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Semiclassical approach to Regge poles trajectories calculations for nonsingular potentials: Thomas–Fermi type

S M Belov[1], N B Avdonina[2,3], Z Felfli[4], M Marletta[5], A Z Msezane[4] and S N Naboko[6]

[1] Department of Mathematics, Duke University, Durham, NC 27708, USA
[2] Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, PA 15260, USA
[3] Department of Electrical Engineering, University of Alaska Fairbanks, Fairbanks, AK 99775, USA
[4] Center for Theoretical Studies of Physical Systems, Clark Atlanta University, Atlanta, GA 30314, USA
[5] School of Mathematics, Cardiff University, Cardiff CF24 4YH, UK
[6] Department of Mathematical Physics, St. Petersburg State University, St. Petersburg, Russia

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Abstract

A simple semiclassical approach, based on the investigation of anti-Stokes line topology, is presented for calculating Regge poles for nonsingular (Thomas–Fermi type) potentials, namely potentials with singularities at the origin weaker than order -2. The anti-Stokes lines for Thomas–Fermi potentials have a more complicated structure than those of singular potentials and require careful application of complex analysis. The explicit solution of the Bohr–Sommerfeld quantization condition is used to obtain approximate Regge poles. We introduce and employ three hypotheses to obtain several terms of the Regge pole approximation.

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1. Introduction

Understanding the role played by dynamic scattering resonances in chemical reactions is crucial in gaining insights into all chemical reactivity. Physical insights are provided by the analysis that identifies complex angular momentum (Regge poles) resonances of the S-matrix in the complex angular momentum (CAM) plane. The energy-dependent Regge-pole positions, l_n and the corresponding residues, r_n where $n = 0, 1, 2, \ldots,$ are the key quantities calculated in the CAM techniques [1]. The position of the Regge pole determines the angular velocity and the angular lifetime of the system, while the residue defines the magnitude of the resonance contribution in the differential cross section (DCS). The main attraction in the CAM methods is that the calculations are based on a rigorous definition of resonances, namely as singularities of the S-matrix.

A recent upsurge in the theoretical investigations of Regge pole trajectories [1–8] (see also [9]) and, most recently, residues [10] for singular scattering potentials, namely potentials more singular than r^{-2} at the origin, has been inspired by developments in heavy-particle collisions [1], chemical reactions and atom–diatom systems [11, 12], cluster physics and small-angle electron DCSs using dispersion relations [13, 14]. The Thomas–Fermi (TF) equation, a delicate nonlinear problem whose solution is determined by unusual boundary conditions [15], is important because all neutral atoms can be described within the TF model by a universal function, the TF function [16] and in nuclear physics in the context of nuclear matter in neutron stars [17]. The importance of TF theory is its exactness in the large-Z limit; consequently, it can be taken as one of the cornerstones of atomic physics [18]. Lieb [18] has summarized what is known rigorously about TF and related theories, including the question of whether the resultant equations have (unique) solutions. Essential mathematical facts about the TF equation have been established [19]. In [20] the TF problem, considered as a variational problem, is shown to be approximately modelled by a simple nonlinear equation for a charge density. TF theory has also been utilized in the analysis of the stability of nonrelativistic and relativistic matter [21, 22]. In [6], it was determined that certain physics problems involving nonsingular potentials could also be investigated readily using the method for singular potentials. Hence the present investigation.

In this paper we use the same anti-Stokes line (aSL) method as in the paper for singular potentials [7]. However, nonsingular potentials (singularity at the origin weaker than order -2) do not satisfy the two hypotheses introduced there. Below, we give assumptions which seem reasonable in the case of TF potentials. It is worth mentioning that the results of this paper can be extended to the case of arbitrary rational potentials. We also demonstrate that the formal solution of the Bohr–Sommerfeld (BS) condition sometimes leads to an incorrect answer, and we give a procedure for finding the region of applicability of the Bohr–Sommerfeld condition for the Thomas–Fermi type potentials. The method of anti-Stokes lines topology reveals and explains such phenomena as false Regge poles: these are solutions of the Bohr–Sommerfeld equation but where the turning points (TPs) are not connected by an anti-Stokes line (connection by an anti-Stokes line is a necessary condition in the application of the Bohr–Sommerfeld condition). The explanation in terms of anti-Stokes lines topology is the following: the connection by an anti-Stokes line of two turning points expands with decreasing energy, and at some energy a triple connection (a connection of three turning points by one anti-Stokes line) appears, and the assumption of the connection of a pair of turning points for the BS equation becomes inapplicable. Comparison with results of direct integration confirms that such solutions of the BS equation do not solve the Schrödinger equation and are false.

