Accurate Regge pole positions and residues determined by phase-amplitude formulae

Nils Andersson†

Department of Theoretical Physics, Thunbergsvägen 3, S-752 38 Uppsala, Sweden

Abstract. Formulae determining Regge pole positions and residues are derived within the phase-amplitude method. Numerical calculations are performed for an optical Lennard–Jones (12, 6) potential using parameters approximating elastic scattering of K, and Li, by HBr. Comparison with previous investigations shows that the phase-amplitude results are very accurate. Hence, the phase-amplitude method provides an important alternative to other methods used to investigate scattering problems in the complex angular momentum representation.

1. Introduction

In elastic scattering theory the collision of two spinless particles is described by the time-independent radial Schrödinger equation

$$\frac{d^2\Psi}{dr^2} + \left\{ \frac{2\mu}{\hbar^2} [E - V(r)] - \frac{l(l+1)}{r^2} \right\} \Psi = 0 \tag{1}$$

where E is the collision energy, μ is the reduced mass of the colliding particles and r is the distance separating them. The potential $V(r)$ is a, possibly complex valued, function describing the interaction. In this investigation we only require that $V(r)$ vanishes asymptotically and that it includes no Coulombic tail. In order to be physically realistic, however, the potential energy function must be attractive at large distances and become strongly repulsive as r decreases.

A general solution to (1) is regular at the origin

$$\Psi(0) = 0 \tag{2}$$

and can be normalized to have the asymptotic form

$$\Psi(r) \sim \exp(-i(kr - l\pi/2)) - S_l \exp(+i(kr - l\pi/2)) \qquad \text{as } r \to +\infty. \tag{3}$$

The quantity $k = (2\mu E)^{1/2}/\hbar$ is the wavenumber and S_l defines the elements of the scattering matrix.

During the last few decades techniques for solving (1) in atomic and molecular physics have been of continuing interest. The quantity of basic physical interest is the differential cross-section which can be expressed in terms of the scattering amplitude.

† Present address: Department of Physics and Astronomy, University of Wales, College of Cardiff, Cardiff CF2 3YB, UK.

Consequently, several methods have been developed to investigate the properties of the scattering amplitude. In the standard representation the angular momentum, l, is a non-negative integer and the scattering amplitude is given by a partial-wave series. However, for collisions involving heavy particles such as atoms or molecules, this series is often slowly convergent and hardly appropriate for practical calculations. In these situations the complex angular momentum representation (see Connor 1980, 1990 or Thylwe 1987 for reviews and further references) has proved to be a powerful alternative. In complex angular momentum theory the energy, E, is treated as a real parameter while the angular momentum, l, is allowed to assume continuous complex values. After a Watson–Sommerfeld transformation the scattering amplitude can be expressed in terms of a background integral and a sum involving the energy-dependent poles of the S-matrix. The great advantage of the complex angular momentum representation is that, in many practical cases, only a few singularities contribute to the pole sum. Poles in the complex l-plane are referred to as Regge poles and it can be shown that there exists an infinite number of such poles for potentials with a repulsive singularity at the origin (i.e. when $r^2V(r)$ diverges as $r \to 0$). At medium and high energies the consecutive poles are separated by a small real part and a relatively large imaginary part.

It follows from (3) that a pole of the S-matrix corresponds to a solution to (1) that fulfils a boundary condition of purely outgoing waves at infinity. This boundary condition cannot be fulfilled unless the angular momentum, or in the standard representation the energy, is complex valued. In effect, the analogue to an investigation of Regge poles, l_n, is the determination of complex energy resonance states.

A determination of the scattering amplitude in the complex angular momentum representation also demands that the residues, r_n, associated with the Regge poles are known. In some neighbourhood of the Regge pole l_n the associated residue is defined by

$$r_n = \lim_{l \to l_n} (l - l_n) S_l. \tag{4}$$

It is clear that, although only a few poles give a significant contribution to the pole sum, the position and residue of each pole must be obtained with a high accuracy if summation is to be a sensible procedure for calculating the scattering amplitude. Most previous investigations have failed to satisfy this demand. This failure is intimately connected with the difficulties of solving the Schrödinger equation for a complex value of the angular momentum.

It has often been realized that direct numerical integration of the Schrödinger equation for a complex valued energy (or angular momentum) involves serious computational difficulties if carried out along the real coordinate axis. This deficiency can, at least to some extent, be avoided through the introduction of complex coordinates. Regge states can be determined by numerical integration of the Schrödinger equation along suitable contours in the complex coordinate plane (Bain *et al* 1975, Sukumar and Bardsley 1975). However, since the integration contours in the standard complex rotation scheme are not unambiguously defined this method is often numerically unstable.

