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Phase-integral formulae in the complex angular momentum (CAM) pole analysis

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Abstract. Formulae for calculating CAM pole positions and corresponding S-matrix residues are derived within the framework of the phase-integral method of Fröman and Fröman. The formulae allow for the use of higher-order approximations with rigorous error estimates. The contributions from two and three isolated turning points are considered, which allows applications in the study of rainbow and diffraction features as well as orbiting phenomena in elastic scattering processes.

1. Introduction

A Regge state for a purely elastic scattering process is an analytical continuation, in the complex angular momentum plane, of a regular solution of the radial Schrödinger equation such that at large distances only outgoing waves are present. To be more specific we write our equation as

$$\mathrm{d}^2\phi_l(r)/\mathrm{d}r^2 + Q^2(r)\phi_l(r) = 0, \tag{1.1}$$

with the function $Q^2(r)$ defined by

$$Q^2(r) \equiv k^2 - U(r) - l(l+1)/r^2. \tag{1.2}$$

Here, $k(>0)$ is the wavenumber pertaining to our particular scattering process and $U(r)$ a so far unspecified isotropic, complex local potential. For a large class of potentials a regular solution of (1.1) quite generally takes the asymptotic form

$$\phi_l(r) \underset{r\to+\infty}{\sim} N_l[\exp(-\mathrm{i}kr + \mathrm{i}\pi l/2) - S_l \exp(\mathrm{i}kr - \mathrm{i}\pi l/2)] \tag{1.3}$$

in some region of the complex l-plane containing the non-negative integers. The quantity N_l in (1.3) is a normalisation constant and S_l is the scattering matrix (or S matrix) element.

We realise that a Regge state must correspond to a pole, at $l = l_m$, say, of the S matrix, a so called Regge or CAM pole. A simple introduction to the non-relativistic theory of CAM poles is given by Thylwe (1983), and more extensive reviews are presented by Nussenzweig (1972), Nörenberg and Weidenmüller (1976) and Connor (1980).

Two quantities of particular interest appear in complex angular momentum theories: the CAM pole position l_m and the corresponding S-matrix residue r_m. In recent investigations (see e.g. Connor *et al* 1979, 1980, Sukumar *et al* 1975, Bosanac

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1978 and references given therein) great effort has been made to simplify the calculations of these quantities and to understand their main behaviour, e.g. as functions of the energy and of the parameters of the potential used. Semiclassical techniques have thereby proved successful and reliable for most applications in the field of heavy-particle elastic scattering.

The purpose of the present paper is to derive accurate formulae for calculating CAM pole positions and S-matrix residues within the framework of the phase-integral method developed by Fröman and Fröman (Fröman and Fröman 1965, 1974a, b, Fröman 1966, 1970). An obvious strength of these formulae is that they allow for a systematic use of higher-order approximations with rigorous error estimates. Furthermore, the formulae are derived to apply to a large class of complex optical model potentials which tend to zero faster than $1/r$, when r tends to infinity.

For the large class of potentials employed throughout the present analysis, there exists in many cases a great number of turning points. However, it will be assumed that not more than three turning points contribute essentially to the properties of S_l in (1.3). The main fields of application of the derived formulae are the investigations of translational rainbow and diffraction features as well as orbiting effects of heavy-particle elastic scattering.

The theoretical foundation of this paper is presented in a work by Thylwe and Fröman (1983), where also the single turning point case is studied in detail. In § 2 we quote an exact phase-integral representation of the scattering matrix, which is derived by Thylwe and Fröman (1983). From this representation one obtains, in a simple way, an exact CAM pole condition and an exact expression for the S-matrix residues. Certain quantities occurring in these expressions, the so called F-matrix elements, are difficult to calulate exactly but can be satisfactorily estimated. Thus, in § 3 we derive approximate expressions for the F-matrix elements, for cases where two or three isolated turning points contribute essentially to the final results. Approximate formulae for CAM pole positions and for the related residues are found in § 4. There we also discuss the pole trajectories, i.e. how the pole positions depend on the energy, and the pole string, i.e. the alignment of poles in the complex l-plane at a given energy. Conclusions are given in § 5.

2. Exact CAM pole condition and S-matrix residues

In a paper by Thylwe and Fröman (1983), hereafter referred to as I, two equivalent representations of the S matrix are derived in terms of the F-matrix elements introduced by Fröman and Fröman (1965). These representations are valid for complex physical potentials as well as for complex angular momenta. In the present context we shall assume the complex r-plane to be cut in such a way that formula (3.27) in I is valid, i.e.

$$S_l = -\mathrm{i}\frac{F_{22}(+0,+\infty)}{F_{21}(+0,+\infty)}\exp\left(2\mathrm{i}\lim_{r\to+\infty}[W(r)-kr+(l+\tfrac{1}{2})\pi/2]\right), \tag{2.1}$$

where $W(r)$ is defined as a contour integral

$$W(r)=\tfrac{1}{2}\int_{\Gamma(r)}\mathrm{d}r'\,q(r') \tag{2.2}$$

of the function $q(r)$ given by equations (3.7)–(3.10c) in I. We shall use the name

transition points for zeros of the first-order expression for $q^2(r)$, i.e. zeros of the function $Q^2_{\text{mod}}(r)$ defined by (3.12*a*) in I. For some of the transition points which become particularly important in the derivation of the formulae we shall use the name turning points. In (2.2) it is assumed that the contour $\Gamma(r)$ circumvents one of the relevant turning points as depicted in figure 1.

The function $q(r)$ in (2.2) is made single valued by the introduction of cuts in the complex r-plane, proceeding away from the turning points toward infinity in the first or fourth quadrant. At the same time the phase of $q(r)$ is defined according to (3.14*a*) in I.

