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On the complex angular momentum theory of scattering

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Abstract. A contribution to the theory of complex angular momentum techniques in the field of atomic and molecular collisions is given. We derive a new, flexible representation of the scattering amplitude on the basis of realistic assumptions for the behaviour of the S matrix in the complex angular momentum plane. The representation has the form of a sum of steepest-descent integrals, S-matrix residue terms and a symmetry-type background integral. The flexibility is due to the presence of two integer parameters which may be chosen conveniently so as to make the residue sums sufficiently convergent and to minimise the total number of important terms.

1. Introduction

The scattering amplitude $f(\theta)$ is a quantity of basic importance in the theory of elastic collisions between particles with an isotropic interaction. Several analytical methods for its computation are developed in standard texts on the subject. In the present paper we discuss some fundamentals of frequently employed real and complex angular momentum descriptions of atomic and molecular collisions. Our results are particularly closely related to three exact representations of the scattering amplitude: the partial-wave representation, the Poisson and Regge representations.

Let us first consider the quantum-mechanical partial-wave representation given by

$$f(\theta)=\frac{\mathrm{i}}{k}\sum_{l=0}^{\infty}(l+\tfrac{1}{2})(1-S_l)P_l(\cos\theta) \tag{1.1}$$

where k is the wavenumber of relative motion, S_l a scattering matrix element and $P_l(\cos\theta)$ a Legendre polynomial. The expansion (1.1) is certainly useful when only a few partial waves contribute. However, for many collisions, typically involving heavy particles, this series is known to be slowly convergent and tedious for practical calculations. Furthermore, when a great number of partial waves contribute, it becomes hopeless to characterise the esential properties of $f(\theta)$ by individual terms in (1.1), since collective effects are unavoidable. The need for analytical techniques, which effectively sum the important contributions in the partial-wave series to a relatively small number of resulting terms, appears obvious. It is with this goal in mind that we shall examine the Poisson and Regge representations as alternatives to (1.1).

The one which is best understood so far is the Poisson representation (see Berry and Mount (1972) and Connor (1980)):

$$f(\theta)=\frac{\mathrm{i}}{k}\sum_{n=-\infty}^{+\infty}(-1)^n\int_0^{\infty}(1-S(\lambda))P_{\lambda-\frac{1}{2}}(\cos\theta)\exp(2\mathrm{i}n\pi\lambda)\lambda\,\mathrm{d}\lambda \tag{1.2}$$

where $\lambda = l+\frac{1}{2}$ is introduced as a continuous variable such that $S(\lambda)=S_l$ and $P_{\lambda-\frac{1}{2}}(\cos\theta)$ is a Legendre function of the first kind. The formula (1.2) has in fact been used as a starting point for the approximate, semiclassical trajectory description of elastic collisions and has, with few exceptions, proved to be rapidly convergent when the representation (1.1) converges slowly. Often only one term ($n=0$) in (1.2) yields sufficiently accurate results. Exceptions may occur at energies which allow the formation of long-lived states (orbiting or resonances) of the interacting particles. Then again the evaluation of $f(\theta)$ becomes cumbersome.

An investigation by Bosanac (1979) suggests, instead, that orbiting and resonance features are well described within a Regge, or complex angular momentum representation. In this representation (see also Connor 1980) one utilises the analytical properties of the terms in the original partial-wave sum, which is suitably converted, via a Watson transform, into a contour integral plus an infinite sum involving the S-matrix residues r_m at the pole positions λ_m. Thus

$$f(\theta)=-\frac{1}{2k}\int_\Gamma (1-S(\lambda))P_{\lambda_n-\frac{1}{2}}(-\cos\theta)\frac{\lambda}{\cos\pi\lambda}\,\mathrm{d}\lambda-\frac{\mathrm{i}\pi}{k}\sum_{m=0}^{\infty} r_m P_{\lambda_m-\frac{1}{2}}(-\cos\theta)\frac{\lambda_m}{\cos\pi\lambda_m} \tag{1.3}$$

where Γ is a path along the imaginary λ axis in the negative direction, with a slightly deformed lower part for strongly singular potentials (see figure 1), and the poles are all in the first quadrant. In order to consider (1.3) as an appropriate representation of $f(\theta)$, one requires that the residue sum converges rapidly (compared with the sums in (1.1) and (1.2)) and that the contour integral can be evaluated conveniently. According to Bosanac (1979), these conditions are satisfied in orbiting collisions for a wide angular range, not too close to the forward direction. Other favourable situations are also encountered (see Connor 1980). Among the known deficiences of (1.3) we shall mention only one, concerning rainbow scattering in atomic collisions,

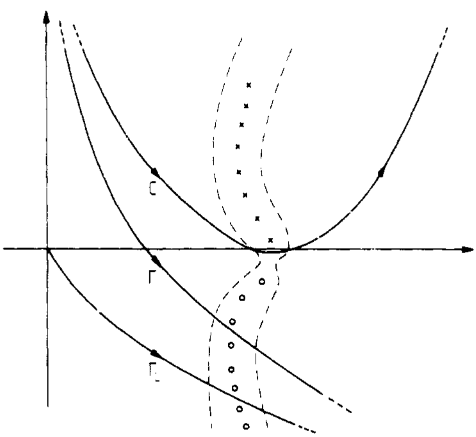

Figure 1. The figure illustrates schematically the location in the half-plane Re $\lambda>0$ of poles ($\times$) and zeros ($\bigcirc$) of the S matrix for an absorptive Lennard-Jones potential. An infinite number of poles and zeros lie along strings, which extends towards infinity in the first and fourth quadrants, respectively. The magnitude of the S matrix varies strongly in the neighbourhood (indicated by the broken curves) of these strings. The integration paths Γ_L, Γ and C are depicted. Integrals which are defined on C may be evaluated by residue sums.

which has been studied by Delos and Carlsson (1975) and Connor and Jakubetz (1978). In that context, serious difficulties in reproducing prominent rainbow features are encountered, because many terms in the residue sum are very large compared with $f(\theta)$ itself, such that considerable cancellation occurs by the summation. On the other hand, the very same features are conveniently described by the use of the Poisson representation (1.2), from which the well known Airy approximation is derived (Connor 1980).

