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The Jost function treated by the F-matrix phase integral method

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Abstract. Exact as well as approximate expressions for the Jost function of a radial barrier transmission problem are derived by the phase-integral method developed by Fröman and Fröman. The resulting formulae are used for calculating the positions and the widths of the quasi-stationary states. To demonstrate the essential features as simply as possible, an s-state in a potential, regular at the origin, is considered, and only the first-order phase-integral formulae are given explicitly, but the generalisation to $l \neq 0$ and arbitrary-order phase-integral approximations is indicated.

1. Introduction

As is well known, the analytic properties of the Jost function are associated with interesting features of the scattering of a quantal particle by a central field of force. Those complex zeros of the Jost function which lie close to the real k-axis are directly related to the sharp resonances due to the existence of quasi-stationary states. The real part of the zero determines the position of the resonance and the imaginary part determines its width. A sharp, narrow resonance corresponds to a small imaginary part of the zero. The imaginary part of the zero determines the probability of decay of the quasi-stationary state, so that a zero with a small imaginary part corresponds to a long-lived quasi-stationary state. The connection between the lifetime of the quasi-stationary state and the imaginary part of the corresponding complex zero of the Jost function was established by Krylov and Fock (1947). This connection was later rediscovered by many authors not aware of the existence of the paper by Krylov and Fock. The actual correct calculation of the complex zero is, however, a very difficult problem. Since the imaginary part cannot be calculated by means of ordinary perturbation theory it seems natural to apply the JWKB approximation, but the usual version of the JWKB method, namely the use of the well known connection formulae, gives no satisfactory possibility of evaluating the complex zeros. This circumstance, which is related to the one-directional nature of the connection formulae at the first and second turning points (cf figure 1(a)), will be clarified in the discussions below our formula (3.20b) in § 3 and at the end of § 4. Furthermore, in the neighbourhood of and above the top of the barrier the usual connection formulae cannot be used. This difficulty was overcome, by the use of exactly soluble model barriers, by Connor (1968, 1973) and Crothers (1976), who derived parabolic connection formulae for tracing a JWKB

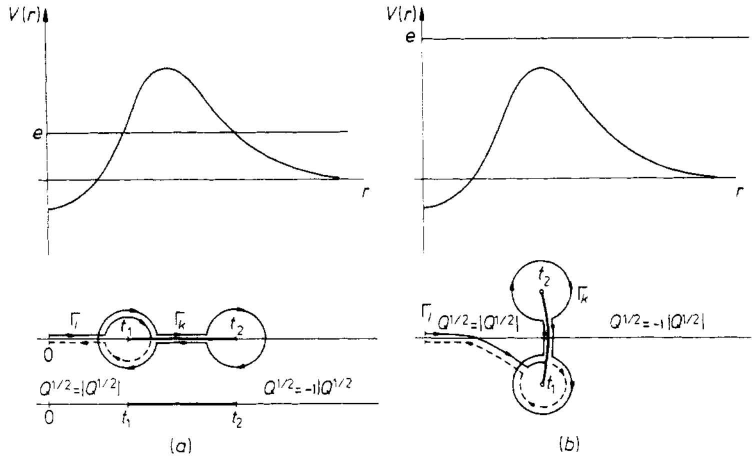

Figure 1. (a) This figure refers to the sub-barrier case. It shows the qualitative behaviour of $V(r)$ and the contours of integration Γ_L and Γ_K. The part of Γ_L which lies on the second Riemann sheet is indicated by a broken curve. The full curve between t_1 and t_2 indicates a cut. The values of $Q^{1/2}$ given in the figure refer to the first Riemann sheet.

(b) This figure refers to the super-barrier case but is otherwise analogous to (a). The point where the cut along the Stokes' line joining t_1 and t_2 crosses the real axis is called s.

solution across the barrier, and by Dickinson (1970), who considered an inverted Morse potential and traced a JWKB solution from one side of the barrier to the other (cf also Miller 1968). However, the formula for the width of a resonance given by Connor (1968, 1973) and Dickinson (1970) (cf. formula (5.14) in the present paper) is not valid near the top of the barrier. The general formula, valid also for that situation, is given in § 5 of the present paper.

Although a rigorous phase-integral expression for the Jost function in the case of the three turning-point problem and real values of the energy E can be obtained directly from equations (33a, b), (43a) and (52b) in the treatment of barrier transmission by Fröman and Fröman (1970), we shall in the present paper not start from those formulae, and we shall only occasionally refer to the notations φ_1, Ω_1 and γ_1 used to express the results in the paper by Fröman and Fröman (1970). It is, however, worthwhile to point out how the Jost function is expressed in terms of those quantities. Therefore, we remark that for real values of the energy, the inverse of the Jost function, i.e. $1/J(k)$, is equal to $\exp(i\varphi_1)/\Omega_1$ times a function which varies only slowly with energy, when the energy-dependent quantity γ_1 is appropriately chosen for the three turning-point problem actually considered, and a convenient modification of the phase-integral approximations is used, if necessary (cf Fröman and Fröman 1974a, 1974b (pp 126–131)). It requires, however, a very careful study of the paper by Fröman and Fröman (1970) to realise this. To make the derivation and the results more easily accessible and directly adapted to scattering and decay problems, we shall therefore in the present paper derive the Jost function in a straightforward way for a particularly simple model and thereby restrict ourselves to the first-order approximation.

According to the phase-integral method (Fröman 1966, 1970; Fröman and Fröman 1965, 1974a, 1974b (pp 126–131)) which will be used in the present paper, the general procedure is to derive first an exact expression for the quantity of interest, i.e. in the present case the Jost function, and then to omit certain small quantities, for which upper bounds can be given (Fröman and Fröman 1965, 1970). In the final formula any convenient order of the kind of phase-integral approximations used (Fröman 1966, 1970; Fröman and Fröman 1974a, 1974b (pp 126–131)) can be chosen. In the present paper we do not aim at generality but will rather strive to bring out the essential points of the general procedure as simply as possible. For this purpose we consider the s-state of a particle in a potential with the shape depicted in figures 1(a) and 1(b). Furthermore, we consider only the first-order phase-integral approximation. Although this approximation is identical with the first order JWKB approximation, the method which we shall use for solving the connection problems (Fröman and Fröman 1965, 1970) makes it possible to derive results which cannot be obtained by means of the usual connection formulae for the first order JWKB approximation.

