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Abstract. It is shown that, when only two turning points are important, the generalised Bohr-Sommerfeld condition for Regge-pole positions can be derived from the behaviour of the semiclassical wavefunctions in a region far from the turning points. The analysis proves that the poles can be accurately determined from the Bohr-Sommerfeld formula also when the turning points lie close together. The implications of the present analysis as to certain asymptotic properties of the semiclassical pole positions and the corresponding pole residues are discussed.

1. Introduction

Semiclassical and phase-integral methods have proved to be useful and accurate tools in the analysis of complex angular momentum poles (Connor 1980). A particular example of the simplicity of semiclassical formulae is given by the generalised Bohr-Sommerfeld condition for the pole positions:

$$\int_{r_{(1)}}^{r_{(2)}} (k^2 - U - (l+\tfrac{1}{2})^2/r^2)^{1/2} \, dr = (n+\tfrac{1}{2})\pi \tag{1}$$

where k is the wavenumber, U the potential (in units of $\hbar^2/2m$), l is the complex angular momentum variable, $r_{(1)}$ and $r_{(2)}$ the two relevant turning points in the complex r plane and n is the quasi-vibrational quantum number labelling the poles.

Apparently, the Bohr-Sommerfeld condition (1) used in the present context is formally identical with the one used to determine the bound states in a simple potential well. One must remember, however, that the potential U in (1) is defined to vanish asymptotically ($r \to +\infty$) and does not necessarily have a well. Furthermore, in complex angular momentum theories, the energy (k^2) is a quantity which is given in advance.

Several authors have derived formula (1) (Brander 1966, Dombey and Jones 1968, Connor *et al* 1976, Knoll and Schaeffer 1976, Thylwe 1983) using different asymptotic techniques. Even higher order quantum corrections can be taken into account (Brander 1966, Thylwe 1983).

In the present paper we shall give another, alternative derivation of (1). It is analogous to Wentzel's proof for the corresponding bound-state problem, a procedure which was rigorously justified some years ago (Fröman and Fröman 1977a, Fröman 1980). This derivation gives some further insight as to the accuracy of the Bohr-

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Sommerfeld formula and indicates that it is, under certain circumstances, far more accurate than can be expected from previous derivations using semiclassical connection formulae for the wavefunction at each turning point.

Generally one agrees that formula (1) improves as the quantum number n gets larger, i.e. the error is somehow associated with the distance between the two turning points $r_{(1)}$ and $r_{(2)}$ in (1). However, in the present analysis it will be apparent that the distance to the nearest transition point other than $r_{(1)}$ and $r_{(2)}$ (lying outside a certain region to which $r_{(1)}$ and $r_{(2)}$ belong) can have the dominant influence on the accuracy of (1).

The main results are derived in § 2. In § 3 we discuss the implications of the present analysis in the study of certain asymptotic properties of pole positions and pole residues.

2. Derivation

In the following derivation of the Bohr–Sommerfeld formula (1) we shall make use of the phase-integral method developed by Fröman and Fröman (1965). Their formulation automatically takes into account higher order corrections to the standard semiclassical (JWKB) results and, furthermore, it keeps track of the errors introduced in replacing the exact solution of the Schrödinger equation by a linear combination of phase-integral wavefunctions.

Consider the radial Schrödinger equation

$$d^2\psi/dr^2 + Q^2(r)\psi = 0 \tag{2}$$

where, with obvious notation,

$$Q^2(r) = k^2 - U - l(l+1)/r^2. \tag{3}$$

The wavenumber k is assumed real and positive, but r, U and l may be complex quantities. U is an analytic function of r in the region of the complex r plane under consideration, except possibly at the origin $r = 0$.

