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Analytic properties of integrals over the continuum as a function of the interaction parameter

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Abstract. The integral of the modulus squared of a radial matrix element, taken over the continuous energy spectrum, is considered as a function of the interaction parameter λ. It is assumed that the matrix element is that of an N-order differential operator with exponentially decreasing coefficients, where $0 \leqslant N \leqslant 2$. The analytic properties of this integral in the neighbourhood of a bound-state appearance threshold λ_0 are investigated. It is shown that the integral has a branch cut on the complex λ plane crossing the physical region (the real axis) at the threshold λ_0. An analytic continuation of the integral into the second Riemann sheet is found, and it is shown that it contains a bound-state term. Thus the corresponding total quantity (the integral over the continuum and the sum over the bound states) is a smooth function of λ. The threshold behaviour of the integral and the bound-state term is considered.

1. Introduction

The problem of analyticity of the physical quantities with respect to the interaction parameter has been considered by many authors (Ebeling *et al* 1976 and references therein). Particular attention has been paid to investigations of the two-body partition function and the second virial coefficient. It has been shown that the analyticity of these quantities is not violated when two-body bound states arise as the interaction parameter is increased.

In this paper we consider the analytic properties of the integral of the modulus of a radial matrix element, taken over the continuum, as a function of the interaction parameter in the neighbourhood of a bound-state appearance threshold. Integrals of this type arise, for example, in radiation theory. The emission and absorption coefficients are expressed in terms of such integrals, if the matrix element under the integral is the dipole one. In this paper we consider a more general case: we assume that the matrix element is that of an N-order differential operator with exponentially decreasing coefficients, where $0 \leqslant N \leqslant 2$. In appendix 1 it is shown that the dipole and kinetic energy matrix elements may be represented in this form. Also the matrix elements of the exponential potentials often used in nuclear calculations are, obviously, the particular case of the matrix element under consideration for $N = 0$.

It is shown below that the integral has a branch cut in the complex plane of the interaction parameter λ, which crosses over the real axis (the physical region) at the point λ_0 corresponding to a bound-state appearance threshold. A discontinuity at the cut is compensated for by a bound-state term, thus the corresponding total quantity (containing both the integral over the continuum and the bound-state term) is a smooth function of λ. It can be considered as an analytic continuation of the integral into the second sheet of the Riemann surface.

For the absorption coefficient these results without the complete proof have been reported (D'yachkov and Kobzev 1981a). For the particular case of radiation processes in the square well potential, the problem of continuity between bound and unbound (virtual and resonant) states is considered in detail by D'yachkov and Kobzev (1981b).

In § 2 we formulate the problem and give the relations needed later on. In particular the wavefunctions are expressed in terms of the regular solutions of the radial Schrödinger equation and the Jost functions. In § 3 the analyticity of the matrix element with the regular solutions is proved. In § 4 an analytic continuation of the integral under consideration into the second Riemann sheet is obtained, and it is shown that it contains a bound-state contribution. The threshold behaviour of the integral and the bound-state term is examined in § 5. The effect of a potential barrier on the threshold behaviour is discussed in appendix 2.

2. Formulation of the problem and preliminaries

Let us consider two spinless non-relativistic particles interacting by means of the potential

$$v(r,\lambda) = v_0(r) + \lambda v_1(r) \tag{1}$$

where $v_{0,1}(r)$ satisfy the condition

$$\int_0^\infty |v_{0,1}(r)|\, \mathrm{e}^{2ar} r\, \mathrm{d}r \leqslant b < \infty, \qquad a>0, \tag{2}$$

and are continuous functions for $r > 0$ with the exception, possibly, of a finite number of the points of finite discontinuities; $v_1(r)$ is an attractive potential, therefore bound states should appear as λ is increased.

This paper is aimed at the investigation of the analytic properties of the quantity given by

$$I = \int_0^{\bar{E}} F(E) |\langle E'|\theta|E\rangle|^2\, \mathrm{d}E, \qquad 0 < \bar{E} \leqslant \infty, \tag{3}$$

as a function of the interaction parameter λ close to a bound-state appearance threshold λ_0. It is assumed that the matrix element in (3) is given by

$$\langle E'|\theta|E\rangle = \sum_{n,n'=0}^{n+n'\leqslant 2} \int_0^\infty A_{nn'}(r) \frac{\partial^n}{\partial r^n} P_l(E,r,\lambda) \frac{\partial^{n'}}{\partial r^{n'}} P_{l'}(E',r,\lambda)\, \mathrm{d}r \tag{4}$$