Another deficiency of the direct numerical integration approach is that a large value of the reduced mass, as in ion-atom collisions, unavoidably leads to rapidly oscillating wavefunctions. In the oscillating region numerical integration requires a large number of integration steps and an accumulation of numerical errors can hardly

be avoided. As discussed by Bosanac (1978), this deficiency can be avoided if the differential equation (1) is replaced by a nonlinear equation whose basic solutions are non-oscillatory.

The use of semiclassical methods have proved to be a reasonably accurate way of investigating the Regge properties of intermolecular potentials (Dombey and Jones 1968, Delos and Carlson 1975, Connor 1972, 1982, Connor *et al* 1976, 1979, 1980). Calculations by Connor *et al* for a Lennard–Jones (12, 6) potential show that Regge pole positions and residues obtained from a uniform WKB treatment are in good agreement with the corresponding numerical integration results, with the accuracy improving as the quantum number n increases. Complex angular momentum techniques have also been successfully developed within the phase-integral method (Thylwe 1983a, b, 1985) and a recent numerical investigation by Amaha and Thylwe (1991) is extremely accurate.

It is well known, however, that the asymptotic nature of the approximate methods restricts their usefulness in problems where many so-called transition points have to be considered. Another deficiency of the approximate calculations is that they lack efficient error control. Reliable numerical integration schemes, where the accuracy can easily be estimated and increased, are therefore necessary complements to any such approximate analysis.

Using a modified Prüfer phase function approach Pajunen and coworkers (1985, 1986, 1988, 1989) have developed a method for evaluating Regge pole positions and residues for singular potentials. The results of Pajunen are numerically more accurate than those obtained by the complex coordinate approach or the WKB method. The Regge pole positions can be accurately and straightforwardly obtained within the Prüfer method. Meanwhile, the formula used by Pajunen to determine the corresponding residues is somewhat confusing. It is equivalent to a formula obtained from a non-uniform WKB treatment. It seems, however, as if a mixture of semiclassical and numerically obtained quantities are used to evaluate this formula. In the opinion of the present author, Pajunen's approach for obtaining residues cannot be considered at all satisfactory.

In a previous paper the phase-amplitude method of Newman and Thorson (1972a, b) – as generalized to the complex coordinate plane—was used to determine accurate quasinormal-mode frequencies for Schwarzschild black holes (Andersson 1992). In this paper phase-amplitude formulae determining the positions and residues of Regge poles will be derived. Numerical calculations will then be performed for an intermolecular potential

$$V(r) = 4\varepsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^{6} \right] - iW \left(\frac{\sigma}{r} \right)^{s} \tag{5}$$

i.e. a Lennard–Jones (12, 6) potential perturbed by an imaginary term proportional to r^{-s}. The imaginary part of this optical potential can be considered as a loss of flux from the elastic channel. Hence, with $W \neq 0$, this potential corresponds to reactive scattering (Thylwe and Fröman 1983). In the present investigation we have introduced the dimensionless quantities

$$K = \frac{E}{\varepsilon} \qquad A = k\sigma \qquad C = \frac{2\mu W \sigma^2}{\hbar^2} = \frac{WA^2}{E}.$$

The parameters will be chosen to approximate scattering of K, and Li, by HBr. These

parameters have been preferred since they are used in a large number of previous investigations, see for example Connor *et al* (1976, 1979, 1980), Pajunen (1988) and Amaha and Thylwe (1991).

2. The phase-amplitude method

By the transformation $z = r/\sigma$ the differential equation (1) can be written

$$\frac{d^2\Psi}{dz^2} + R(z)\Psi = 0 \tag{6}$$

where $R(z)$ is an analytic function of the, possibly complex valued, coordinate z. For the perturbed Lennard–Jones potential, (5), the function $R(z)$ is explicitly given by

$$R(z) = A^2 - \frac{4A^2}{K}\left(\frac{1}{z^{12}} - \frac{1}{z^6}\right) + \frac{iC}{z^s} - \frac{l(l+1)}{z^2}. \tag{7}$$

As mentioned above, the problem of calculating Regge poles, reduces to determining the regular solution to (6) that fulfils the condition of purely outgoing waves at infinity, $z = +\infty$.

In the phase-amplitude method the general solution to (6) is written as a linear combination of the two functions

$$\psi^{\pm} = q^{-1/2}(z)\exp\left\{\pm i\int q(z)\,dz\right\} \tag{8}$$

where the function $q(z)$ can be numerically continued in the complex coordinate plane by integration of the nonlinear differential equation

$$\frac{1}{2q}\frac{d^2q}{dz^2} - \frac{3}{4q^2}\left(\frac{dq}{dz}\right)^2 + q^2 - R(z) = 0. \tag{9}$$

In practice, a convenient scheme for tracing $q(z)$ involves writing (9) as a system of *three* coupled differential equations of the first order, determining also the integral of $q(z)$ along the chosen integration contour (Andersson 1992). In the present investigation this system of differential equations was solved by means of the NAG-routine D02CBF based on a variable step, variable order Adams method.