The phase-integral wavefunctions are defined as follows:

$$f_1(r) = q^{-1/2}(r) \exp(iw(r)) \tag{4a}$$

$$f_2(r) = q^{-1/2}(r) \exp(-iw(r)) \tag{4b}$$

with

$$w(r) = \int^r q(r)\,dr. \tag{5}$$

The general expression for the function $q(r)$ is given by equations (3.6)–(3.9c) in Thylwe and Fröman (1983). In a first-order approximation one only has to assure that the choice of $q(r)$ makes $f_1(r)$ and $f_2(r)$ exact local solutions of (2) at the origin and at infinity. The choice

$$q^2(r) = k^2 - U - (l + \tfrac{1}{2})^2/r^2 \tag{6}$$

satisfies these requirements for most radial problems (Thylwe and Fröman 1983). The relevant complex turning points $r_{(1)}$ and $r_{(2)}$ are now simple zeros of the function $q^2(r)$ in (6). The positions of $r_{(1)}$ and $r_{(2)}$ are not altered when higher order phase-integral approximations are used, even if the function $q(r)$ appearing in equations (4a, b) and (5) is then defined differently (cf Thylwe and Fröman 1983).

According to equations $(3.25a)$ and $(3.25b)$ in Fröman and Fröman (1965) the regular solution ψ of (2) can be written as

$$\psi = a_1(r)f_1(r) + a_2(r)f_2(r) \tag{7a}$$

$$\psi' = a_1(r)f'_1(r) + a_2(r)f'_2(r). \tag{7b}$$

If the 'coefficients' $a_1(r)$ and $a_2(r)$ have been determined at a certain point r', they are given at an arbitrary point r by

$$\begin{pmatrix} a_1(r) \\ a_2(r) \end{pmatrix} = \mathbf{F}(r, r') \begin{pmatrix} a_1(r') \\ a_2(r') \end{pmatrix} \tag{8}$$

the elements of the two by two matrix $\mathbf{F}$ being given by the convergent series expansions $(3.22a)$-$(3.22d)$ in Fröman and Fröman (1965). Useful estimates of these series have been derived in Fröman and Fröman (1965) on the assumption that the points r and r' can be connected by a path Λ in the complex r plane, along which the absolute value of $\exp[iw(r)]$ increases monotonically from r' to r. These so-called basic estimates are given by equations $(4.3a)$-$(4.3d)$ in Fröman and Fröman (1965). They are valid when the quantity μ defined by

$$\mu(r, r') = \int_\Lambda |\varepsilon(r'')q(r'')\,dr''| \tag{9}$$

with

$$\varepsilon(r) = \frac{Q^2 - q^2}{q^2} + \frac{1}{16q^6}\left[5\left(\frac{d}{dr}q^2\right)^2 - 4q^2\frac{d^2}{dr^2}q^2\right] \tag{10}$$

is much smaller than unity.

We now introduce cuts in the complex r plane such that $q(r)$ is single valued, and such that the phase of $q(r)$ can be chosen so that $f_1(r)$ represents an outgoing free (or Coulomb distorted) wave as $r \to +\infty$ as well as it represents the regular solution at the origin. For this purpose we can, for example, utilise the results in Thylwe (1983) as regards the qualitative behaviour of Stokes and anti-Stokes lines associated with the relevant turning point configuration. After an allowed deformation of the cuts shown in figures 5 and 6 in that paper we finally obtain figure 1 in the present work.
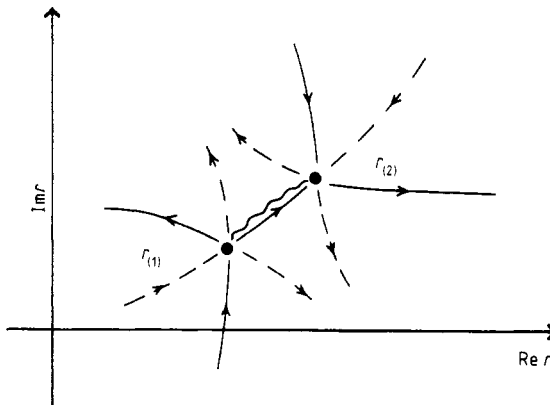

Figure 1. Schematic illustration of the configuration of two turning points and their associated Stokes and anti-Stokes lines for a Regge state (cf Thylwe 1983). The arrows are defined so that $\rightarrow\!\!\!\!\rightarrow\!-$ is the direction for which $i\,dw$ is real and >0 (Stokes line) and $\rightarrow\!-$ is the direction for which dw is real and >0 (anti-Stokes line).