Apparently, a full understanding of the usefulness of the complex angular momentum representation has not yet been reached. Systematic research (along the lines of Connor *et al* (1979, 1980)) concerning the behaviour of poles, λ_m, and residues, r_m, as functions of energy and interaction parameters is particularly important. The effects produced by complex optical-model potentials should also be investigated further.

In the present paper we shall develop a quite general complex angular momentum representation which comprises both the semiclassical trajectory description implied by (1.2) and the Regge pole analysis of (1.3). The derivation is exact and is based on realistic assumptions of the behaviour of the S matrix in the right-hand complex λ plane. The paper proceeds as follows.

In § 2 we outline the basic idea of a Regge pole theory, defining the S matrix, due to a complex interaction potential, for complex angular momenta.

Section 3 is devoted to the study of the S matrix in the complex λ plane. General properties valid for local complex potentials are established. Thus, an extended unitarity condition is given and a reflection symmetry for strongly singular potentials is found. The distribution of poles (and zeros) of the S matrix is discussed.

A transformation of the partial-wave series (1.1) is made in § 4. The procedure is based on analytical properties of the S matrix known for the class of strongly singular potentials, e.g. of the Lennard-Jones type. We end up with a flexible complex angular momentum representation, involving steepest-descent integrals, residue sums and a symmetry-type background integral.

The results are summarised briefly in § 5 and some relations for Legendre functions are listed in the appendix.

2. The complex angular momentum

The basic idea in existing complex angular momentum theories rests on the observation that the radial Schrödinger equation depends in a simple way on the angular momentum quantum number 1, so that one can analyse its solutions for the continuous and even complex values of l. This mathematical technique provides a new device for analysing scattering experiments which also yields a great deal of physical insight. Early developments of complex angular momentum theories for non-relativistic potential scattering (e.g. Newton 1964, de Alfaro and Regge 1965) are nicely summarised by Nussenzveig (1972).

In the present treatment we shall always assume that the wavenumber k of relative motion is real and positive. However, we shall allow the physical model potential $U(r)$ to be a complex function of the relative distance r of the colliding particles. The scattering process in the presence of a complex potential is described by the radial Schrödinger equation

$$\frac{d^2\phi_l(r)}{dr^2}+\left(k^2-U(r)-\frac{l(l+1)}{r^2}\right)\phi_l(r)=0 \qquad (2.1)$$

where conventional notations are used. Restrictions will be imposed on the potential in order to avoid special topics. Thus we exclude non-analytic potentials in the range $r>0$, as well as the presence of Coulombic tails in $U(r)$. Furthermore, we cannot allow potentials which are purely attractive and strongly singular at the origin (cf Frank *et al* 1971). More precisely, we impose the conditions

$$\lim_{\mathrm{Re}\, r\to+\infty} rU(r)=0 \tag{2.2}$$

$$\lim_{r\to+0} |\arg\{r^2U(r)+\delta\}|<\pi \qquad \text{all } \delta>0 \tag{2.3}$$

where in (2.3) we understand the branch $(-\pi, \pi)$ of arg { }. The presence of the positive quantity δ in (2.3) is necessary to allow for purely attractive and weakly singular potentials at the origin. Unless otherwise stated, $U(r)$ may assume arbitrary complex values for $r>0$.

The regular solution of (2.1), fulfilling the boundary condition

$$\phi_l(0)=0 \tag{2.4}$$

at the origin, can be normalised such that its asymptotic form is

$$\phi_l(r) \underset{r\to+\infty}{\sim} \exp(-\mathrm{i}kr+\tfrac{1}{2}\mathrm{i}l\pi)-S_l\exp(\mathrm{i}kr-\tfrac{1}{2}\mathrm{i}l\pi). \tag{2.5}$$

Here S_l defines the element of the elastic scattering matrix (or S matrix) in some region of the complex l plane containing the non-negative integers $l=0, 1, \ldots$. When regular or weakly singular potentials are considered, we must in general restrict l to the half-plane $\mathrm{Re}\, l>-\frac{1}{2}$ (see chapter 9 of Sitenko 1971). For strongly singular potentials, however, the conditions (2.4) and (2.5) can be satisfied without any restrictions on the complex values of l (de Alfaro and Regge 1965). This point is met again in § 3.

