An amplitude-phase approach to calculating Regge-pole positions and residues

2005 J. Phys. A: Math. Gen. 38 5305

(http://iopscience.iop.org/0305-4470/38/23/016)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **38** (2005) 5305–5313 doi:10.1088/0305-4470/38/23/016

An amplitude-phase approach to calculating Regge-pole positions and residues

Karl-Erik Thylwe[1] **and Dmitri Sokolovski**[2]

[1] KTH-Mechanics, Royal Institute of Technology, S-100 44 Stockholm, Sweden
[2] Department of Applied Mathematics, Queen's University, Belfast, BT7 1NN, UK

Received 23 March 2005, in final form 7 April 2005
Published 25 May 2005
Online at stacks.iop.org/JPhysA/38/5305

Abstract

New amplitude-phase formulae for Regge-pole positions and residues are derived. The derivation makes use of certain invariants of the Ermakov–Lewis type. The formulas allow calculation to be made on the real r-axis, with an additional flexibility to optimize its numerical aspects.

PACS numbers: 03.65.Ca, 03.65.Nk, 03.65.Sq, 34.50.−s, 34.80.Bm

1. Introduction

The complex angular momentum theory of potential scattering is a powerful tool for understanding interference effects in elastic, rotationally inelastic and reactive differential cross sections (see [1–3]).

Early analytic and semiclassical methods used for determining Regge-poles positions and residues were developed for specific potential models. Recently, more general approaches for calculating these quantities have been developed [3–10] for a number of diverse applications ranging from reactive atom–molecule collisions [3] to scattering of gravitational waves by relativistic black holes [11]. Among these, the semiclassical calculations [4] are usually accurate, but require detailed knowledge of the potential in the complex coordinate plane. Non-semiclassical approaches include the eigenvalue moment method [7], the use of absorbing potentials [12], direct evaluation of the Jost functions [8] and numerical analytic continuation of the S-matrix into the complex plane of the total angular momentum using the Padé approximants [9, 10]. All these approaches, with the exception of [9, 10] meet with difficulties when extended to several coupled channels or degrees of freedom, while the Padé reconstruction [9, 10] requires dense and highly accurate input data for the poles with large imaginary parts to be reproduced successfully.

It is, therefore, desirable to develop robust numerical methods, which could be applied where approximate approaches lose their accuracy or become cumbersome, e.g., in reactive molecular scattering [10]. The approach based on integrating the Schrödinger equation along the real coordinate axis while adjusting the (complex) value of the total angular momentum

goes back to Burke and Tate [13] and in the present work this method is simplified and generalized. To evaluate the S-matrix, one is required either to accurately estimate the Hankel function with a large complex index [13], or to integrate far into the asymptotic region where the centrifugal barrier can be neglected. The idea of using Milne's amplitude-phase equation (see [14]) to expedite such integration was first suggested in [15], while a more sophisticated amplitude-phase technique for calculating Regge poles can be found in [5]. Applications of similar techniques to bound states calculations can be found in [16, 17].

The purpose of this work is to apply the amplitude-phase method for Regge-pole calculations using the recent amplitude-phase representation of the potential scattering S matrix given in [18]. In its present form, the method does not rely on the use of (semi-classical or quantal) transition points and anti-Stokes' lines that are central to Andersson's approach in [5], but such considerations can be included later. The rest of the paper is organized as follows: in section 2 we present the basic equations of the amplitude-phase method, i.e. the Schrödinger and the Milne equations defining the so-called Ermakov system [19] from which the expression for the S-matrix is derived. The new Regge-pole formulae obtained from the S-matrix representation are given in section 3. An analysis of the choice of matching point is presented in section 4. Numerical results for an attractive square-well potential are analysed in section 5, and section 6 contains our conclusions.