2. Theory

The Thomas–Fermi potential is defined by the function χ obeying the differential equation [23]

$$\frac{\mathrm{d}^2\chi(x)}{\mathrm{d}x^2} = \frac{1}{\sqrt{x}}\chi^{3/2}(x) \tag{1}$$

with the boundary conditions

$$\chi(x) > 0 \qquad x > 0 \tag{2}$$

$$\chi(0) = 1 \tag{3}$$

$$\chi(x) \sim \frac{144}{x^3} \qquad x \to \infty. \tag{4}$$

The dimensionless variable $\chi(x)$ is related to the effective central electrostatic TF potential $q(r)$ in the atom of charge Z through

$$q(r) = \frac{-Z}{r}\chi(x) \tag{5}$$

with $x = rZ^{1/3}/\alpha, \alpha = (1/2)(3\pi/4)^{2/3} \approx 0.885$.

The Majorana solution, considered as a modification of equation (1), but completely different from it, and the Padé approximant approach to the TF problem have been considered recently [15, 24]. Sommerfeld [25] discovered an exact particular solution satisfying only the condition given by equation (4). In this paper we employ a rational function approximation to investigate the behaviour of the turning points, Regge poles and residues at high energy for a specific class of TF potentials denoted by RTF, within the context of complex angular momentum scattering. The RTF potentials give a good numerical approximation to the TF potential defined by equation (5). We present a semiclassical approach for calculating Regge poles for RTF potentials. Unlike the case of singular potentials considered in [7], dealing with RTF potentials is extremely complicated due to the existence of several additional poles (three in our particular case) of the potential which make the anti-Stokes line topology approach very difficult to work with.

This paper is based on three assumptions: (1) the existence of two turning points of the effective potential, responsible for the Regge poles; (2) the connection of these turning points by an anti-Stokes line; and (3) the closeness of the other turning points to the singularities of order one of the potential. These three hypotheses are natural for the RTF potentials and are used to simplify the nonlinear BS equation. Note, that the second assumption is a necessary condition for using the BS equation. Using these assumptions and the Bohr–Sommerfeld condition we find, after simplifications, the first two terms of the series expansion of the Regge poles in powers of $1/k$ (k^2 is the energy). As we show below this series is not a very good approximation and we replace it by another expansion, in which as small parameters we use the distances between the semiclassical turning points and the poles of the potential of order one. By the third hypothesis these distances are small and can be used as small parameters.

Here we consider the Schrödinger equation (in atomic units)

$$\psi'' + 2\left(E - \frac{l(l+1)}{2r^2} - V(r)\right)\psi = 0 \tag{6}$$

where l is complex and E real, with boundary conditions

$$\psi(0) = 0 \tag{7}$$

$$\psi(r) \sim \mathrm{e}^{+\mathrm{i}\sqrt{2E}r} \qquad r \to \infty. \tag{8}$$

Since we plan to consider mostly fast decreasing potentials V, the asymptotic condition at infinity has the standard exponential form. In the Coulomb case as is well known, we have to add an extra logarithmic term. Nontrivial solutions exist for special values of l known as Regge poles [1]. The curves $l(E)$ in the complex plane are called Regge trajectories.

We consider the RTF potential

$$V(r) = \frac{-2Z}{r(1 + aZ^{1/3}r)(1 + bZ^{2/3}r^2)}$$

where Z is the nuclear charge. This form of the potential is an approximation to the solution of the nonlinear diferential equation (1). The exact TF potential has the form of equation (5) (in atomic units). Since the analytic properties of the function $\chi(x)$ are too complicated and, additionally, the TF approach is an approximation itself, it seems reasonable to replace the exact function $\chi(x)$ by its rational approximation. The approximation of the potential by RTF above produces good analytic functions which can be extended to the complex plane. It is similar to that introduced by Tietz [26], but is more convenient for our calculations (note, that the Tietz potential can be considered in a similar way).