where $A_{nn'}(r)$ satisfy

$$\int_0^\infty |A_{nn'}(r)| r^{2-n-n'}\, \mathrm{e}^{2\alpha r}\, \mathrm{d}r \leqslant \beta < \infty, \qquad \alpha > 0, \tag{5}$$

and the condition of continuity similar to that given above for the potential, $P_l(E, r, \lambda)$ is the radial wavefunction satisfying

$$\mathrm{d}^2P/\mathrm{d}r^2 + \{2E - [l(l+1)/r^2] - v(r,\lambda)\}P = 0 \tag{6}$$

and

$$\int_0^\infty P_l(E, r, \lambda) P_l(E', r, \lambda)\, dr = \delta(E - E').$$

We assume that E' in (3) and (4) is related to E by a function $E' = g(E)$, $F(E)$ and $g(E)$ are analytic functions in a certain region enclosing the integration path, $0 \leqslant E \leqslant \bar{E}$, and

$$|g(E)| \geqslant \varepsilon > 0 \tag{7}$$

in this region (it should be noted that condition (7) excludes the case $E' = E$).

Let us consider the regular, $\varphi_l(k, r, \lambda)$, and the irregular, $\chi_l(k, r, \lambda)$, solutions of (6) defined by the boundary conditions (Taylor 1972)

$$\lim_{r\to 0} r^{-l-1}\varphi_l = k^{l+1}[(2l+1)!!]^{-1}, \qquad \lim_{r\to\infty} e^{-ikr}\chi_l = i^{-l}, \tag{8}$$

where $k^2 = 2E$. Then the Jost function can be written as

$$f_l(k, \lambda) = k^{-1}(\chi_l\, \partial\varphi_l/\partial r - \varphi_l\, \partial\chi_l/\partial r).$$

The regular solution is an entire function of k. The Jost function is an analytic function of k for $\operatorname{Im} k > -a$ (Newton 1960, 1966). In the strip $|\operatorname{Im} k| < a$

$$f_l^*(k^*, \lambda^*) = f_l(-k, \lambda). \tag{9}$$

It is known that in the case of a potential $v(r, \lambda) = \lambda v(r)$ satisfying (2), φ_l and f_l are entire functions of λ (Newton 1960, 1966). This result can be easily expanded to the more general case of the potential given by (1).

For scattering states one can write

$$P_l(E, r, \lambda) = (2/\pi k)^{1/2} |f_l(k, \lambda)|^{-1} \varphi_l(k, r, \lambda)$$

and therefore

$$|\langle E'|\theta|E\rangle|^2 = \frac{4Z_{ll'}^2(k, k', \lambda)}{\pi^2 kk' f_l(k, \lambda) f_l(-k, \lambda) f_{l'}(k', \lambda) f_{l'}(-k', \lambda)} \tag{10}$$

where

$$Z_{ll'}(k, k', \lambda) = \sum_{n,n'=0}^{n+n'\leqslant 2} \int_0^\infty A_{nn'}(r) \frac{\partial^n}{\partial r^n}\varphi_l(k, r, \lambda) \frac{\partial^{n'}}{\partial r^{n'}}\varphi_{l'}(k', r, \lambda)\, dr. \tag{11}$$

If E' is a discrete level, $E' = E_0' = \frac{1}{2}k_0'^2 < 0$, then (De Alfaro and Regge 1965)

$$P_{l'}(E_0', r, \lambda) = B_{l'}(k_0', \lambda)\varphi_{l'}(k_0', r, \lambda)$$

where

$$B_{l'}^2(k_0', \lambda) = -4i[(\partial f_{l'}/\partial k')(k_0', \lambda) f_{l'}(-k_0', \lambda)]^{-1}$$

and we get

$$|\langle E_0'|\theta|E\rangle|^2 = -\frac{8i}{\pi k} \frac{Z_{ll'}^2(k, k', \lambda)}{f_l(k, \lambda) f_l(-k, \lambda)(\partial f_{l'}/\partial k')(k_0', \lambda) f_{l'}(-k_0', \lambda)}. \tag{12}$$