It is well known from standard texts that the elastic scattering amplitude $f(\theta)$ for complex potentials can also be obtained from the value of S_l at the non-negative integers $l=0, 1, 2, \ldots$ in accordance with formula (1.1). With the knowledge of $f(\theta)$ one simply obtains the differential cross section $I(\theta)$ and the total cross section σ according to the formulae

$$I(\theta)=|f(\theta)|^2 \tag{2.6}$$

and

$$\sigma=\frac{4\pi}{k}\lim_{\theta\to0}(\mathrm{Im}\, f(\theta)). \tag{2.7}$$

In our approach we shall transform (1.1) with the aid of the Poisson sum formula

$$\sum_{l=0}^{\infty} g(l)=\sum_{n=-\infty}^{+\infty}(-1)^n\int_0^{\infty} g(\lambda-\tfrac{1}{2})\exp(2\mathrm{i}n\pi\lambda)\,\mathrm{d}\lambda \tag{2.8}$$

(see Morse and Feshbach 1953) which yields the Poisson representation (1.2) directly. We then proceed further, in an exact manner, utilising more fully the analytical properties of the summand. In doing so, we must in § 3 make some preliminary studies of the behaviour of the S matrix in the complex l plane (or λ plane) and we shall later take for granted the standard generalisation of the polynomials P_l (cos θ) for $l=0, 1, \ldots$ to the Legendre functions of complex degree (see the appendix).

3. The S matrix

We shall start by establishing bounds for the S matrix in different regions of the complex l plane, providing us with information about the location of possible poles and zeros there. For this purpose, a suitable exact formula which displays the essential dependence of $|S_l|$ on the imaginary part of $U(r)$ and on the complex value of l will be derived. To this end, we consider the radial Schrödinger equation (2.1) together wth its complex conjugate, i.e.

$$\frac{d^2\phi_l^*(r)}{dr^2}+\left(k^2-U^*(r)-\frac{l^*(l^*+1)}{r^2}\right)\phi_l^*(r)=0, \tag{3.1}$$

for $r\geqslant 0$ and $k>0$. Unless otherwise stated, we restrict the values of l to the half-plane $\mathrm{Re}\, l\geqslant -\frac{1}{2}$. However, if the potential is not strongly singular at the origin, one must carefully modify the present treatment on the line $\mathrm{Re}\, l=-\frac{1}{2}$. Our regular solution $\phi_l^*(r)$ satisfies the conditions (cf (2.4) and (2.5))

$$\phi_l^*(0)=0 \tag{3.2}$$

$$\phi_l^*(r)\underset{r\to+\infty}{\sim}\exp(\mathrm{i}kr-\tfrac{1}{2}\mathrm{i}\pi l^*)-S_l^*\exp(-\mathrm{i}kr+\tfrac{1}{2}\mathrm{i}\pi l^*). \tag{3.3}$$

We may form, with the aid of (2.1) and (3.1), the equality

$$\frac{d}{dr}\left(\phi_l^*\frac{d\phi_l}{dr}-\phi_1\frac{d\phi_l^*}{dr}\right)=2\mathrm{i}\,\mathrm{Im}\left(U(r)+\frac{l(l+1)}{r^2}\right)|\phi_l|^2 \tag{3.4}$$

which we integrate from zero to infinity, using (2.4), (2.5), (3.2) and (3.3), to yield the final expression

$$|S_l|^2=\exp(-2\pi\mathrm{Im}\, l)+k^{-1}\exp(-\pi\mathrm{Im}\, l)\int_0^\infty[\mathrm{Im}\, U(r)+2\,(\mathrm{Re}\, 1+\tfrac{1}{2})\,\mathrm{Im}\, l/r^2]|\phi_l|^2\,dr. \tag{3.5}$$

Let us consider *real* potentials, recalling that $k>0$ and $\mathrm{Re}\, l\geqslant-\frac{1}{2}$. Equation (3.5) then reduces to

$$|S_l|^2=\exp(-2\pi\mathrm{Im}\, l)+k^{-1}\exp(-\pi\mathrm{Im}\, l)\int_0^\infty 2(\mathrm{Re}\, l+\tfrac{1}{2})\,\mathrm{Im}\, l/r^2|\phi_l|^2\,dr, \tag{3.6}$$

which on the real l axis further simplifies to the well known unitarity property for the S matrix:

$$|S_l|=1 \qquad (\mathrm{Im}\, l=0). \tag{3.7}$$

Obviously, for a scattering state ($k>0$) no poles or zeros are located on the real axis.

Below the real l axis, $|S_l|^2$ is not larger than the first term on the right-hand side of (3.6), i.e.

$$\begin{aligned}&|S_l|\leqslant\exp(-\pi\mathrm{Im}\, l) &&(\mathrm{Im}\, l<0)\\ &|S_l|=\exp(-\pi\,\mathrm{Im}\, l) &&(\mathrm{Re}\, l=-\tfrac{1}{2}).\end{aligned} \tag{3.8}$$

Above the real l axis, on the other hand, we obtain a lower bound for the S matrix, namely

$$\begin{aligned}&|S_l|\geqslant\exp(-\pi\mathrm{Im}\, l) &&(\mathrm{Im}\, l>0)\\ &|S_l|=\exp(-\pi\mathrm{Im}\, l) &&(\mathrm{Re}\, l=-\tfrac{1}{2}).\end{aligned} \tag{3.9}$$

Hence possible poles must be located above the real l axis and in the half-plane $\operatorname{Re} l > -\frac{1}{2}$, where at the same time no zeros are present.

When an imaginary part is introduced in the potential, we must resort to the formula (3.5). One finds the following general theorems.