2. The S matrix in the amplitude-phase representation

The complex angular momentum analysis is based on the radial Schrödinger equation

$$\frac{\mathrm{d}^2\Psi_\ell(r)}{\mathrm{d}r^2} + \left[\frac{2m}{\hbar^2}\,(E - V(r)) - \frac{\ell(\ell+1)}{r^2}\right]\Psi_\ell(r) = 0, \tag{1}$$

where ℓ is the partial-wave quantum number. The scattering solution is regular at the origin, i.e.

$$\Psi_\ell(0) = 0, \qquad \mathrm{Re}\,\ell > -\tfrac{1}{2}, \tag{2}$$

and it satisfies the asymptotic boundary condition

$$\Psi_\ell(r) \sim N_\ell\left(\mathrm{e}^{-\mathrm{i}[\kappa(r)-\pi\ell/2]} - S_\ell \mathrm{e}^{\mathrm{i}[\kappa(r)-\pi\ell/2]}\right), \qquad r \to +\infty, \tag{3}$$

where N_ℓ is a normalization factor, $\kappa(r) = kr$ if the potential tail vanishes sufficiently fast as $r \to +\infty$, and $\kappa(r) = kr - \eta \ln 2kr$ if the potential contains a Coulomb tail, η being the well-known Sommerfeld parameter. In both cases $\kappa(r)$ satisfies

$$\frac{\mathrm{d}\kappa(r)}{\mathrm{d}r} \to k, \qquad r \to +\infty, \tag{4}$$

with

$$k = \sqrt{\frac{2mE}{\hbar^2}}. \tag{5}$$

The amplitude-phase method makes use also of the particular solution of the nonlinear Milne equation [14]

$$\frac{\mathrm{d}^2 u_\ell}{\mathrm{d}r^2} + \left[\frac{2m}{\hbar^2}\,[E - V(r)] - \frac{\ell(\ell+1)}{r^2}\right]u_\ell = u_\ell^{-3} \tag{6}$$

which tends to a constant in the asymptotic limit of large r,

$$u_\ell(+\infty) = k^{-1/2}. \tag{7}$$

In the present context this 'scattering Milne solution' defines an outgoing Jost solution $\Psi_\ell^+(r)$ given by [18]

$$\Psi_\ell^+(r) = u_\ell(r)\exp\left[\mathrm{i}\int^r u_\ell^{-2}(r')\,\mathrm{d}r'\right] \propto k^{-1/2}\exp(\mathrm{i}kr), \qquad r\to+\infty. \tag{8}$$

With the generalized amplitude-phase method in [18] one derives the S-matrix formula

$$S_\ell = \frac{\Lambda_+(\ell)}{\Lambda_-(\ell)}\exp(2\mathrm{i}\Delta(\ell). \tag{9}$$

In (9) the phase $\Delta(\ell)$ is given by the integral

$$\Delta(\ell) = \lim_{r\to+\infty}\exp\left(\mathrm{i}\left[\int_{r_0}^r u_\ell^{-2}\,\mathrm{d}r - \kappa(r)\right] + \mathrm{i}\pi\ell/2\right), \tag{10}$$

where r_0 is an unspecified phase reference point, $u_\ell(r)$ is the particular scattering solution of the Milne equation and $\kappa(r) = kr$ for short-range potentials, while for a Coulomb-like potential with the Sommerfeld parameter η, $\kappa(r) = \eta\ln(2kr)$ must be used. The quantities $\Lambda_\pm(\ell)$ are the Wronskian- or Ermakov–Lewis-type invariants [19, 20], i.e. quantities independent of the radial variable r. The invariants are expressed in terms of the scattering Milne solution and the regular radial Schrödinger solution as

$$\Lambda_-(\ell) = \left[\Psi'_\ell(r_m)u_\ell(r_m) - \Psi_\ell(r_m)u'_\ell(r_m) - \mathrm{i}\frac{\Psi_\ell(r_m)}{u_\ell(r_m)}\right]\exp\left(\mathrm{i}\int_{r_0}^{r_m} u_\ell^{-2}\,\mathrm{d}r\right), \tag{11a}$$

$$\Lambda_+(\ell) = \left[\Psi'_\ell(r_m)u_\ell(r_m) - \Psi_\ell(r_m)u'_\ell(r_m) + \mathrm{i}\frac{\Psi_\ell(r_m)}{u_\ell(r_m)}\right]\exp\left(-\mathrm{i}\int_{r_0}^{r_m} u_\ell^{-2}\,\mathrm{d}r\right), \tag{11b}$$

where the intermediate point r_m can be chosen at one's convenience, and r_0 is the arbitrary phase reference point mentioned earlier.

