Semiclassical approach for calculating Regge-pole trajectories for singular potentials

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A simple semiclassical approach, based on the investigation of the anti-Stokes line topology is presented for calculating Regge-poles trajectories for singular potentials, viz. potentials more singular than r^{-2} at the origin. It uses the explicit solution of the Bohr-Sommerfeld quantization condition with the *proviso* that the positions of two turning points of the effective potential responsible for the Regge poles be relatively close together. We also demonstrate that due to this closeness the Regge trajectories asymptotically approach parallel equidistant straight lines with a slope of $\cot(\phi/m)$, m being the power and ϕ the argument of the coefficient of the potential. Illustrative results are presented for the polarization and Lennard-Jones potentials.

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I. INTRODUCTION

The complex angular-momentum representation [1], involving Regge-pole calculations, for scattering of heavy particles such as atoms and molecules has achieved great success over the ordinary partial-wave expansion utilizing only non-negative integer values of the angular momentum. Accurate methods for calculating Regge-pole trajectories for potentials more singular than r^{-2} at the origin are needed for collisions involving heavy particles. However, the main difficulty in calculating the Regge-pole trajectories for singular potentials in the complex angular-momentum plane, for real positive values of the energy, stems from the fact that one deals with a singular eigenvalue problem for a non-Hermitian Schrödinger operator with currently no general simple working method.

The study of molecular reactive collisions, both experimental and theoretical, is one of the most active areas of research in chemical physics. Understanding the role that dynamical scattering resonances play in chemical reactions [2], a key to the laser control of reactions and bond selective chemistry, is crucial to gaining insights into all chemical reactivity. Recent advances in both theory and experiment have brought inelastic, particularly reactive atom-diatom collisions to the leading edge of atomic and molecular physics [3–9]. The full understanding of atom-diatom systems, provided by the analysis that identifies complex angular-momentum resonances (Regge poles) of the S matrix for various collision processes [6,9–14], requires insights into the physics of collisions.

Recent Padé-Regge pole analysis of chemical reactions [15] reconstructs the S matrix in the complex plane of the total angular momentum. The generated computer code could be applied to a wide class of reactive or nonreactive atom-diatom collision systems, including the Na^+-Na reaction which has a rich structure [8]. Therefore, accurate, simple, and efficient methods to calculate Regge-pole trajectories are needed. Interestingly, the singular potential method has also been applied successfully in the investigation of the possibility of forming dimer resonances in the He-He collision problem, where the regular potential method [16] proved to be inadequate.

Different methods have been developed for calculating Regge poles. Some of these are as follows: generating converging bounds [17], the semiclassical methods [18], the phase integral method [19], the phase amplitude method [20], the continued fraction method [21], analytical methods for singular potentials [22], the complex harmonic oscillator method [23], the complex eigenvalues method [24], the equivalent dimensional perturbation methods [25], the direct numerical integration of the Schrödinger equation [26,27], and the complex energy methods using the Jost function [16,28]. Many of these methods have been criticized recently [25]. The largest drawback of the semiclassical (WKB) approximation is the difficulty of understanding the behavior of the complex turning points with the attendant anti-Stokes line topology; furthermore, it is cumbersome in application [29]. Hence, the present development.

II. THEORY

A. General

In this paper we present a semiclassical approach for calculating Regge-pole trajectories for singular potentials. It is based on two basic assumptions: (1) The existence of two turning points of the effective potential responsible for the Regge poles, which are relatively close to each other and (2) the connection of these turning points by anti-Stokes lines [30,31]. We also demonstrate that at high energy the Regge-pole trajectories asymptotically approach equidistant parallel straight lines whose slope is related to the parameters of the relevant singular potential.