Consider equation (6) in the form

$$\psi'' + \left(k^2 - \frac{l(l+1)}{r^2} - 2V(r)\right)\psi = 0. \tag{9}$$

Then all results for this equation can be applied to (6) by simple transformations. Our investigation of Regge poles trajectories using the above approximate RTF potential $V(r)$ in equation (9) is more than motivational for the three main reasons: (1) the TF theory can be used with an appropriate TF potential to predict reliably [27] when electrons in the $p-$, $d-$ and $f-$ shells appear, corresponding to Z of 5, 21 and 58, respectively. (2) It is known that when the number of electrons, $N \to \infty$ the TF theory approaches quantum theory and Lieb and collaborators have established that $E^{TF}_{\text{atom}}(\lambda, Z) = Z^{7/3}E^{TF}_{\text{atom}}(\lambda, 1)$, where $N = \lambda Z$, with $0 \leqslant \lambda < 1$ and E^{TF}_{atom} is the ground-state energy of the atom; a similar relation can be written for the density. (3) In [26] the approximate TF potential, similar to ours was used in the Schrödinger equation to obtain the scattering length for low energy elastic electron scattering by atoms. Furthermore we demonstrate that the anti-Stokes lines for the TF potentials have a more complicated structure than that for singular potentials and require careful application of complex analysis.

Let $r_{1,2,3,4,5}$ be the semiclassical turning points of the effective potential $V_{\text{eff}}(r) = V(r) + l(l+1)/2r^2$. These satisfy the following equation:

$$S(r_i, l_n, k) = k^2 - 2V(r_i) - \frac{l_n(l_n+1)}{r_i^2} = 0.$$

We denote by r_1, r_2 the turning points responsible for the Regge poles. Approximate Regge poles can be found by numerical solution of the Bohr–Sommerfeld condition

$$\pi\left(n + \frac{1}{2}\right) = \int_{r_1}^{r_2} \sqrt{S(r, l_n, k)}\,\mathrm{d}r \qquad n = 0, 1, 2, \ldots \tag{10}$$

where the integration, using Newton's method [28] is along the anti-Stokes line: $\operatorname{Im}\int_{r_1}^{r_2} \sqrt{S(r, l_n, k)}\,\mathrm{d}r = 0$, connecting the turning points r_1 and r_2. Thus, the existence of a connecting anti-Stokes line is a necessary condition for the calculation of a Regge pole. Solving the nonlinear equation (10) is non-trivial. The usual way of dealing with it is to look for solutions in the form of a series for large energies k^2. Not surprisingly, this method can perform rather badly (see section 3) for small energies. Our approximation formula for the Regge poles is based on introducing other small parameters Δr_a, $\Delta r_{b\pm}$ below.

2.1. Small parameters

Analysing the position of the turning points of the effective potential we discover that there are always five generally distinct TPs. It is easy to show that for large energies three of the TPs are close to the poles of the effective potential: $-\frac{1}{aZ^{1/3}}, \pm\frac{\mathrm{i}}{\sqrt{b}Z^{1/3}}$. The other two (r_1, r_2), which correspond to the 'closeness' of the RTF potential to the Coulomb one, are close to the origin. Consider an abstract form of the RTF potential

$$V(r) = \frac{C}{r(1+Ar)(1+Br^2)}.$$

Let $r_3 = -\frac{1}{A} + \Delta r_a$, $r_{4,5} = \pm\frac{\mathrm{i}}{\sqrt{B}} + \Delta r_{b\pm}$, where $A = aZ^{1/3}$, $B = bZ^{2/3}$, $C = -2Z$; and all $|\Delta r| \ll 1$. Then for Δr_a we have the equation

$$S(r_3, l, k) = k^2 - \frac{l(l+1)}{1/A^2} + \frac{-C}{\left(-\frac{1}{A}\right)A\Delta r_a\left(1+\frac{B}{A^2}\right)} + CA^3\frac{A^2+3B}{(A^2+B)^2} + O(\Delta r_a) = 0. \tag{11}$$

Solving we obtain an expression for Δr_a:

$$\Delta r_a = -\frac{CA^2}{(A^2+B)\left(k^2 - l(l+1)A^2 + CA^3\frac{A^2+3B}{(A^2+B)^2}\right)}. \tag{12}$$

Similarly, one can obtain approximations for $\Delta r_{b\pm}$:

$$\Delta r_{b\pm} = -\frac{C\sqrt{B}}{2(\sqrt{B}\pm\mathrm{i}A)\left(k^2 + l(l+1)B \pm \frac{\mathrm{i}}{4}BC\frac{3\sqrt{B}\pm 5\mathrm{i}A}{(\sqrt{B}\pm\mathrm{i}A)^2}\right)}.$$

These quantities are small for large values of k. This allows us to use them as small parameters for the decomposition into a series the action integral in equation (8). Also it is easy to check that $r_3 = -\frac{1}{A} + \Delta r_a + O\left(\Delta r_a^3\right)$, $r_{4,5} = \pm\frac{\mathrm{i}}{\sqrt{B}} + \Delta r_{b\pm} + O\left(\Delta r_{b\pm}^3\right)$.