In § 2 we review briefly the derivation of the Fock–Krylov theorem, emphasising certain points which are important for the justification of relations between analytic properties of the Jost function and physical effects in the decay process. In § 3 we derive an exact F-matrix expression for the Jost function. Using estimates of the F-matrix, we obtain in § 4 an approximate expression for the Jost function for real values of k. In § 5 we evaluate the positions and widths of the narrow resonances, and hence the complex zeros (with small negative imaginary parts) of the Jost function, and discuss the results thus obtained in relation to previous results. Previous authors have calculated the resonance width in the first order JWKB approximation (Connor 1968, equation (24); Connor 1973, equation (16a); Dickinson 1970, equation (33)) and have obtained a formula which is, however, not valid for energies close to the top of the barrier. In the present treatment we arrive at the formula (5.13), which is valid also when the resonance lies close to the top of the barrier. In the derivation of the *first order* formulae we aim only at a demonstration of an approach which is more rigorous than those used by previous authors, and which admits of the generalisation of the final results, if needed. The generalisation to l not necessarily equal to zero, as well as to arbitrary order phase-integral approximations, is indicated in § 6. The main conclusions arrived at in the present paper are summarised in § 7.

2. The Fock–Krylov theorem and the Jost function

Let us consider a non-stationary state for a quantal particle which is initially, at the time $t = 0$, located inside a potential well surrounded by a barrier $V(r)$ as shown in figure 1(a) or 1(b). In the present section our aim is to demonstrate the relation between the Jost function and the decay with time of the non-stationary state under consideration. For this demonstration it is sufficient to consider the simplest case when the wavefunction is spherically symmetric (i.e. an s-state) and when there exists no bound state.

Let us denote by $\chi(E, r)$ the time-independent radial wavefunction which satisfies the Schrödinger equation

$$\frac{d^2\chi}{dr^2}+\left(k^2-\frac{2m}{\hbar^2}V(r)\right)\chi=0, \tag{2.1}$$

with obvious notations, and the normalisation condition

$$\int_0^\infty \chi^*(E, r)\chi(E', r)\, dr = \delta(E-E'). \tag{2.2}$$

For later use we note that E can be expressed in terms of k according to the well-known relation

$$E = \hbar^2 k^2/(2m). \tag{2.3}$$

Assuming (as already mentioned) that there can be no bound state in the potential $V(r)$, we can express the time-dependent radial wavefunction of our non-stationary state $\psi(r, t)$ in the form

$$\psi(r, t) = \int_0^\infty C(E)\chi(E, r) \exp(-\mathrm{i}Et/\hbar)\, \mathrm{d}E. \tag{2.4}$$

At $t = 0$ the function $\psi(r, t)$ reduces to the wavefunction $\psi(r, 0)$ of the initial state. For the coefficient $C(E)$ we therefore obtain from (2.4) by means of (2.2) the formula

$$C(E) = \int_0^\infty \chi^*(E, r)\psi(r, 0)\, \mathrm{d}r. \tag{2.5}$$

From the normalisation condition

$$\int_0^\infty |\psi(r, t)|^2\, \mathrm{d}r = 1 \tag{2.6}$$

it follows, with the aid of (2.4) and (2.2), that

$$\int_0^\infty W(E)\, \mathrm{d}E = 1, \tag{2.7}$$

where $W(E)$ is defined by

$$W(E) = |C(E)|^2 \tag{2.8}$$

and gives the energy distribution of the non-stationary state described by the wavefunction (2.4). The probability $P(t)$ of finding, at the time t (>0), the particle still in the initial state is

$$P(t) = |p(t)|^2, \tag{2.9}$$

where

$$p(t) = \int_0^\infty \psi^*(r, 0)\psi(r, t)\, \mathrm{d}r \tag{2.10}$$

is the probability amplitude. Using (2.4), (2.2) and (2.8), we can write (2.10) as

$$p(t) = \int_0^\infty W(E) \exp(-\mathrm{i}Et/\hbar)\, \mathrm{d}E. \tag{2.11}$$

This relation was first proved by Krylov and Fock (1947).

Let us now consider another time-independent continuum wavefunction $\phi(E, r)$ which satisfies the same Schrödinger equation (2.1) as $\chi(E, r)$, but instead of fulfilling the normalisation condition (2.2), $\phi(E, r)$ has by definition the following behaviour at $r = 0$

$$\phi(E, 0) = 0, \qquad \phi'(E, 0) = 1, \tag{2.12}$$

where the prime indicates differentiation with respect to r. Then, if the asymptotic form of $\phi(E, r)$ as $r \to +\infty$ is written

$$\phi(E, r) \sim (2ik)^{-1}(J^*(k)\,\mathrm{e}^{ikr} - J(k)\,\mathrm{e}^{-ikr}), \qquad r \to +\infty, \tag{2.13}$$

$J(k)$ is by definition the Jost function. Since the integral in (2.2) is divergent for $E = E'$, the main contribution to this integral comes from large values of r, and it follows from (2.2), (2.3), (2.13) and the fact that $\chi(E, r)$ differs from $\phi(E, r)$ only by a constant factor, that

$$\chi(E, r) = \left(\frac{2mk}{\pi\hbar^2}\right)^{1/2} \phi(E, r)/J(k), \tag{2.14}$$

if the r-independent phase-factor in $\chi(E, r)$ is chosen conveniently. Inserting (2.14) into (2.5), we get

$$C(E) = \frac{1}{J^*(k)}\left(\frac{2mk}{\pi\hbar^2}\right)^{1/2} \int_0^\infty \phi^*(E, r)\psi(r, 0)\,\mathrm{d}r \tag{2.15}$$

and thus (cf (2.8))

$$W(E) = \frac{1}{|J(k)|^2}\,\frac{2mk}{\pi\hbar^2}\left|\int_0^\infty \phi^*(E, r)\psi(r, 0)\,\mathrm{d}r\right|^2. \tag{2.16}$$

The energy distribution $W(E)$ is thus factorised. The most important factor, which determines the decay with time of the non-stationary state, is $1/|J(k)|^2$. It may depend strongly on the energy. The other factor is, apart from the factor $2mk/\pi\hbar^2$, the square of the absolute value of the integral $\int_0^\infty \phi^*(E, r)\psi(r, 0)\,\mathrm{d}r$, which changes only slowly with energy but depends on the details of the initial wavefunction $\psi(r, 0)$. This function is assumed to be negligible outside the barrier, so actually the integration goes essentially over a finite range of r. For a short-range potential the function $\phi(E, r)$ will be an analytic function of k, and the integral $\int_0^\infty \phi^*(E, r)\psi(r, 0)\,\mathrm{d}r$ will also be an analytic function of k.

