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Improved amplitude-phase method for complex angular momentum analysis

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Abstract

An amplitude-phase formula for the S matrix using *two* Milne solutions and the regular Schrödinger solution is derived. The formula is particularly useful in the analysis of Regge poles located far out in the complex ℓ -plane, particularly for discontinuous scattering potentials. Numerical applications for an attractive square-well potential and an inverse-power potential $\sim r^{-4}$ are presented.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

In this work the scattering matrix for scalar central forces is analysed as a function of complex angular momentum with a new approach to the amplitude-phase method [1, 2] developed from the earliest formulations [3] and a more recent one [4]. In particular, formulae for Regge-pole properties are generalized to account for distant regions of the complex angular momentum plane.

As seen in the current literature [5–12], serious attempts are made to develop methods capable of determining Regge-pole positions and residues without detailed knowledge of the complex properties of the potential and of the topology of so-called Stokes' and anti-Stokes' lines. Applications of existing semiclassical methods of the phase-integral type have proven to give very accurate pole positions and pole residues for the specific potentials considered [13], see also [14]. The main drawback of these semiclassical methods is the requirement of detailed knowledge of Stokes' and anti-Stokes' lines, complex transition points as well as connection formulae. It is interesting to note that perhaps the only exact numerical method [4] that gave superior results for pole positions and residues a decade ago was also exploiting Stokes' and anti-Stokes' lines as well as complex transition points.

The amplitude-phase method [3] effectively uses the solutions of the nonlinear Milne equation to analyse the solutions of the radial Schrödinger equation. Particular Milne

solutions are more or less monotonic as functions of the radial variable r , and by using them the calculations of Schrödinger solutions can be made very accurately. However, the monotonic properties of Milne solutions seem to relate closely to what is known in semiclassical approaches as Stokes' and anti-Stokes' lines. The Andersson approach in [4] is fully exploiting the semiclassical techniques of Stokes' and anti-Stokes' lines, and uses a transformed version of the Milne equation, the q -equation, where $q = u^{-2}$ and u is a Milne solution. As it stands, Andersson's formulation is very specific to the complex behaviour of particular potential models.

The recent amplitude-phase approach in [1, 2] is mainly exploiting certain invariant relations between Schrödinger solutions and Milne solutions. Positions and residues for the leading Regge poles could simply be calculated along the *real* r -axis [2] with this approach. From this point of view the recent version of the amplitude-phase method is easy to implement. However, along the *real* r -axis numerical difficulties will gradually appear for Regge poles located further away from the real ℓ -axis. The present work is focusing on an improvement of the recent flexible amplitude-phase method, so that it can be used for more accurate calculations of Regge poles further out in the complex angular momentum plane without the detailed use of Stokes' and anti-Stokes' lines. Another need for a generalization is the presence of model potentials having one or several points of discontinuity, for which the amplitude-phase method becomes inapplicable or seriously limited in applications; see [2]. Furthermore, the amplitude-phase approach in [1, 2] promises to be generalizable to coupled radial Schrödinger equations since the Ermakov–Lewis invariants are known in this case [15].

Basically, the weak point regarding the accuracy of the approach in [1, 2] is that both the Schrödinger solution and the scattering Milne solution cannot be kept non-oscillating for Regge poles with high quantum numbers. In order to express the S matrix in [1] in terms of non-oscillating quantities, it generally requires more than one Milne solution. A single Milne solution is known to be sufficiently smooth in a limited region of the complex r -plane. This situation can be illustrated on the real r -axis as in figure 1 for a real scattering potential with *two* internal wells. In figure 1 there are three classically allowed regions on the real r -axis corresponding to three semiclassical anti-Stokes' lines, respectively. In each such region there is an ideal, sufficiently smooth Milne solution that is useful also in the neighbouring classically forbidden regions (Stokes' lines). A detailed understanding of the regions of smoothness in the complex plane can be achieved in terms of the semiclassical Stokes' and anti-Stokes' lines associated with complex semi-classical turning points, as explained by Andersson [4].

In section 2 the basic S matrix derived in [1] and [2] is discussed. A generalization of the S matrix formula is derived in section 3, using two particular Milne solutions and valid in a large region of the complex angular momentum plane. Section 4 deals with formulae for determining Regge-pole positions and residues. Numerical applications are discussed in section 5 and conclusions are found in section 6.

2. Basic S matrix

The basic amplitude-phase formula for the S matrix as a function of the complex angular momentum quantum number ℓ is given by [1]

$$S_\ell = \frac{\Lambda_+(u_\ell, \ell)}{\Lambda_-(u_\ell, \ell)} e^{2i\Delta(u_\ell, \ell)}. \quad (1)$$

Equation (1) contains three key quantities; a particular Milne solution u_ℓ (see below), the two 'invariants' $\Lambda_\pm(u_\ell, \ell)$ and a complex phase $\Delta(u_\ell, \ell)$. The quantities $\Lambda_\pm(u_\ell, \ell)$ are obtained