2.2. *Regge poles*

The Bohr–Sommerfeld quantization condition can be written in the following form, which is equivalent to the standard one but better fits our aim:

$$2\pi\left(n+\frac{1}{2}\right) = \int_\Gamma \sqrt{S(r, l_n, k)}\,\mathrm{d}r \qquad n = 0, 1, 2, \ldots. \tag{13}$$

Here the contour Γ must surround the anti-Stokes line connecting the points r_1 and r_2. Cauchy's theorem [29] allows us to transform the contour without changing the value of the integral.

Consider the analytic function $\sqrt{S(r, l_n, k)}$. It has a pole of order 1 at the point $r = 0$ and several branching points of order $\pm\frac{1}{2}$: $\left(-\frac{1}{A}\right)$, $\left(\pm\frac{\mathrm{i}}{\sqrt{B}}\right)$, $r_{1,2,3,4,5}$. In total there are precisely eight branching points (such as 0 for $\sqrt{z}$). At infinity our function is analytic and tends to $+k$ as $|r| \to \infty$. We now produce precisely four cuts (curves on the complex plane) to obtain a well-defined analytic function in the domain excluding these cuts and the origin: (see figure 1). The choice of the cuts is not essential (except the one connecting r_1 and r_2 along the aSL) for our calculations. We can think of them as straight lines (especially for large energies).

Using Cauchy's theorem we can replace our integral along Γ in (13) by the sum of three integrals around the cuts and two residues at points 0 and ∞. This leaves the value of our integral unchanged. In the case of singular potentials this construction was not applied because we assumed the closeness of the turning points r_1 and r_2, which is not true for the case of nonsingular potentials.

$$\int_\Gamma \sqrt{S(r, l_n, k)}\,\mathrm{d}r = \int_{\Gamma_3} \sqrt{S(r, l_n, k)}\,\mathrm{d}r + \int_{\Gamma_4} \sqrt{S(r, l_n, k)}\,\mathrm{d}r + \int_{\Gamma_5} \sqrt{S(r, l_n, k)}\,\mathrm{d}r$$
$$+ 2\pi\mathrm{i}\,\mathrm{res}_{r\to\infty}\sqrt{S(r, l_n, k)} - 2\pi\mathrm{i}\,\mathrm{res}_{r=0}\sqrt{S(r, l_n, k)}.$$

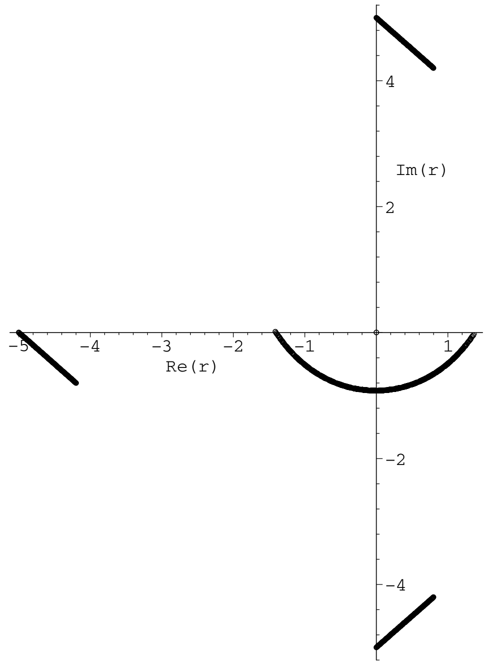

Figure 1. Typical positions of all turning points and singularities of a Thomas–Fermi type potential as well as all cuts.

Let us calculate all the terms in this sum

$$2\pi\mathrm{i}\,\mathrm{res}_{r=0}\sqrt{S(r,l_n,k)} = -2\pi\mathrm{i}\sqrt{-l(l+1)} = 2\pi\sqrt{l(l+1)}$$

$$2\pi\mathrm{i}\,\mathrm{res}_{r\to\infty}\sqrt{S(r,l_n,k)} = \begin{cases} \frac{\pi\mathrm{i}C}{k} & \text{if} \quad A=B=0 \\ 0 & \text{otherwise.} \end{cases}$$

Therefore, the quantization condition has the form

$$-2\pi\left(n+\frac{1}{2}\right) = 2\pi\sqrt{l(l+1)} + \frac{\pi\mathrm{i}C}{k}\delta_{A,0}\delta_{B,0} + \int_{\Gamma_3\cup\Gamma_4\cup\Gamma_5}\sqrt{S(r,l_n,k)}\,\mathrm{d}r$$

where $\delta_{A,0}$ and $\delta_{B,0}$ are the usual Kronecker deltas.