According to (2.9), (2.11) and (2.16) the decay with time of the non-stationary state is governed by the Jost function. This is true even in complicated cases, where there are several close-lying pairs of zeros of the Jost function in the lower half of the complex k plane, as well as other possible singularities. In the simple case when one pair of zeros of the Jost function (in the lower half of the complex k plane and close to the real k axis) is well separated from all other pairs of zeros and singularities, it is possible to separate the contribution of this pair and to obtain a simple formula for the probability $P(t)$ of finding the particle still in the initial state (cf below).

Let us thus consider the simple case, just mentioned, when there is a pair of complex zeros of the Jost function close to the real k axis:

$$k_1 = \eta - \mathrm{i}\alpha, \qquad k_2 = -\eta - \mathrm{i}\alpha, \qquad (\eta > 0, \alpha > 0, \alpha/\eta \ll 1), \tag{2.17}$$

while all other zeros and singularities of $J(k)$ lie far away from the zeros (2.17) under consideration. Assuming k to lie close to one of the zeros (2.17), and writing $J(k)$ in the form

$$J(k) = J_0(k)(k - \eta + \mathrm{i}\alpha)(k + \eta + \mathrm{i}\alpha) = J_0(k)(2m/\hbar^2)(E - E_n + \tfrac{1}{2}\mathrm{i}\Gamma), \tag{2.18}$$

where $J_0(k)$ is a certain function of k (which is almost constant in the small region of k-values under consideration), E is related to k according to (2.3), n is the quantum number associated with the resonance in question, and E_n and Γ are defined by

$$E_n = \frac{\hbar^2}{2m}(\eta^2 + \alpha^2) \tag{2.19}$$

$$\Gamma = \frac{2\hbar^2}{m} k\alpha \approx \frac{2\hbar^2}{m}\eta\alpha, \tag{2.20}$$

we can write (2.16) as follows

$$W(E) = \frac{D(E)}{(E - E_n)^2 + \frac{1}{4}\Gamma^2}, \tag{2.21}$$

where in $D(E)$ we absorb everything except the denominator. If Γ is small compared to the energy level spacing, the factor $[(E - E_n)^2 + \frac{1}{4}\Gamma^2]^{-1}$ in (2.21) changes very rapidly when E passes through E_n, and we can replace $D(E)$ in (2.21) by a constant which, because of (2.7), is equal to $\Gamma/2\pi$. Inserting the resulting expression for $W(E)$ into (2.11), we obtain approximately

$$p(t) = \exp[-\mathrm{i}(E_n - \tfrac{1}{2}\mathrm{i}\Gamma)t/\hbar] = \exp[-\mathrm{i}(E_n t/\hbar) - \Gamma t/2\hbar] \tag{2.22}$$

and hence (cf (2.9))

$$P(t) = \exp(-\Gamma t/\hbar). \tag{2.23}$$

3. Exact expression for the Jost function in terms of the F matrix

In this section we shall let $\psi(r)$ denote a conveniently normalised solution of the time-independent radial Schrödinger equation, which, for convenience, is now written as follows

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}r^2} + Q^2(r)\psi = 0, \tag{3.1}$$

where, for a particle in an s state ($l = 0$) of a potential $V(r)$, we have

$$Q^2(r) = k^2 - \frac{2m}{\hbar^2}V(r) \tag{3.2}$$

with obvious notations. We assume that $V(r)$ is regular at the origin, tends to zero faster than r^{-1} as $r \to +\infty$, and otherwise has the shape depicted in figure 1(a) or 1(b). We recall that k is related to the energy E according to the well-known relation (2.3).

We define a row vector

$$f(r) = (f_1(r), f_2(r)), \tag{3.3}$$

where

$$f_1(r) = Q^{-1/2}(r)\exp(\mathrm{i}w(r)) \tag{3.4a}$$

$$f_2(r) = Q^{-1/2}(r)\exp(-\mathrm{i}w(r)) \tag{3.4b}$$

with

$$w(r) = \int^r Q(r)\,\mathrm{d}r, \tag{3.5}$$

and we introduce a column vector

$$\boldsymbol{a}(r)=\begin{pmatrix}a_1(r)\\ a_2(r)\end{pmatrix}, \tag{3.6}$$

where $a_1(r)$ and $a_2(r)$ are uniquely determined in terms of $\psi(r)$ and $\psi'(r)$ by the requirements

$$\psi(r)=\boldsymbol{f}(r)\boldsymbol{a}(r) \tag{3.7a}$$

$$\psi'(r)=\boldsymbol{f}'(r)\boldsymbol{a}(r), \tag{3.7b}$$

where the prime denotes differentiation with respect to r. Given a solution $\psi(r_0)=\boldsymbol{f}(r_0)\boldsymbol{a}(r_0)$ at a point r_0, the same solution at an arbitrary point r is, according to Fröman and Fröman (1965), given by (3.7a, b) with

$$\boldsymbol{a}(r)=\boldsymbol{F}(r,r_0)\boldsymbol{a}(r_0), \tag{3.8}$$

where $\boldsymbol{F}(r,r_0)$ is a matrix, the elements of which can be expressed as convergent series, admitting of useful estimates of the elements of $\boldsymbol{F}(r,r_0)$.

We consider only unbound states, i.e. the energy of the particle is assumed to be positive but may lie either below or above the top of the barrier. A unified treatment of the cases of sub-barrier and super-barrier transmission is thus given. We assume that the complex r plane has been cut such that $f_1(r)$ and $f_2(r)$, defined by (3.4a, b), are single valued. To make possible the use of results already obtained by Fröman and Fröman (1970), we choose the phase of $Q^{1/2}(r)$ as indicated in figure 1(a), (b). With this choice, when $r\to+\infty$, $f_1(r)$ represents an incoming wave, and $f_2(r)$ represents an outgoing wave.