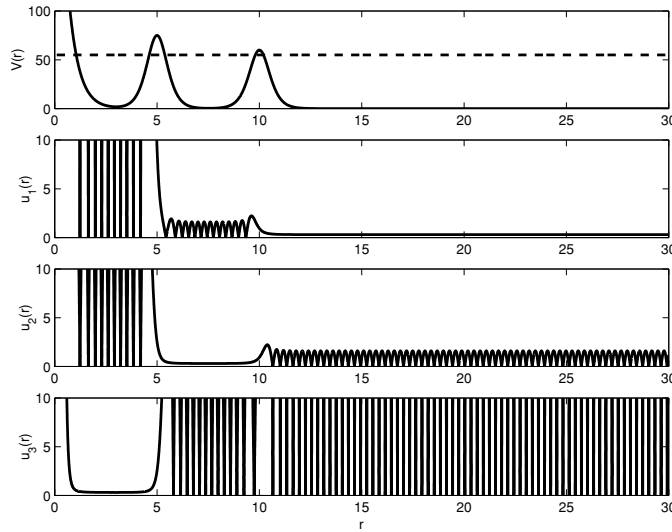


Figure 1. Illustration of typical behaviours of Milne solutions in a multi-well potential. The top subplot shows the scattering potential (solid line) and the energy (dashed line). The remaining subplots show three particular Milne solutions that are non-oscillatory in one of the three classically allowed regions of the real r -axis. In the asymptotic region there is a unique solution $u_1(r)$ that is constant in the limit $r \rightarrow +\infty$. This Milne solution tends to increase towards the first barrier region and becomes oscillatory in the remaining regions as $r \rightarrow +0$. In the outer local well one can find another Milne solution $u_2(r)$ from conditions satisfied by the WKB amplitude there and not too close to any turning point. $u_2(r)$ is numerically useful in an extended region including the neighbouring barriers. Similarly, one can define a smooth Milne solution in the inner local well that is useful in an extended region.

from Wronskian relations, satisfied by Schrödinger solutions, which can also be interpreted as so-called Ermakov–Lewis invariants [16, 17],

$$\Lambda_-(u_\ell, \ell) = \left[\Psi'_\ell(r_m)u_\ell(r_m) - \Psi_\ell(r_m)u'_\ell(r_m) - i \frac{\Psi_\ell(r_m)}{u_\ell(r_m)} \right] e^{i\phi(u_\ell, r_0, r_m)}, \quad (2a)$$

$$\Lambda_+(u_\ell, \ell) = \left[\Psi'_\ell(r_m)u_\ell(r_m) - \Psi_\ell(r_m)u'_\ell(r_m) + i \frac{\Psi_\ell(r_m)}{u_\ell(r_m)} \right] e^{-i\phi(u_\ell, r_0, r_m)}, \quad (2b)$$

with r_m being the (matching) point where the invariants are evaluated.

$\Psi_\ell(r)$ in (2a) and (2b) is the regular Schrödinger scattering solution, i.e.

$$\frac{d^2\Psi_\ell(r)}{dr^2} + \left[\frac{2m}{\hbar^2} (E - V(r)) - \frac{\ell(\ell + 1)}{r^2} \right] \Psi_\ell(r) = 0, \quad (3)$$

where ℓ is the partial-wave quantum number, m is the reduced mass, and $V(r)$ is the scattering potential. The regular solution $\Psi_\ell(r)$ is assumed to satisfy the boundary conditions

$$\Psi_\ell(0) = 0, \quad (4a)$$

$$\Psi_\ell(r) \sim e^{-i[\kappa(r) - \pi\ell/2]} - S_\ell e^{i[\kappa(r) - \pi\ell/2]}, \quad r \rightarrow +\infty, \quad (4b)$$

where $\kappa(r)$ satisfies the relation

$$\frac{d\kappa(r)}{dr} \rightarrow k, \quad r \rightarrow +\infty, \quad (5)$$

with

$$k = \sqrt{\frac{2mE}{\hbar^2}}. \quad (6)$$

In (2a) and (2b) there also appears the particular *scattering* Milne solution satisfying the Milne equation

$$\frac{d^2 u_\ell}{dr^2} + \left[\frac{2m}{\hbar^2} (E - V(r)) - \frac{\ell(\ell+1)}{r^2} \right] u_\ell = u_\ell^{-3}. \quad (7)$$

with the boundary condition

$$u_\ell(+\infty) = k^{-1/2}, \quad \frac{du_\ell(+\infty)}{dr} = 0. \quad (8)$$

The invariants in (2a) and (2b) also contain a phase integral

$$\phi(u_\ell, r_0, r_m) = \int_{r_0}^{r_m} \frac{dr'}{u_\ell^2(r')}, \quad (9)$$

where r_0 is an unspecified reference point, r_m is a matching point, and u_ℓ is the scattering Milne solution mentioned above. Finally, this phase integral with a different upper limit also appears in the overall phase $\Delta(u_\ell, \ell)$ in (1), given by

$$\Delta(u_\ell, \ell) = \lim_{r \rightarrow +\infty} \exp \left(i \left[\int_{r_0}^r u_\ell^{-2} dr - \kappa(r) \right] + i\pi\ell/2 \right). \quad (10)$$

Note that this phase combines with the phases in the ‘invariants’ in (2a) and (2b) to a total phase that is independent of the phase reference point r_0 . Therefore it is convenient to choose $r_0 = r_m$ in applications of the basic S -matrix formula (1). In [2] the basic S -matrix formula was used to derive equations for determining Regge-pole positions and residues on the real r -axis. A detailed discussion on the optimal choice of r_m for numerical purposes can be found in [2].