When going from one choice of reference point, (j), (in the present paper always a turning point) to another, (j'), $W(r)$ changes its value from $W_j(r)$ to $W_{j'}(r)$ related by the equation

$$W_{j'}(r) = W_j(r) + \gamma_{j'j}. \tag{2.3}$$

$\gamma_{j'j}$ is in the first-order phase-integral approximation the phase integral from turning point (j') to (j). In higher-order approximations the integration must proceed along a closed contour $\Gamma_{j'j}$ circumventing both turning points as shown in figure 2, and its value must be halved, i.e.

$$\gamma_{j'j} = \tfrac{1}{2}\int_{\Gamma_{j'j}} \mathrm{d}r\, q(r). \tag{2.4}$$

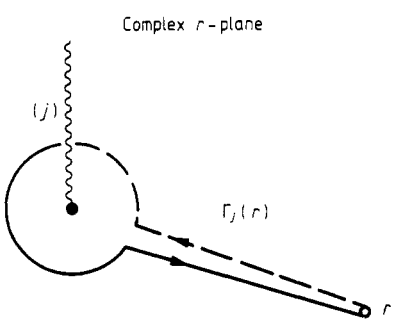

Figure 1. Schematic drawing of the contour $\Gamma_j(r)$ pertaining to a particular choice of reference point (here a turning point (j)) to define the phase integral $W_j(r)$ in (2.2). The contour starts at the point r on the second Riemann sheet, circumvents the turning point (j) and the region where the associated zeros of q, which are present when higher-order approximations are used, are located and ends at the point r on the first Riemann sheet. The cut in the complex r-plane is indicated by the wavy line.

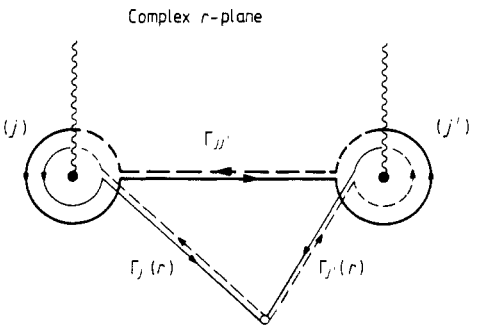

Figure 2. Schematic illustration of the closed contour $\Gamma_{jj'}$ appearing in the definition (2.4) of $\gamma_{jj'}$, and its relation to $\Gamma_j(r)$ and $\Gamma_{j'}(r)$.

From (2.3) one easily notices the relations

$$\gamma_{jj} = 0, \qquad \gamma_{j'j} = -\gamma_{jj'}, \qquad \gamma_{jj''} = \gamma_{jj'} + \gamma_{j'j''}. \tag{2.5a, b, c}$$

The F matrix connecting two arbitrary points r_1 and r_2 changes its value according to the formula

$$\boldsymbol{F}^{(j')}(r_1, r_2) = \boldsymbol{E}^{-1}_{j'j}\boldsymbol{F}^{(j)}(r_1, r_2)\boldsymbol{E}_{j'j} \tag{2.6}$$

where the transformation matrix is given by

$$\boldsymbol{E}_{j'j} \equiv \begin{pmatrix} \exp(\mathrm{i}\gamma_{j'j}) & 0 \\ 0 & \exp(-\mathrm{i}\gamma_{j'j}) \end{pmatrix}. \tag{2.7}$$

The relations (2.5*a–c*) imply the following transformation matrix rules

$$\boldsymbol{E}_{jj} = \mathbf{1}, \qquad \boldsymbol{E}_{jj'}^{-1} = \boldsymbol{E}_{j'j}, \qquad \boldsymbol{E}_{jj''} = \boldsymbol{E}_{jj'}\boldsymbol{E}_{j'j''} = \boldsymbol{E}_{j'j''}\boldsymbol{E}_{jj'}. \tag{2.8a, b, c}$$

As pointed out on p 21 of Fröman and Fröman (1965) only the non-diagonal F-matrix elements alter their values by such a transformation (2.6). In particular we have

$$F_{21}^{(j')}(r_1, r_2) = F_{21}^{(j)}(r_1, r_2)\exp(-2\mathrm{i}\gamma_{jj'}). \tag{2.9}$$

With the aid of (2.3) and (2.9) we observe that the complete S-matrix element in (2.1) is unaffected by a change of reference point, as expected.

If all the phase-integral quantities appearing in (2.1) are finite, it follows that a necessary condition for the S matrix to have a pole is given by

$$F_{21}(+0, +\infty) = 0. \tag{2.10}$$

To be sure that a solution of (2.10) is a pole of the S matrix one must also check that $F_{22}(+0, +\infty)$ does not vanish simultaneously.

If (2.10) defines a simple pole of the S matrix at $l = l_m$, say, then the corresponding residue r_m of S_l is obtained from

$$r_m = \lim_{l \to l_m}\left[-(l - l_m)\mathrm{i}\frac{F_{22}(+0, +\infty)}{F_{21}(+0, +\infty)}\exp\left(2\mathrm{i}\lim_{r\to\infty}[W(r) - kr + (l + \tfrac{1}{2})\pi/2]\right)\right]. \tag{2.11}$$

The generalisation of (2.11) to poles of higher multiplicity is straightforward.

The purpose of the following section is to find approximate analytical expressions for the F-matrix elements occurring in (2.10) and (2.11) for the cases of two and three contributing, isolated turning points. In fact, at least two turning points are required to produce a pole of the S matrix.

3. *F*-matrix elements

In the present section we shall proceed essentially in the same way as in § 4 of I, but we shall extend the treatment to those cases where there are two or even three zeros of $Q^2_{\mathrm{mod}}(r)$ which must be taken into account. Usually the two-turning-point (2T) problem is associated with bound states in a single potential well or, less frequently, penetration through a single barrier, but we shall see that such a configuration is also responsible for CAM poles (or zeros) of the S matrix, even for monotonically repulsive potentials (see Dombey and Jones 1968 and Connor 1980). The three-turning-point (3T) configuration is frequently encountered in the theory of shape resonances from the radial Schrödinger equation.