Consider now a solution $\psi(k,r)$ of (3.1) which is defined by the asymptotic behaviour

$$\psi(k,r)\sim e^{ikr}, \qquad r\to+\infty. \tag{3.9}$$

The Wronskian of this function $\psi(k,r)$ and the function $\phi(E,r)$ introduced in § 2 is $\psi\phi'-\phi\psi'=J(k)$ according to (2.13) and (3.9). Since this Wronskian is independent of r, it can also be evaluated at $r=0$, and in this way one finds that $\psi\phi'-\phi\psi'=\psi(k,0)$ according to (2.12). Comparing the two expressions for the Wronskian, we find that

$$\psi(k,0)=J(k). \tag{3.10}$$

This result will be used presently.

To represent by (3.7a, b) the solution fulfilling (3.9), we put (cf (3.4a, b))

$$a_1(+\infty)=0 \tag{3.11a}$$

$$a_2(+\infty)=Q^{1/2}(+\infty)\exp[\mathrm{i}\lim_{r\to+\infty}(kr+w(r))]. \tag{3.11b}$$

Using (3.8) and (3.11a), we get

$$a_1(0)=F_{12}(0,+\infty)a_2(+\infty) \tag{3.12a}$$

$$a_2(0)=F_{22}(0,+\infty)a_2(+\infty), \tag{3.12b}$$

and hence (cf (3.7a))

$$\psi(k,0)=a_1(0)f_1(0)+a_2(0)f_2(0)=a_2(+\infty)(F_{12}(0,+\infty)f_1(0)+F_{22}(0,+\infty)f_2(0)). \tag{3.13}$$

With due regard to (3.4a, b), (3.11b) and (3.10) we can write (3.13) as follows

$$J(k)=\left(\frac{Q(+\infty)}{Q(0)}\right)^{1/2}\exp[\mathrm{i}\lim_{r\to+\infty}(kr+w(r))]$$
$$\times[F_{12}(0,+\infty)\exp(\mathrm{i}w(0))+F_{22}(0,+\infty)\exp(-\mathrm{i}w(0))]. \tag{3.14}$$

So far k has not been restricted to real values, and the constant lower limit in the integral (3.5) defining $w(r)$ has not been specified. To be able to utilise directly the results obtained by Fröman and Fröman (1970) in their analysis of the barrier transmission problem, we shall from now on assume k to be real, and as the above-mentioned lower limit of integration we shall choose, in the sub-barrier case the classical turning point t_1 (cf figure 1(a)), and in the super-barrier case the point $s-0$, where s is the point where the cut along the Stokes' line between the two complex conjugate transition points t_1 and t_2 crosses the real axis (cf figure 1(b)). With this choice formula (3.14) can be written

$$J(k)=\left(\frac{Q(+\infty)}{Q(0)}\right)^{1/2}\exp(K+\mathrm{i}\lim_{r\to+\infty}(kr-|w_2(r)|))(F_{12}(0,+\infty)\exp(-\mathrm{i}L)$$
$$+F_{22}(0,+\infty)\exp(+\mathrm{i}L)) \tag{3.15}$$

with the notations K, L and $w_2(r)$ defined as follows. The quantity K, which is positive in the sub-barrier case and negative in the super-barrier case, is given by

$$K=\tfrac{1}{2}\mathrm{i}\int_{\Gamma_K}Q(r)\,\mathrm{d}r=\mathrm{i}\int_{t_1}^{t_2}Q(r)\,\mathrm{d}r \tag{3.16}$$

$$=\begin{cases}\mathrm{i}\displaystyle\int_{t_1}^{t_2}Q(r)\,\mathrm{d}r, & \text{sub-barrier case,} \quad (3.16a)\\[2ex] \mathrm{i}\displaystyle\int_{s-0}^{s+0}Q(r)\,\mathrm{d}r, & \text{super-barrier case,} \quad (3.16b)\end{cases}$$

where the contours Γ_K pertinent to the two cases under consideration are depicted in figure 1(a), (b). The integration from t_1 to t_2 shall be performed along the upper edge of the cut between t_1 and t_2 in the sub-barrier case and along the left-hand edge of the cut between t_1 and t_2 in the super-barrier case. The integration from $s-0$ to $s+0$ shall be performed along a path encircling t_2. The quantities L and $w_2(r)$ are defined as (cf figure 1(a), (b)):

$$L=\mathrm{Re}\,\tfrac{1}{2}\int_{\Gamma_L}Q(r)\,\mathrm{d}r=\mathrm{Re}\int_0^{t_1}Q(r)\,\mathrm{d}r \tag{3.17}$$

$$=\begin{cases}\displaystyle\int_0^{t_1}Q(r)\,\mathrm{d}r, & \text{sub-barrier case,} \quad (3.17a)\\[2ex] \displaystyle\int_0^{s-0}Q(r)\,\mathrm{d}r, & \text{super-barrier case,} \quad (3.17b)\end{cases}$$

and

$$w_2(r)=\begin{cases}\displaystyle\int_{t_2}^{r}Q(r)\,\mathrm{d}r & \text{sub-barrier case,} \quad (3.18a)\\[2ex] \displaystyle\int_{s+0}^{r}Q(r)\,\mathrm{d}r & \text{super-barrier case.} \quad (3.18b)\end{cases}$$

Writing, for the sake of simplicity, F_{12} and F_{22} instead of $F_{12}(0, +\infty)$ and $F_{22}(0, +\infty)$, respectively, separating these quantities into amplitude and phase, and noting that $Q^{1/2}(0) = |Q^{1/2}(0)|$ while $Q^{1/2}(+\infty) = -\mathrm{i}|Q^{1/2}(+\infty)|$ (cf figure 1(*a*), (*b*)), we can write (3.15) as follows

$$J(k) = \left|\frac{Q(+\infty)}{Q(0)}\right|^{1/2} \exp(K + \mathrm{i}\Theta)(|F_{12}| \exp(-\mathrm{i}\Phi) - |F_{22}| \exp(+\mathrm{i}\Phi)) \tag{3.19}$$

where

$$\Theta = \lim_{r\to+\infty} (kr - |w_2(r)|) - 3\pi/4 + \tfrac{1}{2} \arg F_{22} + \tfrac{1}{2}(\arg F_{12} - \tfrac{1}{2}\pi) \tag{3.20a}$$

and

$$\Phi = L + \tfrac{1}{2} \arg F_{22} - \tfrac{1}{2}(\arg F_{12} - \tfrac{1}{2}\pi) - 3\pi/4. \tag{3.20b}$$

