$

where  $\mu$  denotes the  $\mu$ -integral along the real axis between  $x_1$  and  $x'_2$ , or between  $x_1$  and  $x_2$ , since the cut in fig. 6.6 in ref. <sup>6)</sup> may evidently be ignored as far as the  $\mu$ -integral is concerned.

The estimates (45b) and (49b) are given in unified form by the relation

$$F_{12}(x_1, x_2) = i \exp \left\{ \frac{1}{2} (|K| - K) \right\} [1 + O(\mu)], \quad (50)$$

which is valid provided  $|K|$  is sufficiently large and the  $\mu$ -integral is performed along a path such as that in fig. 6.4 of ref. <sup>6)</sup> when  $K$  is positive but along the real axis from  $x_1$  to  $x_2$  when  $K$  is negative. Using (50) in the definition (28) of  $\sigma$ , we get the estimate

$$\sigma = O(\mu), \quad (51)$$

which is valid when  $|K|$  is sufficiently large and the  $\mu$ -integral is chosen as described above.

We remark that the estimates (45a, b), which are valid when  $K$  is positive and sufficiently large, can be obtained from (43a, b), (46) and (51).

The estimates given in this section are based on estimates derived in ref. <sup>6)</sup> for the first-order JWKB approximation, but they apply also to the higher-order phase-integral approximations used in the previous sections of the present paper. The conditions for such a generalization to be valid have been discussed elsewhere <sup>7-9)</sup>.

We shall now give some further estimates which will be used in the next section. Provided  $\mu \exp \{\frac{1}{2}(|K|-K)\} \ll 1$  we obtain from (43b)

$$\begin{aligned} |F_{12}| &= [1 + \exp \{-2K\}]^{\frac{1}{2}} [1 + \exp \{-\frac{1}{2}(|K|-K)\} O(\mu)] \\ &= [1 + \exp \{-2K\}]^{\frac{1}{2}} + O(\mu). \end{aligned} \quad (52a)$$

Using this estimate and (43a), we get

$$|F_{12}| + |F_{22}| = [[1 + \exp \{-2K\}]^{\frac{1}{2}} + 1][1 + O(\mu)]. \quad (53a)$$

Recalling the exact relation (23), we note that

$$\frac{|F_{12}| - |F_{22}|^{\frac{1}{2}}}{[1 + \exp \{-2K\}]^{\frac{1}{2}} - 1} = \frac{[1 + \exp \{-2K\}]^{\frac{1}{2}} + 1}{|F_{12}| + |F_{22}|}. \quad (54)$$

Hence, using (53a), we obtain

$$|F_{12}| - |F_{22}| = [[1 + \exp \{-2K\}]^{\frac{1}{2}} - 1][1 + O(\mu)]. \quad (53b)$$

From (23) it also follows that

$$\left| \frac{F_{12}}{F_{22}} \right| = \left[ 1 + \frac{\exp \{-2K\}}{|F_{22}|^2} \right]^{\frac{1}{2}}, \quad (55)$$

which, combined with the estimate (43a), yields

$$\begin{aligned} \left| \frac{F_{12}}{F_{22}} \right| &= [1 + \exp \{-2K\}]^{\frac{1}{2}} [1 + \exp \{-2K - \frac{1}{2}(|K|-K)\} O(\mu)] \\ &= [1 + \exp \{-2K\}]^{\frac{1}{2}} + \exp \{-2K\} O(\mu). \end{aligned} \quad (52b)$$

#### 4. Approximate expressions for the wave function

The estimates given in sect. 3 can be used for obtaining approximate analytic formulae for the wave function from the exact expressions given in sect. 2. Since our interest in the present paper is focused on two particular cases, namely the case when the wave function is given as a standing wave to the left of the barrier and the case when the wave function is given as an outgoing wave to the right of the barrier, we shall write down explicitly and discuss the results corresponding to these two situations only.

##### 4.1. WAVE FUNCTION GIVEN AS A STANDING WAVE TO THE LEFT OF THE BARRIER

4.1.1. *Positive or negative K.* In subsect. 2.1.2 we imposed the condition that the wave function is given as a standing wave, eq. (30a), to the left of the barrier. To the right of the barrier it is then represented by (30b) with  $\Omega_1$  and  $\varphi_1$  given by (33a, b).