The single-turning-point (1T) situation illustrated in figure 3 is characterised in detail in I. When there is more than one turning point influencing essentially the behaviour of the S matrix, we expect at least one of the conditions in § 4 of I,

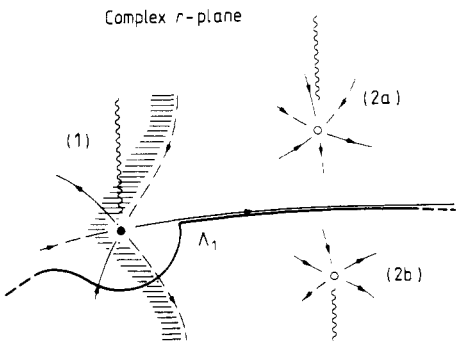

Figure 3. Schematic drawing of the path Λ which is used for approximating the F-matrix elements when only a single complex turning point has to be taken into account. The remote part of the path Λ_1 is not explicitly shown, since the treatment in that region is the same for all cases considered and given previously in I. Relevant Stokes' lines (broken) and anti-Stokes' lines (full) are indicated, with arrows pointing in the direction for which $\mathrm{id}w>0$ and $\mathrm{d}w>0$, respectively. The single-turning-point situation can be disturbed by an approach of a second turning point in two topologically different ways. These are also shown in the figure.

characterising a 1T problem, to be violated. It is reasonable to expect that the very first assumption that loses its justification is the one concerning the smallness of the μ integral along the path Λ_1, depicted in figure 3, while at the same time nothing else is drastically changed. For example, the turning point (1) still has the status of being the innermost one with respect to the origin. It means that the μ integral starts to get large only on the part of Λ_1 which coincides with the 'free' anti-Stokes line of (1), due to the presence of the second turning point.

In figure 3 the two possible topologies are shown which can arise when a 1T configuration is essentially perturbed by a well separated turning point (2). The situation where (2) approaches the 'free' anti-Stokes line from below is met in the study of zeros of S_l in the complex l-plane and will not be analysed in detail here. Figure 4 shows schematically a sequence of configurations which are topologically equivalent with figures 4(a) and 4(e), indicating the breaking down limits of the topology. The understanding of the configurations in figure 4 is an important part in our study before we add the complications of a third turning point.

When a well isolated turning point is situated in the shaded area in figure 3 and no other turning points are present, then the F matrix can be estimated in exactly the same way as in the 1T case. We notice that it is merely the existence of a 1T path Λ_1, along which the μ integral is much smaller than unity, which characterises this case, not the presence alone of other turning points.

Let us now turn to the configuration in figure 4(a) which illustrates the limiting case where 1T and 2T treatments meet. In the present analysis where only well separated transition points are considered there must not be any significant difference between a 1T and a 2T treatment of figure 4(a). In other words, the contribution from (2) must be exponentially small compared with that from (1).

In figure 4(b) we observe that the anti-Stokes line emerging from (1) and extending to the right towards infinity comes closer to the second turning point. For this situation the μ integral along the 1T path Λ_1 is no longer a small quantity compared with unity. Clearly both zeros of $Q^2_{\mathrm{mod}}(r)$ must then be taken into account, and a new path Λ_2

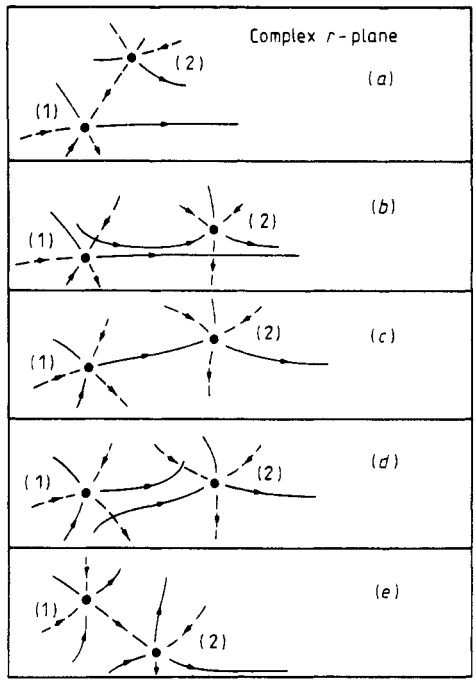

Figure 4. Schematic illustrations of topologically equivalent configurations (a)–(e) of two well separated turning points. The importance of turning point (2) increases from being insignificant in (a) to become entirely dominant in configuration (e).

must be constructed which circumvents each zero, crossing the emerging anti-Stokes lines at sufficiently large distance from the corresponding turning points (see below).

Analogous arguments apply also to the situations illustrated in figures 4(c), (d). Furthermore, we can see in figure 4(d) that the right-hand turning point tends to be the dominating one, and that (1) no longer has a 'free' anti-Stokes line. Finally the role of (1) has become insignificant in the limiting case shown in figure 4(e).

In § 3.1 we investigate in more detail the 2T problem, as it is relevant for the CAM poles of the S matrix. With our introductory considerations in mind we can concentrate our study on the situations shown in figures 4(b)–(d). The other configurations can be handled by 1T estimates of the F matrix. It turns out that figure 4(c) represents the relevant 2T configuration which can produce CAM poles in the S matrix. In § 3.2 a third turning point is introduced so as to 'perturb' the 2T configuration and the important approximative matrix elements $F_{21}(+0, +\infty)$ and $F_{22}(+0, +\infty)$ in (2.1) are derived.

3.1. Two well separated turning points

The purpose of this subsection is to obtain the approximate matrix $\boldsymbol{F}(+0, +\infty)$ for the situations in figures 4(b)–(d). We start with the situation in figure 4(b) which is specified by the condition $|\exp(i\gamma_{12})| \leqslant 1$. To obtain approximate expressions for the F-matrix elements we can either use a 1T estimate, corresponding to the path Λ_1, or a 2T estimate, corresponding to the path Λ_2, both paths being drawn schematically in figure 5.