3. Analytic properties of $Z_{ll'}(k, k', \lambda)$

In order to show that $Z_{ll'}(k, k', \lambda)$ is an analytic function of k, k' and λ we use the standard method. To prove the existence and the analytic properties of φ_l, one uses the iterative solution of the integral equation equivalent to (6) with (8) (Newton 1960, 1966, De Alfaro and Regge 1965)

$$\varphi_l(k, r, \lambda) = \sum_{m=0}^{\infty} \varphi_l^{(m)}, \qquad \varphi_l^{(0)} = u_l(kr),$$

$$\varphi_l^{(m)}(k, r, \lambda) = \int_0^r g_l(k, r, r') v(r', \lambda) \varphi_l^{(m-1)}(k, r', \lambda)\, \mathrm{d}r', \qquad m \geqslant 1,$$

$$g_l(k, r, r') = k^{-1}(u_l(kr')v_l(kr) - u_l(kr)v_l(kr')), \qquad r' \leqslant r,$$

where u_l and v_l are the Ricatti–Bessel functions

$$u_l(z) = (\tfrac{1}{2}\pi z)^{1/2} J_{l+1/2}(z), \qquad v_l(z) = (\tfrac{1}{2}\pi z)^{1/2} N_{l+1/2}(z).$$

The bounds

$$|\varphi_l^{(m)}(k, r, \lambda)| \leqslant C_l^{m+1} \frac{\exp(|\nu| r)}{m!} \left(\frac{|k| r}{1 + |k| r}\right)^{l+1} \left(\int_0^r \frac{r'}{1 + |k| r'} |v(r', \lambda)|\, \mathrm{d}r'\right)^m,$$

$$|\varphi_l(k, r, \lambda)| \leqslant C_l\, \mathrm{e}^{|\nu| r} \left(\frac{|k| r}{1 + |k| r}\right)^{l+1} \exp\left(C_l \int_0^r \frac{r'}{1 + |k| r'} |v(r', \lambda)|\, \mathrm{d}r'\right)$$
$$\leqslant C_l |k| r \exp(C_l b(1 + |\lambda|) + |\nu| r),$$

where $\nu = \operatorname{Im} k$ and C_l is constant, are valid (Newton 1960).

We get an analogous representation for the first derivative $\partial\varphi_l/\partial r$. Using the well known properties of the Ricatti–Bessel functions we find

$$\partial g_l(k, r, r')/\partial r = h_l(k, r, r') - (l/r) g_l(k, r, r'), \qquad r' \leqslant r,$$

$$h_l(k, r, r') = u_l(kr')v_{l-1}(kr) - u_{l-1}(kr)v_l(kr'), \qquad r' \leqslant r,$$

$$\partial\varphi_l^{(m)}/\partial r = \xi_l^{(m)} - (l/r)\varphi_l^{(m)}, \qquad \xi_l^{(0)} = k u_{l-1}(kr),$$

$$\xi_l^{(m)}(k, r, \lambda) = \int_0^r h_l(k, r, r') v(r', \lambda) \varphi_l^{(m-1)}(k, r', \lambda)\, \mathrm{d}r', \qquad m \geqslant 1.$$

Thus, we obtain

$$\partial\varphi_l/\partial r = \xi_l - (l/r)\varphi_l$$

where

$$\xi_l = \sum_{m=0}^{\infty} \xi_l^{(m)}$$

Using the known bounds for the Ricatti–Bessel functions we can easily obtain for $r' \leqslant r$

$$|h_l(k, r, r')| \leqslant C_l \left(\frac{|k| r}{1 + |k| r}\right)^l \left(\frac{|k| r'}{1 + |k| r'}\right)^{-l} \exp[|\nu|(r - r')]$$

and therefore

$$|\xi_l^{(m)}(k, r, \lambda)| \leqslant C_l^{m+1} \frac{\exp(|\nu| r)}{m!} |k| \left(\frac{|k| r}{1 + |k| r}\right)^l \left(\int_0^r \frac{r'}{1 + |k| r'} |v(r', \lambda)|\, \mathrm{d}r'\right)^m.$$

Then we can conclude that ξ_l and consequently $\partial\varphi_l/\partial r$ are entire functions of k and λ. Also we have the bound

$$\partial\varphi_l(k, r, \lambda)/\partial r \leq C_l|k| \exp[C_l b(1+|\lambda|)+|\nu|r].$$

For the second derivative we obtain

$$|\partial^2\varphi_l/\partial r^2| \leq [|k|^2 r^2 + l(l+1) + d(1+|\lambda|)]C_l|k|r^{-1} \exp[C_l b(1+|\lambda|)+|\nu|r].$$