The functions (8) provide two linearly independent solutions to (6) for all possible choices of initial conditions for $q(z)$. However, it is computationally desirable that the function $q(z)$ is non-oscillatory. A smooth behaviour of $q(z)$ is, to some extent, guaranteed from the use of accurate asymptotic initial conditions (Andersson 1992). In the asymptotic region we therefore replace $q(z)$ with an explicit expression obtained from the arbitrary-order phase-integral approximation, see Fröman and Fröman (1991) for references. The phase-integral expression for $q(z)$ is accurate when z is far away from all transition points, i.e. zeros and poles of $R(z)$. In practice, there are other possible ways to obtain appropriate initial values for the numerical integration of (9), e.g. power series expansions. In the present analysis the phase-integral approximation has been preferred since it provides functions with a very high accuracy when the order of approximation is increased. We consider the phase-
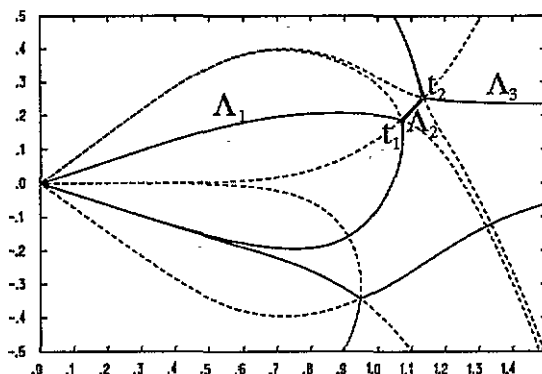
Figure 1. The pattern of semiclassical anti-Stokes (fulldrawn) and Stokes (dashed) lines for the Lennard–Jones (12, 6) potential (5) and parameters corresponding to $n = 0$ in table 1. The transition points considered in the analysis are t_1 and t_2. Integration contours used are Λ_1, Λ_2 and Λ_3.

integral function replacing $q(z)$ asymptotically to be chosen such that ψ^+ fulfils the boundary condition determining a Regge state at infinity.

In order to avoid oscillations in $q(z)$ it is also convenient to consider the pattern of semiclassical anti-Stokes lines, see figure 1 and the discussion in appendix 1. These are contours along which the quantity $R^{1/2}(z)\, dz$ is purely real. It is convenient to replace the physical boundary conditions (on the real coordinate axis) with boundary conditions on such anti-Stokes lines (Andersson 1992). On the anti-Stokes line Λ_3, emanating from t_2 towards infinity, the solution ψ^+ corresponds to an outgoing wave. For $|z|$ very large it can be shown, using semiclassical theory, that this solution corresponds to the desired behaviour on the real axis. It can also be proved that a solution corresponding to a wave travelling away from the transition point t_1 along the contour Λ_1 corresponds to an exponentially decaying solution on the Stokes line emerging from t_1 towards the origin. In effect, such a solution agrees with the condition of regularity at the origin.

Consequently, we trace the solution to (6) along an integration path $\Lambda = \Lambda_1 + \Lambda_2 + \Lambda_3$ consisting of anti-Stokes lines and joining the origin with $z = \infty$ (figure 1). Then the differential equation (9) has to be integrated through the region close to two transition points, t_1 and t_2. No other transition points are of relevance in the analysis. It is important to note that the integration contours are, in a sense, well defined. Thus we avoid the ambiguities of any standard complex rotation scheme. In this investigation the integration contours are constructed such that Λ_1 approximates the anti-Stokes line that emerges from the innermost of the two transition points considered, t_1, towards the origin. Meanwhile, Λ_3 is a straight line approximating the anti-Stokes line that emerges from the outermost transition point, t_2, towards infinity. The contour Λ_2 is a straight line joining t_1 with t_2.