The 1T estimate (cf equations (4.14*a*, *b*) in I) yields the result

$$\boldsymbol{F}^{(1)}(+0, +\infty) = \begin{pmatrix} \overline{} & \overline{} \\ -\mathrm{i}+\mathrm{O}(\mu_1) & 1+\mathrm{O}(\mu_1) \end{pmatrix}, \tag{3.1}$$

or, with the aid of (2.6),

$$\boldsymbol{F}^{(2)}(+0, +\infty) = \begin{pmatrix} \overline{} & \overline{} \\ (-\mathrm{i}+\mathrm{O}(\mu_1))\exp(-2\mathrm{i}\gamma_{12}) & 1+\mathrm{O}(\mu_1) \end{pmatrix}, \tag{3.8}$$

depending on the choice of reference point for the phase integrals. Note that the relevant (single) turning point in the estimates (3.1) and (3.2) is (1), while 2 does not satisfy condition (iii) in I required for a single turning point. The μ-integral μ_1 in (3.1)–(3.2) is calculated along the entire path Λ_1. We observe that two F-matrix elements are unknown according to these estimates. However, for our purposes only the 21- and 22-elements are of interest.

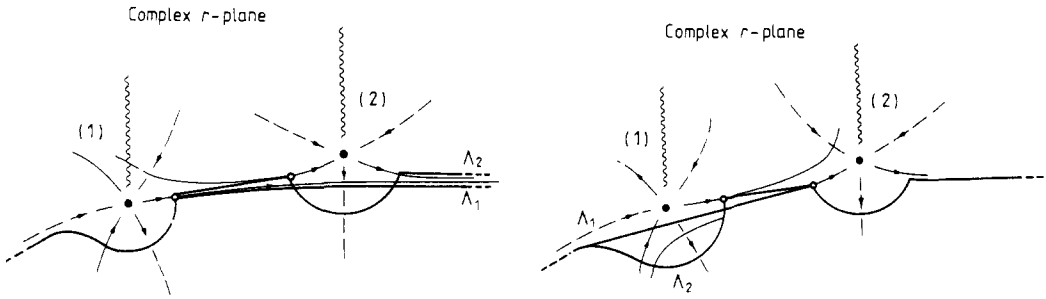

Figure 5 and **figure 6.** The figures show, for the situations depicted in figure 4(*b*) and (*d*) respectively, the paths Λ_1 and Λ_2, along which the F-matrix elements are approximated. The small circles indicate the positions a (leftmost) and b (rightmost) in (3.3).

To obtain the 2T approximation we make use of the multiplication rule for the F matrices and write

$$\boldsymbol{F}(+0, +\infty) = \boldsymbol{F}(+0, a)\boldsymbol{F}(a, b)\boldsymbol{F}(b, +\infty). \tag{3.3}$$

The intermediate points a and b are indicated in figure 5. Following the treatment in I, we estimate each matrix in (3.3). We thereby use results given in the work by Fröman and Fröman (1965), namely the basic estimates (4.3*a*)–(4.3*d*) and the inverse of the matrix in (7.5*b*). The latter shows the effect of circumventing a zero in the complex r plane via two neighbouring anti-Stokes lines of the type used in figure 5. It should be emphasised that the formula (7.5*b*) just mentioned is valid only if $W(r)$ is defined by the contour of integration pertinent to the turning point of interest.

The first matrix to the right of (3.3) is found to be of the same form as the 1T estimates in (3.1)–(3.2), i.e. with the reference point at (2),

$$\boldsymbol{F}^{(2)}(+0, a) = \begin{pmatrix} \overline{} & \overline{} \\ (-\mathrm{i}+\mathrm{O}(\mu_2'))\exp(-2\mathrm{i}\gamma_{12}) & 1+\mathrm{O}(\mu_2') \end{pmatrix}, \tag{3.4}$$

μ_2' being the μ integral calculated along the part of Λ_2 connecting $+0$ and a. Again we notice that two matrix elements are unknown.

The second matrix $\boldsymbol{F}(a, b)$ can be studied with the aid of the basic estimates. Recalling the fact that $|\exp(\mathrm{i}\gamma_{12})| \leqslant 1$, we obtain the result ($a$ and b are lying on

anti-Stokes lines emerging from (1) and (2), respectively)

$$\boldsymbol{F}^{(2)}(a, b) = \begin{pmatrix} 1+O(\mu_2'') & O(\mu_2'') \\ O(\mu_2'')\,e^{-2i\gamma_{12}} & 1+O(\mu_2'')(1+O(\mu_2'')\,e^{-2i\gamma_{12}}) \end{pmatrix}, \tag{3.5}$$

where μ_2'' is to be calculated along the part of Λ_2 connecting a and b.

Taking the inverse of the matrix (7.5b) in the work by Fröman and Fröman (1965) and using properties of the F matrix analogous to those displayed in equations (4.4)–(4.9) in I, we easily obtain the estimate of $\boldsymbol{F}(b, +\infty)$. Hence, we find

$$\boldsymbol{F}^{(2)}(b, +\infty) = \begin{pmatrix} 1+O(\mu_2''') & O(\mu_2''') \\ -i+O(\mu_2''') & 1+O(\mu_2''') \end{pmatrix}, \tag{3.6}$$

with the appropriate μ-integral estimate of the correction terms.

Inserting (3.4)–(3.6) into (3.3) we arrive at the final 2T expression

$$\boldsymbol{F}^{(2)}(+0, +\infty) = \begin{pmatrix} - & - \\ -i(1+e^{-2i\gamma_{12}})+O(\mu_2)\,e^{-2i\gamma_{12}} & 1+O(\mu_2)\,e^{-2i\gamma_{12}} \end{pmatrix}, \tag{3.7}$$

where the μ integral is to be calculated along the entire path Λ_2. We observe that the error term $O(\mu_2)\exp(-2i\gamma_{12})$ in (3.7) may become large when $|\exp(i\gamma_{12})|$ decreases so that apparently no reliable result can be obtained for the 22-element from (3.7). However, when $|\exp(i\gamma_{12})|$ is sufficiently small the 1T estimate (3.2) is adequate and we see that the 22-element is approximately unity also in this case. The 21-element in (3.7) reduces smoothly to the 1T result in (3.2) as $|\exp(i\gamma_{12})|$ tends to zero.