From the semiclassical consideration the equidistant parallel straight-line behavior should be the consequence of the crucial simplification of the Bohr-Sommerfeld condition, which gives the quantization of the trajectories. The correct simplification of the condition results from the assumption of the relative closeness of the relevant semiclassical turning points in the complex plane of the variable r. This hypothesis seems to be a natural instrument for the investigation of the

Regge trajectories for large values of the energy. It enables us to replace the very complicated nonlinear Bohr-Sommerfeld equation by much simpler equations corresponding to the decomposition into series of the action integral near the turning points. According to the semiclassical approach, relative closeness implies that the distance between the pair of turning points generating the Regge poles is much less than their distance from the origin. (Note that at high energy turning points usually are close to the origin.)

The second hypothesis in our approach, namely, the connection of the pair of turning points which are close to each other by an anti-Stokes line [30,31] is a necessary condition for solving the Bohr-Sommerfeld quantization condition in the high-energy asymptotic behavior of Regge-pole trajectories. We also need a more detailed analysis of the anti-Stokes line topology for the calculation of higher-order terms of the asymptotic behavior. The structure of the anti-Stokes line is rather complicated, even for the case of simple potentials. We will restrict ourselves here to the first two terms. A more general detailed presentation, which includes higher-order terms than the second is forthcoming [32].

It should be mentioned that the idea of the localization of the particle at the bottom of the effective potential, for the calculation of the leading term of the asymptotic behavior of the poles has been utilized [25] within the framework of the dimensional scaling approach. In that approach the leading term of the $1/k$ expansion (k^2 is the scaled energy) of the Regge pole was found by minimizing the effective potential, while the higher-order terms were evaluated by a perturbation approach. In this paper we present a semiclassical method to obtain the higher-order correction in the $1/k$ expansion. We also give the semiclassical verification for the approach of the paper [25], based on the topology of the anti-Stokes lines.

Here we consider the Schrödinger equation as an eigenvalue problem for the complex angular momentum $l=l_n(k)$ with the given positive energy $k^2>0$. The solution of this equation, with the regular boundary condition for the wave function $\Psi(l_n(k),r)$ [33] at the origin and the condition that at infinity $\Psi(l_n(k),r)$ is an outgoing plane wave leads, in general, to the complex values of $l_n(k)$ ($n=0,1,2,\ldots$). Our method is applied to potentials $V(r)=C(r)/r^m (m>2)$ near the origin with $C(r)$ being a finite smooth function of r. We assume that $V(r)\to 0$ for $r\to\infty$.

The semiclassical condition can be satisfied if we consider the semiclassical turning points $r_{1,2}$ in the effective potential $V_{eff}=-V(r)-l(l+1)/r^2$ to be close to each other in the complex r plane. The leading term l_n^0 of the Regge pole of $l_n(k)$ can be obtained immediately from the system of equations (the turning points $r_{1,2}$ are assumed to coincide with the value r_0)

$$S(r_0,l_n^0,k)=k^2-V(r_0)-\left[\frac{\left(l_n^0+\frac{1}{2}\right)}{r_0}\right]^2=0 \tag{1}$$

$$\left(\frac{\partial S(r_0,l_n^0,k)}{\partial r}\right)=\left(-\frac{dV(r)}{dr}+2\frac{\left(l_n^0+\frac{1}{2}\right)^2}{r^3}\right)_{r=r_0}=0, \tag{2}$$

where we have used the standard replacement $l(l+1)$ by $(l+1/2)^2$.

To obtain the next term in the approximation of $l_n(k)$ we assume that the positions of the turning points $r_{1,2}$ do not coincide but are close together so that

$$r_{1,2}=r_0(1\pm\tfrac{1}{2}\Delta), \quad |\Delta|\ll 1 \quad \text{for } k\to\infty, \tag{3}$$

where $r_{1,2}$ are solutions of the equation

$$S(r,l_n,k)=k^2-V(r_{1,2})-\left[\frac{\left(l_n+\frac{1}{2}\right)}{r_{1,2}}\right]^2=0 \tag{4}$$

with

$$\left(l_n+\frac{1}{2}\right)^2=\left(l_n^0+\frac{1}{2}\right)^2(1+\delta), \quad \delta\propto\Delta^2. \tag{5}$$