At the origin we thus have

$$\psi \mathop{=}_{r \to +0} a_1 f_1(r) \tag{11}$$

where a_1 is an undetermined normalisation factor. Using the relation (8) and the inversion formula for $\mathbf{F}$ (see equation (3.20) in Fröman and Fröman (1965)) we find the exact representation at infinity

$$\psi \mathop{=}_{r \to +\infty} a_1 (F_{22}(+0, +\infty) f_1(r) - F_{21}(+0, +\infty) f_2(r)). \tag{12}$$

F_{21} and F_{22} are here independent of r, since the potential U as well as the function $q(r)$ are such that $f_1(r)$ and $f_2(r)$ are exact solutions in the limit $r \to +\infty$.

Let us further specify a particular exact Regge state corresponding to the wavefunction ψ_n with $l = l_n$, say, which satisfies the exact pole condition (cf equation (2.10) in Thylwe (1983))

$$F_{21}(+0, +\infty) = 0 \tag{13}$$

or, equivalently,

$$\psi_n \mathop{=}_{r \to +\infty} b_1 f_1(r) \qquad b_1 = a_1 F_{22}(+0, +\infty). \tag{14}$$

The next step is to show that ψ_n is approximately proportional to $f_1(r)$ also in a certain simply connected region in the r plane, which contains the points $+0$ and $+\infty$ and which surrounds the two relevant turning points. In a previous investigation by the present author (Thylwe 1983) the key assumption is that the two turning points are well separated so that an accurate phase-integral representation of ψ in terms of a linear combination of $f_1(r)$ and $f_2(r)$ exists in a region between $r_{(1)}$ and $r_{(2)}$. We shall relax this assumption here and instead require that $r_{(1)}$ and $r_{(2)}$ are well separated from *other transition points* which may be present.

Such a requirement assures the existence of a certain band B (see figure 2), surrounding the two turning points, where $q^2(r)$ is approximately a quadratic function of r, putting

$$q^2(r) \approx c_1(r - r_c)^2 + c_2 \qquad (r \text{ in } B) \tag{15}$$

with $c_{1,2}$ being constants and r_c located at half the distance between $r_{(1)}$ and $r_{(2)}$. The orientation of important Stokes and anti-Stokes lines in B is then easily established, even quantitatively, if $c_{1,2}$ are known (see figure 2). The two Stokes lines with arrows pointing outwards (the direction for which $i\,dw$ is real and >0 so that $|\exp(iw)|$ grows) divide the band B into two halves B_L and B_R (L = left and R = right) as shown in figure 2. From the assumptions in Thylwe (1983) of a two-turning-point Regge-pole configuration it follows that there exists a path Λ_L, along which $|\exp(iw)|$ is non-decreasing as one moves from $+0$ to any point in B_L (see figure 2). Similarly, any point in B_R can be reached from $+\infty$ by a path Λ_R, along which $|\exp(iw)|$ is non-decreasing, except for a remote part of finite length, proceeding orthogonally to the real axis. It is realised that these requirements agree with the monotonicity properties discussed in § 3 in Thylwe (1983) except possibly in the neighbourhood of the turning points $r_{(1)}$ and $r_{(2)}$.
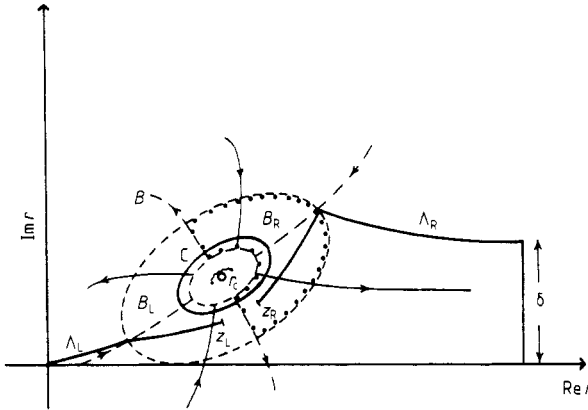
Figure 2. The figure shows the relevant Stokes and anti-Stokes lines in a deformed circular region B ($= B_L \cup B_R$) surrounding the two turning points which may lie close together but should be well separated from other transition points. The paths Λ_L and Λ_R, used for tracing the phase-integral wavefunctions from $+0$ and $+\infty$ to arbitrary points $z_L \in B_L$ and $z_R \in B_R$, respectively, are indicated. The vertical part of Λ_R is eventually shifted towards infinity in the same way as discussed in § 4 in Thylwe and Fröman (1983). C is a closed contour of integration appearing in equation (27).