3. Application to the Regge-pole calculations

It is readily seen that the Regge poles, i.e. the poles of the S matrix in the complex ℓ-plane, may arise from the zeros of the denominator of equation (9) and are then determined by the condition

$$\Lambda_-(\ell_n) = 0. \tag{12}$$

In the neighbourhood of a pole ℓ_n the expansion of $\Lambda_-(\ell)$ is

$$\Lambda_-(\ell) \approx \frac{\partial\Lambda_-(\ell_n)}{\partial\ell}(\ell - \ell_n), \tag{13}$$

so that the expression for the residue takes the form

$$\rho_n = \mathrm{Res}_{\ell=\ell_n} S_\ell = \frac{\Lambda_+(\ell_n)}{\partial\Lambda_-(\ell_n)/\partial\ell}\,\mathrm{e}^{2\mathrm{i}\Delta_{\ell_n}}. \tag{14}$$

It is convenient to choose the reference point r_0 to coincide with the point r_m where the invariants $\Lambda_\pm(\ell)$ are calculated. The phase integrals in (11a) and (11b) then vanish and the Regge-pole condition becomes

$$\Lambda_-(\ell_n) = \Psi'_{\ell_n}u_{\ell_n} - \Psi_{\ell_n}u'_{\ell_n} - \mathrm{i}\frac{\Psi_{\ell_n}}{u_{\ell_n}} = 0, \tag{15}$$

so that

$$\Lambda_+(\ell_n) = 2\mathrm{i}\frac{\Psi_{\ell_n}}{u_{\ell_n}}, \tag{16}$$

and

$$\rho_n = \frac{2\mathrm{i}\Psi_{\ell_n}}{u_{\ell_n}(\partial\Lambda_-(\ell_n)/\partial\ell)}\exp\left(2\mathrm{i}\Delta_{\ell_n}\right). \tag{17}$$

It may also be convenient to rewrite the Regge-pole condition as

$$\Lambda_-(\ell_n)\Big/\left(\Psi_{\ell_n}u_{\ell_n}\right) = \frac{\Psi'_{\ell_n}}{\Psi_{\ell_n}} - \frac{u'_{\ell_n}}{u_{\ell_n}} - \mathrm{i}\frac{1}{u^2_{\ell_n}} = 0. \tag{18}$$

Equation (18) expresses that the logarithmic derivative of the regular radial solution $\Psi_\ell(r)$ matches the logarithmic derivative of the outgoing Jost solution $\Psi^+_\ell(r)$, expressed in terms of the Milne amplitude $u_\ell(r)$, at some matching point r_m. The particular solution $u_\ell(r)$ satisfying (7) is, typically, a slowly varying function away from the origin and can be accurately obtained by integrating from the far asymptotic region. In addition, for $\mathrm{Re}\,\ell > -\frac{1}{2}$ the regular radial solution can be easily integrated from the origin outwards, so that equations (12) and (14) provide a convenient numerical tool for evaluating both the poles positions and the residues. The optimal numerical choice of the matching point r_m will be further discussed in section 4.