For the situation defined in figure 4(d) we have that $|\exp(i\gamma_{12})| \geqslant 1$. Again we have the possibility to perform a 1T estimate and a 2T estimate, where the alternative paths Λ_1 and Λ_2, respectively, to be used are depicted in figure 6. The 1T estimate (along Λ_1) yields

$$\boldsymbol{F}^{(2)}(+0, +\infty) = \begin{pmatrix} - & - \\ -i+O(\mu_1) & 1+O(\mu_1) \end{pmatrix}, \tag{3.8}$$

where the μ integral is calculated along the entire path Λ_1. We expect μ_1 to become large when the quantity $|\exp(i\gamma_{12})|$ tends to unity, and in that situation we must take into account also the turning point (1).

The 2T estimate is obtained by the use of the matrix product in (3.3). The first and third matrices on the right-hand side of (3.3) are estimated in precisely the same way as before, yielding the results (3.4) and (3.6), respectively.

To obtain the estimate of the second matrix on the right-hand side of (3.3) we apply the basic estimates to the matrix $\boldsymbol{F}(b, a)$ and then we use the inversion formula (equation (3.20) in Fröman and Fröman 1965) to achieve the desired result. We get

$$\boldsymbol{F}^{(2)}(a, b) = \begin{pmatrix} 1+O(\mu_2'')(1+O(\mu_2))\,e^{2i\gamma_{12}} & O(\mu_2'')\,e^{2i\gamma_{12}} \\ O(\mu_2'') & 1+O(\mu_2'') \end{pmatrix}. \tag{3.9}$$

Inserting (3.4), (3.6) and (3.9) into (3.3) we obtain

$$\boldsymbol{F}^{(2)}(+0, +\infty) = \begin{pmatrix} - & - \\ -i[1+\exp(-2i\gamma_{12})]+O(\mu_2) & 1+O(\mu_2) \end{pmatrix}, \tag{3.10}$$

which is valid provided $|\exp(i\gamma_{12})| \geqslant 1$.

Equation (3.10) reduces to the 1T result (3.8) in the limit $|\exp(i\gamma_{12})| \to \infty$, but now the adequate turning point is (2).

If the μ integral is sufficiently small we can use the same approximate expression for the F matrix, obtained by neglecting terms proportional to μ_2 in (3.7) and (3.10),

$$\boldsymbol{F}^{(2)}(+0, +\infty) \simeq \begin{pmatrix} \overline{} & \overline{} \\ -i[1+\exp(-2i\gamma_{12})] & 1 \end{pmatrix}. \tag{3.11}$$

This formula can be used as long as the topology of the Stokes and anti-Stokes lines required for its derivation is unaffected. This means (cf figures 4, 5 and 6) that one has to check the phase integral γ_{12} so that $\mathrm{Re}(\gamma_{12})$ never becomes negative. At the boundary $\mathrm{Re}(\gamma_{12}) = 0$ (see figures 4(*a*), (*e*)), which defines the Stokes set, the two turning points lie on the same Stokes line and one should use the 1T formulae (3.1) or (3.2).

3.2. Three well separated turning points

Let us now assume that the influence from a third turning point (3) becomes significant and that the 2T configuration is only slightly disturbed (see figure 7). Of course, one could imagine the third turning point to be situated in many different ways, relative to the other two turning points. However, by reasons of symmetry, we may still assume, without loss of generality, that (1) possesses the status of the innermost turning point.

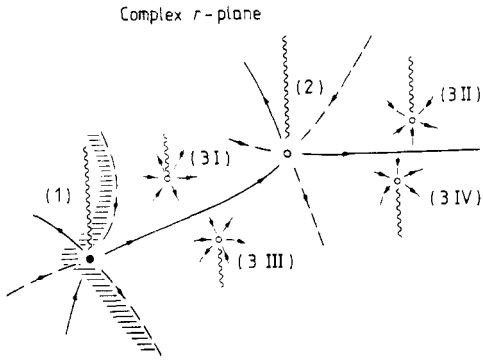

Figure 7. The figure shows the four possible ways, (I)–(IV), a well isolated third turning point (3) disturbs a two-turning-point configuration of (1) and (2), typical for a Regge state. The status of (1) as being the innermost turning point is assumed not to be affected by the introduction of (3).

What happens when the 2T treatment breaks down is that the μ integral calculated along the path Λ_2 becomes comparable to unity or larger. This fact means, within the semiclassical frame of validity, that a third turning point comes close to the part of Λ_2 lying between (1) and (2) or the one extending towards infinity. In figure 7 we have indicated the four possible ways in which the 2T configuration can be perturbed by a well isolated third turning point (3).

Two of the four 3T configurations thus created, namely (I) and (II), have the same topology and lead to identical results. Hence, we concentrate on (I), (III) and (IV) below. The configuration (III) is often encountered in CAM analysis of radial scattering problems where a single centrifugal barrier can be formed in the real effective potential.

However, (I) and (IV) correspond to more complicated situations where the physical potential may be complex or possess several barriers.

For clarity we shall in the following omit correction terms proportional to the pertinent μ-integrals. In the situation (I) we define a path Λ_3 which circumvents the three turning points as in figure 8(I) and which will be used to derive the relevant F-matrix elements.