The corrections Δ and δ are obtained from the Bohr-Sommerfeld condition

$$\pi\left(n+\frac{1}{2}\right)=\int_{r_1}^{r_2}\sqrt{S(r,l_n,k)}\,dr, \quad n=0,1,2,\ldots. \tag{6}$$

In Eq. (5) we integrate along the anti-Stokes line: $\mathrm{Im}\int_{r_1}^{r_2}\sqrt{S(r,l_n,k)}dt=0$, connecting the turning points r_1 and r_2, i.e., the connection by the anti-Stokes line is the necessary condition to obtain the Regge-pole trajectories. From Eqs. (1) and assuming that other solutions of Eq. (3) are different from r_0, we obtain

$$\pi\left(n+\frac{1}{2}\right)=r_0^{-m/2}\left(\frac{\partial^2 r^m S(r,l_n^0,k)}{2\partial r^2}\right)^{1/2}\int_{r_1}^{r_2}\sqrt{(r-r_1)(r-r_2)}\,dr. \tag{7}$$

The integral can be easily calculated

$$\int_{r_1}^{r_2}\sqrt{(r-r_1)(r-r_2)}\,dr=\pm i\frac{\pi}{8}(r_2-r_1)^2. \tag{8}$$

From Eqs. (2) and (6) we obtain

$$\pi\left(n+\frac{1}{2}\right)=\pm i\frac{\pi}{8}r_0^{(4-m)/2}\Delta^2\left(\frac{\partial^2 r^m S(r,l_n^0,k)}{2\partial r^2}\right)^{1/2}_{r=r_0}. \tag{9}$$

In Secs. II and III we derive analytical expressions for Regge-pole trajectories for the $V(r)=C/r^m$, $(m>2)$ potential [particularly the polarization potential $V(r)=C/r^4$], and for the Lennard-Jones potential. We show that in both cases the trajectories approach parallel equidistant straight lines in the high-energy limit.

B. Regge-pole trajectories for the $V(r)=C/r^m$ potential

Here we consider the singular potential $V(r)=C/r^m$, ($m>2$). For such a potential the system of equations, Eqs. (1), is satisfied for

$$r_0^2=\frac{\left(l_n^0+\frac{1}{2}\right)^2}{k^2}\,\frac{m-2}{m} \tag{10}$$

and the zero-order Regge pole is

$$l_n^0=-\tfrac{1}{2}+[-C(m-2)/2]^{1/m}\sqrt{m/(m-2)}\;\;k^{1-2/m}. \tag{11}$$

Note that r_0 is small for large k. The next-order term is obtained from the Bohr-Sommerfeld condition, Eq. (8). A straightforward calculation of the derivative in Eq. (8) yields

$$\pi\left(n+\frac{1}{2}\right)=\pm i\frac{\pi}{8}kr_0\Delta^2\sqrt{m}. \tag{12}$$

Substituting either of $r_{1,2}$ from Eq. (2) and $(l_n+1/2)^2$ from Eq. (4) with r_0 and l_n^0 given by Eqs. (9) and (10), respectively, into the first of Eqs. (1) we find the relationship between the corrections Δ and δ (to an accuracy of Δ^2) given by

$$\Delta^2=\frac{4\delta}{m-2}. \tag{13}$$

Choosing the $(+)$ sign for Δ^2, we obtain from Eqs. (9) and (11)

$$\Delta^2=8i\frac{\left(n+\frac{1}{2}\right)}{\left(l_n^0+\frac{1}{2}\right)\sqrt{m-2}}. \tag{14}$$

Combining Eqs. (4), (10), (12), and (13) we obtain the Regge-pole positions

$$l_n+\tfrac{1}{2}\cong[-C(m-2)/2]^{1/m}\sqrt{m/(m-2)}\;\;k^{1-2/m}+i(n+\tfrac{1}{2})\sqrt{m-2}. \tag{15}$$

This formula coincides with that of Connor [1] for the power-like potentials. It gives another confirmation of the validity of Connor's formula over that of Tiktopoulos [34]. For the polarization potential $[V(r)=C/r^4]$, Eq. (14) corresponds to that of Vrinceanu *et al.* [29].