The quantity $\frac{1}{2} \arg F_{22} - \frac{1}{2}(\arg F_{12} - \frac{1}{2}\pi)$ appearing in the right-hand member of (3.20*b*) is the quantity which Fröman and Fröman (1970) denoted by $\gamma_1^{(0)}$. Well below the top of the barrier this quantity is very small, but it is still dangerous to neglect it close to a sharp resonance, since, due to the largeness of the factor $\exp\{K\}$ in (3.19), this negligence will in general imply that the resulting formula for $J(k)$ will lead to a displacement of the resonance from its actual position by a very large number of half-widths. This has been shown by Fröman and Fröman (1970) and clearly illustrated for an exactly soluble model by Lundborg (1977). However, it is in general not necessary to know the numerical value of the small quantity $\frac{1}{2} \arg F_{22} - \frac{1}{2}(\arg F_{12} - \frac{1}{2}\pi)$ but only to be aware of the existence of this small correction quantity which is only slightly energy-dependent. The appearance of the quantity $\frac{1}{2} \arg F_{22} - \frac{1}{2}(\arg F_{12} - \frac{1}{2}\pi)$ in the expression (3.20*b*) for Φ is, for energies well below the top of the barrier, closely related to the one-directional nature of the connection formulae at the first and second turning points. This one-directedness thus reflects itself, in the present context, as the above-mentioned displacement of the sharp resonance.

Formula (3.19) can be written as follows

$$J(k) = \left|\frac{Q(+\infty)}{Q(0)}\right|^{1/2} \exp(K + \mathrm{i}\Theta)[(|F_{12}| - |F_{22}|) \cos\Phi - \mathrm{i}(|F_{12}| + |F_{22}|) \sin\Phi]. \tag{3.21}$$

This formula can then be written

$$J(k) = |J(k)| \exp(-\mathrm{i}\delta) \tag{3.22}$$

where

$$|J(k)| = \left|\frac{Q(+\infty)}{Q(0)}\right|^{1/2} |F_{12}F_{22}|^{1/2} \Lambda \exp(K) \left(1 + \frac{\sin^2\Phi}{\Lambda^2/4}\right)^{1/2}, \tag{3.23}$$

Λ being a positive quantity (cf (3.26)) defined by

$$\Lambda = \left|\frac{F_{12}}{F_{22}}\right|^{+1/2} - \left|\frac{F_{12}}{F_{22}}\right|^{-1/2}, \tag{3.24}$$

and

$$\delta = \tan^{-1}\left(\frac{|F_{12}|/|F_{22}| + 1}{|F_{12}|/|F_{22}| - 1} \tan\Phi\right) - \Theta, \tag{3.25}$$

$\tan^{-1}$ lying in the same quadrant as Φ. Since k is real, the quantities $|F_{12}|$ and $|F_{22}|$, which appear in the above formulae, are related to each other according to the relation (23) in the analysis of barrier transmission by Fröman and Fröman (1970), i.e.

$$|F_{12}|^2 = |F_{22}|^2 + \exp(-2K). \tag{3.26}$$

4. Approximate expressions for the Jost function on the real k-axis

As in the last part of § 3 we shall in the present section restrict ourselves to real values of k, since the results obtained by Fröman and Fröman (1970), parts of which we shall now use, are restricted to real values of the energy. According to the estimates (43a, b), (52b) and (53b) in that paper we have, after omission of small correction terms,

$$|F_{22}| \approx 1 \tag{4.1}$$

$$|F_{12}| \approx (1+\exp(-2K))^{1/2} \tag{4.2}$$

$$|F_{12}/F_{22}| \approx (1+\exp(-2K))^{1/2} \tag{4.3}$$

$$|F_{12}| - |F_{22}| \approx (1+\exp(-2K))^{1/2} - 1 = \frac{\exp(-2K)}{1+(1+\exp(-2K))^{1/2}} \tag{4.4}$$

$$\tfrac{1}{2}\arg F_{22} \pm \tfrac{1}{2}(\arg F_{12} - \tfrac{1}{2}\pi) \approx \pm\sigma \tag{4.5}$$

where, by definition,

$$\sigma = \tfrac{1}{2}(\arg F_{12} - \tfrac{1}{2}\pi). \tag{4.6}$$

According to equations (10) and (10a) in Fröman *et al* (1972) (see also references therein) σ is for the first-order phase-integral approximation given by the formula

$$\sigma \approx \frac{1}{2}\left[-\arg\Gamma\left(\frac{1}{2}+\mathrm{i}\frac{K}{\pi}\right) + \frac{K}{\pi}\ln\left|\frac{K}{\pi}\right| - \frac{K}{\pi}\right], \tag{4.7}$$

where Γ is the gamma function. This formula has been obtained by means of a comparison equation method for connecting the first-order JWKB solutions on opposite sides of the top of a barrier which has approximately parabolic shape, when the energy is close to that of the top of the barrier. For such energies the 'parabolic' connection formulae thus obtained can be used in both directions.

Inserting (4.5), with the upper signs, into (3.20a), we obtain

$$\Theta \approx \lim_{r\to+\infty}(kr - |w_2(r)|) - 3\pi/4 + \sigma, \tag{4.8}$$

where σ is given by the approximate formula (4.7). Inserting (4.3) into (3.24), we get

$$\Lambda \approx (1+\exp(-2K))^{+1/4} - (1+\exp(-2K))^{-1/4}, \tag{4.9}$$

and by means of (3.24) and (4.4) we obtain the following approximate formula for another quantity appearing in (3.23):

$$|F_{12}F_{22}|^{1/2}\Lambda\exp K = (|F_{12}| - |F_{22}|)\exp K \approx \frac{\exp(-K)}{1+(1+\exp(-2K))^{1/2}}. \tag{4.10}$$

Inserting (4.1), (4.2) and (4.8) into (3.19), we obtain

$$J(k) \approx \left|\frac{Q(+\infty)}{Q(0)}\right|^{1/2} \exp\{i[\lim_{r\to+\infty}(kr-|w_2(r)|)-3\pi/4+\sigma]\}$$
$$\times([\exp(2K)+1]^{1/2}\exp(-i\Phi)-\exp(K)\exp(+i\Phi)). \tag{4.11}$$