As pointed out in the introduction, the main weakness with the S -matrix formula using a single matching point is that both the Schrödinger solution and the single Milne solution cannot be kept non-oscillating for multi-well potentials. Particularly, the oscillations in the Milne solutions should be avoided if possible. A few oscillations in the Schrödinger solution are less alarming. In the complex angular momentum theory for smooth potentials, one can in many cases identify a ‘complex local well’ where the Schrödinger solution behaves oscillatory like in a real local well. This means that Regge poles with high quantum numbers become difficult to compute using a single matching point.

A typical such two-turning-point situation that generates a Regge pole is illustrated in figure 2. Most of the fundamental quantal interference occurs along the anti-Stokes’ lines that almost connect the turning points of the complex well. It therefore becomes increasingly difficult to obtain the relevant information of the Milne solution and the Schrödinger solution on the real r -axis if the complex well is located far from the real r -axis.

To add further flexibility to the method a second matching point is introduced in the subsequent section.

3. The S matrix expressed in terms of two Milne solutions

In this section a second Milne solution v_ℓ is introduced, which, as it turns out, will modify the invariants $\Lambda_\pm(u_\ell, \ell)$ in the basic S -matrix formula (1).

It is well known in the amplitude-phase theory that each Milne solution u_ℓ and v_ℓ defines a pair of particular (fundamental) solutions of the Schrödinger equation written as

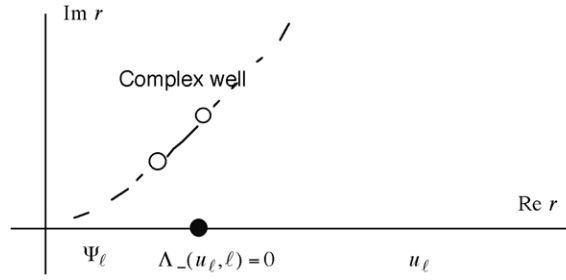


Figure 2. Illustration of a complex well defined by two complex turning points (open circles) and an anti-Stokes’ line joining them. Quantal interference in the complex well may result in the formation of a Regge state with purely outgoing travelling waves ‘leaking’ out to infinity $r \rightarrow +\infty$. A typical matching point on the real axis (solid circle) is indicated, where $\Lambda_{-}(u_{\ell}, \ell)$ in the Regge-pole condition is to be evaluated.

$$F^{\pm}(u_{\ell}, r_0, r) = u_{\ell}(r) e^{\pm i\phi(u_{\ell}, r_0, r)}, \quad \phi(u_{\ell}, r_0, r) = \int_{r_0}^r \frac{dr'}{u_{\ell}^2(r')}, \quad (11a)$$

$$F^{\pm}(v_{\ell}, r_0, r) = v_{\ell}(r) e^{\pm i\phi(v_{\ell}, r_0, r)}, \quad \phi(v_{\ell}, r_0, r) = \int_{r_0}^r \frac{dr'}{v_{\ell}^2(r')}, \quad (11b)$$

respectively. The amplitude-phase solutions of the Schrödinger equation $F^{+}(u_{\ell}, r_0, r)$ and $F^{-}(u_{\ell}, r_0, r)$ in [1] that are used to derive the basic S matrix in (1) can be expressed as a linear combination of the ‘intermediate’ solutions $F^{+}(v_{\ell}, r_0, r)$ and $F^{-}(v_{\ell}, r_0, r)$, i.e.

$$\begin{aligned} F^{+}(u_{\ell}, r_0, r) &= M_{11}F^{+}(v_{\ell}, r_0, r) + M_{21}F^{-}(v_{\ell}, r_0, r), \\ F^{-}(u_{\ell}, r_0, r) &= M_{12}F^{+}(v_{\ell}, r_0, r) + M_{22}F^{-}(v_{\ell}, r_0, r), \end{aligned} \quad (12)$$

where it is assumed that v_{ℓ} is more nicely behaved than u_{ℓ} in some important ‘intermediate’ region of the complex r -plane.

The relation between both pairs of solutions is determined next. Let the reference point r_0 be identical to the matching point for the amplitude-phase solutions (11a) and (11b), i.e. $r = r_0$. The four explicit matching equations are given by

$$\begin{aligned} u_{\ell}(r_0) &= M_{11}v_{\ell}(r_0) + M_{21}v_{\ell}(r_0), \\ u_{\ell}(r_0) &= M_{12}v_{\ell}(r_0) + M_{22}v_{\ell}(r_0), \\ u'_{\ell}(r_0) + iu_{\ell}^{-1}(r_0) &= M_{11}(v'_{\ell}(r_0) + iv_{\ell}^{-1}(r_0)) + M_{21}(v'_{\ell}(r_0) - iv_{\ell}^{-1}(r_0)), \\ u'_{\ell}(r_0) - iu_{\ell}^{-1}(r_0) &= M_{12}(v'_{\ell}(r_0) + iv_{\ell}^{-1}(r_0)) + M_{22}(v'_{\ell}(r_0) - iv_{\ell}^{-1}(r_0)), \end{aligned} \quad (13)$$

where M_{ij} can be solved as elements in the matrix

$$\mathbf{M} = \begin{pmatrix} \frac{1}{2}(-i\mathcal{P} + \mathcal{Q} + \mathcal{Q}^{-1}) & \frac{1}{2}(-i\mathcal{P} + \mathcal{Q} - \mathcal{Q}^{-1}) \\ \frac{1}{2}(i\mathcal{P} + \mathcal{Q} - \mathcal{Q}^{-1}) & \frac{1}{2}(i\mathcal{P} + \mathcal{Q} + \mathcal{Q}^{-1}) \end{pmatrix}, \quad (14)$$

with

$$\mathcal{Q} = u_{\ell}(r_0)/v_{\ell}(r_0), \quad \mathcal{P} = v_{\ell}(r_0)u'_{\ell}(r_0) - v'_{\ell}(r_0)u_{\ell}(r_0). \quad (15)$$