One may argue that figure 1 suggests other—perhaps as convenient—choices of integration contours. It may be worthwhile to clarify the reason why these possibilities have been discarded. The argument requires some knowledge of how an approximate solution, i.e. a linear combination of the two solutions (8) with $q(z)$ approximated by $R^{1/2}(z)$, will change if continued in the complex coordinate plane. It is known that the linear combination must change as a zero of $R(z)$ is circumvented. Specifically, the

coefficient of the solution that is exponentially small will change rapidly as a semiclassical Stokes line (along which $R^{1/2}(z)\,dz$ is purely imaginary) is crossed. This is known as Stokes phenomenon. Let us first see what this implies should we want to continue a given solution to (6) along the real coordinate axis. In doing so, it is clear from figure 1 that, we must cross two Stokes lines; one emanating from the transition point t_1 and the other from t_2. Hence, the effect of these two points must be considered. It is also worth pointing out that if one continues the solution along the lower one of the two anti-Stokes lines that goes from t_1 to the origin the same argument implies that a third transition point (approximately at $0.9-0.35\,i$) should be accounted for. Hence, that choice would be more complicated. Finally, it is not possible to discard the two transition points t_1 and t_2 and instead match the numerical solutions, as integrated from infinity and the origin, at the third transition point in figure 1. Because of the first argument above, the effect of t_1 and t_2 should still be considered.

3. Regge pole positions

The desired solution to (6) on the anti-Stokes line Λ_1 of figure 1 can be written

$$\Psi_1 = a_1^+ \psi_1^+ \tag{10}$$

where a_1^+ is a constant and we have introduced subscripts to indicate on which integration contour the quantities are numerically determined. For all points on Λ_1, the function ψ_1^+ (i.e. $q_1(z)$) is obtained by numerical integration of (9). However, a simple semiclassical argument (outlined in appendix 1) suggests that the numerically determined function $q(z)$ will not remain nicely behaving if it is continued through the region close to the transition point t_1. Hence, it is preferable to match the above solution to another one at t_1 using the requirement that a solution to (6) (and its derivative) be continuous. It then follows that, on the contour Λ_2 the solution Ψ_1 can be expressed in terms of the function $q_2(z)$ (which is determined by integration from a point on Λ_2), and we have

$$\Psi_1 = a_1^+ \frac{q_2^{1/2}(t_1)}{q_1^{1/2}(t_1)\cos\theta_1} q_2^{-1/2}(z) \cos\left(\int_{t_1}^z q_2(z)\,dz - \theta_1\right). \tag{11}$$

Note that we have used the transition point t_1 as matching point of the two solutions. The connection phase θ_1 is given by the implicit relation

$$q_2\tan\theta_1 = iq_1 - \frac{1}{2}\left(\frac{1}{q_1}\frac{dq_1}{dz} - \frac{1}{q_2}\frac{dq_2}{dz}\right) \qquad z = t_1. \tag{12}$$

In the evaluation of this formula we assume that the necessary branch cuts extend along the imaginary axis from $\tan\theta_1 = \pm i$ towards the positive and negative infinity, respectively. In practice, this means that the real part of θ_1 is close to $\pi/3$ while the imaginary part is small.

It is important to note that initial conditions for the determination of the function $q_1(z)$ are chosen such that ψ_1^+ has the desired behaviour on Λ_1. Meanwhile, there is no boundary condition determining initial conditions for the function $q_2(z)$. However, although (11) arises from the matching of two different solutions at the transition point t_1, it expresses the function Ψ_1 in terms of the, more or less, arbitrary function $q_2(z)$. Therefore, initial conditions determining $q_2(z)$ can be chosen in any convenient

way. It is, of course, still desirable that the function is non-oscillatory. We have used the first order phase-integral approximation (which is equivalent to the WKB approximation) to initiate the determination of $q_2(z)$. The integration of (9) was then continued from the midpoint of the contour Λ_2 towards the two transition points.

On the other hand, the general solution to (6) on the contour Λ_3 is

$$\Psi_3 = a_3^+ \psi_3^+ + a_3^- \psi_3^- \tag{13}$$

where a_3^+ and a_3^- are constants. It is straightforward to verify that, the corresponding solution in a point on Λ_2 can be written

$$\Psi_3 = (a_3^+ + a_3^-) \frac{q_2^{1/2}(t_2)}{q_3^{1/2}(t_2) \cos \theta_2} q_2^{-1/2}(z) \cos \left(\int_{t_2}^z q_2(z)\, \mathrm{d}z - \theta_2 \right). \tag{14}$$

The connection phase θ_2 is given by

$$q_2 \tan \theta_2 = \frac{1}{a_3^+ + a_3^-} \left[a_3^+ \left\{ iq_3 - \frac{1}{2} \left(\frac{1}{q_3} \frac{\mathrm{d}q_3}{\mathrm{d}z} - \frac{1}{q_2} \frac{\mathrm{d}q_2}{\mathrm{d}z} \right) \right\} \right.$$
$$\left. + a_3^- \left\{ -iq_3 - \frac{1}{2} \left(\frac{1}{q_3} \frac{\mathrm{d}q_3}{\mathrm{d}z} - \frac{1}{q_2} \frac{\mathrm{d}q_2}{\mathrm{d}z} \right) \right\} \right] \tag{15}$$

where all quantities are to be evaluated at the transition point t_2.