4. The choice of the matching point

The present section deals with the unspecified matching point r_m and some problems encountered when it is used at (or near) the boundary points. Consider the choice of the matching point r_m for short ranged potentials such that $V(r) \approx 0$ for $r > R$. For r_m in the far asymptotic region ($r_m \gg R$) such that $u_l(r) \approx k^{-1/2}$, equation (18) reduces to the simplified boundary condition for Ψ_l,

$$(\mathrm{d}/\mathrm{d}r - \mathrm{i}k)\Psi_l(r_m) = 0. \tag{19}$$

This choice is, however, impractical as it requires an accurate integration of the Schrödinger equation over a region which can be large, owing to the slow convergence of the Hankel functions to their exponential form, and where Ψ_l is highly oscillatory. It is more convenient to choose r_m just outside the range of the potential, $r_m > R$, in which case $u_\ell(r_m)$ contains no information about the scattering dynamics and serves solely to represent the Hankel function $h^1_\ell(kr)$ describing the outgoing wave in the potential-free region. Unlike $h^1_\ell(kr)$, $u_\ell(r)$ usually varies slowly, which allows for the accurate integration of the Milne equation [14, 15]. If the matching point is chosen inside the potential range, $r_m < R$, Ψ_ℓ contains the information about the inner part of the potential, $r < r_m$, while the scattering by its tail and the potential-free region is described by $u_\ell(r)$. Finally, r_m could in principle be chosen close to 0 (or the potential wall in the case of a hard sphere) so that the scattering problem is described purely in terms of the Milne equation (6). Such a choice is now studied in some detail.

Relation (8) can be inverted by solving equation (18) in order to express $u_\ell(r)$ in terms of $\Psi^{-2}_\ell(r')$. This yields

$$u_\ell(r) = \Psi_\ell(r)\left[C' - 2\mathrm{i}\int^r \Psi^{-2}_\ell(r')\,\mathrm{d}r'\right]^{1/2} \tag{20}$$

and

$$\int^r u^{-2}_\ell(r')\,\mathrm{d}r = \frac{\mathrm{i}}{2}\log\left[C' - 2\mathrm{i}\int^r \Psi^{-2}_\ell(r')\,\mathrm{d}r'\right] + C'', \tag{21}$$

where C' and C'' are arbitrary constants. Equation (20) suggests that $u_\ell(r)$ may, due to the presence of the integral of Ψ_ℓ^{-2}, have a singularity near a zero of $\Psi_\ell(r)$. Assuming the matching point r_m is chosen at the boundary point where the regular Schrödinger solution vanishes, the regular Schrödinger solution is written as

$$\Psi_\ell(r) \approx (r - r_m)^{\alpha+1}, \qquad r \to r_m, \tag{22}$$

where $r_m = 0$ and $\alpha = \ell$ for regular singular potentials and $r_m = R$ and $\alpha = 0$ for hard sphere potentials. It follows from (20) that

$$u_\ell(r) \approx \left[\frac{\mathrm{i}}{\alpha + 1/2}\right]^{1/2} (r - r_m)^{1/2}, \qquad r \to r_m, \quad \mathrm{Re}\,\alpha > -\frac{1}{2}, \tag{23}$$

so that the singular behaviour of $u_\ell(r)$ at the inner-boundary matching point is of the square root type, $u_\ell(r_m) = 0$ and $u'_\ell(r_m) = \infty$ for any exponent such that $\mathrm{Re}\,\alpha > -1/2$. A further problem arises when the phase $\int^r u_\ell^{-2}\mathrm{d}r$ has to be computed for this choice of matching point r_m. From (23) one obtains

$$\mathrm{i}\int^r u_\ell^{-2}\,\mathrm{d}r \approx C''' + (\alpha + 1/2)\ln(r - r_m),\ r \to r_m, \qquad \mathrm{Re}\,\alpha > -\frac{1}{2}, \tag{24}$$

where C''' is an integration constant. It is readily seen that

$$\exp\left(\mathrm{i}\int^r u_\ell^{-2}\,\mathrm{d}r\right) \sim (r - r_m)^{\alpha+1/2}, \qquad r \to r_m, \quad \mathrm{Re}\,\alpha > -\frac{1}{2}. \tag{25}$$

Thus, for a 'soft' potential, dominated at the origin by the centrifugal barrier, the Milne solution must vanish at $r = 0$, and for a hard sphere potential the Milne solution must vanish at its boundary $r = R$. Finally, for a strongly repulsive 'hard' potential,

$$V(r) \approx gr^{-n}, \qquad n > 2, \qquad r \to 0 \tag{26}$$

one has the accurate WKB approximation for the regular solution [21]

$$\Psi_\ell(r) \sim r^{n/4}\exp[-2g^{1/2}r^{1-n/2}/(n-2)], \qquad r \to +0. \tag{27}$$