If, for a given l such that $\operatorname{Im} l \leqslant 0$, the complex potential satisfies the condition

$$\int_0^\infty \operatorname{Im} U(r)|\phi_l|^2 \,\mathrm{d}r \leqslant 0, \tag{3.10}$$

then also

$$|S_l| \leqslant \exp(-\pi \operatorname{Im} l). \tag{3.11}$$

Furthermore, if for a given l such that $\operatorname{Im} l \geqslant 0$, the potential satisfies

$$\int_0^\infty \operatorname{Im} U(r)|\phi_l|^2 \,\mathrm{d}r \geqslant 0, \tag{3.12}$$

then also

$$|S_l| \geqslant \exp(-\pi \operatorname{Im} l). \tag{3.13}$$

In particular, for purely absorptive potentials, i.e. $\operatorname{Im} U(r) \leqslant 0$ $(r \geqslant 0)$, we conclude that all possible poles lie above the real l axis. However, the zeros are no longer forced to lie below the real axis, as was the case for real potentials (cf (3.7)–(3.9)). Thus it is possible that some zeros are situated on the real l axis and/or above it, and then they may cause drastic changes in the S-matrix element in (1.1). Indeed, in heavy-ion scattering problems (see, e.g., Nörenberg and Weidenmüller 1976, McVoy 1971) these zeros may be responsible for diffraction oscillations in the differential cross section $I(\theta)$. It is interesting to note that the upward displacement of the zeros is not a general feature implied by absorptive potentials. Connor *et al* (1979) and Thylwe (1981) have shown that Lennard–Jones-type potentials, often used in atom–atom collision models, cause a downward shift of the zeros of S_l at rainbow energies, while at the same time its poles tend to move closer to the real l axis as the absorption increases.

Next we shall derive an extended unitarity property for the S matrix, which will allow a one-to-one correspondence to be established between its zeros and its poles. Let $\hat{\phi}_l(r)$ denote a particular regular solution of the Schrödinger equation with the potential $U(r)$ replaced by $U^*(r)$, i.e. $\hat{\phi}_l(r)$ satisfies

$$\frac{\mathrm{d}^2\hat{\phi}_l(r)}{\mathrm{d}r^2} + \left(k^2 - U^*(r) - \frac{l(l+1)}{r^2}\right)\hat{\Phi}_l(r) = 0 \tag{3.14}$$

and the boundary condition

$$\hat{\phi}_l(0) = 0 \tag{3.15}$$

and has the asymptotic form

$$\hat{\phi}_l(r) \underset{r\to\infty}{\sim} \exp(-\mathrm{i}kr + \tfrac{1}{2}\mathrm{i}\pi l) - \hat{S}_l \exp(\mathrm{i}kr - \tfrac{1}{2}\mathrm{i}\pi l) \tag{3.16}$$

where $\hat{S}_1$ is the scattering matrix element pertaining to the potential $U^*(r)$. One now observes, from (3.14) and (3.1), that the two regular solutions $\hat{\phi}_{l^*}$ and ϕ_l^* satisfy the same differential equation and, hence, must be proportional. To determine the factor of proportionality we can, for instance, compare the terms representing outgoing waves in their asymptotic forms (3.16) and (3.3), respectively. We then find that

$$\hat{\phi}_{l^*}(r) = -\hat{S}_{l^*}\phi_l^*(r), \tag{3.17}$$

which, with due regard also to the terms representing incoming waves, results in an extended unitary condition

$$\hat{S}_{l^*}S_l^* = 1. \tag{3.18}$$

For real potentials we obviously have $\hat{S}_l \equiv S_l$, so that (3.18) reduces to

$$S_{l^*}S_l^* = 1. \tag{3.19}$$

An immediate consequence of (3.19) is that zeros and poles of S_l produced by real potentials lie symmetrically about the real l axis, each pole at a certain position corresponding to a zero at the complex conjugate position, and *vice versa*. When complex potentials are employed we find instead

$$l_{\text{zero}}(U) = l^*_{\text{pole}}(U^*), \tag{3.20}$$

i.e. a zero produced by the potential $U(r)$ is located at the complex conjugate of the position of a pole produced by the complex conjugate potential $U^*(r)$.

Finally we derive the well known reflection symmetry of S_l with respect to the point $l = -\frac{1}{2}$, valid only for strongly singular complex potentials (e.g. of the Lennard–Jones type). For this class of potentials, the regular solution of (2.1), and thus the S matrix, can be directly continued to the left-half-plane $\operatorname{Re} l \leqslant -\frac{1}{2}$, without violating the regularity of the solution at $r = 0$. Observing that equation (2.1) is invariant under the substitution $l \to -l-1$, we find that ϕ_l and ϕ_{-l-1} are both regular solutions satisfying the same differential equation and, therefore, must be proportional. This implies that their asymptotic forms and hence also S_l and S_{-l-1} must be proportional as well. One easily verifies that

$$S_{-l-1} = \exp[-\mathrm{i}2\pi(l+\tfrac{1}{2})]S_l, \tag{3.21}$$

which is the desired reflection property of the S matrix.

4. The elastic scattering amplitude

Throughout the present section we use instead of l the complex variable λ, related to l by

$$\lambda \equiv l + \tfrac{1}{2}, \tag{4.1}$$

and transform the elastic scattering amplitude (1.1) with the aid of Poisson's sum formula (2.8), obtaining immediately the Poisson representation

$$f(\theta) = \frac{\mathrm{i}}{k}\sum_{n=-\infty}^{+\infty}(-1)^n\int_0^\infty (1-S(\lambda))P_{\lambda-\frac{1}{2}}(\cos\theta)\exp(2\mathrm{i}n\pi\lambda)\lambda\,\mathrm{d}\lambda. \tag{4.2}$$

Here $S(\lambda)$ denotes the analytically continued scattering matrix element S_l and $P_{\lambda-\frac{1}{2}}(\cos\theta)$ is the Legendre function of the first kind of complex degree (see the appendix). The alternative procedure of applying a Watson transform would be equivalent for our purpose (cf Nussenzweig 1969). However, the Poisson representation (4.2) stays closer to the traditional semiclassical techniques (Berry and Mount 1972).