Using (43a), (52a) and (53a, b), we obtain from (33a, b) the formulae

$$\begin{aligned} \Omega_1 = & ([\exp \{2K\} + 1]^{\frac{1}{2}} - \exp \{K\}) \\ & \times \left\{ 1 + \left( \frac{\sin(\gamma_1 - \gamma_1^{(0)})}{\frac{1}{2}[1 + \exp \{-2K\}]^{+\frac{1}{2}} - \frac{1}{2}[1 + \exp \{-2K\}]^{-\frac{1}{2}}} \right)^2 \right\}^{\frac{1}{2}} \\ & \times [1 + \exp \{\frac{1}{2}(|K| - K)\} O(\mu)], \end{aligned} \quad (56a)$$

$$\varphi_1 = \text{arctg} \left\{ \frac{[1 + \exp \{-2K\}]^{+\frac{1}{2}} - [1 + \exp \{-2K\}]^{-\frac{1}{2}}}{[1 + \exp \{-2K\}]^{+\frac{1}{2}} + [1 + \exp \{-2K\}]^{-\frac{1}{2}}} \text{tg} [\frac{1}{2}\pi - (\gamma_1 - \gamma_1^{(0)})] \right\} + O(\mu), \quad (56b)$$

with arctg chosen such that  $\varphi_1$  lies in the same quadrant as  $\frac{1}{2}\pi - (\gamma_1 - \gamma_1^{(0)})$  and  $\gamma_1^{(0)}$  defined by

$$\gamma_1^{(0)} = -(\sigma - \frac{1}{2} \arg F_{22}). \quad (57)$$

From (33b) we also obtain the alternative formula

$$\begin{aligned} \varphi_1 = & -(n - \frac{1}{2})\pi \\ & - \text{arctg} \left\{ \frac{[1 + \exp \{-2K\}]^{+\frac{1}{2}} + [1 + \exp \{-2K\}]^{-\frac{1}{2}}}{[1 + \exp \{-2K\}]^{+\frac{1}{2}} - [1 + \exp \{-2K\}]^{-\frac{1}{2}}} \text{tg} (\gamma_1 - \gamma_1^{(0)}) \right\} + O(\mu), \end{aligned} \quad (56b')$$

where arctg takes its principal value, and  $n$  is an integer (positive, negative or zero) chosen such that

$$|\gamma_1 - (\gamma_1^{(0)} + n\pi)| \leq \frac{1}{2}\pi. \quad (58)$$

From (57) and (43a) we obtain

$$\gamma_1^{(0)} = -\sigma + \exp \{\frac{1}{2}(|K| - K)\} O(\mu) \approx -\sigma. \quad (59)$$

This formula is useful for a rough calculation of  $\gamma_1^{(0)}$ , but, since the resonances (cf. below) are very narrow if  $K$  is positive and large, it is often too crude to be used in (56a, b, b') when  $\gamma_1 - \gamma_1^{(0)}$  is close to an integer multiple of  $\pi$ .

Let us keep the points  $x_1$  and  $x_2$  fixed, and let also the energy of the particle be fixed, while the phase  $\gamma_1$  of the standing wave (30a) to the left of the barrier is varied. The quantities  $K$  and  $\gamma_1^{(0)}$  are then constants. When  $\gamma_1$  is equal to  $\gamma_1^{(0)}$  or differs from  $\gamma_1^{(0)}$  by an integer multiple of  $\pi$ , the quantity  $\Omega_1$ , with the error term in (56a) neglected, takes its minimum value, which according to (30a, b) means that the ratio between the amplitude of the wave function to the left of the barrier and the amplitude to the right of the barrier takes its largest possible value. If the region to the left of the barrier lies inside some atomic system, and the region to the right of the barrier lies outside this system, the above mentioned values of  $\gamma_1$  therefore correspond to resonances for the physical system considered. The formulae (30a, b), (56a, b, b') with the error terms neglected, and (57) give a detailed description of the wave function in the presence of a potential barrier. The shape of the resonance curve is completely determined by these formulae. In principle, so is also its position, but the definition (57) of  $\gamma_1^{(0)}$

contains the quantity  $\frac{1}{2} \arg F_{22}$  which, although it is small compared to unity, is in general large compared to the half-width  $\Delta\gamma$  of the resonance when  $K$  is positive (unless one uses phase-integral approximations of high order) and cannot be calculated within the framework of the phase-integral approximations. Thus our approximate formulae (56a, b, b'), with the error terms neglected, give a very satisfactory description of the resonance curve except that the position of the resonance may differ from that calculated from the approximate formula (59) by a quantity which is small compared to unity but large compared to the half-width of the resonance.