Here we have used the bound

$$|v_{0,1}(r)|r^2 \leq d < \infty$$

which follows from (2) and the condition of the continuity. Thus we can write for $0 \leq n+n' \leq 2$

$$\begin{aligned}|A_{nn'}(r)(\partial^n/\partial r^n)\varphi_l(k, r, \lambda)(\partial^{n'}/\partial r^{n'})\varphi_{l'}(k', r, \lambda)|&\\ \leq C_l C_{l'}|kk'|r^{2-n-n'}|A_{nn'}(r)| \exp[(C_l+C_{l'})b(1+|\lambda|)+(|\nu|+|\nu'|)r]&\\ \times\{1+\delta_{n2}[-1+l(l+1)+|k|^2r^2+d(1+|\lambda|)]&\\ +\delta_{n'2}[-1+l'(l'+1)+|k'|^2r^2+d(1+|\lambda|)]\}.&\end{aligned}$$

As a result the integrand in (11) is an entire function of k, k' and λ for fixed $r \geq 0$, and it is a continuous function of r for fixed k, k' and λ. It is bounded in the product of any closed regions on the k, k', λ planes and the positive half of the r axis. Furthermore, if $|\nu|+|\nu'| < 2\alpha$ then the limit

$$\lim_{\substack{\rho\to 0\\ R\to\infty}} \int_\rho^R \left|A_{nn'}(r)\frac{\partial^n}{\partial r^n}\varphi_l(k, r, \lambda)\frac{\partial^{n'}}{\partial r^{n'}}\varphi_{l'}(k', r, \lambda)\right| dr \tag{13}$$

exists and is finite. Thus, if

$$|\mathrm{Im}\, k|+|\mathrm{Im}\, k'| < 2\alpha, \tag{14}$$

then $Z_{ll'}(k, k', \lambda)$ is an entire function of λ and an analytic function of k and k' (Markushevitz 1978).

If $E' = E'_0 < 0$ is a discrete level then the conditions (14) and (5) can be weakened. In this case $\varphi_{l'}$ and $\chi_{l'}$ are multiples of one another:

$$\varphi_{l'}(k'_0, r, \lambda) = c\chi_{l'}(k'_0, r, \lambda).$$

In order to prove the convergence of (13) at the upper end, we can use the bound

$$|\partial^{n'}\chi_{l'}(k'_0, r, \lambda)/\partial r^{n'}| \leq C_{l'}|k'_0|^{n'} \exp[C_{l'}b(1+|\lambda|)-\mathrm{Im}\, k'_0 r], \qquad 0 \leq n' \leq 2,$$

which is valid for $k \neq 0$ and large enough r, and is obtained by the method above. Therefore (14) can be substituted by

$$|\mathrm{Im}\, k| - \mathrm{Im}\, k'_0 < 2\alpha.$$

Since $k'_0 = \mathrm{i}|k'_0|$ we have the condition

$$|\mathrm{Im}\, k| - |k'_0| < 2\alpha.$$

If we restrict ourselves to the strip $|\mathrm{Im}\, k| \leq \zeta_1 < \zeta$, where $\zeta = \min k'_0(\lambda)$ in the neighbourhood of λ_0 (we exclude the accidental case of the degeneration $k'_0 = k_0 = 0$ at λ_0), then we can consider operators with the coefficients $A_{nn'}(r)$ increased exponentially so that $2\alpha > \zeta_1 - \zeta$.

4. Analytic continuation of $I(\lambda)$

Inserting (10) into (3), we can write

$$I(\lambda)=\int_{-\bar{k}}^{\bar{k}} \frac{2F(k^2/2)Z_{ll'}^2(k,k',\lambda)}{\pi^2 k' f_l(k,\lambda) f_l(-k,\lambda) f_{l'}(k',\lambda) f_{l'}(-k',\lambda)}\,\mathrm{d}k \tag{15}$$

where $\bar{k}=(2\bar{E})^{1/2}$, $k'=[g(k^2/2)]^{1/2}\equiv\eta(k)$. Taking into account (7), we can conclude that $\eta(k)$ is an analytic function in a certain region enclosing the integration path $-\bar{k}\leqslant k\leqslant\bar{k}$. It is easily seen that (15) is an analytic function of λ with the exception of branch cuts along the trajectories of the zeros of $f_l(k,\lambda)$ and $f_{l'}(\eta(k),\lambda)$ for real k running from $-\bar{k}$ to $\bar{k}$. It is known that $f_l(k,\lambda)$ cannot vanish for real λ and real $k\neq 0$ (Newton 1960, 1966). Therefore, according to (7), the branch cut originated from zeros of $f_{l'}(\eta(k),\lambda)$ does not cross the real λ axis and lies off it. Since we are interested in physical (real) values of λ, this cut may be disregarded. The branch cut originated from zeros of $f_l(k,\lambda)$ is symmetric with respect to the real λ axis. It crosses over the λ axis at the point λ_0 corresponding to a bound-state appearance threshold. Discontinuity of $I(\lambda)$ at the branch cut is connected with the fact that poles of the integrand in (15) (the zeros of $f_l(\pm k,\lambda)$) cross over the integration path (the real k axis).