The obvious condition that the two functions (11) and (14), determining the solution to (6) on the contour Λ_2, must be identical (except for a constant factor) implies that

$$\int_{t_1}^{t_2} q_2(z)\, \mathrm{d}z = n\pi + \theta_1 - \theta_2 \qquad n = 0, 1, 2, \ldots \tag{16}$$

when the boundary condition of outgoing waves at infinity is imposed this can be written

$$\int_{t_1}^{t} q_2(z)\, \mathrm{d}z = n\pi + \theta_1 - \theta_{2,n} \qquad n = 0, 1, 2, \ldots \tag{17}$$

where n is an integer labelling the Regge poles. The quantity $\theta_{2,n}$ (corresponding to the nth Regge state) is given by (15) with $a_3^- = 0$.

It is important to note that each complex eigenvalue l_n of (17) is unambiguously associated with a quantum number n. This is not the case in many standard numerical integration schemes. In effect, the condition (17) does not demand an accurate initial guess for the eigenvalue in order to be computationally efficient.

4. Residues

To obtain the residue, r_n, corresponding to a Regge pole position l_n, the definition (15) can be rewritten

$$\frac{a_3^+}{a_3^-} = \frac{q_2(\tan \theta_2 - \tan \theta_{2,n}) + 2 iq_3}{q_2(\tan \theta_{2,n} - \tan \theta_2)}$$

$$\approx 2 i \left(\frac{q_3}{q_2} \right)_{t_2} \frac{1}{\tan \theta_{2,n} - \tan \theta_2} \qquad \text{as } l \to l_n \tag{18}$$

since $\theta_2 = \theta_{2,n}$ for a Regge state. By expanding this expression in a Taylor series around the nth Regge pole position, l_n, we have

$$\frac{a_3^+}{a_3^-} \approx 2i \left(\frac{q_3}{q_2}\right)_{t_2} \cos^2\theta_{2,n} \left[\frac{\partial D_n}{\partial l}\right]^{-1} \frac{1}{l - l_n} \tag{19}$$

where $D_n(l)$ is defined by

$$D_n(l) = \theta_{2,n} - \theta_2 \tag{20}$$

However, since θ_2 is defined by (15) for any value of l we can use (16) to replace θ_2 in the above formula. We then have

$$D_n(l) = \int_{t_1}^{t_2} q_2(z)\,dz - n\pi - \theta_1 + \theta_{2,n} \tag{21}$$

which vanishes for a Regge state according to our condition (17). The partial derivative in (19) is formally given by

$$\frac{\partial D_n}{\partial l} = \int_{t_1}^{t_2} \frac{\partial q_2}{\partial l}\,dz - \frac{\partial\theta_1}{\partial\lambda} + \frac{\partial\theta_{2,n}}{\partial l}. \tag{22}$$

It is important to note that the last two terms in this expression are non-zero. This is since the connection phases θ_i depend on the initial conditions used for the integration of (9) and the actual position of each transition point. In effect, θ_i will depend on the value of l.

It can be identified from (3) and (13) that the desired S-matrix element is given by

$$S_l = -\left(\frac{a_3^+}{a_3^-}\right)\exp(2i\delta_l)$$

$$= -2i\left(\frac{q_3}{q_2}\right)_{t_2}\cos^2\theta_{2,n}\left[\frac{\partial D_n}{\partial l}\right]^{-1}\frac{1}{l - l_n}\exp(2i\delta_l). \tag{23}$$

The asymptotic phase, δ_l, is defined by

$$\int_{t_3}^{z} q_3(z)\,dz \to Az - l\frac{\pi}{2} + \delta_l \qquad z \to +\infty. \tag{24}$$

Consequently we obtain, after comparison with (4), a phase-amplitude formula for the residue

$$r_n = -2i\left(\frac{q_3}{q_2}\right)_{t_3}\cos^2\theta_{2,n}\left[\frac{\partial D_n}{\partial l}\right]^{-1}_{l = l_n}\exp(2i\delta_l). \tag{25}$$

5. Numerical results and conclusions

The phase-amplitude formulae, (17) and (25), determining the Regge pole positions and the associated residues have been applied to potentials of the Lennard–Jones (12, 6) type. Calculations have been made for the potential (5) and parameters

Table 1. The first 15 Regge pole positions and residues for the potential (5) and parameters $A = 141.425$, $K = 5$, $C = 0$, $s = 0$ approximating non-reactive scattering of K by HBr. The power of ten by which the entry for the residue should be multiplied is given in a parenthesis..