Generally speaking, Eq. (10) or Eq. (14) gives m different series of Regge trajectories corresponding to the choice of the appropriate root of the first of Eqs. (1). The proper branch should be chosen on the basis of the anti-Stokes line topology analysis. Note that in order to apply the semiclassical method, the close turning points are to be connected by anti-Stokes lines [30,31] for the values l_n from Eq. (14). Our calculations for the polarization potential show that the right choice corresponds to the minimum value of $[-C(m-2)/2]^{1/m}$.

From Eq. (14) the asymptotic equidistant linear behavior of the Regge trajectories at high energy can be easily explained. Introducing the appropriate notations, we have for Eq. (14)

$$l_n+\tfrac{1}{2}=k^{1-2/m}(-C)^{1/m}\alpha_m+i(n+\tfrac{1}{2})\beta_m, \tag{16}$$

where $\alpha_m=[(m-2)/2]^{1/m}$ and $\beta_m=\sqrt{m-2}$ (for proper positive values α_m and β_m, depending only on m). Define $\arg(-C)=\phi$, then

$$\mathrm{Re}(l_n)=k^{1-2/m}\alpha_m(|C|)^{1/m}\cos(\phi/m)-\tfrac{1}{2}, \tag{17}$$

$$\mathrm{Im}(l_n)=k^{1-2/m}\alpha_m(|C|)^{1/m}\sin(\phi/m)+(n+\tfrac{1}{2})\beta_m. \tag{18}$$

Equations (16) and (17) reduce to

$$\mathrm{Re}(l_n)=\cot(\phi/m)\mathrm{Im}(l_n)-\tfrac{1}{2}-\cot(\phi/m)\beta_m(n+\tfrac{1}{2}). \tag{19}$$

For the specific case of the polarization potential, we have from Eq. (18)

$$\mathrm{Re}(l_n)=\cot(\phi/4)[\mathrm{Im}(l_n)-(n+\tfrac{1}{2})\sqrt{2}]-\tfrac{1}{2}. \tag{20}$$

Equation (18) is the linear equation for the Regge trajectories. It is clear from Eq. (18) that all Regge trajectories have the same slope ϕ/m and the distance between the lines corresponding to $n=0,1,2,\ldots$ is equal to $\cot(\phi/m)\beta_m$ and is again the same for all Regge trajectories. We note that Eq. (18) for the case of the polarization potential, viz. Eq. (19) was obtained previously [1,29] by different methods. The equidistant linear behavior of the asymptotics of the Regge trajectories was noted and presented in Ref. [29]. However, to the best of our knowledge the explanation of the behavior is given for the first time here.

C. The Lennard-Jones potential

The same method can be applied to the calculation of the Regge-pole trajectories for the Lennard-Jones potential

$$V(r)=4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12}-\left(\frac{\sigma}{r}\right)^{6}\right],\quad \sigma>0, \tag{21}$$

where the parameter $\epsilon>0$ is the well's depth. The exact turning points equation is

$$\left(\frac{r}{\sigma}\right)^{12}-\frac{a}{\sigma^2}\left(\frac{r}{\sigma}\right)^{10}-\frac{4\epsilon}{k^2}\left[1-\left(\frac{r}{\sigma}\right)^{6}\right]=0 \tag{22}$$

with $a=(l+1/2)^2/k^2$. From the system of Eqs. (1) we obtain

$$\left(\frac{\sigma}{r}\right)^6=\frac{4\epsilon}{k^2}\pm\sqrt{\left(\frac{4\epsilon}{k^2}\right)^2-\frac{20\epsilon}{k^2}}. \tag{23}$$