In the simple situation of the Coulomb potential $q(r) = \frac{C}{r}$ there are no cuts at all, we have $A = B = 0$, and our formula immediately gives

$$-2\pi\left(n+\frac{1}{2}\right) = 2\pi\sqrt{l(l+1)} + \frac{\pi\mathrm{i}C}{k} \approx 2\pi\left(l+\frac{1}{2}\right) + \frac{\pi\mathrm{i}C}{k}$$

and hence

$$l = -n-1-\frac{\mathrm{i}C}{2k} = -n-1+\frac{\mathrm{i}Z}{k}$$

which is the exact formula for the Coulomb potential [4, 30].

We now deal with the contour integrals. By Cauchy's theorem the integral over Γ_3 can be reduced to two integrals along a straight line connecting the zero at r_3 to the pole $-\frac{1}{A}$. We now use equation (11) and make the change of variable $r = -\frac{1}{A} + t\Delta r_a$. Finally, we use equation (12) to combine all the terms under the square root to obtain

$$S\left(-\frac{1}{A}+t\Delta r_a, l_n, k\right) = \frac{t-1}{t}\frac{-CA^2}{(A^2+B)\Delta r_a} + O(\Delta r_a)$$

and

$$\int_{\Gamma_3} \sqrt{S(r, l_n, k)}\, \mathrm{d}r = \pm 2\Delta r_a \int_0^1 \sqrt{\frac{t-1}{t} \frac{-CA^2}{(A^2+B)\Delta r_a} + O(\Delta r_a)}\, \mathrm{d}t$$
$$= \pm \pi \mathrm{i} A \sqrt{\frac{-C\Delta r_a}{(A^2+B)}} + O\big(\Delta r_a^{5/2}\big).$$

Similarly

$$S\left(\pm \frac{\mathrm{i}}{\sqrt{B}} + t\Delta r_{b\pm}, l_n, k\right) = \frac{t-1}{t} \frac{-C\sqrt{B}\Delta r_{b\pm}}{2(\sqrt{B} \pm \mathrm{i}A)} + O(\Delta r_{b\pm})$$

and

$$\int_{\Gamma_{4,5}} \sqrt{S(r, l_n, k)}\, \mathrm{d}r = \pm 2\Delta r_{b\pm} \int_0^1 \sqrt{\frac{t-1}{t} \frac{-C\sqrt{B}\Delta r_{b\pm}}{2(\sqrt{B} \pm \mathrm{i}A)} + O(\Delta r_{b\pm})}\, \mathrm{d}t$$
$$= \pm \pi \mathrm{i} \sqrt{\frac{-C\sqrt{B}}{2(\sqrt{B} \pm \mathrm{i}A)\Delta r_{b\pm}}} + O\big(\Delta r_{b\pm}^{5/2}\big).$$

So,

$$l_n = -n - 1 \pm \frac{\mathrm{i}A}{2} \sqrt{\frac{-C\Delta r_a}{A^2+B}} \pm \frac{\mathrm{i}}{2} \sqrt{\frac{-C\sqrt{B}\Delta r_{b+}}{2(\sqrt{B}+\mathrm{i}A)}} \pm \frac{\mathrm{i}}{2} \sqrt{\frac{-C\sqrt{B}\Delta r_{b-}}{2(\sqrt{B}-\mathrm{i}A)}} + O\left(\frac{1}{k^5}\right). \tag{14}$$

The choice of signs comes from comparing the results of the direct integration of the Schrödinger equation or using the given asymptotics $\mathrm{e}^{+\mathrm{i}kr}$ as $r \to \infty$. This choice of the asymptotics determines a unique branch of the multivalued function by a standard procedure. Thus all the signs in the previous equation should be taken as +, and we obtain

$$l_n = -n - 1 + \frac{\mathrm{i}A}{2} \sqrt{\frac{-C\Delta r_a}{A^2+B}} + \frac{\mathrm{i}}{2} \sqrt{\frac{-C\sqrt{B}\Delta r_{b+}}{2(\sqrt{B}+\mathrm{i}A)}} + \frac{\mathrm{i}}{2} \sqrt{\frac{-C\sqrt{B}\Delta r_{b-}}{2(\sqrt{B}-\mathrm{i}A)}} + O\left(\frac{1}{k^5}\right). \tag{15}$$