The F matrix connecting an arbitrary point z_L, say, in B_L with the origin can easily be estimated along Λ_L with the aid of the basic estimates mentioned previously. We find

$$\mathbf{F}(z_L, +0) = \begin{pmatrix} 1 + O(\mu_L) & - \\ O(\mu_L)|\exp(2iw(z_L))| & - \end{pmatrix} \tag{16}$$

where μ_L is the μ integral calculated along Λ_L. The two unknown elements in (16) will not enter into our derivation, as will be seen presently. Applying (4a), (4b), (7a), (8), (11) and (16), we get

$$\psi_n(z_L) = a_1 f_1(z_L)(1 + O(\mu_L)) \qquad (z_L \text{ in } B_L). \tag{17}$$

The matrix $\mathbf{F}(z_R, +\infty)$ must, however, be considered as a product of the matrices $\mathbf{F}(z_R, +\infty + i\delta)$ and $\mathbf{F}(+\infty + i\delta, +\infty)$, where δ denotes the length of the remote vertical part of Λ_R when this part is shifted towards infinity (see figure 2). According to equation (4.9) in Thylwe and Fröman (1983) we find that the latter matrix is exactly equal to a unit matrix. For the remaining matrix in the product we make use of the basic estimates again, thus obtaining

$\mathbf{F}(z_R, +\infty) =$

$$\begin{pmatrix} 1 + O(\mu_R) & O(\mu_R)|\exp[-2iw(+\infty + i\delta)]| \\ O(\mu_R)|\exp(2iw(z_R))| & 1 + O(\mu_R)(1 + O(\mu_R)|\exp[2i(w(z_R) - w(+\infty + i\delta))]|) \end{pmatrix} \tag{18}$$

which, together with equations (4a, b), (7a), (8) and (14), gives

$$\psi_n(z_R) = b_1 f_1(z_R)(1 + O(\mu_R)) \qquad (z_R \text{ in } B_R). \tag{19}$$

We observe that the regions B_L and B_R have a common boundary on which formulae (17) and (19) are valid. Since the exact solution ψ_n is continuous there, we conclude

from (17) and (19):

$$b_1 = a_1(1 + O(\mu)) \tag{20}$$

and according to (14):

$$F_{22}(+0, +\infty) = 1 + O(\mu) \tag{21}$$

where μ is calculated along a joint path $\Lambda = \Lambda_L \cup \Lambda_R$ which connects $+0$ and $+\infty$. Furthermore, we have established an approximate wavefunction with control of the error in the whole of region B (and in some region connecting B with $+0$ and $+\infty$):

$$\psi_n(r) = a_1 f_1(r)(1 + O(\mu)) \qquad (r \text{ in } B). \tag{22}$$

From (7b) it also follows

$$\psi'_n(r) = a_1 f'_1(r)(1 + O(\mu)) \qquad (r \text{ in } B). \tag{23}$$

We shall now see that, in order to derive (1), it is sufficient to have these approximate Regge state wavefunctions only in the surrounding band B, the size of which is determined by the presence of transition points other than $r_{(1)}$ and $r_{(2)}$. There are of course other such transition points present. (At the origin, for example, $q^2(r)$ has a higher-order pole of the type r^{-m}, with m an integer not smaller than 2 (see equation (6) and examples given by Connor et al (1980).) The exact wavefunction $\psi(r)$ may have singularities in connection with them without violating the present derivation. Thus, having established that $\psi_n(r)$ is approximately represented by $a_1 f_1(r)$ in the whole band B, we can utilise Wentzels's line of argument (see § 4 in Fröman and Fröman 1977a). To this end we recall some properties of the exact wavefunction and its derivative.