The expression under the square-root sign can be denoted by [29]

$$D=\sqrt{4-\frac{5k^2}{\epsilon}}=\pm\frac{k\sqrt{5}i}{\epsilon}\sqrt{1-\frac{4\epsilon}{5k^2}}. \tag{24}$$

Equation (22) then reduces to

$$\left(\frac{r}{\sigma}\right)^6=\frac{4\epsilon}{k^2}\left(1\pm\frac{D}{2}\right). \tag{25}$$

The appropriate branch is chosen such that $D\to i\sqrt{(5/\epsilon)}k$ as $k\to\infty$. This choice immediately dictates the selection of the $(-)$ sign in Eq. (24). However, the choice of the correct branch between the two can be checked numerically through the investigation of the anti-Stokes lines connection of the corresponding turning points [32].

From the expression for D we have

$$D^2=4-\frac{5k^2}{\epsilon}, \tag{26}$$

so that

$$\frac{4\epsilon}{k^2}=\frac{20}{(2-D)(2+D)} \tag{27}$$

and, hence

$$\left(\frac{r}{\sigma}\right)^6=\frac{10}{2+D}. \tag{28}$$

Equation (27) gives the approximate value of both turning points (r_1 and r_2) under our hypothesis of their relative closeness. This leads to the expression for the leading term of the Regge-pole trajectories, which is obtained by using Eq. (27) in Eq. (21),

$$\left(l_n^0+\frac{1}{2}\right)^2=6k^2\sigma^2\left(\frac{2}{2+D}\right)^{1/3}\left(\frac{3-D}{2-D}\right). \tag{29}$$

For the next correction we use the modified Eq. (8) in the form

$$\pi\left(n+\frac{1}{2}\right)=\pm i\frac{\pi}{8}\sigma^2(\sigma r_0)^6\left(\frac{\partial^2\left(\frac{r}{\sigma}\right)^{12}S(r,l_n^0,k)}{2\partial r^2}\right)^{1/2}_{r_0}$$
$$\times\left(\frac{r_2}{\sigma}-\frac{r_1}{\sigma}\right)^2, \tag{30}$$

where $r_{1,2}$ are defined by

$$\left(\frac{r_{1,2}}{\sigma}\right)^6=\frac{10}{2+D}\left(1\pm\frac{1}{2}\Delta\right) \tag{31}$$

[compare with Eq. (2)].

Performing the differentiation of the function $S(r,l_n^0,k)$, given by the first of Eqs. (1), with the Lennard-Jones potential $V(r)$ from Eq. (20), we have with accuracy $O(1/k^{5/12})$

$$l_n\approx-\tfrac{1}{2}+(-20\epsilon)^{1/12}k^{5/6}\sqrt{\tfrac{6}{5}}\sigma+i\sqrt{10}(n+\tfrac{1}{2}). \tag{32}$$

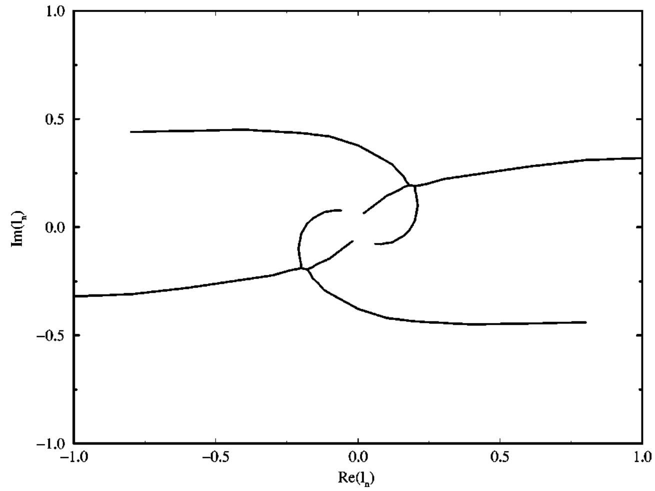

FIG. 1. Anti-Stokes line topology for the polarization potential $V(r)=2/r^4$ for $k=20$ and $n=7$. The four turning points generating the Regge pole $l_7=4.818\,296+i5.288\,306$ are given in Table I.