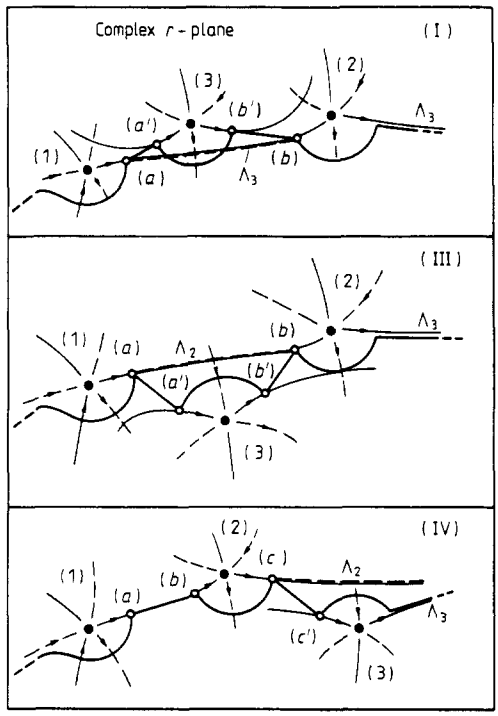

Figure 8. Schematic drawing of how the paths Λ_2 and Λ_3 are to be constructed for the situations (I), (III) and (IV) in figure 7.

The F matrix is conveniently factorised in the following way

$$\boldsymbol{F}(+0, +\infty) = \boldsymbol{F}(+0, a)\boldsymbol{F}(a, a')\boldsymbol{F}(a', b')\boldsymbol{F}(b', b)\boldsymbol{F}(b, +\infty). \tag{3.12}$$

Here $\boldsymbol{F}(+0, a)$ and $\boldsymbol{F}(b, +\infty)$ are given, again, by (3.4) and (3.6), respectively. Because of the third turning point, $\boldsymbol{F}(a, b)$ in (3.3) is no longer approximately a unit matrix. Recalling that $\boldsymbol{F}(a, a')$ and $\boldsymbol{F}(b', b)$ in (3.12) are approximately unit matrices (from the basic estimates of Fröman and Fröman (1965) and the discussion following (3.7) above), we now find that $\boldsymbol{F}(a, b)$ is replaced essentially by the matrix $\boldsymbol{F}(a', b')$. On taking the inverse of the matrix given by equation (7.5b) in Fröman and Fröman (1965) and transforming the phase reference point to (2), we get

$$\boldsymbol{F}^{(2)}(a, b) \simeq \begin{pmatrix} 1 & 0 \\ -\mathrm{i}\exp(-2\mathrm{i}\gamma_{32}) & 1 \end{pmatrix} \qquad \text{(I)}. \tag{3.13}$$

We see that (3.19) reduces to a unit matrix if $|\exp(-2\mathrm{i}\gamma_{32})|$ vanishes, i.e. if the third turning point is pushed away, far up in the complex r-plane, and thus giving us back

the 2T approximation. Combining (3.4), (3.6) and (34.13), we finally find

$$\boldsymbol{F}^{(2)}(+0, +\infty) \simeq \begin{pmatrix} \overline{} & \overline{} \\ -\mathrm{i}(1+\mathrm{e}^{-2\mathrm{i}\gamma_{12}}+\mathrm{e}^{-2\mathrm{i}\gamma_{32}}) & 1 \end{pmatrix} \qquad \text{(I)}, \tag{3.14}$$

where irrelevant correction terms proportional to the μ integral, calculated along Λ_3, are neglected. This result is also obtained for the situation (II) mentioned above, if the turning points are properly relabelled.

The analysis of the situation (III) in figure 7 is analogous to (I) and we can use the same factorisation (3.18). Because of the different orientation of Stokes and anti-Stokes lines of the third turning point (see figure 8(III)) we use here formula (7.5*a*) in Fröman and Fröman (1965) for the matrix $\boldsymbol{F}(a', b')$, leading to

$$\boldsymbol{F}^{(2)}(a, b) \simeq \begin{pmatrix} 1 & \mathrm{i}\exp(2\mathrm{i}\gamma_{32}) \\ 0 & 1 \end{pmatrix} \qquad \text{(III)}. \tag{3.15}$$

The matrix (3.15) reduces to unity if $|\exp(\mathrm{i}\gamma_{32})|$ vanishes, which is the case when (3) is pushed away downwards in the complex r-plane. The complete F matrix becomes

$$\boldsymbol{F}^{(2)}(+0, +\infty) \simeq \begin{pmatrix} \overline{} & \overline{} \\ -\mathrm{i}(1+\mathrm{e}^{-2\mathrm{i}\gamma_{12}}+\mathrm{e}^{-2\mathrm{i}\gamma_{13}}) & 1+\mathrm{e}^{-2\mathrm{i}\gamma_{13}} \end{pmatrix} \qquad \text{(III)}. \tag{3.16}$$

Configuration (III) is frequently met in CAM analysis of scattering systems described by a single-well radial potential where (2) and (3) correspond to the turning points at the complex centrifugal barrier. In § 4 we shall discuss this case further and derive useful formulae for calculating the properties of the CAM poles.

In figure 8(IV) we have constructed Λ_3 for the final case (IV). The factorisation now reads

$$\boldsymbol{F}(+0, +\infty) = \boldsymbol{F}(+0, a)\boldsymbol{F}(a, b)\boldsymbol{F}(b, c)\boldsymbol{F}(c, c')\boldsymbol{F}(c', +\infty). \tag{3.17}$$

For the product of the three first matrices to the right of equation (3.17) we have essentially the 2T formula

$$\boldsymbol{F}^{(2)}(+0, c) \simeq \begin{pmatrix} \overline{} & \overline{} \\ -\mathrm{i}(1+\exp(-2\mathrm{i}\gamma_{12})) & 1 \end{pmatrix} \qquad \text{(IV)}. \tag{3.18}$$