The exact regular solution ψ_n is an analytic function of the complex radial variable r in the band B and the region surrounded by B. We note that ψ_n is analytic at the turning points $r_{(1)}$ and $r_{(2)}$ even though the phase-integral approximants $f_{1,2}(r)$ are not. Furthermore, ψ_n has precisely n simple zeros (for the nth Regge state), located in a region between $r_{(1)}$ and $r_{(2)}$ which in our case is surrounded by B. In the same region under consideration, the quotient ψ'_n/ψ_n is an analytic function of r with simple poles of residue 1 at the n zeros of ψ_n. If C is a closed contour in the same region which encircles the n zeros of ψ_n in the positive sense, we obtain from Cauchy's residue theorem

$$\oint_C (\psi'_n/\psi_n)\, dr = 2\pi i n \tag{24}$$

which is an exact formula, since ψ_n is an exact 'eigenfunction' for the corresponding Regge state.

The contour C can, of course, be deformed to lie in the region B, where the approximate expressions for ψ_n and ψ'_n, i.e. equations (22) and (23), respectively, are valid. From (4a), (22) and (23) we thus obtain the following expression for the integrand:

$$(\psi'_n/\psi_n) = -(d/dr) \ln q^{1/2} + iq + O(\mu). \tag{25}$$

Since the approximand in (25) is a slowly varying function on the contour C (cf equation (15)), it can be used, without introducing further errors, to evaluate the integral in (24) approximately, thus yielding (recall that $q(r)$ is single valued in B but

$q^{1/2}(r)$ is not; it changes the sign after one completed turn along C):

$$-\pi i + i \oint_C q(r)\, dr + O(\mu) = 2\pi i n. \tag{26}$$

Hence

$$\tfrac{1}{2} \oint_C q(r)\, dr = (n + \tfrac{1}{2})\pi + O(\mu). \tag{27}$$

If $q(r)$ is chosen according to equation (6), which is a first-order phase-integral expression, C may be condensed onto the lips of the cut joining $r_{(1)}$ and $r_{(2)}$, thus giving us the Bohr–Sommerfeld condition (1) with an additional measure of the error. The μ integral in (27) is, however, still associated with the original contour which was lying in B. As such, this μ integral may be arbitrarily small, depending on some arbitrarily large parameter in the Schrödinger equation, even if the phase-integral distance between $r_{(1)}$ and $r_{(2)}$ and, hence, the quantum number n is not large. On the other hand, along a 'traditional' connection path, which circumvents each turning point separately (see, for example, Thylwe 1983), the quantity μ cannot be made arbitrarily small unless $n \to \infty$. This distinction is fundamental for the analytical investigations of, for example, the high-energy behaviour of Regge-pole trajectories using the Bohr–Sommerfeld formula (Thylwe 1985) (see also related numerical studies by Connor *et al* 1976, 1979, 1980).

3. Discussion

The derivation above widens the validity of the Bohr–Sommerfeld Regge-pole condition so that it is no longer essentially a large quantum number n formula, even if a 'traditional' derivation of it suggests that it is the case. Such an extended validity of the well known semiclassical two-turning-point formula for the corresponding pole residues (Brander 1966, Knoll and Schaeffer 1976, Connor *et al* 1976, Thylwe 1983) would also be desired because of its explicit simplicity, but has not been found. In the present discussion we shall give strong evidence for the existing residue formula (contrary to equations (1) or (27)) being correct (μ is arbitrarily small) only in the large quantum number limit, and not in any other asymptotic limit independent of n. To this end we shall see how the assumptions and arguments of § 2 fail to improve the validity of the residue formula, given e.g. by equation (4.18) in Thylwe (1983), beyond the usual requirement of well separated turning points $r_{(1)}$ and $r_{(2)}$ (i.e. large n).