For fixed energy and fixed points  $x_1$  and  $x_2$ , i.e. for fixed values of  $K$  and  $\gamma_1^{(0)}$ , it follows from (56a) that the total half-width of a resonance, i.e. the difference between the two values of  $\gamma_1$  on opposite sides of a resonance for which the square of  $\Omega_1$  is equal to twice its value at resonance, is

$$\Delta\gamma_1 = 2 \arcsin \left\{ \frac{1}{2} \left[ [1 + \exp \{-2K\}]^{+\frac{1}{2}} - [1 + \exp \{-2K\}]^{-\frac{1}{2}} \right] \right\}. \quad (60)$$

We shall still consider the general case when  $K$  may be positive or negative, but we shall now assume that  $\gamma_1$  is not too close to a value corresponding to resonance, which according to (59) means that  $\gamma_1 + \sigma$  is not too close to an integer multiple of  $\pi$ . More precisely, we shall assume that

$$\mu \exp \left\{ \frac{1}{2} (|K| - K) \right\} \ll |\gamma_1 + \sigma - n\pi| \leq \frac{1}{2}\pi, \quad (61)$$

where  $n$  is an integer chosen such that the last inequality in (61) is fulfilled. Because of (59) we have the formulae

$$\begin{aligned} \sin(\gamma_1 - \gamma_1^{(0)}) &= \left[ 1 + (\exp \left\{ \frac{1}{2} (|K| - K) \right\} O(\mu))^2 + \frac{\exp \left\{ \frac{1}{2} (|K| - K) \right\} O(\mu)}{\operatorname{tg}(\gamma_1 + \sigma)} \right] \sin(\gamma_1 + \sigma), \quad (62a) \end{aligned}$$

$$\begin{aligned} \operatorname{tg} \left[ \frac{1}{2}\pi - (\gamma_1 - \gamma_1^{(0)}) \right] &= \left[ 1 + \frac{\exp \left\{ \frac{1}{2} (|K| - K) \right\} O(\mu)}{\operatorname{tg}(\gamma_1 + \sigma)} \right] \left\{ \operatorname{tg} \left[ \frac{1}{2}\pi - (\gamma_1 + \sigma) \right] + \exp \left\{ \frac{1}{2} (|K| - K) \right\} O(\mu) \right\}. \quad (62b) \end{aligned}$$

Substituting (62a, b) into (56a, b), and noting that

$$\frac{\exp \left\{ \frac{1}{2} (|K| - K) \right\} O(\mu)}{\operatorname{tg}(\gamma_1 + \sigma)} + \exp \left\{ \frac{1}{2} (|K| - K) \right\} O(\mu) = \frac{\exp \left\{ \frac{1}{2} (|K| - K) \right\} O(\mu)}{|\gamma_1 + \sigma - n\pi|},$$

we get

$$\begin{aligned} \Omega_1 &= \left( [\exp \{2K\} + 1]^{\frac{1}{2}} - \exp \{K\} \right) \\ &\quad \times \left\{ 1 + \left( \frac{\sin(\gamma_1 + \sigma)}{\frac{1}{2} [1 + \exp \{-2K\}]^{+\frac{1}{2}} - \frac{1}{2} [1 + \exp \{-2K\}]^{-\frac{1}{2}}} \right)^2 \right\}^{\frac{1}{2}} \\ &\quad \times \left[ 1 + \frac{\exp \left\{ \frac{1}{2} (|K| - K) \right\} O(\mu)}{|\gamma_1 + \sigma - n\pi|} \right], \quad (63a) \end{aligned}$$