Furthermore, $\boldsymbol{F}(c, c')$ is again approximately the unit matrix and $\boldsymbol{F}(c', +\infty)$ is obtained from (7.5*a*) in Fröman and Fröman (1965) together with (2.6) (cf equation (3.15)). Thus

$$\boldsymbol{F}^{(2)}(c, +\infty) \simeq \begin{pmatrix} 1 & \mathrm{i}\exp(2\mathrm{i}\gamma_{32}) \\ 0 & 1 \end{pmatrix} \qquad \text{(IV)}, \tag{3.19}$$

and by combining (3.18) and (3.19) we find

$$\boldsymbol{F}^{(2)}(+0, +\infty) \simeq \begin{pmatrix} \overline{} & \overline{} \\ -\mathrm{i}(1+\mathrm{e}^{-2\mathrm{i}\gamma_{12}}) & 1+\mathrm{e}^{2\mathrm{i}\gamma_{32}}(1+\mathrm{e}^{-2\mathrm{i}\gamma_{12}}) \end{pmatrix} \qquad \text{(IV)}. \tag{3.20}$$

If we compare (3.20) with the 2T result (3.11) we notice a change due to the third turning point only in the 22-element. This was not the case in the situation (III) above for which (3.16) shows a change in both the 21- and 22-elements. One might ask oneself if this difference between (3.16) and (3.20) results in an inconsistency at the common limiting configuration of validity where $\mathrm{i}\gamma_{23} = \mathrm{Re}(\mathrm{i}\gamma_{23}) > 0$.

Again the explanation must be that, for well separated turning points, the difference between two distinct topologies is numerically insignificant there. If a situation is encountered where significant discontinuities occur at the Stokes set, i.e. those complex values of l which produce limiting configurations, then the turning points can no longer be considered as well separated.

Instead, to resolve the problem one has to invoke some uniformisation procedure (see e.g. Bárány and Crothers 1983 and Connor 1968) for the particular critical subsystem of turning points.

4. Approximate CAM pole condition and S-matrix residues

Throughout this section we shall assume that l belongs to a certain region of the complex angular momentum plane which corresponds to the topology of turning points shown in figure 8(III). The relevant F-matrix elements are then given in equation (3.16). Inserting (3.16) into (2.1) we find the approximate phase-integral expression for the S matrix

$$S_l = \frac{1+\exp(-2i\gamma_{13})}{1+\exp(-2i\gamma_{12})+\exp(-2i\gamma_{13})}\exp(2i\eta_l), \tag{4.1}$$

with the phase shift η_l calculated from the turning point (2) according to the formula

$$\eta_l = \lim_{r\to+\infty}(W_2(r)-kr)+(l+\tfrac{1}{2})\pi/2. \tag{4.2}$$

Equation (4.1) (or, equivalently, (2.10) together with (3.16)) immediately yields an approximate condition for obtaining the positions of the CAM poles of the S matrix. The condition reads

$$D(l, m, E) = 0, \tag{4.3}$$

where in (4.3) D is the denominator of (4.1) written in the form

$$D(l, m, E) \equiv \exp(-2i\gamma_{12})+\exp(-2i\gamma_{13})-\exp(-2i\pi(m+\tfrac{1}{2})), \tag{4.4}$$

with $m = 0, 1, \ldots$. Negative integers m in (4.4) are excluded because (4.3) would then require at least one of the phase integrals to have a negative real part, which is inconsistent with the topology in figure 8(III).

Condition (4.3) is to be solved with respect to l holding the energy and the integer m at fixed values. There are expected to be many, and even an infinite number of solutions $l_m(E)$ to (4.3) for most collisional systems of heavy particles (Connor 1980).

In some neighbourhood of a CAM pole $l = l_m$, which we assume to be simple, the S matrix takes the form

$$S_l \underset{l\to l_m}{\sim} \frac{r_m(E)}{l-l_m(E)}, \tag{4.5}$$

where $r_m(E)$ is the residue corresponding to the pole at $l = l_m(E)$. An approximate expression for r_m is found directly from (4.1) by expanding the denominator D around the pole position. We have

$$r_m(E) = -\frac{\exp[-2i\gamma_{12}(l_m(E))]}{(\partial D/\partial l)_{l=l_m(E)}}\exp(2i\eta_{l_m(E)}), \tag{4.6}$$

where from (4.4)

$$\left(\frac{\partial}{\partial l}D\right)_{l=l_m(E)} = -2i\left[\exp[-2i\gamma_{12}(l_m(E))]\left(\frac{\partial}{\partial l}\gamma_{12}\right)_{l=l_m(E)}\right.$$
$$\left.+\exp[-2i\gamma_{13}(l_m(E))]\left(\frac{\partial}{\partial l}\gamma_{13}\right)_{l=l_m(E)}\right]. \tag{4.7}$$

The calculation in (4.7) of the partial derivative of the closed loop integrals defining the γ's may seem to be very tedious when higher-order phase integral approximations are used. However, we can apply the general formula, for the derivative of $q(r)$ with respect to a parameter, derived by Fröman (1974), i.e.

$$\frac{\partial}{\partial\kappa}\gamma \simeq \tfrac{1}{4}\oint_\Gamma \mathrm{d}r\, q^{-1}(\kappa; r)(\partial/\partial\kappa)Q^2(\kappa; r), \tag{4.8}$$

where in our case only $\kappa \equiv l, E$ are relevant. The function Q^2 appears in the radial Schrödinger equation and is given by (1.2). It is required that the closed path Γ in (4.8) stays outside the regions around each turning point where zeros of q are situated (see a discussion in § 3 in I).

As is obvious from (4.3), the CAM pole positions can be considered as function of both the pole number m and the energy E. Thus, at a given energy, the poles are situated on a so called pole string, defined semiclassically by the continuous parameter m in (4.3). Alternatively, given an integer m to specify a particular pole, $l_m(E)$ describes a certain path (pole trajectory) in the complex l-plane, as the energy is varied (see figure 9).

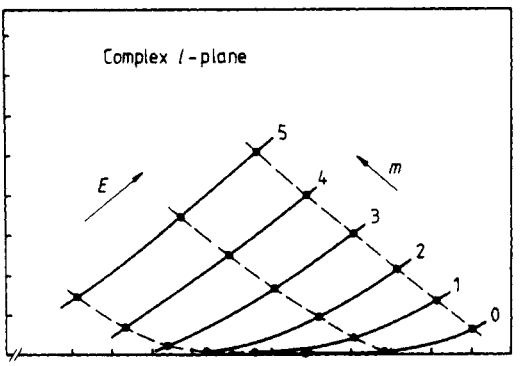

Figure 9. The figure shows typical locations of CAM poles at different energies. The pole strings (broken curves) and pole trajectories (full curves) are indicated.