This expression agrees with the first two terms of Eq. (23) in paper [29]. Note, that the same result can be obtained for the potential $V(r)=4\epsilon(\sigma/r)^{12}$ (see Sec. I). This is not surprising since at high energy the largest contribution comes from the internal part of the potential well, and the influence of the second term of the Lennard-Jones potential Eq. (19) is of a smaller order [our estimation [32] shows that the order is $O(1/k^{1/6})$].

III. RESULTS

Figure 1 shows the anti-Stokes line topology for the polarization potential $V(r)=2/r^4$ for $k=20$ and $n=7$. The four turning points generating the Regge pole $l_7=4.818\,296+i5.288\,306$ are given in Table I. The upper turning points are very close to each other and are almost connected by an anti-Stokes line. This approximate, rather than complete, connection is due to a small error in the true Regge-pole calculations by the Newton method we used. The diagram is obviously symmetric with respect to the origin. Other anti-Stokes lines, except those connecting the two pairs of turning points, are either tending to infinity or approaching the origin. The close pair of turning points generating the Regge pole is clearly manifest in Fig. 1.

Figure 2 shows the linear behavior of the Regge trajecto-

TABLE I. Turning points generating the Regge pole $l_7=4.818\,295\,895+i5.288\,305\,825$ for the polarization potential $V(r)=2/r^4$ with $k=20$ and $n=7$.

	Real part	Imaginary part
r_1	-0.1767215688	-0.1966888754
r_2	0.1767215688	$+0.1966888754$
r_3	-0.1989215566	-0.1787275944
r_4	0.1989215566	$+0.1787275944$

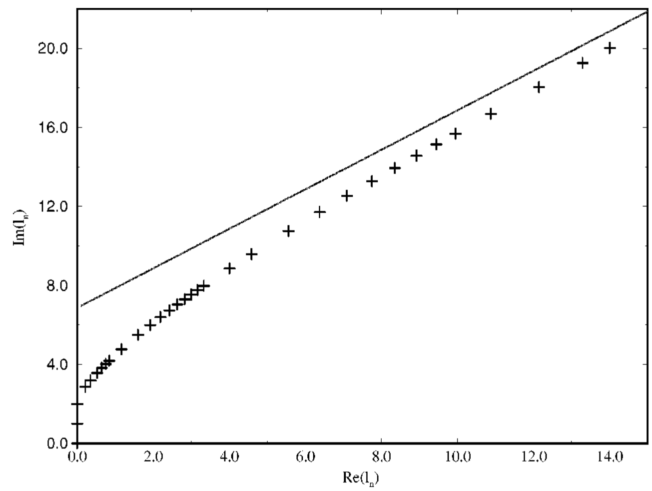

FIG. 2. Linear behavior of the Regge trajectories in the complex angular-momentum plane for the polarization potential $V(r)=1/r^4$ for $n=4$ and k varying from 0.05 through 200.

ries in the complex angular-momentum plane, for $V(r)=1/r^4$ with $n=4$ and k varying from 0.05 through 200. The straight line is according to the asymptotic formula, Eq. (15), while the dotted curve is the numerical solution of the Bohr-Sommerfeld equation, Eq. (5). It was used in Newton's method [35] for solving the Bohr-Sommerfeld equation for l. Clearly, for high energy the asymptotically linear character of the Regge trajectory is evident and is consistent with our Eq. (15). For this case the slope of the line is $\cot(\pi/4)$. There are many more lines corresponding to different values of n.