n	Re l_n	Im l_n	Re r_n	Im r_n
0	180.01194 802439	21.21891 512843	5.77470 7026	4.53347 6997 (5)
1	179.23898 784084	24.03474 884056	−1.23424 0659	−6.22386 4836 (6)
2	178.52289 375120	26.89009 534776	−1.43769 2536	2.06831 7707 (7)
3	177.86657 699632	29.78018 810164	6.16778 2768	−0.35239 6135 (7)
4	177.27239 060119	32.70007 684278	−6.09585 0924	−8.71245 4078 (7)
5	176.74212 599615	35.64469 252487	−0.69323 0414	1.19833 6299 (8)
6	176.27701 612317	38.60891 259111	1.40395 7405	0.30107 3710 (8)
7	175.87774 600573	41.58762 560819	0.02984 8349	−1.23374 7247 (8)
8	175.54447 127345	44.57579 387606	−9.06964 9267	0.31460 3272 (7)
9	175.27684 460365	47.56851 246641	−0.20692 0990	5.86207 6012 (7)
10	175.07404 953509	50.56106 317230	3.31864 2495	0.78875 4079 (7)
11	174.93484 067442	53.54896 204117	0.96384 8910	−1.54572 4035 (7)
12	174.85758 898894	56.52799 946735	−4.87737 1648	−7.67831 9456 (6)
13	174.84033 067693	59.49427 219168	−4.31626 1216	−0.00021 8985 (6)
14	174.88081 803256	62.44420 694809	−1.24300 4897	1.53338 1216 (6)

$A = 141.425$, $K = 5$, $C = 0$, $s = 0$ (Connor *et al* 1976, Pajunen 1988), and $A = 141.425$, $K = 5$, $C = 2 \times 10^4$, $s = 12$ (Connor *et al* 1979, Pajunen 1988) which correspond to elastic scattering of K by HBr. The numerical results are presented in tables 1 and 2, respectively. Calculations have also been performed for parameter values $A = 53.401$, $K = 2.462$, $C = 1 \times 10^4$, $s = 20$ (Connor *et al* 1979, Pajunen 1988) corresponding to elastic scattering of Li by HBr. The Regge pole positions and residues for these parameters are in table 3. All the results in the tables are expected to be accurate, except for a slight uncertainty (due to round-off errors) in the last digit.

Table 2. The first 15 Regge pole positions and residues for the potential (5) and parameters $A = 141.425$, $K = 5.0$, $C = 2 \times 10^4$, $s = 12$ approximating reactive scattering of K by HBr. The power of ten by which the entry for the residue should be multiplied is given in a parenthesis.

n	Re l_n	Im l_n	Re r_n	Im r_n
0	192.35701 697690	19.37323 330320	2.08395 1558	−1.49212 8626 (3)
1	191.93607 835206	22.12443 748969	−1.78193 1999	−1.13573 5056 (4)
2	191.56072 720963	24.89339 580341	−2.27252 0918	8.11446 8711 (4)
3	191.23218 694799	27.67707 027566	2.17497 6156	0.15156 3186 (5)
4	190.95136 366049	30.47234 119133	−0.16757 3003	−4.14007 2331 (5)
5	190.71884 466553	33.27604 719548	−6.20061 3172	0.34254 4551 (5)
6	190.53490 240589	36.08502 423372	0.20350 9419	7.69436 5625 (5)
7	190.39950 338703	38.89614 260236	7.99851 2591	1.66105 5919 (5)
8	190.31232 171283	41.70634 143972	3.51857 1971	−6.76911 6268 (5)
9	190.27275 667267	44.51266 007291	−4.23406 8115	−4.81153 0446 (5)
10	190.27995 374713	47.31226 574202	−4.77076 8399	1.26093 6118 (5)
11	190.33282 833766	50.10247 735007	−1.03185 0301	3.38354 8388 (5)
12	190.43009 149304	52.88078 502310	1.41416 8689	1.93114 6426 (5)
13	190.57027 690451	55.64486 540219	1.54003 1274	0.14783 9427 (5)
14	190.75176 846855	58.39259 271994	7.59019 4586	−5.96279 2417 (4)

Table 3. The first 15 Regge pole positions and residues for the potential (5) and parameters $A = 53.401$, $K = 2.462$, $C = 1 \times 10^4$, $s = 20$ approximating reactive scattering of K of HBr. The power of ten by which the entry for the residue should be multiplied is given in a parenthesis.