This approximate formula can also be written in the alternative form (3.22) with the following expressions for $|J(k)|$ and δ, which are readily obtained from (3.23), (3.25), (4.3), (4.8), (4.9) and (4.10),

$$|J(k)| \approx \left|\frac{Q(+\infty)}{Q(0)}\right|^{1/2} \frac{\exp(-K)}{1+(1+\exp(-2K))^{1/2}}$$
$$\times\left(1+\left(\frac{\sin\Phi}{\frac{1}{2}(1+\exp(-2K))^{+1/4}-\frac{1}{2}(1+\exp(-2K))^{-1/4}}\right)^2\right)^{1/2} \tag{4.12}$$

and

$$\delta \approx \tan^{-1}\left(\frac{(1+\exp(-2K))^{+1/4}+(1+\exp(-2K))^{-1/4}}{(1+\exp(-2K))^{+1/4}-(1+\exp(-2K))^{-1/4}}\tan\Phi\right)$$
$$-\lim_{r\to+\infty}(kr-|w_2(r)|)+3\pi/4-\sigma. \tag{4.13}$$

We recall that several of the formulae used for obtaining (4.12) and (4.13) were derived on the assumption that k is real. We also emphasise that close to a sharp resonance the quantity $\frac{1}{2}\arg F_{22}-\frac{1}{2}(\arg F_{12}-\frac{1}{2}\pi)$ in the expression (3.20b) for Φ can in general not be neglected or replaced by the approximate expression obtained from (4.5), with the lower signs, and (4.7), for if this is done, and if the resulting approximate expression for Φ is used in the expression for the Jost function, the position of a sharp resonance is in general shifted from its correct position by a very large number of half-widths. The reason for this fact, which, as has already been mentioned, is closely related to the one-directional nature of the connection formulae at the first and second turning points, when the energy lies well below the top of the barrier, is that at the resonance there is a cancellation of two large terms in the expression (3.19) or (4.11) for the Jost function.

5. The positions and widths of the quasi-stationary states

From (3.23) we obtain

$$\frac{1}{|J(k)|^2} = \left|\frac{Q(0)}{Q(+\infty)}\right| \frac{\exp(-2K)}{4|F_{12}F_{22}|}\xi, \tag{5.1}$$

where

$$\xi = \frac{1}{\Lambda^2/4+\sin^2\Phi} \tag{5.2}$$

is the factor on the right-hand side of (5.1) that accounts for the resonance effect, while the other factors there vary slowly over the energy interval in which the resonance occurs. From (4.9) it follows that Λ increases as K decreases, i.e. as E increases, and that $\Lambda = 2^{1/4}-2^{-1/4} \approx 0{\cdot}35$ at the top of the barrier. Due to the smallness of Λ when

$K \gtrsim 0$ the quantity ξ, which is the most important factor in (5.1), has fairly sharp peaks when Φ changes, while Λ is kept constant. The maxima of ξ occur when

$$\Phi = n\pi, \; n = 0, 1, 2, \ldots . \tag{5.3}$$

The positions E_n of the quasi-stationary states are obtained from this condition.

The half-width, Γ, of a peak on the energy scale can be obtained as follows. Neglecting the energy dependence, over the width of the resonance, of Λ as well as of all factors except ξ on the right-hand side of (5.1), we realise with the aid of (5.2) that the half-width on the Φ-scale is $\Delta\Phi = 2\sin^{-1}(\Lambda/2)$. For $K \gtrsim 0$ the quantity Λ is so small ($\lesssim 0{\cdot}35$) that $\sin(\Lambda/2)$ can approximately be replaced by $\Lambda/2$, and hence we get $\Delta\Phi \approx \Lambda$. To convert this half-width on the Φ-scale to the energy scale we divide by $(\mathrm{d}\Phi/\mathrm{d}E)_{E=E_n}$, obtaining

$$\Gamma \approx \frac{\Lambda}{(\mathrm{d}\Phi/\mathrm{d}E)_{E=E_n}}. \tag{5.4}$$

This formula increases in accuracy the narrower the resonance is, but is also approximately valid close to the top of the barrier, where the resonances are comparatively broad.

Provided the peak is not too broad, one can easily derive a simple, well known formula for its shape. To do this we assume E to be close to E_n and note that then (cf (5.3))

$$\sin\Phi = (-1)^n \sin(\Phi - n\pi) \approx (-1)^n(\Phi - n\pi) \approx (-1)^n (\mathrm{d}\Phi/\mathrm{d}E)_{E=E_n}(E - E_n) \tag{5.5}$$

to the first order in $E - E_n$. Assuming this approximate formula to be valid over the whole width of the peak, and inserting it into (5.2), we get for the line shape the Lorentzian expression

$$\xi = \frac{1/(\mathrm{d}\Phi/\mathrm{d}E)^2_{E=E_n}}{\Gamma^2/4 + (E - E_n)^2}, \tag{5.6}$$

where Γ is given by (5.4).

From (3.20b) and (4.5), with the lower signs, it follows that

$$(\mathrm{d}\Phi/\mathrm{d}E)_{E=E_n} \approx \frac{T}{2\hbar} - (\mathrm{d}\sigma/\mathrm{d}E)_{E=E_n} \tag{5.7}$$

where T is defined by

$$T = 2\hbar(\mathrm{d}L/\mathrm{d}E)_{E=E_n}. \tag{5.8}$$

We emphasise that the last term on the right-hand side of (5.7) is very important when the energy is close to that of the top of the barrier but is otherwise negligible. Using (3.17), (3.2) and (2.3), we can write (5.8) as follows

$$T = 2\frac{m}{\hbar}\mathrm{Re}\left(\frac{1}{2}\int_{\Gamma_L}\frac{\mathrm{d}r}{Q(r)}\right)_{E=E_n} = 2\frac{m}{\hbar}\mathrm{Re}\left(\int_0^{t_1}\frac{\mathrm{d}r}{Q(r)}\right)_{E=E_n}. \tag{5.8$'$}$$

In the case of sub-barrier penetration T is the classical period of a complete oscillation of the particle back and forth between the origin and the classical rning point t_1. To evaluate $\mathrm{d}\sigma/\mathrm{d}E$, appearing in (5.7), we write $\mathrm{d}\sigma/\mathrm{d}E = (\mathrm{d}\sigma/\mathrm{d}K)(\mathrm{d}K/\mathrm{d}E)$ when the first-order phase-integral approximation is used. For $\mathrm{d}K/\mathrm{d}E$ we obtain, with the aid of (3.16), (3.2) and (2.3), the first-order formula

$$\frac{\mathrm{d}K}{\mathrm{d}E}=\mathrm{i}\frac{m}{2\hbar^2}\int_{\Gamma_K}\frac{\mathrm{d}r}{Q(r)}=\mathrm{i}\frac{m}{\hbar^2}\int_{t_1}^{t_2}\frac{\mathrm{d}r}{Q(r)}. \tag{5.9}$$