Using the expressions for Δr_a and Δr_b, we obtain the first three terms of the expansion l_n in powers of $1/k$

$$l_n = -n - 1 + \frac{c_1}{k} + \frac{c_2}{k^3} + c_3 + O\left(\frac{1}{k^5}\right) \tag{16}$$

where the coefficients c_1, c_2, c_3 can easily be obtained from equation (15), e.g.

$$c_1 = -\frac{CA^2\mathrm{i}}{2(A^2+B)} - \frac{C\sqrt{B}}{4(A-\mathrm{i}\sqrt{B})} + \frac{C\sqrt{B}}{4(A+\mathrm{i}\sqrt{B})} = -\frac{C\mathrm{i}}{2} = Z\mathrm{i} \tag{17}$$

$$c_2 = -\frac{\mathrm{i}C}{4}(n(n+1)(A^2-B) - CA) \tag{18}$$

$$c_3 = \frac{C^2}{8}(2n+1)(A^2-B). \tag{19}$$

Going back to the RTF potential with $A = aZ^{1/3}$, $B = bZ^{2/3}$ and $C = -2Z$, we obtain the corrected l_n

$$l_n = -n - 1 + \frac{Z\mathrm{i}}{k} + \frac{\mathrm{i}Z^{5/3}(n(n+1)(a^2-b) + 2aZ^{2/3})}{2k^3} + \frac{Z^{8/3}(2n+1)(a^2-b)}{2k^4} + O\left(\frac{1}{k^5}\right). \tag{20}$$

It is clear from this formula that at high energies the RP trajectories merge with the trajectories of the Coulomb potential ($a = b = 0$).

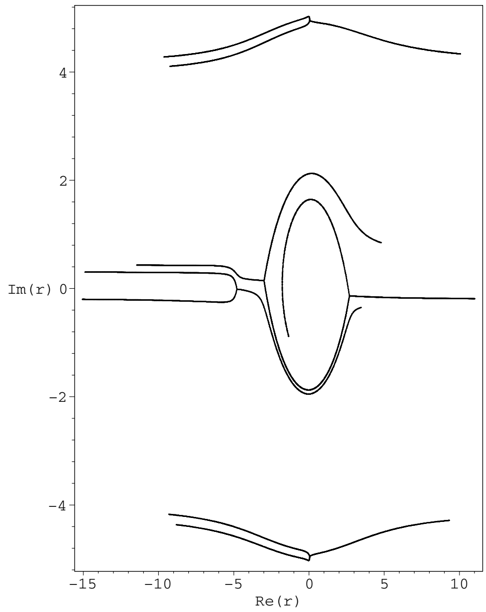

Figure 2. Anti-Stokes line topology for the RTF potential $V(r) = -\frac{1}{r(1+0.2r)(1+0.04r^2)}$ for $k = 2$ and $n = 5$. The five points generating the Regge pole $l_5 = -6.019\,884\,954 + \mathrm{i}0.267\,807\,0513$ are given in table 1.

Table 1. Five points generating the Regge pole $l_5 = -6.019\,884\,954 + \mathrm{i}0.267\,807\,0513$.

	Real part	Imaginary part
r_1	$-2.986\,037\,291$	$0.145\,475\,8971$
r_2	$2.686\,283\,188$	$-0.136\,926\,2214$
r_3	$-4.799\,075\,077$	$-0.010\,926\,043\,24$
r_4	$0.048\,351\,064\,56$	$-4.951\,326\,218$
r_5	$0.050\,478\,115\,67$	$4.953\,702\,585$

3. Results

Figure 1 shows the typical positions of all turning points and singularities of the potential, as well as all cuts. There are four poles and five TPs of the RTF potential. Three of the TPs are located next to the poles (each pole is connected to the closely located TP by a cut) and the other two generate Regge poles (connected by a cut to each other). So there is a total of four cuts.

Figure 2 shows the anti-Stokes line topology for the RTF potential with $a = 0.2$, $b = 0.04$ and $Z = 1$: $V(r) = -\frac{1}{r(1+0.2r)(1+0.04r^2)}$ for $k = 2.0$ and $n = 5$. The five points generating the Regge pole $l_5 = -6.019\,884\,954 + \mathrm{i}0.267\,807\,0513$ are given in table 1. The points r_1 and r_2 are almost connected by an anti-Stokes line. The connection is not complete due to an error in the calculation by the Newton method of solving the Bohr–Sommerfeld condition. The central part of the picture is typical of a Coulomb potential. For large energies the RTF potential is very similar to the Coulomb potential. This can be explained by the fact that the two turning points generating the Regge pole are close to the origin and the other three singularities of the potential do not affect the connection by an anti-Stokes line.