The linear relation (12) is now determined with the coefficients satisfying

$$\det \mathbf{M} = 1. \quad (16)$$

To proceed, the basic invariants $\Lambda_{\mp}(u_{\ell}, \ell)$ can be expressed in terms of the new pair of solutions (11b) using (12) together with the linearity of Wronskian determinants. One obtains

$$\Lambda_{-}(u_{\ell}, \ell) = M_{11}\Lambda_{-}(v_{\ell}, \ell) + M_{21}\Lambda_{+}(v_{\ell}, \ell), \quad (17a)$$

$$\Lambda_{+}(u_{\ell}, \ell) = M_{12}\Lambda_{-}(v_{\ell}, \ell) + M_{22}\Lambda_{+}(v_{\ell}, \ell), \quad (17b)$$

where

$$\Lambda_{-}(v_{\ell}, \ell) = \left[\Psi'_{\ell}(r_m)v_{\ell}(r_m) - \Psi_{\ell}(r_m)v'_{\ell}(r_m) - i\frac{\Psi_{\ell}(r_m)}{v_{\ell}(r_m)} \right] e^{i\phi(v_{\ell}, r_0, r_m)}, \quad (18a)$$

$$\Lambda_{+}(v_{\ell}, \ell) = \left[\Psi'_{\ell}(r_m)v_{\ell}(r_m) - \Psi_{\ell}(r_m)v'_{\ell}(r_m) + i\frac{\Psi_{\ell}(r_m)}{v_{\ell}(r_m)} \right] e^{-i\phi(v_{\ell}, r_0, r_m)}. \quad (18b)$$

Finally, the S matrix (1) can be expressed in terms of two Milne solutions and a regular Schrödinger solution as

$$S_{\ell} = \frac{M_{12}\Lambda_{-}(v_{\ell}, \ell) + M_{22}\Lambda_{+}(v_{\ell}, \ell)}{M_{11}\Lambda_{-}(v_{\ell}, \ell) + M_{21}\Lambda_{+}(v_{\ell}, \ell)} e^{2i\Delta(u_{\ell}, \ell)}. \quad (19)$$

Note that the asymptotic phase $\Delta(u_{\ell}, \ell)$ in (19) is still expressed in terms of the ‘scattering Milne solution’ u_{ℓ} , whilst the original quantities $\Lambda_{\pm}(u_{\ell}, \ell)$ are instead given in terms of the ‘intermediate Milne solution’ v_{ℓ} .

The new S -matrix formula (19) is valid and accurate for values of ℓ in a large region of the complex ℓ -plane including the real ℓ -axis. If the Schrödinger solution and the Milne solutions are real on the real r -axis for real values of ℓ , it is clear that $\Lambda_{\pm}^{*}(v_{\ell}, \ell) = \Lambda_{\mp}(v_{\ell}, \ell)$, $M_{11}^{*} = M_{22}$ and $M_{21}^{*} = M_{12}$, so that (19) in this case be written in a complex unitary way.

4. Determination of Regge-pole positions and residues

In the present section the basic Regge-pole formulae are modified with the use of the ‘intermediate’ Milne solution v_{ℓ} .

The basic Regge-pole condition from (1) is given by

$$\Lambda_{-}(u_{\ell}, \ell_n) = 0. \quad (20)$$

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

$$\Lambda_{-}(u_{\ell}, \ell) \approx \frac{\partial \Lambda_{-}(u_{\ell_n}, \ell_n)}{\partial \ell} (\ell - \ell_n), \quad (21)$$

so that the expression for the residue takes the form

$$\rho_n = \text{Res}_{\ell=\ell_n} S_{\ell} = \frac{\Lambda_{+}(u_{\ell_n}, \ell_n)}{\partial \Lambda_{-}(u_{\ell_n}, \ell_n) / \partial \ell} e^{2i\Delta(u_{\ell}, \ell)}. \quad (22)$$

The basic formulae above were discussed in [2].

The two-Milne-function condition for Regge poles becomes

$$(\Lambda_{-}(u_{\ell_n}, \ell_n) =)M_{11}\Lambda_{-}(v_{\ell_n}, \ell_n) + M_{21}\Lambda_{+}(v_{\ell_n}, \ell_n) = 0, \quad (23)$$

where v_{ℓ} and Ψ_{ℓ} are considered to be the main important functions, whereas u_{ℓ} will appear in the ‘coefficients’ M_{ij} . From this condition alone one has the relation between $\Lambda_{+}(v_{\ell_n}, \ell_n)$ and $\Lambda_{-}(v_{\ell_n}, \ell_n)$ given by

$$\Lambda_{+}(v_{\ell_n}, \ell_n) = -\frac{M_{11}\Lambda_{-}(v_{\ell_n}, \ell_n)}{M_{21}}. \quad (24)$$

Hence, the numerators in (1) and (19) reduce at the poles to

$$\Lambda_+(u_{\ell_n}, \ell_n) = (-M_{21}M_{12} + M_{22}M_{11}) \frac{1}{M_{11}} \Lambda_+(v_{\ell_n}, \ell_n), \quad (25)$$

which according to (16) simplifies to

$$\Lambda_+(u_{\ell_n}, \ell_n) = \frac{1}{M_{11}} \Lambda_+(v_{\ell_n}, \ell_n). \quad (26)$$