Let us divide the sum in (4.2) into three parts, i.e.

$$f(\theta)=f_0+f_1+f_2 \tag{4.3}$$

where

$$f_0\equiv\frac{\mathrm{i}}{k}\int_0^\infty (1-S(\lambda))P_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\ \mathrm{d}\lambda \tag{4.4}$$

$$f_1\equiv\frac{\mathrm{i}}{k}\sum_{n=1}^{\infty}(-1)^n\int_0^\infty (1-S(\lambda))P_{\lambda-\frac{1}{2}}(\cos\theta)\exp(2\mathrm{i}n\pi\lambda)\lambda\ \mathrm{d}\lambda \tag{4.5}$$

$$f_2\equiv\frac{\mathrm{i}}{k}\sum_{n=1}^{\infty}(-1)^n\int_0^\infty (1-S(\lambda))P_{\lambda-\frac{1}{2}}(\cos\theta)\exp(-2\mathrm{i}n\pi\lambda)\lambda\ \mathrm{d}\lambda. \tag{4.6}$$

In (4.6) we have replaced the original sum over negative integers n by a sum over positive ones.

To proceed further we shall assume that the scattering process to be studied belongs to the category defined below.

For the case under investigation we assume the following properties of the analytical function $S(\lambda)$ (see figure 1).

(*a*) $S(\lambda)$ is meromorphic with simple poles in the first quadrant (cf de Alfaro and Regge 1965).

(*b*) $|S(\lambda)|\leq\exp(-\pi\,\mathrm{Im}\,\lambda)$ as $|\lambda|\to+\infty$ along the imaginary axis, or arbitrarily close to this line (cf equation (3.5)).

(*c*) $S(\lambda)\to1+\mathrm{O}(1/\lambda)$ as $|\lambda|\to+\infty$ to the right of a certain region containing the poles and zeros (see figure 1).

We merely state without proof that this category comprises scattering on strongly singular non-emittive potentials, e.g. of the Lennard–Jones type (see Dombey and Jones 1968, Brander 1966).

The properties (*a*)–(*c*) together with the properties of the Legendre functions listed in the appendix are sufficient for the present analysis of the scattering amplitude $f(\theta)$ at all angles except possibly $\theta=0$ and π where special care is required. Let us study f_0, f_1 and f_2 separately.

The term f_0 in (4.3), which in primitive semiclassical theories is taken as a basic approximation of $f(\theta)$ itself, can be treated as follows. Inserting equation (A.2) from the appendix into (4.4), we first obtain

$$f_0=\frac{\mathrm{i}}{k}\int_0^\infty (1-S(\lambda))Q^{(-)}_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\ \mathrm{d}\lambda+\frac{\mathrm{i}}{k}\int_0^\infty (1-S(\lambda))Q^{(+)}_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\ \mathrm{d}\lambda. \tag{4.7}$$

The first of the integrals in (4.7) can be evaluated along a contour Γ_{L} in the fourth quadrant (see figure 1), starting at the origin and terminating at infinity to the right of the zeros of $S(\lambda)$. On this contour the integral can be separated into two convergent parts, one of which can be evaluated along the negative imaginary axis, or, with the substitution $\lambda\to-\lambda$, along the positive imaginary axis. We now have

$$f_0=\frac{\mathrm{i}}{k}\int_0^{\mathrm{i}\infty} Q^{(-)}_{-\lambda-\frac{1}{2}}(\cos\theta)\lambda\ \mathrm{d}\lambda-\frac{\mathrm{i}}{k}\int_{\Gamma_{\mathrm{L}}} S(\lambda)Q^{(-)}_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\ \mathrm{d}\lambda$$
$$+\frac{\mathrm{i}}{k}\int_0^\infty (1-S(\lambda))Q^{(+)}_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\ \mathrm{d}\lambda. \tag{4.8}$$

To the last integral we add and subtract the finite contribution from a path along the positive imaginary axis, and form a contour integral along a curve C (see figure 1), which starts at $+i\infty$, circumvents the pole region and terminates at infinity to the right of it. The contour integral obtained is split into two parts, of which only the one containing $S(\lambda)$ gives a non-zero contribution. Finally, f_0 takes the form

$$\begin{aligned} f_0 = \frac{i}{k}\int_0^{i\infty} Q^{(-)}_{-\lambda-\frac{1}{2}}(\cos\theta)\lambda\, d\lambda - \frac{i}{k}\int_{\Gamma_L} S(\lambda)Q^{(-)}_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\, d\lambda \\ -\frac{i}{k}\int_C S(\lambda)Q^{(+)}_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\, d\lambda + \frac{i}{k}\int_0^{i\infty} Q^{(+)}_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\, d\lambda \\ -\frac{i}{k}\int_0^{i\infty} S(\lambda)Q^{(+)}_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\, d\lambda. \end{aligned} \tag{4.9}$$