Figure 3 shows the anti-Stokes lines topology for the Lennard-Jones potential $V(r)=r^{-12}-r^{-6}$ for $k=10.0$ and $n=2$, when l is a Regge pole given by $l_2=-6.534\,711+i1.870\,983$. The 12 turning points generating l_2 are given in Table II. Again the figure is symmetric with respect to the origin. Among the 12 turning points displayed, only the two upper ones are connected by an anti-Stokes line. These points are relatively close to each other. All the remaining pairs of turning points, except the two symmetric ones, are not connected by anti-Stokes lines since the anti-Stokes lines originating at these turning points are either going to infinity or to the origin. Figure 3(b) depicts the anti-Stokes line topology for the same Lennard-Jones potential as in Fig. 3(a), for $k=10.0$ and $n=2$, but when l_2 is not a Regge pole and is given by $l=-2.708\,857-i0.337\,874$. The corresponding turning points are given in Table III. Here no two turning points are connected by an anti-Stokes line, consistent with our second hypothesis.

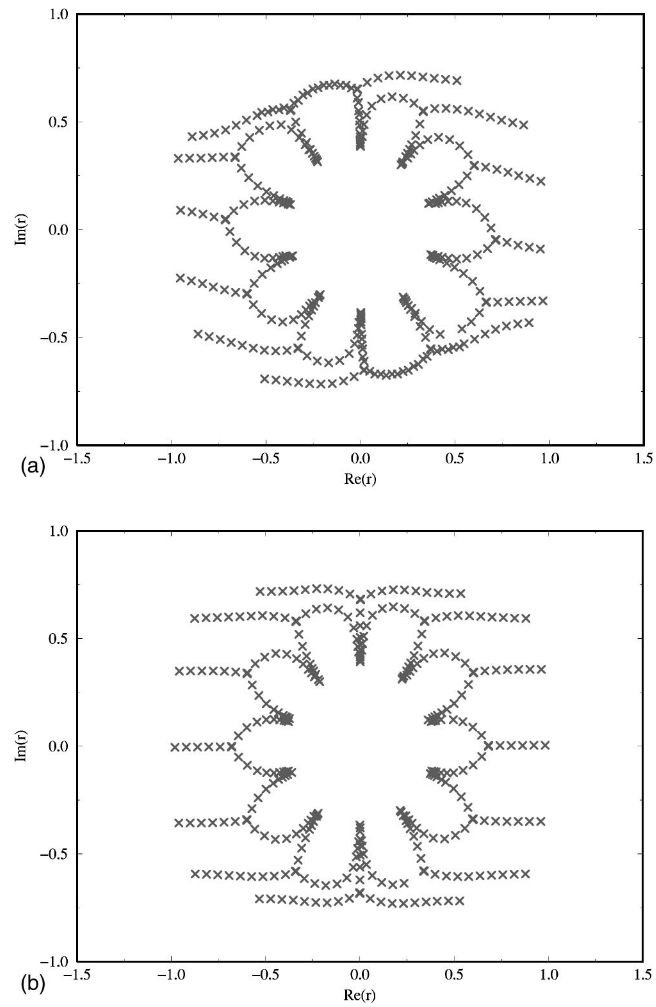

FIG. 3. (a) Anti-Stokes line topology for the Lennard-Jones potential $V(r)=r^{-12}-r^{-6}$ for $k=10.0$ and $n=2$, when l is a Regge pole given by $l_2=-6.534\,711+i1.870\,983$. The 12 turning points generating l_2 are given in Table II. (b) Anti-Stokes line topology for the same Lennard-Jones potential as in (a) for $k=10.0$ and $n=2$, but when l_2 is not a Regge pole and given by $l_2=-2.708\,857-i0.337\,874$. The corresponding turning points are given in Table III.