The basic residue formula (22) can thus be expressed, with the new relations (23) and (26), as

$$\rho_n = \left\{ \frac{\Lambda_+(v_\ell, \ell)}{M_{11} \partial [M_{11} \Lambda_-(v_\ell, \ell) + M_{21} \Lambda_+(v_\ell, \ell)] / \partial \ell} \right\}_{\ell=\ell_n} e^{2i\Delta(u_{\ell_n}, \ell_n)}. \quad (27)$$

A more detailed Regge-pole condition is obtained if the quantities $\Lambda_\pm(v_\ell, \ell)$ are written as

$$\Lambda_\pm(v_\ell, \ell) = a_\pm e^{\pm i\gamma}, \quad (28)$$

with

$$a_\pm = v_\ell(r_m) \Psi'_\ell(r_m) - v'_\ell(r_m) \Psi_\ell(r_m) \pm i \frac{\Psi_\ell(r_m)}{v_\ell(r_m)}, \quad (29a)$$

and

$$\gamma = \phi(v_\ell, r_m, r_0). \quad (29b)$$

According to (29b) the integration of the intermediate Milne solution in γ is formally performed from the 'inner' matching point r_m (involving the Schrödinger solution) to the 'outer' matching point r_0 (involving the scattering Milne solution). The real part of γ should in general be positive by this definition.

The S -matrix denominator in (1) and (19) can now be expressed as

$$\Lambda_-(u_\ell, \ell) = M_{21} a_+ e^{i\gamma} \left[1 + \frac{M_{11} a_-}{M_{21} a_+} e^{-2i\gamma} \right], \quad (30)$$

so that at a Regge pole $\ell = \ell_n$

$$\left[-\frac{M_{11} a_-}{M_{21} a_+} e^{-2i\gamma} \right]_{\ell=\ell_n} = 1. \quad (31)$$

Using (31) when expanding $\Lambda_-(u_\ell, \ell)$ near the poles, one gets

$$\begin{aligned} \Lambda_-(u_\ell, \ell) &\approx (M_{21} a_+ e^{i\gamma})_{\ell=\ell_n} \left[\frac{M_{11} a_-}{M_{21} a_+} e^{-2i\gamma} \right]_{\ell=\ell_n} \left\{ \frac{\partial \left[\frac{M_{11} a_-}{M_{21} a_+} \right] / \partial \ell}{\left[\frac{M_{11} a_-}{M_{21} a_+} \right]} - 2i \frac{\partial \gamma}{\partial \ell} \right\}_{\ell=\ell_n} (\ell - \ell_n) \\ &= (M_{21} a_+ e^{i\gamma})_{\ell=\ell_n} \left\{ 2i \frac{\partial \gamma}{\partial \ell} - \frac{\partial \left[\frac{M_{11} a_-}{M_{21} a_+} \right] / \partial \ell}{\left[\frac{M_{11} a_-}{M_{21} a_+} \right]} \right\}_{\ell=\ell_n} (\ell - \ell_n). \end{aligned} \quad (32)$$

With the use of (28) the residue formula (27) can be written as

$$\rho_n = \left\{ M_{11} M_{21} \left[2i \frac{\partial \gamma}{\partial \ell} + \frac{\partial}{\partial \ell} \ln \left(\frac{M_{21} a_+}{M_{11} a_-} \right) \right] \right\}_{\ell=\ell_n}^{-1} e^{2i\Delta(u_{\ell_n}, \ell_n)}. \quad (33)$$

Note that the Regge-pole condition (31) may also be put in the form of a semiclassical-type quantization condition

$$\gamma = \left[n + 1 + \frac{1}{2i\pi} \ln \left(-\frac{M_{11} a_-}{M_{21} a_+} \right) \right] \pi, \quad n = 0, 1, 2, \dots \quad (34)$$

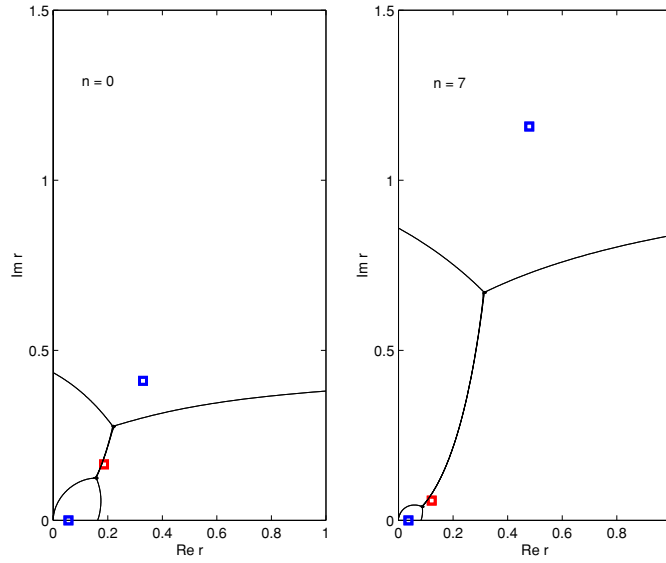


Figure 3. Illustration of the semiclassical transition points and their anti-Stokes' lines for two Regge poles, $\ell_0 = 4.8289 + i6.0137$ and $\ell_7 = 5.9079 + i13.3783$, corresponding to a repulsive r^{-4} -potential. For the leading pole ℓ_0 the two turning points lie close to the (ℓ -dependent) minimum (small square) of a complex well in which the Schrödinger wavefunction describes the lowest quasi-bound state. The two matching points (also small squares) are here chosen outside the complex well. A similar situation is given for the Regge pole ℓ_7 in the right subplot. In this case the Schrödinger wavefunction has seven almost exact nodes between the turning points, but the 'intermediate' Milne solution is non-oscillating there. Note that the local minimum (small square) of the complex well does not lie exactly on the anti-Stokes' line joining the turning points.