For $\mathrm{d}\sigma/\mathrm{d}K$ we obtain from (4.7) the following first-order formula:

$$\frac{\mathrm{d}\sigma}{\mathrm{d}K}\approx\frac{1}{2\pi}\left(\ln|K/\pi|-\frac{\mathrm{d}\arg\Gamma(\frac{1}{2}+\mathrm{i}K/\pi)}{\mathrm{d}(K/\pi)}\right)$$

$$=\frac{1}{2\pi}[\ln|K/\pi|-\mathrm{Re}\;\psi(\tfrac{1}{2}+\mathrm{i}K/\pi)] \tag{5.10}$$

where (cf Abramowitz and Stegun 1965, 6.1.27)

$$\psi(z)=\frac{\mathrm{d}\ln\Gamma(z)}{\mathrm{d}z}=\frac{\Gamma'(z)}{\Gamma(z)}. \tag{5.11}$$

For $|K|<\pi/2$ we can expand $\psi(\frac{1}{2}+\mathrm{i}K/\pi)$ in a Taylor series around $K=0$. Taking the real part of the resulting series, we obtain (cf Abramowitz and Stegun 1965, 6.3.3 and 6.4.4)

$$\mathrm{Re}\;\psi(\tfrac{1}{2}+\mathrm{i}K/\pi)=\psi\left(\frac{1}{2}\right)+\sum_{\nu=1}^{\infty}\frac{(-1)^{\nu}}{(2\nu)!}\psi^{(2\nu)}\left(\frac{1}{2}\right)\left(\frac{K}{\pi}\right)^{2\nu}$$

$$=-(\gamma+2\ln 2)+\sum_{\nu=1}^{\infty}(-1)^{\nu-1}(2^{2\nu+1}-1)\zeta(2\nu+1)\left(\frac{K}{\pi}\right)^{2\nu}, \tag{5.12}$$

where γ is Euler's constant and ζ is Riemann's zeta function. The first few terms in this series are (cf Abramowitz and Stegun 1965, 6.3.3 and Table 23.3)

$$\mathrm{Re}\;\psi(\tfrac{1}{2}+\mathrm{i}K/\pi)=-1{\cdot}9635+2{\cdot}1036\,(2K/\pi)^2-2{\cdot}0090\,(2K/\pi)^4+\ldots. \tag{5.12'}$$

Inserting (4.9) and (5.7) into (5.4), we get

$$\Gamma\approx\frac{2\hbar[(1+\exp(-2K))^{+1/4}-(1+\exp(-2K))^{-1/4}]}{|T-2\hbar(\mathrm{d}\sigma/\mathrm{d}E)_{E=E_n}|}. \tag{5.13}$$

For K, T and $\mathrm{d}\sigma/\mathrm{d}E=(\mathrm{d}\sigma/\mathrm{d}K)(\mathrm{d}K/\mathrm{d}E)$ we have the formulae (3.16), (5.8′), (5.10) with (5.12′), and (5.9).

The formula for the half-width derived by Connor (1968, equation (24); 1973, equation (16*a*)), on the assumption of a parabolic barrier, and by Dickinson (1970, equation (33)), on the assumption of an inverted Morse potential, reads in our notation

$$\Gamma\approx\frac{\hbar\ln(1+\exp(-2K))}{T}. \tag{5.14}$$

This formula can, however, be used only well below the top of the barrier (cf Connor 1976, pp 135–136), where it agrees approximately with our formula (5.13). In this case $\exp(-2K)\ll 1$, and (5.13) as well as (5.14) simplify into

$$\Gamma\approx\hbar\exp(-2K)/T. \tag{5.15}$$

For energies close to the top of the barrier the numerators in (5.13) and (5.14) still have approximately the same numerical values (since $2\;(2^{1/4}-2^{-1/4})=0{\cdot}697$ and $\ln 2=$

0·693), whereas the denominators differ considerably. As the energy approaches the top of the barrier, the denominator in (5.14), which is the classical oscillation time T, tends to infinity, while the denominator in the correct formula (5.13) remains finite. From (5.14) one would therefore draw the erroneous conclusion that a resonance at the top of the barrier would have the width $\Gamma = 0$, i.e. that it would be infinitely sharp.

Recalling (3.20b), we can write the resonance condition (5.3) as follows

$$L + \tfrac{1}{2}\arg F_{22} - \tfrac{1}{2}(\arg F_{12} - \tfrac{1}{2}\pi) = (n + \tfrac{3}{4})\pi, \qquad n = 0, 1, 2, \ldots. \tag{5.16}$$

Inserting (4.5), with the lower signs, into (5.16), we obtain

$$L - \sigma \approx (n + \tfrac{3}{4})\pi, \qquad n = 0, 1, 2, \ldots. \tag{5.17}$$

As concerns the location of the quasi-stationary levels obtained from (5.17), we should note that, since we use the first-order JWKB approximation, the positions of the levels will in general be displaced by many half-widths Γ. Only by using higher-order phase-integral approximations can one expect to get the position of a level with an accuracy of the order of Γ or better. (See Fröman and Fröman 1970 pp 620–621.)

Considering a narrow resonance, we shall finally express our results in terms of zeros of the Jost function. The value of the resonance energy E_n is approximately obtained from the resonance condition (5.17), where σ will be neglected since the resonance is assumed to be narrow, i.e. from the condition

$$L = (n + \tfrac{3}{4})\pi, \qquad n = 0, 1, 2, \ldots. \tag{5.18}$$

We emphasise that the error in the value E_n thus obtained is in general very large compared to Γ, although small compared to the spacing of the energy levels. Since the resonance is assumed to be narrow, $\exp(-2K)$ is small compared to unity, and $2\hbar\, \mathrm{d}\sigma/\mathrm{d}E$ can be put equal to zero in the denominator of formula (5.13), which therefore simplifies into (5.15). Solving (2.19) and (2.20) with respect to η and α, we obtain

$$\eta \approx \frac{1}{2}\left[\frac{2m}{\hbar^2}\left(E_n + \frac{1}{2}\Gamma\right)\right]^{1/2} + \frac{1}{2}\left[\frac{2m}{\hbar^2}\left(E_n - \frac{1}{2}\Gamma\right)\right]^{1/2} \approx \left(\frac{2mE_n}{\hbar^2}\right)^{1/2} \tag{5.19}$$

and

$$\alpha \approx \frac{1}{2}\left[\frac{2m}{\hbar^2}\left(E_n + \frac{1}{2}\Gamma\right)\right]^{1/2} - \frac{1}{2}\left[\frac{2m}{\hbar^2}\left(E_n - \frac{1}{2}\Gamma\right)\right]^{1/2} \approx \frac{1}{4}\Gamma\left(\frac{2m}{\hbar^2 E_n}\right)^{1/2} \approx \frac{\Gamma}{4E_n}\eta. \tag{5.20}$$