Inserting equation (27) into equation (20), one finds

$$u_\ell(r) \approx (-1/g)^{1/4}r^{n/4}, \qquad r \to +0. \tag{28}$$

Note that in all cases the Milne solution, representing the Regge state, must vanish at the left boundary, thus rendering the $1/u_\ell^3$-term in equation (6) infinite. Also, the derivative of the Milne solution will diverge there (with the exception of singular potentials with $n = 4k, k = 1, 2, 3, \ldots$) thus presenting possible additional difficulties for numerical integration. Thus, it is desirable to choose the matching point away from the left boundary, in order to avoid the divergences, yet sufficiently close to utilize the non-oscillating character of u_ℓ.

5. The model and numerical results

The method is applied to an attractive square-well potential model defined by

$$\begin{aligned} V(r) &= -V_0, \quad 0 \leqslant r \leqslant R, \\ &= 0, \quad r > R. \end{aligned} \tag{29}$$

This model potential allows for a rigorous comparison with results from an analytic closed-form expression of the S-matrix (see formula (30) below). Physically this model corresponds, for example, to the scattering of electro-magnetic waves from a spherical water droplet [1].

Table 1. Resonance Regge-pole positions determined by a square-well potential with depth $V_0 = 200$ and range $R = 1$ at an energy of $E = 100$.

n	ℓ_n (amplitude-phase)	ℓ_n (Padé)
0	13.395 33 + 0.007 64i	13.283 + 0.007i
1	10.038 67 + 0.205 72i	10.042 + 0.218i
2	7.087 65 + 0.407 71i	7.077 + 0.383i
3	4.480 02 + 0.454 83i	4.551 + 0.437i
4	2.150 60 + 0.450 65i	2.344 + 0.547i
5	0.024 52 + 0.427 64i	0.609 + 0.585i

The corresponding semiclassical Regge representation for the scattering amplitude was recently studied in [10]. The Regge pole structure for $V(r)$ contains narrow and broad resonances, located below and above the centrifugal barrier, respectively, as well as a sequence of the diffraction poles associated with the scattering off the sharp cut-off [1]. In this section we will calculate the positions and residues for the resonance poles for the model with $V_0 = 200$, $R = 1$, and the scattering energy $E = 100$ with units such that $2m/\hbar^2 = 1$. The results will be compared with the values obtained by constructing a [9/9] Padé approximant [10] from the S-matrix computed for the first 19 partial waves, $\ell = 0, 1, \ldots, 19$.

For the potential (29) the obvious matching point is $r_m = R$, at which the regular Schrödinger solution should not be exactly zero for a Regge state (see the preceding section). Unfortunately, other ways to choose the matching point are not possible in the present formulation.

The regular Schrödinger solution is integrated from a point sufficiently near $r = 0$ to $r = R$, for an initial guess of the Regge-pole position ℓ_n. In the present case the initial guesses are provided by the set of pole positions calculated with the Padé approximant, specified above. The Milne solution is integrated from a large value $r \approx 10^8$ to the matching point $r = R$, where the Regge pole condition is tested and a new initial guess is estimated by the Newton iteration scheme. The iteration process stops when the absolute value of the Newton correction of the pole position is less than a given number; here 10^{-6} is used.

An additional check of the accuracy of the numerical results can be done using the analytic S-matrix formula for the square-well potential [1]

$$S_\ell = -\frac{H^{(2)}_{\ell+/2}(\beta)}{H^{(1)}_{\ell+/2}(\beta)} \left\{ \frac{\ln' H^{(2)}_{\ell+/2}(\beta) - N \ln' J_{\ell+/2}(\alpha)}{\ln' H^{(1)}_{\ell+/2}(\beta) - N \ln' J_{\ell+/2}(\alpha)} \right\}, \tag{30}$$

where $H^{(1,2)}_{\ell+/2}(\beta)$ are the cylindrical Hankel functions and $J_{\ell+/2}(\alpha)$ is the cylindrical Bessel function. $\ln'$ denotes the logarithmic derivative with respect to the arguments $\alpha = \sqrt{E + V_0}R$ and $\beta = \sqrt{E}R$, and $N = \alpha/\beta$.