$$\varphi_1 = \operatorname{arctg} \left\{ \frac{[1 + \exp \{-2K\}]^{+\frac{1}{4}} - [1 + \exp \{-2K\}]^{-\frac{1}{4}}}{[1 + \exp \{-2K\}]^{+\frac{1}{4}} + [1 + \exp \{-2K\}]^{-\frac{1}{4}}} \operatorname{tg} \left[ \frac{1}{2}\pi - (\gamma_1 + \sigma) \right] \right\} + \frac{\exp \{ \frac{1}{2}(|K| - K) \} O(\mu)}{|\gamma_1 + \sigma - n\pi|}, \quad (63b)$$

where  $\operatorname{arctg}$  shall be chosen such that  $\varphi_1$  lies in the same quadrant as  $\frac{1}{2}\pi - (\gamma_1 - \gamma_1^{(0)})$ .

4.1.2. *Sufficiently large positive K.* When the path of integration for defining the  $\mu$ -integral is chosen as presupposed in (46), we obtain from (56a) the formula

$$\Omega_1 = \frac{1}{2} \exp \{-K\} \left[ 1 + \left( \frac{\sin(\gamma_1 - \gamma_1^{(0)})}{\frac{1}{4} \exp \{-2K\}} \right)^2 \right]^{\frac{1}{4}} [1 + O(\mu)] \quad (64a)$$

and from (56b, b') the formulae

$$\varphi_1 = \operatorname{arctg} \left\{ \frac{1}{4} \exp \{-2K\} \operatorname{tg} \left[ \frac{1}{2}\pi - (\gamma_1 - \gamma_1^{(0)}) \right] \right\} + O(\mu), \quad (64b)$$

$$\varphi_1 = -(n - \frac{1}{2})\pi - \operatorname{arctg} \frac{\operatorname{tg}(\gamma_1 - \gamma_1^{(0)})}{\frac{1}{4} \exp \{-2K\}} + O(\mu), \quad (64b')$$

where  $n$  is chosen according to (58).

For fixed energy and fixed points  $x_1$  and  $x_2$  the quantities  $K$  and  $\gamma_1^{(0)}$  are constant. From (64a, b) we can then draw the following conclusions. When  $\gamma_1$  increases monotonically,  $\Omega_1$  passes through a series of narrow and deep minima (the resonances). When  $\gamma_1$  passes through a value corresponding to a resonance, the phase  $\varphi_1$  decreases very rapidly and changes its value by  $-\pi$  in a  $\gamma_1$  interval a few times larger than  $\exp \{-2K\}$ , but between the resonances  $\varphi_1$  is approximately constant and close to an integer multiple of  $\pi$ . The formula (60) for the total half-width  $\Delta\gamma_1$  of a resonance becomes

$$\Delta\gamma_1 \approx \frac{1}{2} \exp \{-2K\}. \quad (65)$$

Since this half-width is very small (e.g. in problems in nuclear physics), it is important to have approximate analytic formulae for determining the positions, widths and shapes of the resonances. In many cases it would be hard to calculate the positions of the resonances by a reasonable amount of purely numerical work without a theoretical knowledge of the resonances.

We recall that the quantity  $\gamma_1^{(0)}$  appearing in (64a, b, b') is defined by the exact formula (57). Since we are considering the case when  $K$  is positive and sufficiently large, we obtain from (59) and (51) the estimate

$$\gamma_1^{(0)} = O(\mu) \approx 0, \quad (66)$$

which can be used for approximate localization of the resonances but is in general too crude to be used in (64a, b, b') when  $\gamma_1$  is close to  $\gamma_1^{(0)} + n\pi$ .

We shall now consider two particular cases. In the case when

$$|\gamma_1 - (\gamma_1^{(0)} + n\pi)| \ll \frac{1}{4} \exp \{-2K\} \quad (67)$$

formulae (64a, b') yield

$$\Omega_1 = \frac{1}{2} \exp \{-K\} \left\{ 1 + \left[ \mathbf{O} \left( \frac{|\gamma_1 - (\gamma_1^{(0)} + n\pi)|}{\frac{1}{4} \exp \{-2K\}} \right) \right]^2 + \mathbf{O}(\mu) \right\}, \quad (68a)$$

$$\varphi_1 = -(n - \frac{1}{2})\pi + \mathbf{O} \left( \frac{|\gamma_1 - (\gamma_1^{(0)} + n\pi)|}{\frac{1}{4} \exp \{-2K\}} \right) + \mathbf{O}(\mu). \quad (68b)$$