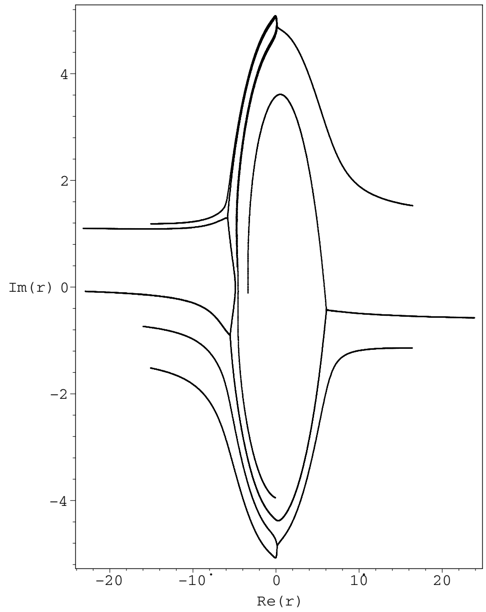

Figure 3. Anti-Stokes line topology for the RTF potential $V(r) = -\frac{1}{r(1+0.2r)(1+0.04r^2)}$ for $k = 0.8359$ and $n = 5$. The five points generating the Regge pole $l_5 = -5.697\,128\,644 + \mathrm{i}0.343\,059\,6507$ are given in table 2.

Table 2. Five points generating the Regge pole $l_5 = -5.697\,1286\,44 + \mathrm{i}0.343\,059\,6507$

	Real part	Imaginary part
r_1	6.060 138 392	−0.427 908 6239
r_2	−5.827 882 440	1.303 898 691
r_3	−5.525 389 875	−0.901 629 3692
r_4	0.135 956 4202	−4.850 630 477
r_5	0.157 177 5032	4.876 269 779

Figure 3 shows the anti-Stokes line topology for the same RTF potential with $k = 0.8359, l_5 = -5.697\,128\,644 + \mathrm{i}0.343\,059\,6507$. Here three turning points are connected by an anti-Stokes line. Such a triple connection signifies that: either we have to pick another pair of turning points or choose another value n or both. This triple connection is a condition which determines whether or not the Bohr–Sommerfeld equation is still valid for the chosen pair of turning points. The initial choice of the turning points for large energies is easy since the turning points responsible for the Regge poles tend to the origin when the energy becomes huge. So the connection of these TPs by aSL is close to the origin too. With decreasing energy, this aSL expands and at some value of the energy touches one of the other three turning points. This is a signal that the formal solution of the BS equation is no longer applicable and we have to change the pair of TPs in the integral in the BS condition equation (10) and possibly n as well.

Figure 4 shows three partial Regge trajectories for the RTF potential $V(r) = -\frac{20}{r(1+0.027\,144\,176\,17r)(1+7.368\,062\,997r^2)}$ $(Z = 10, a = 0.0126, b = 1.5874)$ with $n = 5$. This figure demonstrates very good agreement among the results of direct integration of the