The absolute value of the denominator in the embraced factor in the analytic formula (30) is approximately 10^{-5} for the pole positions obtained in the present amplitude-phase calculations. In table 1 the pole positions of the amplitude-phase method are presented with five decimals and in the order of decreasing real parts. The less accurate pole positions given by the Padé method that led to converging results for the amplitude-phase method are presented with tree decimals. The corresponding pole residues are given in table 2.

The pole number n, which semiclassically corresponds to the number of intermediate complex-r nodes (zeros) of the wavefunction, cannot be simply deduced from the Regge-pole condition (15) and is assigned by studying the regular wavefunctions on the real r-axis. In table 1 one notes that the $n = 0$ is a 'narrow' resonance, typically located below the top of

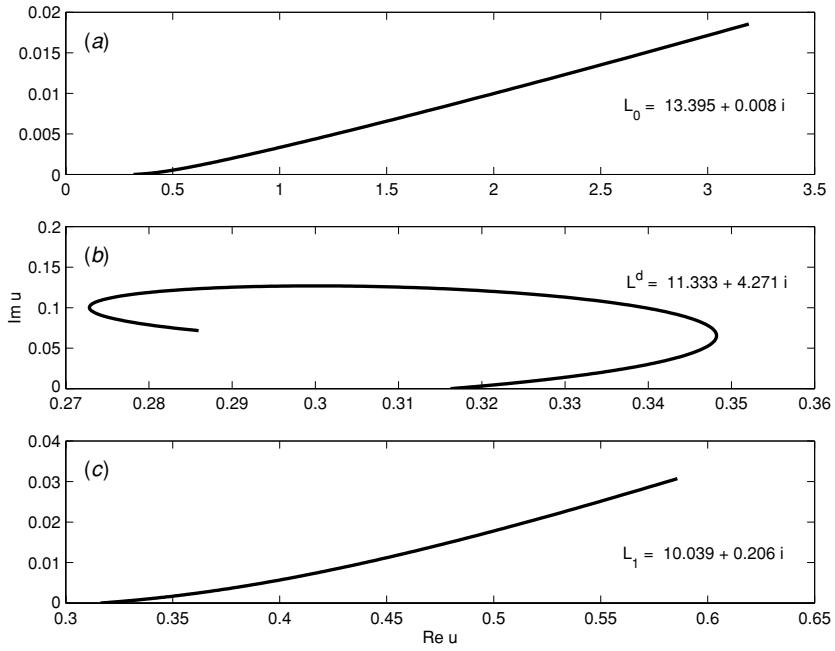

Figure 1. Illustration of the complex Milne solutions corresponding to the resonance Regge poles with $n = 0, 1$, in the tables and also to the leading diffraction pole (31). The imaginary part of $u_\ell(r)$ is plotted against its real part for Regge state.

Table 2. Residues corresponding to the Regge poles in table 1.

n	ρ_n (amplitude-phase)	ρ_n (Padé)
0	0.0004 + 0.0153i	0.0002 + 0.013i
1	0.2769 + 0.2549i	0.30 + 0.27i
2	−0.3093 − 0.4131i	−0.28 − 0.39i
3	0.3647 − 0.2351i	0.34 − 0.23i
4	0.3515 + 0.0821i	0.35 + 0.04i
5	0.2662 + 0.1538i	0.20 − 0.16i

the centrifugal barrier, whereas the rest represent the 'broad' resonances close to or above the barrier top [1]. Unitarity of the S-matrix requires that each pole be complemented by a symmetric Regge zero in the fourth quadrant of the complex ℓ-plane. Accordingly, the narrow $n = 0$ pole is almost cancelled by its zero and has a relatively small residue. The broad poles with $n > 0$ have larger residues of the same order and, unlike the narrow resonance significantly affect the angular distribution.