The non-negative integer n enters in (34) as a (quasi-vibrational) quantum number, i.e. the pole number that defines a string of poles in the complex ℓ -plane. The ground state (leading Regge pole) $n = 0$ corresponds to the smallest possible value of γ with a positive real part and that satisfies the condition (31). It is known that the particular Milne solution satisfying

$$v_\ell(r) \approx \left[\frac{2m}{\hbar^2} (E - V(r)) - \frac{\ell(\ell + 1)}{r^2} \right]^{-1/4}, \quad (35)$$

near the 'bottom' of the complex well will stay well behaved and monotonically increasing as r tends to either of the turning points of the complex well and beyond (see [18, 19]).

Formula (34) is most effective if the matching points are chosen so that the 'coefficients' M_{ij} and a_\pm become almost like constants. This can be realized assuming that v_ℓ becomes large beyond the complex-well turning points; the scattering Milne solution remains almost constant in the outer (upper right) region and the Schrödinger solution is kept small in the inner (lower left) region away from the complex well. By choosing the matching points r_0 and r_m outside the complex well, as indicated by small squares in figure 3, it is then possible to realize the following limiting case

$$M_{21} \approx -M_{11} \approx \frac{1}{2}(i\mathcal{P} - \mathcal{Q}^{-1}), \quad \mathcal{Q} = \frac{u_{\ell_n}(r_0)}{v_{\ell_n}(r_0)} \ll 1, \quad (36)$$

$$a_- \approx a_+ \approx v_\ell(r_m)\Psi'_\ell(r_m) - v'_\ell(r_m)\Psi_\ell(r_m), \quad \frac{\Psi_\ell(r_m)}{v_\ell(r_m)} \ll 1, \quad (37)$$

so that (34) can be approximated by

$$\gamma \approx (n + 1)\pi, \quad \frac{\Psi_\ell(r_m)}{v_\ell(r_m)} \ll 1, \quad \frac{u_{\ell_n}(r_0)}{v_{\ell_n}(r_0)} \ll 1. \tag{38}$$

This Regge-pole condition (38) appears to be identical to the one used by Korsch *et al* [19] for localizing complex energy poles. Here γ is an integral of an exact quantal momentum function v_ℓ^{-2} where the integration extends from deep inside the classically forbidden region on the side of the complex well close to the origin, across the well, and far into the classically forbidden region on the other side of the complex well.

5. Numerical applications

Two cases of Regge states are considered in the present section: those of a repulsive inverse-power potential $\sim r^{-4}$, and those of a discontinuous square-well potential. All calculations in this section are performed with units such that $2m/\hbar^2 = 1$. A numerical tolerance of 3×10^{-14} is used in the calculations and convergence of the Regge-pole condition is accepted when corrections in ℓ are smaller than 3×10^{-12} .

The purpose of this section is to demonstrate that the amplitude-phase method is a powerful numerical tool also with a minimum knowledge of the complex behaviour of the potentials. However, anti-Stokes' lines are calculated for an illustrative purpose and to add a deeper understanding from a semiclassical point of view.

5.1. $V(r) = \alpha^2 r^{-4}$

Handy *et al* [6, 7] studied Regge-pole positions and residues for this potential with

$$\alpha^2 = 2, \quad E = 400. \tag{39}$$

The so-called eigenvalue moment method [6, 7] produces highly accurate results for both positions and residues of the Regge poles.

Two analytic results are useful in the Newton iteration procedure for finding the Regge-pole positions. The potential-free turning point

$$t_0 = \frac{[\ell(\ell + 1)]^{1/2}}{k} \tag{40}$$

is a valuable reference point for trying out one of the matching points in the complex r -plane. Another point of interest in the complex plane is a possible minimum in the complex well. A quick calculation gives

$$\frac{d}{dr} \left(\frac{\alpha^2}{r^4} + \frac{\ell(\ell + 1)}{r^2} \right) = 0 \quad \Rightarrow \quad (r =) t_m = i \left(\frac{2\alpha^2}{\ell(\ell + 1)} \right)^{1/2}. \tag{41}$$

The complex points t_0 and t_m define a line that should be reasonably close to the complex well. For the leading pole, ℓ_0 , it is expected that the turning points of the complex well lie close to the minimum t_m . A rough estimate ℓ_* of ℓ_0 can be obtained by solving $t_0 = t_m$, which gives $\ell_* \approx k^{1/2}(2\alpha^2)^{1/4} e^{i\pi/4}$. A more sophisticated semiclassical estimate [20] gives

$$\ell_n + 1/2 \approx 2^{1/2} e^{i\pi/4} \chi + 2^{1/2} (n + 1/2)i + 2^{1/2} (n + 1/2)^2 e^{-i\pi/4} \chi^{-1}, \quad \left| \frac{n + 1/2}{\chi} \right| \ll 1, \tag{42}$$

where $n = 0, 1, 2, \dots$ is the pole number, and

$$\chi = k^{1/2}(\alpha^2)^{1/4}. \tag{43}$$

Table 1. Positions and residues of the Regge poles corresponding to the repulsive potential $V(r) = \alpha^2 r^{-4}$ and energy $E = 400$. The marked digits (underlined) differ from those in a corresponding table in [6] that comprises the first eight poles ($n = 0, 1, \dots, 7$). Note that the residues given in the table in [6] have been multiplied by the imaginary unit before the comparison is made.