Approximate expressions for the pole strings and pole trajectories can provide accurate inputs in the numerical root searching procedure which solves (4.3) for some new values of m and/or E. On a local scale one can use a linear approximation. Let us, for example, assume that a CAM pole has been found at $l = l_m(E)$, say. The pole $l_{m'}(E')$ is then by a linear approximation given as

$$l_{m'}(E') \simeq l_m(E) + s_m(E)(m'-m) + t_m(E)(E'-E), \tag{4.9}$$

with

$$s_m(E) \equiv \mathrm{d}l_m(E)/\mathrm{d}m, \tag{4.10}$$

$$t_m(E) \equiv \mathrm{d}l_m(E)/\mathrm{d}E. \tag{4.11}$$

Phase-integral formulae can be obtained for the local linear coefficients $s_m(E)$ and $t_m(E)$ of the string and trajectory, respectively, starting from the implicit relation (4.3), i.e. in our case:

$$D(l_m(E), m, E) = 0. \tag{4.12}$$

Firstly, (4.12) holds identically along the string, so that

$$\frac{\mathrm{d}}{\mathrm{d}m} D \equiv \frac{\partial}{\partial m} D + \left(\frac{\partial}{\partial l} D\right)_{l=l_m(E)} s_m(E) = 0. \tag{4.13}$$

With the aid of (4.4), (4.13) reduces to

$$s_m(E) = -\frac{2\pi \mathrm{i}}{(\partial D/\partial l)_{l=l_m(E)}} \exp[-2\mathrm{i}\pi(m+\tfrac{1}{2})], \tag{4.14}$$

where, of course, m must be a non-negative integer for $l_m(E)$ to represent a true pole position. Again the denominator in (4.14) is given by (4.7) and (4.8).

Similarly, we can differentiate (4.12) with respect to the energy E, keeping m constant, with the result

$$t_m(E) = -(\partial D/\partial E)_{l=l_m(E)}/(\partial D/\partial l)_{l=l_m(E)}. \tag{4.15}$$

Here the numerator takes the explicit form

$$\left(\frac{\partial}{\partial E} D\right)_{l=l_m(E)} = -2\mathrm{i}\Big[\exp[-2\mathrm{i}\gamma_{12}(l_m(E))]\left(\frac{\partial}{\partial E}\gamma_{12}\right)_{l=l_m(E)} + \exp[-2\mathrm{i}\gamma_{13}(l_m(E))]\left(\frac{\partial}{\partial E}\gamma_{13}\right)_{l=l_m(E)}\Big], \tag{4.16}$$

which together with (4.7) and (4.8) specifies the phase-integral expression for $t_m(E)$.

The formulae derived in this section can be considerably simplified if the contribution from the third turning point has become insignificant. The procedure is quite straightforward and amounts to the neglect of (putting to zero) the exponential $\exp(-2\mathrm{i}\gamma_{13})$ where it appears in equations (4.1), (4.4), (4.7) and (4.16). Thus the CAM pole condition (4.3) reduces to the Bohr–Sommerfeld form

$$\gamma_{12} = (m+\tfrac{1}{2})\pi, \qquad m = 0, 1, \ldots. \tag{4.17}$$

Furthermore, the formulae for calculating $r_m(E)$, $s_m(E)$ and $t_m(E)$ in the 2T limit are given by

$$r_m(E) = (1/2\mathrm{i})[\exp(2\mathrm{i}\eta_{l_m(E)})]/(\partial\,\gamma_{12}/\partial l)_{l=l_m(E)}, \tag{4.18}$$

$$s_m(E) = \pi/(\partial\gamma_{12}/\partial l)_{l=l_m(E)}, \tag{4.19}$$

$$t_m(E) = -(\partial\gamma_{12}/\partial E)_{l=l_m(E)}/(\partial\gamma_{12}/\partial l)_{l=l_m(E)}, \tag{4.20}$$

respectively.

We finally point out that our formulae, in the first-order phase-integral approximation, for the CAM pole condition and the residues agree in the 2T limit with those of Connor (1980), Dombey and Jones (1968) and Brander (1966), and that they generally seem to be equivalent to the complex trajectory results of Knoll and Schaeffer (1976).

5. Conclusions

In the present paper we have derived a 3T phase-integral expression for the S matrix, valid in regions of the complex l-plane where S has poles, whose derivation required essentially:

(i) the turning points (1), (2) and (3) must be sufficiently isolated, i.e. $|\gamma_{12}|$, $|\gamma_{13}|$ and $|\gamma_{32}|$ large enough;

(ii) the mutual orientation of turning points must be topologically equivalent to figure 8(III), i.e. $\mathrm{Re}(\gamma_{12})$, $\mathrm{Re}(\gamma_{13})$ and $\mathrm{Re}(\gamma_{32}) > 0$.

It is not very difficult to check that the use of the S-matrix expression obtained is consistent with the conditions (i) and (ii) above. If (i) and (ii) are not satisfied, one should be careful. For example, when a particular l-value is very close to a Stokes set (usually a line) in the complex l-plane, where a phase integral becomes purely imaginary, one has to make sure that the discontinuity across the Stokes set, introduced by the switching to the relevant formula on the other side, is insignificantly small. If this is not the case a uniform treatment must be employed.

From our S-matrix formula we derived a complex angular momentum pole condition and expressions for the pole residues. We discussed further the local behaviour of pole strings and pole trajectories.

Our main results generalise those of Knoll and Schaeffer (1976) in that higher-order quantum corrections are systematically included in the formalism. In the 2T limit our formulae agree also with results of a partly uniform treatment of Connor (1980) and an asymptotic analysis of Brander (1966).

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