Let us continue $I(\lambda)$ into the second Riemann sheet and consider the physical meaning of the continuation. For this purpose the integration contour should be deformed in order that the poles do not cross over it. The trajectories of zeros of the Jost function for real λ are well known (see e.g. Demkov and Drukarev 1965, Newton 1966, Taylor 1972). The zeros of $f_l(k,\lambda)$ and $f_l(-k,\lambda)$ from two sides of the integration contour tend to coalesce in the origin $k=0$ as $\lambda\to\lambda_0$, and the contour becomes pinched between these poles of the integrand. Consequently we must go round the point λ_0. Figure 1(a) shows the trajectories of the zeros of $f_l(\pm k,\lambda)$ for the circular path in the upper half of the λ plane, figure 1(b) shows the trajectories for the circular path in the lower half-plane. The corresponding deformations of the integration contour are given in figures 2(a) and (b). The analytic continuation of $I(\lambda)$ into the second

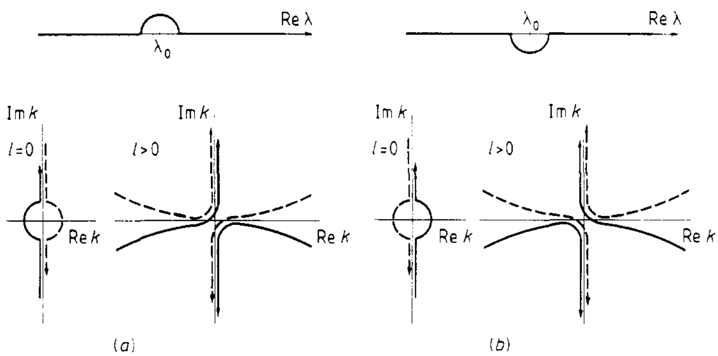

Figure 1. Trajectories of the zeros of $f_l(k,\lambda)$ (full curves) and $f_l(-k,\lambda)$ (broken curves) for two circular paths around the threshold point λ_0: (a) above and (b) below it.

sheet defined by the deformed contour integration can be written as

$$I_c(\lambda)=I(\lambda)+I_0(\lambda)$$

where $I(\lambda)$ is the first-sheet branch given by (15), $I_0(\lambda)$ is the difference of the residues

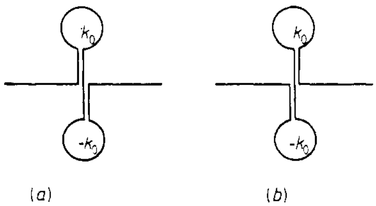

Figure 2. Deformations of the integration contour corresponding to the circular paths (*a*) above λ_0 and (*b*) below λ_0.

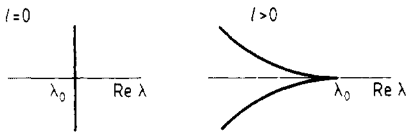

Figure 3. The branch cuts of $I(\lambda)$ corresponding to bound states of $l = 0$ and $l > 0$.

of the integrand at the poles $\pm k_0$ (i.e. at the zeros of $f_l(\pm k, \lambda)$):

$$I_0(\lambda) = 2\pi \mathrm{i}(R(-k_0) - R(k_0))$$

(we assume that the poles remain in the region of analyticity of f_l, F and η). Obviously $I_0(\lambda)$ does not depend on the circular path around λ_0. Therefore we may put

$$I_c(\lambda_0) = \lim_{\varepsilon \to 0} I(\lambda_0 - \varepsilon) = \lim_{\varepsilon \to 0} (I(\lambda_0 + \varepsilon) + I_0(\lambda_0 + \varepsilon)).$$

Since the integrand in (15) is an even function of k, the residues are equal in value but opposite in sign. Thus, we get

$$I_0(\lambda) = \frac{8\mathrm{i}F(E_0)Z^2_{ll'}(k_0, k', \lambda)}{\pi k'(\partial f_l/\partial k)(k_0, \lambda) f_l(-k_0, \lambda) f_{l'}(k', \lambda) f_{l'}(-k', \lambda)}$$

where $E_0 = \frac{1}{2}k_0^2$ is the bound state energy, $k' = \eta(k_0)$. A comparison with (12) gives

$$I_0(\lambda) = F(E_0)|\langle E'|\theta|E_0\rangle|^2.$$

Thus, I_0 is the bound-state contribution.