In the case when

$$\frac{1}{4} \exp \{-2K\} \ll |\gamma_1 - (\gamma_1^{(0)} + n\pi)| \leq \frac{1}{2}\pi \quad (69)$$

formulae (64a, b') yield

$$\Omega_1 = 2 \exp \{K\} |\sin(\gamma_1 - \gamma_1^{(0)})| \left\{ 1 + \left[ \mathbf{O} \left( \frac{\frac{1}{4} \exp \{-2K\}}{|\gamma_1 - (\gamma_1^{(0)} + n\pi)|} \right) \right]^2 + \mathbf{O}(\mu) \right\}, \quad (70a)$$

$$\varphi_1 = - \left[ n - \frac{1}{2} \left( 1 - \frac{\gamma_1 - (\gamma_1^{(0)} + n\pi)}{|\gamma_1 - (\gamma_1^{(0)} + n\pi)|} \right) \right] \pi + \mathbf{O} \left( \frac{\frac{1}{4} \exp \{-2K\}}{|\operatorname{tg}(\gamma_1 - \gamma_1^{(0)})|} \right) + \mathbf{O}(\mu). \quad (70b)$$

Thus

$$\begin{aligned} \Omega_1 &\approx 2 \exp \{K\} |\sin(\gamma_1 - \gamma_1^{(0)})|, & \varphi_1 &\approx -(n-1)\pi \\ &\text{when } -\frac{1}{2}\pi \leq \gamma_1 - (\gamma_1^{(0)} + n\pi) \ll -\frac{1}{4} \exp \{-2K\}, \end{aligned} \quad (71a)$$

$$\begin{aligned} \Omega_1 &\approx \frac{1}{2} \exp \{-K\}, & \varphi_1 &\approx -(n - \frac{1}{2})\pi \\ &\text{when } |\gamma_1 - (\gamma_1^{(0)} + n\pi)| \ll \frac{1}{4} \exp \{-2K\}, \end{aligned} \quad (71b)$$

$$\begin{aligned} \Omega_1 &\approx 2 \exp \{K\} |\sin(\gamma_1 - \gamma_1^{(0)})|, & \varphi_1 &\approx -n\pi \\ &\text{when } \frac{1}{4} \exp \{-2K\} \ll \gamma_1 - (\gamma_1^{(0)} + n\pi) \leq \frac{1}{2}\pi. \end{aligned} \quad (71c)$$

Recalling (30a, b), we realize from (71b) that at resonance the amplitude of the standing wave  $q^{-\frac{1}{2}} \cos [\dots]$  to the left of the barrier is larger than that to the right of the barrier by the factor  $2 \exp \{K\}$ , while from (71a, c) and (66) it follows that off resonance the amplitude to the right of the barrier is larger than that to the left of the barrier by the factor  $2 \exp \{K\} |\sin \gamma_1|$ . The phase of the wave function (30a, b) to the right of the barrier is at resonance obtained from (71b), (43a) and (51), while off resonance it is obtained from (71a, c), (43a) and (51).

The formulae (30a, b) and (71a, b, c) may be further illuminated as follows. Referring to one of the connection formulae in ref. <sup>8)</sup>, we note that when the wave function inside the barrier is positive and increasing in the direction from the left-hand towards the right-hand classical turning point, the phase of the wave function to the right of the barrier is approximately equal to  $|w_2(x_2)| - \frac{1}{4}\pi$  in agreement with (30b), (43a), (51) and (71a, c). On the other hand, from the same connection formula it

follows that for a wave function which inside the barrier is positive and increasing in the direction from the right-hand towards the left-hand classical turning point the phase of the wave function to the left of the barrier is approximately equal to  $|w_1(x_1)| - \frac{1}{4}\pi$  in agreement with (30a) and (66) with due regard to (30b) and (71a, b, c).