Next we consider the term f_1 given by (4.5). Adding and subtracting to each integral the finite contribution from a path along the positive imaginary axis, we get

$$\begin{aligned} f_1 = \frac{i}{k}\sum_{n=1}^{\infty}(-1)^n \int_C (1-S(\lambda))P_{\lambda-\frac{1}{2}}(\cos\theta)\exp(2in\pi\lambda)\lambda\, d\lambda \\ -\frac{i}{2k}\int_0^{i\infty} (1-S(\lambda))P_{\lambda-\frac{1}{2}}(\cos\theta)\frac{\exp(i\pi\lambda)}{\cos\pi\lambda}\lambda\, d\lambda \end{aligned} \tag{4.10}$$

where the order of summation and integration is reversed in the last integral and the identity

$$\sum_{n=1}^{\infty}(-1)^m \exp(2in\pi\lambda) = -\frac{1}{2}\frac{\exp(i\pi\lambda)}{\cos\pi\lambda} \qquad \text{Im} \geq 0,\ \lambda \neq \tfrac{1}{2}, \tfrac{3}{2}, \ldots \tag{4.11}$$

has been utilised. The contour C in (4.10) is the same as before. In (4.10) the first integral separates into its two additive parts, the first of which yields zero contribution. The second integral in (4.10) is likewise divided into its two parts. To the second of these parts we add and subtract the convergent integral

$$\frac{i}{2k}\int_0^{i\infty} S(\lambda)P_{\lambda-\frac{1}{2}}(\cos\theta)\frac{\exp(-i\pi\lambda)}{\cos\pi\lambda}\lambda\, d\lambda.$$

The term f_1 now takes the form

$$\begin{aligned} f_1 = -\frac{i}{k}\sum_{n=1}^{\infty}(-1)^n \int_C S(\lambda)P_{\lambda-\frac{1}{2}}(\cos\theta)\exp(2in\pi\lambda)\lambda\, d\lambda \\ -\frac{i}{2k}\int_0^{i\infty} P_{\lambda-\frac{1}{2}}(\cos\theta)\frac{\exp(i\pi\lambda)}{\cos\pi\lambda}\lambda\, d\lambda + \frac{i}{k}\int_0^{i\infty} S(\lambda)P_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\, d\lambda \\ -\frac{i}{2k}\int_0^{i\infty} S(\lambda)P_{\lambda-\frac{1}{2}}(\cos\theta)\frac{\exp(-i\pi\lambda)}{\cos\pi\lambda}\lambda\, d\lambda. \end{aligned} \tag{4.12}$$

Finally, in the expression (4.6) for f_2 we deform the path of integration to coincide with the negative imaginary axis and perform the sum over the integers n using

$$\sum_{n=1}^{\infty}(-1)^n \exp(-2in\pi\lambda) = -\frac{1}{2}\frac{\exp(-i\pi\lambda)}{\cos\pi\lambda} \qquad \text{Im}\,\lambda \leq 0,\ \lambda \neq \tfrac{1}{2}, \tfrac{3}{2}, \ldots \tag{4.13}$$

which yields

$$f_2 = -\frac{\mathrm{i}}{2k}\int_0^{-\mathrm{i}\infty} P_{\lambda-\frac{1}{2}}(\cos\theta)\frac{\exp(-\mathrm{i}\pi\lambda)}{\cos\pi\lambda}\lambda\,\mathrm{d}\lambda + \frac{\mathrm{i}}{2k}\int_0^{-\mathrm{i}\infty} S(\lambda)P_{\lambda-\frac{1}{2}}(\cos\theta)\frac{\exp(-\mathrm{i}\pi\lambda)}{\cos\pi\lambda}\lambda\,\mathrm{d}\lambda. \tag{4.14}$$

Making the substitution $\lambda \to -\lambda$ in the first of these integrals, we arrive at the formula

$$f_2 = -\frac{\mathrm{i}}{2k}\int_0^{\mathrm{i}\infty} P_{\lambda-\frac{1}{2}}(\cos\theta)\frac{\exp(\mathrm{i}\pi\lambda)}{\cos\pi\lambda}\lambda\,\mathrm{d}\lambda + \frac{\mathrm{i}}{2k}\int_0^{-\mathrm{i}\infty} S(\lambda)P_{\lambda-\frac{1}{2}}(\cos\theta)\frac{\exp(-\mathrm{i}\pi\lambda)}{\cos\pi\lambda}\lambda\,\mathrm{d}\lambda. \tag{4.15}$$

Here we have also utilised the property (A.3) as well as the symmetric nature of $\cos\pi\lambda$.

By the insertion of (4.9), (4.12) and (4.15) into (4.3) and with the aid of (A.2), we find for $f(\theta)$

$$\begin{aligned} f(\theta) = &-\frac{\mathrm{i}}{k}\int_\Gamma S(\lambda)Q^{(-)}_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\,\mathrm{d}\lambda - \frac{\mathrm{i}}{k}\int_C S(\lambda)Q^{(+)}_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\,\mathrm{d}\lambda \\ &-\frac{\mathrm{i}}{k}\sum_{n=1}^{\infty}(-1)^n\int_C S(\lambda)[Q^{(-)}_{\lambda-\frac{1}{2}}(\cos\theta)+Q^{(+)}_{\lambda-\frac{1}{2}}(\cos\theta)]\exp(2\mathrm{i}n\pi\lambda)\lambda\,\mathrm{d}\lambda \\ &+\frac{\mathrm{i}}{2k}\int_{+\mathrm{i}\infty}^{-\mathrm{i}\infty} S(\lambda)P_{\lambda-\frac{1}{2}}(\cos\theta)\frac{\exp(-\mathrm{i}\pi\lambda)}{\cos\pi\lambda}\lambda\,\mathrm{d}\lambda \\ &+\frac{\mathrm{i}}{k}\int_0^{\mathrm{i}\infty}\left(Q^{(-)}_{-\lambda-\frac{1}{2}}(\cos\theta)+Q^{(+)}_{\lambda-\frac{1}{2}}(\cos\theta)-\frac{\exp(\mathrm{i}\pi\lambda)}{\cos\pi\lambda}P_{\lambda-\frac{1}{2}}(\cos\theta)\right)\lambda\,\mathrm{d}\lambda \end{aligned} \tag{4.16}$$