If E' is a discrete level, alterations of the obtained equations are clear.

We have obtained the result which, from the physical point of view, is explicit. An analytic continuation of (3) into the region above a bound-state appearance threshold should contain the contribution of the bound state.

5. Threshold behaviour of $I(\lambda)$

In this section we wish to examine the behaviour of $I(\lambda)$ near the threshold λ_0. Firstly we find the shape of the branch cut, $\lambda(k)$, in the neighbourhood of λ_0, using a method analogous to that presented by Ostrovsky and Solovyov (1972). Writing the Jost function as

$$f_l(k, \lambda) = K_l(k^2, \lambda) + \mathrm{i}k^{2l+1} L_l(k^2, \lambda)$$

where K_l and L_l are real-valued functions for k^2 and λ both real (Drukarev 1963), we expand K_l and L_l in a double power series of both k^2 and $\lambda - \lambda_0$. Since $f_l(0, \lambda_0) = 0$, we find

$$\lambda(k) = \lambda_0 - (\boldsymbol{K}_l^{(10)}/\boldsymbol{K}_l^{(01)})k^2 - \mathrm{i}(L_l^{(00)}/\boldsymbol{K}_l^{(01)})k^{2l+1} + \mathrm{O}(k^s) \qquad (16)$$

where $K_l^{(mn)} = \partial^{m+n} K_l / \partial(k^2)^m \, \partial\lambda^n$ at $k^2 = 0$, $\lambda = \lambda_0$ and the same for $L_l^{(mn)}$ too, $s = 3$ for $l = 0$ and $s = 4$ for $l > 0$. Therefore, for $l = 0$ the branch cut crosses the real λ axis at right angles, for $l > 0$ it is tangential to the λ axis and has the shape of a beak. Inverting (20), we have for $l > 0$

$$k_0^2(\lambda) = -(K_l^{(01)}/K_l^{(10)})(\lambda - \lambda_0).$$

Consequently $K_l^{(10)}/K_l^{(01)} > 0$, since $E_0 = \frac{1}{2}k_0^2 < 0$ for $\lambda - \lambda_0 > 0$. Thus we know the direction of the beak. Figure 3 shows the crossing of the branch cut with the real λ axis for two cases: $l = 0$ and $l > 0$.

We now consider the behaviour of $I(\lambda)$ near λ_0. It should be noted that $Z_{ll}^2(k_0, k', \lambda) = \mathrm{O}(k_0^{2l+2})$ as follows from (8). Taking into account that $f_l(-k_0, \lambda) = -2\mathrm{i}k_0^{2l+1} L_l(k_0, \lambda)$, and using again the expansion of L_l, we get the jump of $I(\lambda)$ at the threshold

$$\Delta I(\lambda_0) = -\lim_{\varepsilon \to 0} I_0(\lambda_0 + \varepsilon) = \begin{cases} 0, & l = 0, \\ -\dfrac{2Q_{ll'}(k', \lambda_0)}{\pi k' K_l^{(10)} L_l^{(00)}}, & l > 0, \end{cases}$$

where

$$Q_{ll'}(k', \lambda) = \lim_{k \to 0} \frac{F(k^2/2) Z_{ll'}^2(k, k', \lambda)}{k^{2(l+1)} f_{l'}(\eta(k), \lambda) f_{l'}(-\eta(k), \lambda)}.$$

For $l > 0$ the jump of $I(\lambda)$ is related to the fact that the shape resonance due to the centrifugal barrier becomes a bound state at the threshold λ_0. In the region below λ_0 it makes a contribution to the integral $I(\lambda)$. At the threshold λ_0 the bound state contribution I_0 is separated from the scattering state contribution $I(\lambda)$ (D'yachkov 1981).