We shall now discuss the wave function inside the potential barrier. From (71a, c) it follows that  $\Omega_1 \approx 1$  when  $\gamma_1 - (\gamma_1^{(0)} + n\pi)$  is equal to  $-\frac{1}{2} \exp \{-K\}$  and  $+\frac{1}{2} \exp\{-K\}$ . Since the barrier is assumed to be thick and the function  $q^{-\frac{1}{2}}(x)$  is slowly varying, it is evident that when  $\gamma_1$  is so close to  $(\gamma_1^{(0)} + n\pi) - \frac{1}{2} \exp \{-K\}$  that  $\Omega_1$  is of the order of magnitude unity, the wave function cannot be monotonic inside the barrier. The same is true for values of  $\gamma_1$  sufficiently close to  $(\gamma_1^{(0)} + n\pi) + \frac{1}{2} \exp \{-K\}$ . From the wave equation (1) it follows that in a classically forbidden region of the real axis the absolute value of a real wave function  $\psi$  cannot be constant or have a maximum. When  $\gamma_1$  takes values sufficiently close to either of the values  $(\gamma_1^{(0)} + n\pi) - \frac{1}{2} \exp \{-K\}$  or  $(\gamma_1^{(0)} + n\pi) + \frac{1}{2} \exp \{-K\}$ , the absolute value of the wave function  $\psi(x)$  must therefore have a single minimum inside the potential barrier.

Let us now consider two cases in which it is possible to obtain simple approximate formulae for the wave function inside the potential barrier.

Consider first the case when we are not too far from a resonance. More precisely we assume that

$$|\gamma_1 - (\gamma_1^{(0)} + n\pi)| \ll \frac{\frac{1}{4} \exp \{-2K\}}{\mu}, \tag{72}$$

where  $\mu$  denotes the  $\mu$ -integral along a convenient path [see fig. 6.4 in ref. <sup>6</sup>] from  $x_1$  to  $x_2$ . From (64b), (72) and (46) it follows that  $\varphi_1$  and, because of (43a) and (51), also  $\varphi_1 - (\sigma + \frac{1}{2} \arg F_{22})$  differ from an integer multiple of  $\pi$  by quantities which are much larger than  $\mu$ . Because of (30b) and one of the connection formulae discussed in chapter 8 of ref. <sup>6</sup>) and in ref. <sup>8</sup>) we therefore have the approximate formula

$$\psi(x_0) \approx \Omega_1 \sin \varphi_1 |q^{-\frac{1}{2}}(x_0)| \exp \{|w_2(x_0)|\}, \quad w_2(x_0) = \frac{1}{2} \int_{\Gamma_0 - \Gamma_K} q(z) dz \tag{73}$$

for the wave function inside the barrier. We remark that from (64a), (72) and (46), and the assumption that  $\mu$  is small compared to unity it follows that  $\Omega_1$  is small compared to  $\frac{1}{2} \exp \{-K\}/\mu$ , i.e. small compared to  $\exp \{K\}$ .

Consider then the case when we are not too close to a resonance. More precisely we assume that

$$|\gamma_1 - (\gamma_1^{(0)} + n\pi)| \gg \mu, \tag{74}$$

where  $n$  is an integer fulfilling (58), and  $\mu$  denotes the  $\mu$ -integral along a convenient path [cf. fig. 6.4 in ref. <sup>6</sup>] from the point  $x_1$  to a point  $x_0$  on the real axis inside the potential barrier. Because of (66) we can replace (58) and (74) by the condition

$$\frac{1}{2}\pi + O(\mu) > |\gamma_1 - n\pi| \gg \mu. \tag{74'}$$

From (30a), (74'), and one of the connection formulae discussed in chapter 8 of

ref. <sup>6</sup>) and in ref. <sup>8</sup>), it follows that

$$\psi(x_0) \approx \sin \gamma_1 |q^{-\frac{1}{2}}(x_0)| \exp \{ |w_1(x_0)| \}, \quad w_1(x_0) = \frac{1}{2} \int_{\Gamma_0} q(z) dz. \quad (75)$$

We remark that from (64a), (74) and (46) it follows that  $\Omega_1$  is much larger than  $2 \exp \{ K \} \mu$ .