The amplitude-phase method also located the leading 'diffraction pole' [1] with

$$\ell^d = 11.333\,39 + 4.270\,62\mathrm{i}, \quad \rho^d = 0.4969 - 0.2495\mathrm{i}, \tag{31}$$

not reproduced by the [9/9] Padé approximant. The diffraction pole defines a decaying surface wave with a narrow angular range in the forward direction. For this state, the Milne solution in figure 1(b), initially real and equal to $k^{-1/2}$ with $k = \sqrt{E}$, remains almost constant (note the difference in the scale between figures 1(a), (b) and (c), but with a tendency to become non-monotonic.

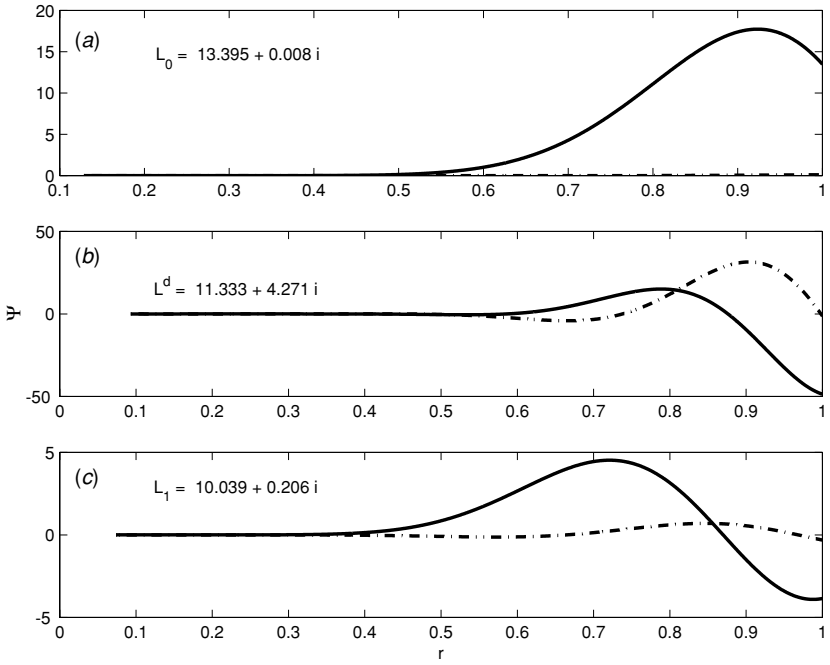

Figure 2. Illustration of the r-behaviour of the regular Schrödinger solutions corresponding to the resonance Regge poles labelled with $n = 0, 1$, in the tables and also the leading diffraction pole (31). The solid lines represent the real parts of the solutions and the dashed-dotted ones represent the imaginary parts.

Finally, figure 2 shows the behaviour of the regular Schrödinger wavefunctions in the interior region $r < R$ for $n = 0, 1$ and for the diffraction Regge state (31). Comparing the $n = 1$ resonance wavefunction with that for the diffraction surface state, one notes that they have the same number of nodes (i.e. one) in their real parts. This problem of distinguishing and classifying complex (Regge) states is typical for a non-semiclassical approach. Note, however, the present amplitude-phase method may (in principle) be extended to include all semiclassical ingredients in order to make the classification of states easier. Thus, for the present problem it is possible to use the contours of the semiclassical Stokes'- and anti-Stokes' lines and for each anti-Stokes' line find an appropriate Milne function that is strictly monotonic in its complex radial behaviour.

6. Conclusions

The main achievement of the present work is the demonstration of a method for calculating Regge-pole positions and residues by using the real r axis. The formulation of the present amplitude-phase method, based on recent studies of the invariants of Ermakov systems of equations, contains a flexibility in the choice of a 'matching point', which allows us to optimize and simplify the numerical calculations for smooth potentials. However, for the discontinuous potential studied in section 5 this flexibility could not be utilized.