where the contour Γ in the first integral is composed of the positive imaginary axis and the path Γ_L and runs, suitably deformed, in the downward direction. According to (A.6), the last integral in (4.16) is identically zero. The last but one integral, which is evaluated along $\mathrm{Re}\,\lambda = 0$ and hence has the nature of a so-called background I, say, can be put into the form

$$I = \frac{\mathrm{i}}{2k}\int_0^{\mathrm{i}\infty}(\exp(2\mathrm{i}\pi\lambda)S(-\lambda)-S(\lambda))P_{\lambda-\frac{1}{2}}(\cos\theta)\frac{\exp(-\mathrm{i}\pi\lambda)}{\cos\pi\lambda}\lambda\,\mathrm{d}\lambda. \tag{4.17}$$

By virtue of the reflection property (3.23), this symmetry-type background integral, I, is identically zero for strongly singular potentials (e.g. of the Lennard–Jones type). However, since we have not explicitly assumed the potential to be strongly singular in the derivation of (4.16), the term (4.17) should be retained in the final formulae. Thus we find that the elastic scattering amplitude $f(\theta)$ may be expressed in terms of two infinite sums of contour integrals and a symmetry-type background integral:

$$f(\theta) = \sum_{n=0}^{\infty} f_n^{(-)}(\theta) + \sum_{n=0}^{\infty} f_n^{(+)}(\theta) + I \tag{4.18}$$

where I is given by (4.17) and where

$$f_0^{(-)}(\theta) = -\frac{\mathrm{i}}{k}\int_\Gamma S(\lambda)Q^{(-)}_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\,\mathrm{d}\lambda \tag{4.19}$$

$$f_0^{(+)}(\theta) = -\frac{\mathrm{i}}{k}\int_{\mathrm{C}} S(\lambda)Q^{(+)}_{\lambda-\frac{1}{2}}(\cos\theta)\lambda\,\mathrm{d}\lambda \tag{4.20}$$

$$f_n^{(\pm)}(\theta) = -\frac{\mathrm{i}}{k}\int_{\mathrm{C}} (-1)^n S(\lambda)Q^{(\pm)}_{\lambda-\frac{1}{2}}(\cos\theta)\exp(2\mathrm{i}n\pi\lambda)\lambda\,\mathrm{d}\lambda \qquad n \geqslant 1. \tag{4.21}$$

The formulae (4.18)–(4.21) constitute an exact, modified version of the Poisson representation (4.2) of $f(\theta)$. We shall mention some advantages of (4.18) over (4.2), which are expected to be of great importance for developing accurate approximation schemes in heavy-particle scattering.

(i) The terms with negative integers n are eliminated in (4.18). In existing semi-classical treatments they are neglected as being dynamically not allowed.

(ii) The non-dynamical term in the Poisson integrals, due to the presence of the unscattered plane wave, is similarly removed. This is frequently done by using the closure relation for the Legendre polynomials in (1.1), with the result that the integrands in (4.2) diverge as $\lambda \to +\infty$.

(iii) The new integrals are defined on infinite contours in the complex λ plane. This point makes (4.18) well suited for a semiclassical trajectory approximation which takes into account complex saddles originating from classically forbidden events or from a complex physical potential.

There is another important consequence of (iii) which we shall develop in some more detail here. The integrals in (4.20) and (4.21), which are defined along the contour C (see figure 1), may, if convenient, be closed at infinity and evaluated as S-matrix residue sums. In this way the infinite sum of integrals in (4.18) can be resummed analytically. To see this, let us define an arbitrary infinite sum of such integrals, namely

$$f^{(\pm)}_{\mathrm{P},N_\pm}(\theta) \equiv \sum_{n=N_\pm}^{\infty} f_n^{(\pm)}(\theta) \qquad N_+ \geqslant 0,\ N_- \geqslant 1 \tag{4.22}$$

where the subscript P refers to the contribution from the poles of $S(\lambda)$. If the procedure of closing the contour C is justified (cf Dombey and Jones 1968), we find

$$f^{(\pm)}_{\mathrm{P},N_\pm}(\theta) = (-1)^{N_\pm}\frac{\pi}{k}\sum_{m=0}^{\infty} r_m Q^{(\pm)}_{\lambda_m-\frac{1}{2}}(\cos\theta)\frac{\exp[\mathrm{i}(2N_\pm - 1)\pi\lambda_m]}{\cos\pi\lambda_m}\lambda_m. \tag{4.23}$$

Here r_m is the residue of $S(\lambda)$ at the pole λ_m. As a result, the elastic scattering amplitude takes the form

$$f(\theta) = \sum_{n=0}^{N_- -1} f_n^{(-)}(\theta) + \sum_{n=0}^{N_+ -1} f_n^{(+)}(\theta) + f^{(-)}_{\mathrm{P},N_-}(\theta) + f^{(+)}_{\mathrm{P},N_+}(\theta) + I. \tag{4.24}$$

The integers N_- and N_+ in (4.24) may be chosen conveniently. For example, the choice $N_- = N_+ = \infty$ would give us back (4.18), which was shown to be a modified Poisson representation (4.2). At the other extreme we can choose $N_- = 1$ and $N_+ = 0$, the maximal pole representation, and with the aid of (A.2)–(A.5) regain the Regge pole representation (1.3). Thereby we find that the background integral in (1.3) is identical to the sum of $f_0^{(-)}(\theta)$ and I, the latter being zero if the S matrix satisfies the reflection symmetry (3.21).