We shall in some more detail consider the case when the condition (74') is fulfilled, which means that  $\gamma_1$  is not too close to a value corresponding to a resonance. Because of (66) and in analogy to (62a, b) we have the formulae

$$\sin (\gamma_1 - \gamma_1^{(0)}) = \left[ 1 + O(\mu^2) + \frac{O(\mu)}{\operatorname{tg} \gamma_1} \right] \sin \gamma_1, \quad (76a)$$

$$\operatorname{tg} \left[ \frac{1}{2} \pi - (\gamma_1 - \gamma_1^{(0)}) \right] = \left[ 1 + \frac{O(\mu)}{\operatorname{tg} \gamma_1} \right] \{ \operatorname{tg} (\frac{1}{2} \pi - \gamma_1) + O(\mu) \}. \quad (76b)$$

Substituting (76a, b) into (64a, b), we get [cf. (63a, b)]

$$\Omega_1 = \frac{1}{2} \exp \{ -K \} \left\{ 1 + \left( \frac{\sin \gamma_1}{\frac{1}{2} \exp \{ -2K \}} \right)^2 \right\}^{\frac{1}{2}} \left[ 1 + \frac{O(\mu)}{|\gamma_1 - n\pi|} \right], \quad (77a)$$

$$\varphi_1 = \operatorname{arctg} \left\{ \frac{1}{4} \exp \{ -2K \} \operatorname{tg} (\frac{1}{2} \pi - \gamma_1) \right\} + \frac{O(\mu)}{|\gamma_1 - n\pi|}, \quad (77b)$$

where  $\operatorname{arctg}$  is to be chosen such that  $\varphi_1$  lies in the same quadrant as  $\frac{1}{2} \pi - (\gamma_1 - \gamma_1^{(0)})$ . Remembering (74') and (46), we can write (77a, b) as follows

$$\Omega_1 = 2 \exp \{ K \} |\sin \gamma_1| \left[ 1 + \frac{O(\mu)}{|\gamma_1 - n\pi|} \right], \quad (78a)$$

$$\varphi_1 = - \left[ n - \frac{1}{2} \left( 1 - \frac{\gamma_1 - (\gamma_1^{(0)} + n\pi)}{|\gamma_1 - (\gamma_1^{(0)} + n\pi)|} \right) \right] \pi + \frac{O(\mu)}{|\gamma_1 - n\pi|}, \quad (78b)$$

cf. (70a, b).

#### 4.2. WAVE FUNCTION GIVEN AS AN OUTGOING WAVE TO THE RIGHT OF THE BARRIER

Using the estimates (43a) and (52a), with the error terms neglected, we can write eqs. (41a, b) as follows

$$\psi(x_2) = |q^{-\frac{1}{2}}(x_2)| \exp \{ +i[|w_2(x_2)| + \frac{1}{4}\pi] \}, \quad (79a)$$

$$\begin{aligned} \psi(x_1) \approx & [\exp \{ 2K \} + 1]^{\frac{1}{2}} |q^{-\frac{1}{2}}(x_1)| \exp \{ -i[|w_1(x_1)| - \frac{1}{4}\pi - 2\sigma] \} \\ & + \exp \{ K \} |q^{-\frac{1}{2}}(x_1)| \exp \{ +i[|w_1(x_1)| - \frac{1}{4}\pi] \}. \end{aligned} \quad (79b)$$

In this formula  $\sigma$  can be neglected unless the energy of the particle is close to the energy corresponding to the top of the barrier.

For the first-order JWKB approximation the reflection and transmission coefficients,  $R$  and  $T$ , are given by the approximate formulae (9.12a, b) in ref. <sup>6)</sup>, which according to pp. 98-99 in ref. <sup>6)</sup> apply to both positive and negative values of  $K$ . For the higher-order phase-integral approximations used in the present paper  $R$  and  $T$  are still given by the same formulae, i.e.

$$R \approx \frac{\exp \{2K\}}{1 + \exp \{2K\}}, \quad (80a)$$

$$T \approx \frac{1}{1 + \exp \{2K\}}, \quad (80b)$$

where  $K$  is now defined by eq. (12). The relative errors in these formulae for  $R$  and  $T$  are at the most of the orders of magnitude  $\mu \exp \{-\frac{1}{2}(|K| - K) - 2K\}$  and  $\mu \exp \{-\frac{1}{2}(|K| - K)\}$ , respectively, as is easily seen from the exact formulae (9.9a, b) in ref. <sup>6)</sup> and the estimates (52a, b) in the present paper.

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