In an analogous way we can find that $\mathrm{d}I_0/\mathrm{d}\lambda$ is finite at the threshold λ_0 for all l except $l = 1$. For $l = 1$ $\mathrm{d}I_0/\mathrm{d}\lambda$ increases as $|k_0|^{-1} = (K_l^{(10)}/K_l^{(01)})^{1/2}(\lambda - \lambda_0)^{-1/2}$ when $\lambda \to \lambda_0$ $(\lambda > \lambda_0)$ (cf (17)). The following equations show the behaviour of $\mathrm{d}I_0/\mathrm{d}\lambda$ at λ_0 (the limits are the right-hand ones):

$$\lim_{\lambda \to \lambda_0} \frac{\mathrm{d}I_0}{\mathrm{d}\lambda} = \frac{4}{\pi k'} \frac{K_0^{(01)}}{(L_0^{(00)})^3} Q_{0l'}(k', \lambda_0), \qquad l = 0,$$

$$\lim_{\lambda \to \lambda_0} (\lambda - \lambda_0)^{1/2} \frac{\mathrm{d}I_0}{\mathrm{d}\lambda} = \frac{3L_1^{(01)} Q_{1l'}(k', \lambda_0)}{2\pi k' (K_1^{(10)})^{3/2} K_1^{(20)} (K_1^{(01)})^{1/2}}, \qquad l = 1,$$

$$\lim_{\lambda \to \lambda_0} \frac{\mathrm{d}I_0}{\mathrm{d}\lambda} = \frac{2}{\pi k'} (K_l^{(10)} L_l^{(00)})^{-1} \left\{ \frac{\partial Q_{ll'}}{\partial\lambda}(k', \lambda_0) - \frac{Q_{ll'}(k', \lambda_0)}{K_l^{(10)} L_l^{(00)}} \left[\frac{\partial}{\partial\lambda} \left(\frac{\partial K_l}{\partial k^2}(0, \lambda) L_l(0, \lambda) \right) \right] \bigg|_{\lambda = \lambda_0} - \frac{K_l^{(01)}}{K_l^{(10)}} \left(\frac{K_l^{(20)}}{K_l^{(10)}} + \frac{L_l^{(10)}}{L_l^{(00)}} \right) \right\}, \qquad l \geq 2,$$

where $k' = \eta(0)$.

Schematically the threshold behaviour of $I(\lambda)$ and $I_0(\lambda)$ are shown in figure 4.

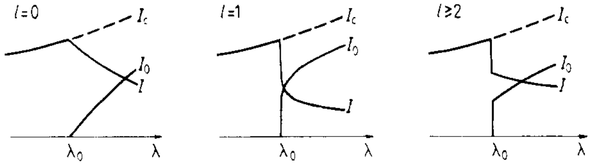

Figure 4. Behaviour of the scattering state, $I(\lambda)$, and the bound state, $I_0(\lambda)$, contributions near the appearance threshold λ_0 of a bound state of angular momentum $l = 0$, $l = 1$ or $l \geqslant 2$.

6. Conclusions

We have considered a function of the interaction parameter, $I(\lambda)$, given by the integral (3) over the continuous spectrum, and found its analyticity properties in the neighbourhood of a bound-state appearance threshold λ_0. We have shown that $I(\lambda)$ has a branch cut crossing the physical region (the real λ axis) at the threshold λ_0, and found its shape near the point λ_0. The quantity $I(\lambda)$, as a function of real λ, has a discontinuity at the threshold corresponding to a bound state of angular momentum $l > 0$. At the threshold corresponding to $l = 0$ there is only a discontinuity of the first derivative. The discontinuity is compensated for by a bound-state term. Thus, the total quantity taking into account both the bound and the scattering state contributions is a smooth function of λ. Figure 4 shows the threshold behaviour of the scattering and the bound-state contributions to the total quantity. We have shown that the total quantity is an analytic continuation of $I(\lambda)$ into the second sheet of the Riemann surface. The analyticity of the physical quantity given by the integral (sum) of type (3) over the total energy spectrum (continuous and discrete) allows the use of perturbation methods with respect to powers of the interaction parameter. In particular these methods are possible in the case when a bound state appears or disappears as a result of a perturbation in the potential.

A jump of $I(\lambda)$ at the threshold corresponding to a bound state of $l > 0$ is connected with the fact that the resonance due to the centrifugal barrier becomes a bound state and goes out of the integration region in (3). But, if a potential has a barrier, then resonance is also possible for $l = 0$. An effect of such resonance on the threshold behaviour of $I(\lambda)$ is discussed in appendix 2.

Finally we wish to make the following remark. We have assumed that $F(E)$ in (3) is an analytic function in a certain region enclosing the integration contour. However, if $F(E)$ has a singularity at the contour, for example $F(E) \sim (E - E')^{-1}$, we can divide the integration path into two parts: from nought to $\bar{E}_1$ and from $\bar{E}_1$ to $\bar{E}$, where $\bar{E}_1 < E'$ (the condition (7) is significant). Then the results of this paper are valid for the first of the integrals. Moreover, one can easily see that the results are independent of the upper integration limit.