n	$\mathrm{Re}\, l_n$	$\mathrm{Im}\, l_n$	$\mathrm{Re}\, r_n$	$\mathrm{Im}\, r_n$
0	76.93675 231616	4.67764 625857	−4.28736 7297	−1.01170 5778 (1)
1	76.69124 265644	7.52121 295041	0.65225 7503	2.04056 7134 (2)
2	76.56189 829690	10.36977 300855	3.56214 6457	−2.75296 8656 (2)
3	76.53938 446616	13.21475 768514	−4.06064 6289	−4.04478 0153 (2)
4	76.61961 547167	16.04755 421752	−4.03848 0246	3.30486 3805 (2)
5	76.79887 476652	18.85793 028405	1.31335 3152	3.55492 4352 (2)
6	77.07176 956914	21.63532 394264	2.33123 8271	0.46802 1776 (2)
7	77.43099 573032	24.37014 940204	1.15573 6076	−0.79312 5378 (2)
8	77.86781 466543	27.05457 084008	2.36262 2158	−7.18850 3120 (1)
9	78.37270 846800	29.68280 726378	−0.66496 8333	−4.09789 3701 (1)
10	78.93598 862116	32.25111 745195	−1.12288 5120	−2.02355 7723 (1)
11	79.54827 512074	34.75759 521965	−9.00300 0026	−9.80654 3178 (0)
12	80.20082 902290	37.20187 189039	−6.19982 1250	−5.01964 7693 (0)
13	80.88575 206699	39.58479 191223	−4.12040 9880	−2.83810 3758 (0)
14	81.59607 923553	41.90810 247845	−2.75158 2950	−1.80244 6287 (0)

In practice, the Regge pole positions were found by iterating (17) in the complex l-plane using Müller's method. The residues were then determined from (25). The partial derivative of $D_n(l)$ with respect to l, required for the evaluation of (25), may be calculated by means of numerical differentiation of (17). Alternatively, the system of first-order differential equations corresponding to (9) can be extended to determine also the partial derivative of $q(z)$ with respect to l. This is, although computationally faster and conceptually more accurate, not a simple method because of the complexity of the higher-order phase-integral expressions used to initiate the numerical integration. If, however, only reasonably accurate results are required the latter approach should be preferred.

Semiclassical and complex coordinate methods have been used by Connor *et al* (1976, 1979) to determine the Regge pole positions and residues for the potential (5) and the above parameters. Recently Pajunen (1988) used the Prüfer approach to investigate the problem. Our results were primarily compared to those of Pajunen (1988) for two reasons: first, they are claimed to be of higher accuracy than those of Connor *et al*; secondly, the Prüfer method of Pajunen is based on numerical integration of a slowly varying phase, and is therefore similar to the phase-amplitude method of the present paper. A comparison with the results obtained by Pajunen (1988) shows that the Regge pole positions obtained by Pajunen are confirmed and increased in accuracy by at least six digits by the present treatment. For each residue, Pajunen's result generally agrees with that obtained from (25) to three decimal places. In a few cases the discrepancy is in the fourth decimal place (which is the accuracy quoted by Pajunen), but there are also cases where it is larger. However, it is clear from the pole positions that the numerical accuracy of the present treatment is much higher than that used by Pajunen. Moreover, while Pajunen's method for obtaining the residues is rather *ad hoc* (it is at least not properly described) our residues are determined from (25) which followed from a rigorous derivation. Hence, we believe that the present results should be trusted.

It is obvious from tables 1–3 that the phase-amplitude method yields very accurate numerical results for the Regge pole problem. In fact, the present treatment is much more accurate than any previously published investigation. The only exception is recent phase-integral calculations in high orders of approximation by Amaha and Thylwe (1991). The phase-amplitude results presented in our tables are in complete agreement with those of the phase-integral calculations. Hence, the high accuracy of both methods is confirmed. However, it is conceivable that the phase-amplitude approach will be reliable also in situations where the phase-integral method can not be used. When several transition points lie close to each other the accuracy of the phase-integral method will be poor. The phase-amplitude method should not suffer from this deficiency.

We conclude that the Regge pole problem can straightforwardly be solved within the phase-amplitude method. Formulae determining the Regge pole positions and the corresponding residues have been derived. The results obtained from these formulae are of very high numerical accuracy. The phase-amplitude method must therefore be considered as an important alternative to any other numerical integration scheme or approximate analysis.

Appendix 1. On the occurence of oscillations in $q(z)$

In this appendix we argue that oscillations in $q(z)$ are unavoidable if the integration of (9) is continued through a zero of $R(z)$. We consider the situation depicted in figure 1, and assume that two exact solutions to the Schrödinger equation (6) can be represented by the two functions (8) on the anti-Stokes line Λ_3. The function $q(z)$ can then be expressed in terms of these two solutions, i.e.

$$q(z) = \frac{1}{\psi^+ \psi^-}. \tag{26}$$

Well away from the transition point, however, we have

$$\psi^+ \approx R^{-1/4}(z) \exp\left[+i \int_{t_2}^{z} R^{1/2}(z)\, dz \right] \tag{27}$$

and

$$\psi^- \approx R^{-1/4}(z) \exp\left[-i \int_{t_2}^{z} R^{1/2}(z)\, dz \right] \tag{28}$$

with the lower limit of integration chosen to be the transition point t_2. (In the analysis below we consider the case where $R^{1/2}(z)\, dz$ is positive and increasing as we move

away from the transition point t_2 along Λ_3.) It follows from (26) that the numerically determined function $q(z)$ is not essentially more oscillating than $R^{1/2}(z)$. At least not as long as the approximate solutions (27) and (28) remain valid.