n	ℓ_n	ρ_n
0	4.828 946 803 <u>678</u> + 6.013 713 550 104i	0.031 274 035 06 + 0.102 004 304 24i
1	4.925 902 544 668 + 7.295 011 652 620i	0.110 588 013 <u>52</u> + 0.109 396 476 <u>55</u> i
2	5.067 366 792 145 + 8.468 178 243 369i	0.149 632 536 76 + 0.079 705 047 <u>72</u> i
3	5.228 355 421 678 + 9.557 720 099 833i	0.162 037 454 <u>29</u> + 0.051 363 433 <u>22</u> i
4	5.397 261 497 <u>165</u> + 10.582 006 552 146i	0.162 896 173 <u>78</u> + 0.030 661 151 <u>41</u> i
5	5.568 460 400 97 <u>8</u> + 11.554 236 518 880i	0.159 363 616 20 + 0.016 371 580 <u>35</u> i
6	5.739 137 652 223 + 12.483 976 816 193i	0.154 421 441 <u>55</u> + 0.006 550 629 <u>99</u> i
7	5.907 870 381 072 + 13.378 312 553 437i	0.149 267 497 <u>98</u> - 0.000 276 077 <u>37</u> i
8	6.073 956 213 732 + 14.242 616 101 411i	0.144 360 904 95 - 0.005 094 574 58i
9	6.237 078 466 712 + 15.081 053 103 543i	0.139 854 640 55 - 0.008 547 120 46i
10	6.397 131 350 226 + 15.896 919 297 825i	0.135 775 674 30 - 0.011 053 689 42i

Figure 3 shows the semiclassical turning points and the associated anti-Stokes' lines forming a 'complex well' in the first quadrant of the ℓ -plane. As the pole number increases, the well becomes wider. Three more points are shown in the figure: the inner matching point r_m , the outer matching point r_0 and the complex minimum t_0 , which lies between the turning points and close to the anti-Stokes' line joining the turning points. Not shown in the figure is the 'potential-free' turning point t_0 , which turns out to be a good approximation of the true upper turning point.

In the calculations the matching point r_0 can be chosen to lie some distance from t_0 away from the minimum t_m . The inner matching point r_m is chosen to be on the other side of t_m , closer to the real axis and the origin. The Schrödinger equation is integrated from close to the origin, near the real axis, along a straight line to r_m . Then the intermediate Milne solution is integrated from $r = t_m$ back to r_m , so that $\Lambda_{\pm}(v_{\ell}, \ell)$ is calculated and part of the phase γ is collected. The initial conditions in this integration are set from (35) at $r = t_m$ where $dv_{\ell}(r_m)/dr = 0$. To proceed, the inner Milne equation is integrated up to r_0 where the calculation of γ is completed. The scattering Milne solution is finally calculated from some large distance ($\text{Re } r \rightarrow +\infty$), along a straight line up to r_0 , where the coefficients M_{11} and M_{21} are determined. The Regge-pole condition is evaluated as well as the ℓ -derivative of this condition, and a better initial guess is determined. The procedure is repeated until convergence is found (see table 1).

5.2. $V(r) = -V_0, 0 < r \leq R$ and $V(r) = 0, r > R$

This potential was discussed in [2] for the case $R = 1, E = 100, V_0 = 200$. The basic Regge-pole formulae were used on the real r -axis and successfully located the narrow and broad resonance poles as well as the leading diffraction pole. A theoretically interesting aspect of this potential is the break up of the pole string into two branches, which makes the identification of a pole with a unique pole number impossible.

The single matching point used in [2] had to be chosen at the cut-off $r = R$ and the flexibility of the method was thereby limited. It mainly affected the search for the diffraction poles far from the real ℓ -axis. With two matching points the numerical situation is improved, so that further diffraction poles can be located.

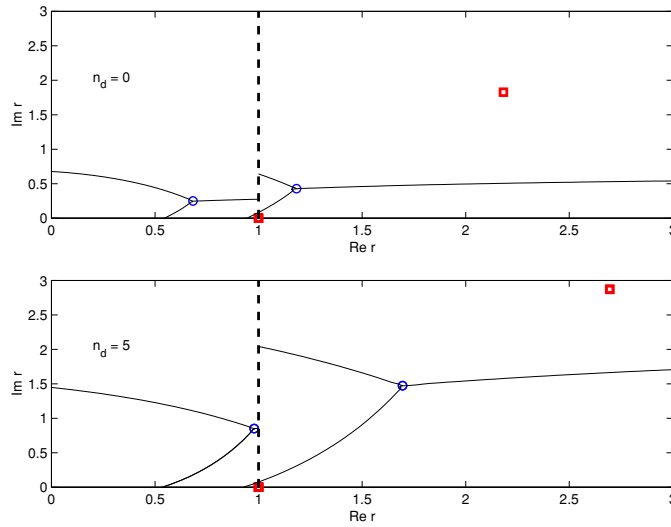


Figure 4. Illustration of the discontinuous complex wells forming diffraction Regge states. A vertical cut is introduced in the complex r -plane from the real axis at $r = R$.