It should be emphasized that, except for discontinuous potentials, the method contains the option of using complex-valued matching points (in order to avoid numerical integration of oscillatory functions) and of using several complex matching points when many barriers of the

effective real (smooth) potential is present. Such improvements may be needed if important Regge poles are located far out in the complex plane, but it requires more than one Milne solution to describe the regular wavefunction in a subdivided outer region. Improvements of this kind have been made and will soon be published elsewhere.

Further applications of the amplitude-phase method, such as calculations of Siegert states [22], accurate evaluation of the Bessel functions of complex index and extensions to multichannel scattering will be considered in future work.

Acknowledgments

One of us (DS) is grateful to KET for his hospitality during the stay in Stockholm, and to the EPSRC (UK) for the support of the project through the Grant GR/S03799/01.

References

[1] Adams J A 2002 *Phys. Rep.* **356** 229–365
[2] Connor J N L 1990 *J. Chem. Soc. Faraday Trans.* **86** 1627
[3] Sokolovski D, Connor J N L and Schatz G C 1995 *J. Chem. Phys.* **103** 5979
[4] Connor J N L 1973 *Mol. Phys.* **25** 1469
Connor J N L 1968 *Mol. Phys.* **15** 621
Connor J N L 1972 *Mol. Phys.* **23** 717
Dombey N and Jones R H 1968 *J. Math. Phys.* **9** 986
Delos J B and Carlson C E 1975 *Phys. Rev.* A **11** 210
Amaha A and Thylwe K-E 1991 *Phys. Rev.* A **44** 4203
Fröman N and Fröman P O 1991 *Phys. Rev.* **43** 3563
[5] Andersson N 1993 *J. Phys. A: Math. Gen.* **26** 5085
[6] Kais S and Herschbach D R 1993 *J. Chem. Phys.* **98** 3990
[7] Handy C R and Msezane A Z 2001 *J. Phys. A: Math. Gen.* **34** L531
Handy C R, Msezane A Z and Yan Z 2002 *J. Phys. A: Math. Gen.* **35** 6359
[8] Sofianos S A, Rakityansky S A and Massen S E 1999 *Phys. Rev.* A **60** 337
[9] Vrinceanu D, Msezane A Z, Bessis D, Connor J N L and Sokolovski D 2000 *Chem. Phys. Lett.* **324** 311
[10] Sokolovski D and Msezane A Z 2004 *Phys. Rev.* A **70** 032710
[11] Andersson N and Thylwe K-E 1993 *Class. Quantum Grav.* **11** 2991
[12] Sokolovski D, Tully C and Crothers D S F 1998 *J. Phys. A: Math. Gen.* **31** 6525
[13] Burke P J and Tate C 1969 *Comput. Phys. Commun.* **1** 97
[14] Milne W E 1930 *Phys. Rev.* **35** 863
[15] Wheeler J A 1937 *Phys. Rev.* **52** 1123
[16] Korsch H J and Laurent H 1981 *J. Phys. B: At. Mol. Phys.* **14** 4213
[17] Matzkin A 2000 *Phys. Rev.* A **63** 012103
Matzkin A 2001 *J. Phys. A: Math. Gen.* **34** 7833
[18] Thylwe K-E 2004 *J. Phys. A: Math. Gen.* **37** L589
[19] Ermakov V P 1880 *Univ. Izv. Kiev Serie III* **9** 1
Lewis H R 1967 *Phys. Rev. Lett.* **18** 510
Lewis H R 1967 *Phys. Rev. Lett.* **18** 636 (erratum)
Lewis H R 1968 *J. Math. Phys.* **9** 1976
[20] Thylwe K-E 2002 *J. Phys. A: Math. Gen.* **35** 4359
[21] Frank W M, Land D J and Spector R M 1971 *Rev. Mod. Phys.* **43** 36-98
[22] Sitnikov G V and Tolstikhin O I 2003 *Phys. Rev.* A **67** 032714