Appendix 1

As is well known, the dipole matrix element can be written in three forms: length, velocity and acceleration. We use the last. For a potential satisfying (2) the acceleration form of the radial matrix element is expressed by the equation ($l' = l \pm 1$)

$$\int_0^\infty P_l(E,r)\frac{\mathrm{d}v}{\mathrm{d}r}P_{l'}(E',r)\,\mathrm{d}r = \int_0^\infty v(r)\left(P_l(E,r)\frac{\partial P_{l'}(E',r)}{\partial r} + \frac{\partial P_l(E,r)}{\partial r}P_{l'}(E',r)\right)\mathrm{d}r$$

which coincides with (4) if we put $A_{01} = A_{10} = v(r)$, $A_{00} = A_{20} = A_{02} = 0$, $\alpha = a$, $\beta = b$.

Let us assume that $v(r)$ behaves as $r^{-1+\varepsilon}$, where $\varepsilon > 0$, near the origin. Then the matrix element of the kinetic energy operator, $T = -\frac{1}{2}\nabla^2$, can be also expressed by (4). We have (the operator ∇ in parentheses acts only on a function in the same brackets)

$$\langle E'|T|E\rangle = \frac{\langle E'|\nabla^2 H - H\nabla^2|E\rangle}{2(E'-E)} = \frac{\langle E'|(\nabla^2 v) + 2(\nabla v)\nabla|E\rangle}{4(E'-E)}$$

where $H = -\frac{1}{2}(\nabla^2 - v(r))$. Next

$$\langle E'|(\nabla^2 v)|E\rangle = \delta_{ll'}\int_0^\infty P_l(E,r)P_l(E',r)\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{1}{r^2}\frac{\mathrm{d}v}{\mathrm{d}r}\right)\mathrm{d}r$$

$$= \delta_{ll'}\int_0^\infty \frac{\mathrm{d}v}{\mathrm{d}r}\left(\frac{2}{r}P_l(E,r)P_l(E',r) - P_l(E,r)\frac{\partial P_l(E',r)}{\partial r} - \frac{\partial P_l(E,r)}{\partial r}P_l(E',r)\right)\mathrm{d}r,$$

$$\langle E'|(\nabla v)\nabla|E\rangle = \delta_{ll'}\int_0^\infty \frac{\mathrm{d}v}{\mathrm{d}r}\left(\frac{\partial P_l(E,r)}{\partial r} - \frac{P_l(E,r)}{r}\right)P_l(E',r)\,\mathrm{d}r.$$

Consequently for $l' = l$

$$\langle E'|T|E\rangle = \frac{1}{4(E-E')}\int_0^\infty \frac{\mathrm{d}v}{\mathrm{d}r}\left(P_l(E,r)\frac{\partial P_l(E',r)}{\partial r} - \frac{\partial P_l(E,r)}{\partial r}P_l(E',r)\right)\mathrm{d}r$$

$$= \frac{1}{4(E-E')}\int_0^\infty v(r)\left(P_l(E,r)\frac{\partial^2 P_l(E',r)}{\partial r^2} - \frac{\partial^2 P_l(E,r)}{\partial r^2}P_l(E',r)\right)\mathrm{d}r.$$

Appendix 2

We now wish to discuss the effect of a potential barrier on the threshold behaviour of $I(\lambda)$. The threshold behaviour depends on the behaviour of the wavefunction at zero energy, i.e., ultimately, on the barrier penetrability at $E = 0$.

As is well known, the resonant level in a potential well surrounded by a barrier becomes a bound one as the well is deepened. If the barrier penetrability reduces to zero at $E = 0$, then the resonance becomes directly a bound state (the zeros of the Jost function corresponding to the resonance coalesce on the real k axis in the origin) (Demkov and Drukarev 1965, Newton 1966). This takes place in the case of the centrifugal barrier ($l > 0$) considered in this paper. For $l = 0$ the barrier penetrability at $E = 0$ is non-zero; this is a consequence of equation (2). Therefore there is an intermediate region of λ corresponding to virtual state (the zeros of the Jost function coalesce on the negative imaginary axis). In this case the threshold behaviour is transitional between those shown in figures 4(a) and (b). It should be, evidently, similar to that presented in figure 5.

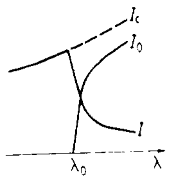

Figure 5. The threshold behaviour of $I(\lambda)$ and $I_0(\lambda)$ in the case of a potential barrier of non-zero penetrability at $E = 0$.

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