In this model the turning points are easily calculated. For the exterior region it is given by

$$t_0 = \left[\frac{\hbar^2 \ell(\ell + 1)}{2mE} \right]^{1/2}, \quad t_0 > R. \tag{44}$$

Similarly, for the interior region

$$t_1 = \left[\frac{\hbar^2 \ell(\ell + 1)}{2m(E + V_0)} \right]^{1/2}, \quad t_1 \leq R. \tag{45}$$

The minimum of the ‘complex well’ is simply $t_m = R$ but the derivative of the potential is not zero if $\ell \neq 0$.

The diffraction Regge states are expected not to penetrate far into the well, so an inner matching point is chosen at the cut-off, $r_m = R$. An outer matching point is chosen on the other side of the outer turning point, $|r_0| > |t_0|$. The integration of the ‘inner’ Milne solution is performed directly from the inner matching point to the outer one. Initial values are taken from (35) with $V(r_m) = 0$, and recalling that the derivative is different from zero.

The ‘complex well’ forming the Regge states is distorted by the discontinuity (see figure 4). When the Regge-pole condition is written in the form (34), one can identify the pole number n . It turns out that the leading diffraction Regge state can be associated from (34) with a ‘diffraction pole number’ $n = n_d = 0$, but the correction term $\frac{1}{2i\pi} \ln \left(-\frac{M_{11}a_-}{M_{21}a_+} \right) \approx \frac{1}{2i\pi} \ln \left(\frac{a_-}{a_+} \right)$ has a significant contribution. This correction term does not change very much for the first ten diffraction poles, so there is a significant phase contribution in the Regge-pole condition coming from the wavefunction inside the physical potential well. The diffraction pole number n_d thus only measures the exterior phase range of the wavefunction in the complex well.

The first ten Regge-pole positions and residues are collected in table 2. The accuracy of the Regge-pole positions has been estimated by the use of an exact analytic S -matrix formula [21]

$$S_\ell = -\frac{H_{\ell+1/2}^{(2)}(\beta)}{H_{\ell+1/2}^{(1)}(\beta)} \left\{ \frac{\ln' H_{\ell+1/2}^{(2)}(\beta) - N \ln' J_{\ell+1/2}(\alpha)}{\ln' H_{\ell+1/2}^{(1)}(\beta) - N \ln' J_{\ell+1/2}(\alpha)} \right\}, \tag{46}$$

Table 2. Positions and residues of the Regge poles corresponding to the square-well potential with depth $V_0 = 200$, range $R = 1$ and energy $E = 100$. The diffraction quantum number n_d refers to the exterior part of the complex well between the cut-off radius and the exterior turning point t_0 .

n_d	ℓ_{n_d}	ρ_{n_d}
0	11.333 393 287 195 + 4.270 620 759 476i	0.496 873 978 – 0.249 479 259i
1	12.669 435 728 597 + 6.957 733 153 068i	0.379 681 354 – 0.188 248 823i
2	13.765 512 772 354 + 9.172 616 815 414i	0.330 577 906 – 0.163 100 991i
3	14.738 345 065 276 + 11.153 023 759 918i	0.301 900 287 – 0.147 563 957i
4	15.629 045 882 295 + 12.985 159 188 194i	0.282 365 037 – 0.136 498 088i
5	16.458 995 199 668 + 14.711 739 815 656i	0.267 865 181 – 0.128 021 820i
6	17.241 313 808 844 + 16.357 763 669 615i	0.256 500 990 – 0.121 228 049i
7	17.984 839 238 296 + 17.939 432 712 660i	0.247 253 635 – 0.115 608 976i
8	18.695 897 676 687 + 19.467 998 658 989i	0.239 519 234 – 0.110 852 102i
9	19.379 219 050 331 + 20.951 674 770 197i	0.232 913 091 – 0.106 751 976i

where $H_{\ell+1/2}^{(1,2)}(\beta)$ are the cylindrical Hankel functions and $J_{\ell+1/2}(\alpha)$ is the cylindrical Bessel function. \ln' denotes the logarithmic derivative with respect to the arguments $\alpha = \sqrt{\frac{2m}{\hbar^2}(E + V_0)}R$ and $\beta = \sqrt{\frac{2mE}{\hbar^2}}R$, and $N = \alpha/\beta$. By inserting the amplitude-phase results for the pole positions in the denominator of the embraced factor in (46), and numerically obtaining an approximate ℓ -derivative for this denominator, the pole positions were found to be accurate with 11–12 significant decimals.

The accuracy of the residues in table 2 is more difficult to estimate. The phase $\Delta(u_\ell, \ell)$ in the residue formula needs to be calculated from a large distance $r > 10^4$ up to the outer matching point r_0 .

6. Conclusions and discussions

It has been shown that the basic formula of the S matrix, derived from Ermakov–Lewis invariants, can be generalized to include two Milne solutions. The applicability of this amplitude-phase method is thereby generalized to be more flexible so that it can handle more distant Regge poles with large pole numbers. No particular knowledge of the Stokes' and anti-Stokes' lines is required for using this method, but such considerations are no doubt very valuable for accurate numerical computations.

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