Let us consider the following exact relation:

$$r_n = \frac{k}{(l_n + \tfrac{1}{2})} \left(\int_{+0}^{+\infty} \psi_n^2 r^{-2}\, dr \right)^{-1} \tag{28}$$

where r_n is the residue corresponding to the pole at $l = l_n$ and ψ_n is the pertaining Regge-state wavefunction normalised so that, with obvious notation,

$$\psi_n \underset{r \to +\infty}{\sim} \exp(ikr - i\eta \ln 2kr - il\pi/2). \tag{29}$$

Equation (28) is a modified version of equation (10.4) in Newton (1964) and is valid for the most common case of first-order poles.

The relevant question here is whether or not one can successfully use in (28) the representation (22) for ψ_n to evaluate the integral $\int \psi_n^2 r^{-2} \, dr$. As pointed out by Fröman and Fröman (1977b) for the analogous bound state problem, this is a very dangerous procedure which is likely to lead to completely wrong results. The fundamental reason being that the integrand is exponentially large and oscillating on an integration path which is deformed to avoid both turning points $r_{(1)}$ and $r_{(2)}$. The accumulated absolute error is, therefore, generally larger than the value of the integral itself. Thus, a blind application of the assumptions in § 2 would probably be fatal and, moreover, it does not lead to the wanted semiclassical expression which should be a good approximation, at least in the large n limit.

To obtain the desired semiclassical residue formula, it seems unavoidable to use the approximate wavefunction in a region between the two turning points where, of course, the coefficient of the component $f_2(r)$ must also be determined. But this is just the 'traditional' approach which may give a vanishing μ integral only in the limit $n \to \infty$. It should be possible, however, to improve the two-turning-point formula itself by using uniform techniques (allowing the proximity of $r_{(1)}$ and $r_{(2)}$) and slightly modify the error analysis.

The results of the present paper are obviously of decisive importance for analytical investigations of asymptotic properties of Regge poles using semiclassical and phase-integral formulae. For Lennard–Jones type potentials it has been explicitly shown that the Bohr–Sommerfeld formula (1), and all higher-order phase-integral versions of it, correctly yield the terms in the high-energy and strong potential core expansion of all pole positions (Thylwe 1985). Such expansions cannot be derived for the pole residues from the semiclassical analysis unless uniform techniques are invoked.

These conclusions confirm several already published numerical investigations by Connor and co-workers (Connor *et al* 1976, 1979, 1980), who compared exact and semiclassical pole positions and residues for numerous interaction potentials.

References

Brander O 1966 *Ark. Fys.* **32** 131–65
Connor J N L 1980 *Semiclassical Methods in Molecular Scattering and Spectroscopy* ed M S Child (Dortrecht: Riedel) pp 45–107
Connor J N L, Jakubetz W, Mackay D C and Sukumar C V 1980 *J. Phys. B: At. Mol. Phys.* **13** 1823–37
Connor J N L, Jakubetz W and Sukumar C V 1976 *J. Phys. B: At. Math. Phys.* **9** 1783–99
Connor J N L, Mackay D C and Sukumar C V 1979 *J. Phys. B: At. Mol. Phys.* **12** L515–9
Dombey N and Jones R H 1968 *J. Math. Phys.* **9** 986–95
Fröman N 1980 *Semiclassical Methods in Molecular Scattering and Spectroscopy* ed M S Child (Dortrecht: D Riedel) pp 1–44
Fröman N and Fröman P O 1965 *JWKB-Approximation, Contribution to the Theory* (Amsterdam: North-Holland)
——— 1977a *J. Math. Phys.* **18** 96–9
——— 1977b *J. Math. Phys.* **18** 903–6

Knoll J and Schaeffer R 1976 *Ann. Phys., NY* **97** 307-66
Newton R G 1964 *The Complex j-Plane* (New York: Benjamin)
Thylwe K-E 1983 *J. Phys. A: Math. Gen.* **16** 3325-40
—— 1985 to be published
Thylwe K-E and Fröman N 1983 *Ann. Phys., NY* **150** 413-31