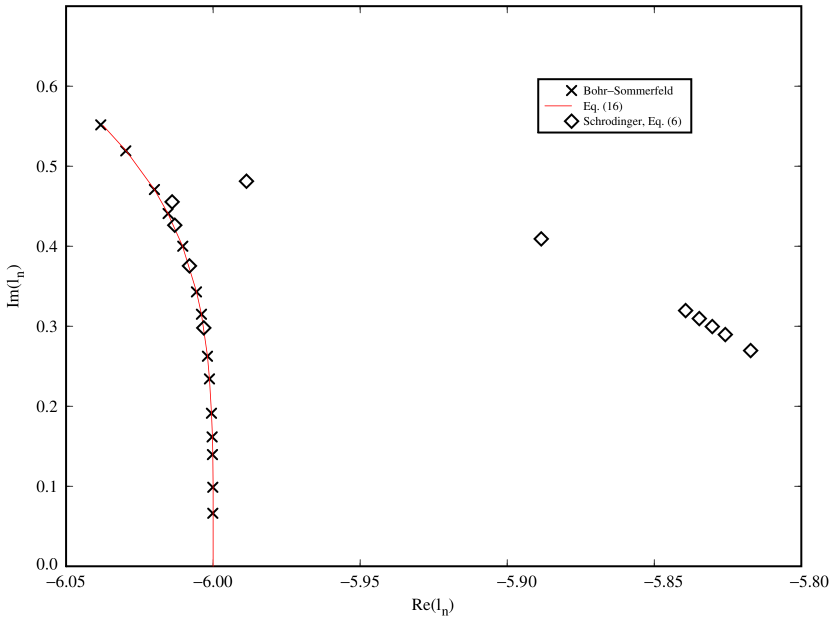

Figure 4. Three partial Regge trajectories for the RTF potential $V(r) = -\frac{20}{r(1+0.027\,144\,176\,17r)(1+7.368\,062\,997r^2)}$ ($Z = 10, a = 0.0126, b = 1.5874$) with $n = 5$. One of the partial trajectories (crosses) is calculated from solving the Bohr–Sommerfeld condition ($k = 10$ through 150). Diamonds represent the results of direct integration of the Schrödinger equation ($k = 4.5$ through 30) while dashes are the results obtained using equation (16) ($k = 20$ through 150).

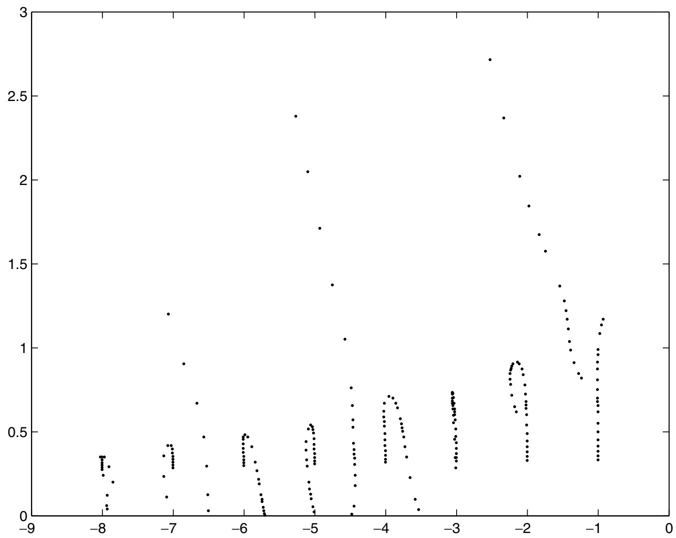

Figure 5. Sequence of partial Regge trajectories for the RTF potential $V(r) = -\frac{20}{r(1+0.027\,144\,176\,17r)(1+7.368\,062\,997r^2)}$ ($a = 0.0126, b = 1.5874, z = 10$) with n varying from 0 to 7 and k varying from 4.5 to 30.

Schrödinger equation (diamonds), solving the BS equation (crosses), and using the formula given by equation (16) (dashes) for high energies ($k = 20$ through to 150). Then, with decreasing energy, the RT goes to the right away from the predicted values. So the formal solution of the BS equation is not valid and the pair of TPs and the number n have to be changed in the BS condition, equation (10). Also, it is clear that the usual approach of decomposing into a series in powers of $1/k$ requires more terms to give a good accuracy.

Figure 5 reveals partial Regge trajectories for the RTF potential of figure 4 as solutions of the Schrödinger equation. As expected, most of them have negative almost integer real parts for large energies. This corresponds to different integer n from 0 through 7 as k varies from 4.5 to 30 in the BS condition. For smaller energies some trajectories turn right and others turn left. All of them tend to go to the real line as k approaches ∞. There are three unusual trajectories which do not seem to be bounded as energies becomes infinitely large. These curves and why the Regge trajectories turn right or left need further investigation.

4. Discussion and conclusion

In our investigation of Regge poles trajectories for the complicated nonsingular such as the Thomas–Fermi type potentials we discovered a simple and powerful semiclassical method, based on the investigation of anti-Stokes line topology. The interesting result has been found that in contrast to the case of singular potentials, the anti-Stokes lines topology for the Thomas–Fermi potentials is very complicated and requires a careful application of complex analysis. For large energies three of the five turning points are close to the poles of the effective potential. This permitted the introduction of the concept of small parameters for decomposing into a series the action integral (Bohr–Sommerfeld quantization condition).

Using Cauchy's theorem, we evaluated the resulting contour integrals to obtain an approximate expression for the Regge poles, which with the appropriate choice of the parameters of the effective potential reduces to the well-known result for the Coulomb potential. We also discovered that the Bohr–Sommerfeld condition at low E can result in a triple connection, implying the failure of our assumption of connectivity. We conclude by noting that the Regge poles trajectories for other rational approximations of the Thomas–Fermi potential can be investigated similarly to the present approach.

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