In the flexible complex angular momentum representation (4.24), the main result of this study, all choices of N_- and N_+ will lead to exact results. However, the total number of significantly large terms in (4.24) may be quite different, initiating a need for an 'optimal' representation of $f(\theta)$. We shall not enter here into details of how this problem can be solved, but merely state some useful observations made on the convergence and magnitude of the residue terms only, as given by equation (4.23):

(iv) $f^{(-)}_{\mathrm{P},N_-}(\theta)$ becomes more strongly convergent (but possibly of smaller magnitude and hence of less importance) if the integer N_- is increased. Furthermore, the convergence depends on the scattering angle in such a way that smaller θ are favoured.

(v) $f^{(+)}_{\mathrm{P},N_+}(\theta)$ becomes more strongly convergent (but possibly also of smaller magnitude and hence of less importance) if the integer N_+ is increased. Larger scattering angles θ are favoured here.

(vi) Both residue sums become of equal magnitude if either $N_-=N_+$ and θ approaches the forward angle, or $N_-=N_++1$ and θ approaches the backward angle.

5. Conclusion

In this paper we have developed a complex angular momentum theory for treating atomic and molecular elastic collisions. The S matrix produced by complex potentials was defined for complex values of the angular momentum quantum number, and the distribution of its poles and zeros there was discussed without using Jost functions. An extended unitarity condition was found which displays an unique correspondence between poles and zeros. Finally we were able to derive a new flexible representation of the scattering amplitude, containing sums of contour integrals and S-matrix residues as well as two integer parameters which can be adjusted so as too minimise the total number of large terms.

The representation is especially suited for a semiclassical (or semiquantal) analysis of low-energy differential cross sections, taking into account in a convenient way the contribution from possible resonances.

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Appendix. Legendre functions

The Legendre polynomials have a standard analytical continuation, based on the Legendre differential equation (Robin 1958). Let $P_{\lambda-\frac{1}{2}}(\cos\theta)$ and $Q_{\lambda-\frac{1}{2}}(\cos\theta)$ denote the Legendre functions of the first and second kind, respectively, and let $Q^{(-)}_{\lambda-\frac{1}{2}}(\cos\theta)$ and $Q^{(+)}_{\lambda-\frac{1}{2}}(\cos\theta)$ be defined by

$$Q^{(\mp)}_{\lambda-\frac{1}{2}}(\cos\theta)=\tfrac{1}{2}\left(P_{\lambda-\frac{1}{2}}(\cos\theta)\pm\frac{2\mathrm{i}}{\pi}Q_{\lambda-\frac{1}{2}}(\cos\theta)\right). \tag{A.1}$$

The following relations are given by Robin (1958) and Nussenzweig (1969):

$$P_{\lambda-\frac{1}{2}}(\cos\theta)=Q^{(-)}_{\lambda-\frac{1}{2}}(\cos\theta)+Q^{(+)}_{\lambda-\frac{1}{2}}(\cos\theta) \tag{A.2}$$

$$P_{\lambda-\frac{1}{2}}(\cos\theta)=P_{-\lambda-\frac{1}{2}}(\cos\theta) \tag{A.3}$$

$$P_{\lambda-\frac{1}{2}}(-\cos\theta)=\mathrm{i}\exp(-\mathrm{i}\pi\lambda)P_{\lambda-\frac{1}{2}}(\cos\theta)-2\mathrm{i}\cos\pi\lambda Q^{(-)}_{\lambda-\frac{1}{2}}(\cos\theta) \tag{A.4}$$

$$P_{\lambda-\frac{1}{2}}(-\cos\theta)=-\mathrm{i}\exp(\mathrm{i}\pi\lambda)P_{\lambda-\frac{1}{2}}(\cos\theta)+2\mathrm{i}\cos\pi\lambda Q^{(+)}_{\lambda-\frac{1}{2}}(\cos\theta). \tag{A.5}$$

With the aid of (A.3)–(A.5) one may show the useful identity

$$\exp(\mathrm{i}\pi\lambda)P_{\lambda-\frac{1}{2}}(\cos\theta)-(Q^{(+)}_{\lambda-\frac{1}{2}}(\cos\theta)+Q^{(-)}_{-\lambda-\frac{1}{2}}(\cos\theta))\cos\pi\lambda=0. \tag{A.6}$$

Both functions $Q^{(-)}_{\lambda-\frac{1}{2}}(\cos\theta)$ and $Q^{(+)}_{\lambda-\frac{1}{2}}(\cos\theta)$ have poles in the λ plane at negative half-integer λ values ($\equiv l+\frac{1}{2}$). These poles cancel and are not present in $P_{\lambda-\frac{1}{2}}(\cos\theta)$. Furthermore, for θ not too close to 0 and π, the asymptotic ($|\lambda|\theta \gg 1$) behaviour of the functions $Q^{(\mp)}$ is given by

$$Q^{(\mp)}_{\lambda-\frac{1}{2}}(\cos\theta)=\frac{\exp[\mp\mathrm{i}(\lambda\theta-\frac{1}{4}\pi)]}{(2\pi\lambda\sin\theta)^{1/2}}(1+\mathrm{O}(\lambda^{-1})). \tag{A.7}$$

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