If $q(z)$ is numerically continued through the region surrounding the transition point t_2 onto the anti-Stokes line Λ_2 of figure 1 the two solutions ψ^+ and ψ^- will change according to the Stokes phenomenon. From, for example, chapter 7 in Fröman and Fröman (1965) it follows that the two approximate solutions are properly represented by

$$\psi^+ \approx R^{-1/4}(z) \exp\left[+i \int_{t_2}^{z} R^{1/2}(z)\,dz\right] - iR^{-1/4}(z) \exp\left[-i \int_{t_2}^{z} R^{1/2}(z)\,dz\right] \tag{29}$$

and

$$\psi^- \approx R^{-1/4}(z) \exp\left[-i \int_{t_2}^{z} R^{1/2}(z)\,dz\right] \tag{30}$$

for z well away from the transition point t_2 on Λ_2. These expressions, together with (26), imply that the exact function $q(z)$ (as numerically continued from a point on the anti-Stokes line Λ_3) has the approximate behaviour

$$q(z) \approx R^{1/2}(z) \left(1 - i \exp\left[-2i \int_{t_2}^{z} R^{1/2}(z)\,dz\right]\right)^{-1}. \tag{31}$$

Hence, oscillations in the function $q(z)$ must appear after continuation onto the anti-Stokes line Λ_2.

References

Amaha A and Thylwe K E 1991 *Phys. Rev.* A **44**, 4203–9
Andersson N 1992 *Proc. R. Soc. Lond.* A **439** 47–58
Bain R A, Bardsley J N, Junker B R and Sukumar C V 1975 *J. Phys. B:* 7 2189–202
Bosanac S 1978 *J. Math. Phys.* **19** 789–97
Connor, J N L 1972 *Mol. Phys.* **23** 717–35
—— 1980 *Semiclassical Methods in Molecular Scattering and Spectroscopy* ed M S Child NATO ASI Series C vol 53 (Dordrecht, Riedel) pp. 45–107
—— 1982 *J. Phys. B* **15** 1683–92
—— 1990 *J. Chem. Soc. Faraday Trans.* **86** 1627–40
Connor J N L, Jakubetz W and Sukumar C V 1976 *J. Phys. B* **9** 1783–99
Connor J N L, Mackay D C and Sukumar C V 1979 *J. Phys. B* **12** L515–9
Connor J N L, Jakubetz W, Mackay D C and Sukumar C V 1980 *J. Phys. B* **13** 1823–37
Delos J B and Carlson C E 1975 *Phys. Rev.* A **11** 210–20
Dombey N and Jones R H 1968 *J. Math. Phys.* **9** 986–95
Fröman N and Fröman P O 1965 *JWKB Aproximation, Contributions to the Theory* (Amsterdam, North-Holland).
—— 1991 *Forty More Years of Ramifications: Spectral Asymptotics and its Applications* eds S A Fulling and F J Narcowich (Discourses in Mathematics and its Applications no 1, Texas A&M University) pp 121–59
Newman W I and Thorson W R 1972a *Phys. Rev. Lett.* **29** 1350–3
—— 1972b *Can. J. Phys.* **50** 2997–3022
Pajunen P 1988 *J. Chem. Phys.* **88** 4268–72
—— 1989 *J. Comp. Phys.* **82** 16–28
Pajunen P and Luppi J 1985 *J. Chem. Phys.* **82** 5118–20
Pajunen P and Tienari J 1986 *J. Comp. Phys.* **65** 159–69

Sukumar C V and Bardsley J N 1975 *J. Phys. B:* **8** 568–76
Thylwe K E and Fröman N 1983 *Ann. Phys.* **150** 413–31
Thylwe K E 1983a *J. Phys. A: Math. Gen.* **16** 1141–53
—— 1983b *J. Phys. A* **16** 3325–40
—— 1985 *J. Phys. A* **18** 3445–53
—— 1987 *Resonances—the Unifying Route Towards the Formulation of Dynamical processes* eds E Brändas
    and N Elander *(Springer Lecture Notes in Physics 325)* pp 281–311