IV. CONCLUSION AND DISCUSSION

The need for more powerful, simple, and efficient methods for calculating Regge-pole trajectories for singular potentials, particularly for application to collision problems in the Bose-Einstein condensation and resonance scattering, has inspired this paper. Here we have developed a simple approach for the calculation of Regge trajectories for singular potentials to augment the few existing analytical and numerical methods, many of which have been criticized recently [25]. It is based on two self-consistent hypotheses: (1) relative closeness of the two turning points generating the Regge trajectories (this hypothesis is compatible with the dimensional scaling approach [25]) and (2) connection or approximate connection of these two turning points by an anti-Stokes line. When applied to the standard polarization and Lennard-Jones potentials, our expressions yield results that are in excellent agreement with those of other analytical and numerical calculations of Regge-pole trajectories.

By examining the anti-Stokes line topology of turning points in the complex r plane, even for complicated potentials such as the Lennard-Jones potential, connected turning points can be readily identified [see Figs. 3(a) and 3(b)] and the integration path in the complex r plane can be defined. This problem of determining which turning points are connected by anti-Stokes lines had plagued the semiclassical

TABLE II. Turning points generating the Regge pole $l_2 = -6.534\,710\,753 + i1.870\,983\,399$ for the Lennard-Jones potential $V(r) = r^{-12} - r^{-6}$ with $k = 10$ and $n = 2$.

	Real part	Imaginary part
r_1	−0.7158204177	+0.04685172418
r_2	−0.6649891582	+0.3358233039
r_3	−0.6016085508	−0.2973002704
r_4	−0.3703911337	+0.5543339621
r_5	−0.3313257974	−0.5495790559
r_6	−0.01792718343	+0.6515177685
r_7	0.01792718343	−0.6515177685
r_8	0.3313257974	+0.5495790559
r_9	0.3703911337	−0.5543339621
r_{10}	0.6016085508	+0.2973002704
r_{11}	0.6649891582	−0.3358233039
r_{12}	0.7158204177	−0.04685172418

TABLE III. Turning points generating the non-Regge pole $l_2 = -5.510\,696\,693 + i2.894\,997\,458\,1$ for the Lennard-Jones potential used in Fig. 3(a) with $k = 8$ and $n = 2$.

	Real part	Imaginary part
r_1	−0.6811080930	−0.001884306551
r_2	−0.6010191104	−0.3420704396
r_3	−0.5988337916	+0.3387919023
r_4	−0.3418052508	−0.5812956748
r_5	−0.3387881141	+0.5797935133
r_6	−0.001770041012	−0.6814218018
r_7	0.001770041012	+0.6814218018
r_8	0.3387881141	−0.5797935133
r_9	0.3418052508	+0.5812956748
r_{10}	0.5988337916	−0.3387919023
r_{11}	0.6010191104	+0.3420704396
r_{12}	0.6811080930	+0.001884306551

methods, thereby limiting their deserved utility. In the present development we are able to identify even "false Regge poles," i.e., poles that satisfy the Bohr-Sommerfeld quantization condition but do not satisfy the Schrödinger equation.

We have demonstrated the validity of our hypotheses by the numerical calculation of the anti-Stokes line topology for the polarization and the Lennard-Jones potentials. The wave function $\Psi(l_n(k),r)$ when analytically continued to the complex r plane, is concentrated along the anti-Stokes line where it has an oscillatory character. It exponentially decreases along the anti-Stokes line, which connects one of the turning points with the origin. Thus, the asymptotic straight-line behavior of the Regge trajectories can be explained in terms of the sharp localization of the wave function in a very small region of the complex r plane, which implies the closeness of the turning points generating the trajectory.

Generally, for the calculation of scattering differential and integral cross sections for atoms, accurate Regge-pole positions and the corresponding residues are needed. However, for the recently developed Padé-Regge pole analysis [15] of chemical reactions in which the S matrix is analytically continued to the complex angular-momentum plane to identify resonances and for the generalized Lassettre expansion [36] for the calculation of small-angle electron-scattering differential cross sections [37], only accurate Regge-pole positions are required. These, together with the difficulty of understanding the behavior of complex turning points and the accompanying anti-Stokes line topology, inherent in the semiclassical description of scattering processes, have motivated the present development. The expressions for the residues will be ready for presentation with the general formulas.

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