Because of what is said immediately below formula (5.18) about the inaccuracy of E_n, as obtained from (5.18), the corresponding error in the value of η, obtained from (5.19), is in general very large compared with α, although small compared to η. By increasing the order of the phase-integral approximations one may diminish the error in η, so that it may become as small as Γ or perhaps even smaller. The capability and the restriction of the phase-integral method as regards the determination of the pair of well separated zeros (2.17) of the Jost function associated with the resonance under consideration is thus demonstrated.

6. Generalisation

We shall now indicate how the results presented in the previous sections can be generalised to the case that the physical potential $V(r)$ is either regular or has a

Coulomb singularity at the origin and that the angular momentum quantum number l may be different from zero. In the radial Schrödinger equation (3.1) the function $Q^2(r)$ is then given by

$$Q^2(r) = k^2 - \frac{2m}{\hbar^2} V(r) - \frac{l(l+1)}{r^2}. \tag{6.1}$$

Defining

$$Q^2_{\text{mod}}(r) = Q^2(r) - \frac{1}{4r^2} = k^2 - \frac{2m}{\hbar^2} V(r) - \frac{(1+\frac{1}{2})^2}{r^2}, \tag{6.2}$$

we introduce modified phase-integral approximations of arbitrary order according to Fröman and Fröman (1974a, 1974b (pp 126–131)). The reason for this is that we want the phase-integral approximations to be valid also at the origin. With the expression (6.2) for $Q^2_{\text{mod}}(r)$ there are two generalised classical turning points associated with the potential well in the case of sub-barrier penetration. As the energy increases and the super-barrier case is reached, the left generalised classical turning point remains, but the right one goes over into one of the two generalised transition points associated with the underdense barrier. The analysis of the barrier transmission problem made by Fröman and Fröman (1970) can then be taken over directly. In fact, except for a factor which changes smoothly with energy, the inverse of the complex conjugate of the Jost function, i.e. $1/J^*(k)$, is given by the inverse of the expression $\Omega_1 \exp(\mathrm{i}\varphi_1)$, obtained by Fröman and Fröman (1970, equation (31)), for real values of k. In this expression we define K by the first equality in our formula (3.16) but with $Q(r)$ replaced by $q(r)$, we note that (cf Fröman and Fröman 1970, equations (28) and (57))

$$-(\sigma - \tfrac{1}{2}\arg F_{22}) = \tfrac{1}{2}\arg F_{22} - \tfrac{1}{2}(\arg F_{12} - \tfrac{1}{2}\pi) = \gamma_1^{(0)}, \tag{6.3}$$

and we put

$$\gamma_1 = \tfrac{1}{2}\pi - L, \tag{6.4}$$

where L is defined by the first equality in our formula (3.17) but with $Q(r)$ replaced by $q(r)$ and Γ_L replaced by a closed loop around the two generalised classical turning points associated with the potential well (in the sub-barrier case) or around the generalised classical turning point and one of the generalised transition points associated with the barrier (in the super-barrier case). The quantities Ω_1 and φ_1 are given by the explicit formulae (33*a*, *b*) and (56*a*, *b*) in the analysis by Fröman and Fröman (1970). If we replace our definition (3.20*b*) by (cf (6.3) and (6.4))

$$\Phi = \gamma_1^{(0)} - \gamma_1 = L + \tfrac{1}{2}\arg F_{22} - \tfrac{1}{2}(\arg F_{12} - \tfrac{1}{2}\pi) - \tfrac{1}{2}\pi, \tag{6.5}$$

our formula (5.2) for the essential factor in $1/|J(k)|^2$ remains valid, Λ being still given by (4.9); cf formula (60) in the paper by Fröman and Fröman (1970). With the expression (6.5) for Φ our formula (5.3) for the positions of the resonances also remains valid. Consequently (5.17) and (5.18) remain valid, if $(n+\frac{3}{4})\pi$ is replaced by $(n+\frac{1}{2})\pi$. Also (5.13) remains valid, if T is defined by (5.8) but with the definition of L changed as described above. For calculating $\mathrm{d}L/\mathrm{d}E$ in (5.8) one then uses formulae (23) or (26) in a paper by Fröman (1974), the use of the former formula being necessary if the energy is close to the top of the barrier. For calculating $\mathrm{d}\sigma/\mathrm{d}E$ in (5.13), when higher-order phase-integral approximations are used, one uses formulae (10) and (10*a*, *b*, *c*) given by Fröman *et al* (1972).

7. Conclusions

We have considered in detail the quantal decay of an s state of a particle in a potential with the shapes shown in figures 1(a) and 1(b). With the aid of the Fock–Krylov theorem we demonstrated in § 2 how the decay with time of this non-stationary state can be expressed in terms of the Jost function. Using, in the F matrix phase-integral method developed by Fröman and Fröman (1965), the first order JWKB functions defined by (3.4a, b) with (3.5), we derived in § 3 for the Jost function $J(k)$ the exact expression given by equations (3.22)–(3.25) and (3.20a, b), which is valid when k is real, whether the energy E lies below or above the top of the barrier. Omitting, in this expression, small correction terms, we obtained in § 4 the approximate formulae (4.12) and (4.13) with (4.7) for the quantities $|J(k)|$ and δ in (3.22). For the widths and positions of the quasi-stationary states we obtained in § 5 the approximate formulae (5.13) and (5.17), and we emphasised that for a narrow resonance (when the energy lies well below the top of the barrier) the error in the energy level position E_n obtained from (5.17) is in general very large compared with the energy level width Γ, although small compared to the spacing of the energy levels. The generalisation to the case that the physical potential $V(r)$ is either regular or has a Coulomb singularity at the origin and that the angular momentum quantum number l may be different from zero was indicated in § 6.

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