Analytical accurate Regge-trajectory calculation for singular potentials

D. Vrinceanu,[1,2] A. Z. Msezane,[1] and D. Bessis[1]
[1]*Center for Theoretical Studies of Physical Systems, Clark Atlanta University, Atlanta, Georgia 30314*
[2]*School of Physics, Georgia Institute of Technology, Atlanta, Georgia 30332*
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An entirely analytical method for computing Regge-pole trajectories for singular potentials (potentials diverging faster than r^{-2} at the origin) is presented. Explicit results are presented for polarization ($1/r^4$) and Lennard-Jones (6,12) potentials. Numerical precision of the calculations is fully controlled and often better than the state of the art numerical methods. The present method combines two different analytical approaches. The first one obtains a perturbation expansion of the Regge trajectories in terms of an appropriate parameter. Then the convergence of the resulting asymptotic series is improved through Padé approximations. Highly accurate results are then possible within a wide range of energies. For typical parameters used in the literature, the two-term expansion, for which explicit formulas are presented, gives at least five digits of accuracy, while higher approximations give up to 14 digits of accuracy.

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I. INTRODUCTION

For scattering involving heavy particles, such as atoms and molecules, the ordinary partial wave expansion utilizing only non-negative integer values of the angular momentum is often slowly convergent and hardly appropriate for numerical calculation. The complex angular momentum representation [1], which involves Regge-pole calculations, has proved to be the adequate answer.

In the case of singular potentials, the main difficulty in computing a Regge-pole position in the complex angular momentum plane, for real positive values of the energy, comes from the fact that this problem is a singular eigenvalue problem for a non-Hermitean Schrödinger operator. Currently, no general working method is available that can provide a sufficiently accurate and simple analytic expression for the Regge-pole positions. The most accurate methods published, to our knowledge, are purely numerical; see, for the latest work, [2]. They have various degrees of complexities as well as accuracy.

The understanding of collisional processes involving heavy particles, which are important in laser isotope separation, astrophysics, plasma physics, and molecular processes, requires the calculation of differential and integral cross sections (DCSs, ICSs). In Regge-pole theory, the evaluation of the DCSs requires a knowledge of such quantities as Regge-pole positions and their corresponding residues. Currently, there are several calculational approaches, of varying degrees of accuracy, used to calculate Regge poles. Some of them are the following: direct numerical integration of the Schrodinger equation [3,4], semiclassical WKB approximation [1,5,6], transformation of the Schrodinger equation into a nonlinear form [7], dimensional scaling procedure [8,9], phase-integral methods [10], and phase-amplitude methods [11].

The first two methods have been criticized [7]. The direct method is slow because it involves the integration of a wave function and it is numerically unstable due to the accumulation of errors. The largest drawback of the WKB approximation is the difficulty of understanding the behavior of the complex turning points with the attendant problem of the Stokes lines topology; furthermore, it is cumbersome in application. Although it has yielded reasonably accurate results with accuracy increasing with the Regge-pole index n, there is no general scheme to achieve a given *a priori* accuracy in this approach. The disadvantages of transforming the Schrödinger equation into a nonlinear form are that derivatives of the potential appear and the corresponding Hankel functions must be determined very accurately. Incidentally, the Jost function [2] approach for singular potentials, which is essentially a variation of the WKB method, suffers problems similar to some of the methods above since it also employs derivatives of the potential and uses coordinate rotation.

Phase-integral methods [10] and phase-amplitude methods [11] give very accurate results. However, they do not provide deep insight into the analytic structure of the Regge-pole trajectories and lack wide energy range analytic expressions for the Regge-pole positions.

Analytic expressions, like the complex harmonic oscillator formula [12], have been improved by direct $\hbar$ expansion [13]. But because no accelerator of convergence has been applied to those analytic expressions, the range of application of such formulas is restricted. Equivalent dimensional perturbation methods [8,9] make use of Padé approximations but as a pure numerical tool and not to build analytic continued fractions.

The present paper presents a general method for finding the Regge poles for any singular potential within a wide range of energies. Two important steps are tackled to obtain analytic formulas that are able to provide any desired precision. The first one consists of obtaining a perturbation expansion of the Regge trajectories in terms of an appropriate parameter. The convergence of the resulting asymptotic series is improved through Padé approximations, which is the second step in this approach. Highly accurate results are then possible by increasing the number of terms in the expansion until the desired accuracy level is reached. Two examples are used to demonstrate the application of the general framework described in this paper: the polarization ($1/r^4$) and Lennard-Jones (6,12) potentials.

II. BASIC FORMULATION

The Regge pole is defined as a ''generalized'' bound state, when both the energy and the angular momentum can have complex values. The position of the Regge pole in the complex angular momentum (CAM) space, when the energy is a real number, describes the Regge trajectory (RT). If the potential is less singular at the origin than the centrifugal barrier potential, the RT's are closed curves in the CAM space because in the limit of infinite positive, or negative, energy the Regge poles accumulate to a finite complex angular momentum. When the potential is singular, diverging at the origin faster than r^{-2}, the RT goes asymptotically to infinity along a given direction in CAM space.

The radial Schrödinger equation for the system with the reduced mass μ, energy $E=\hbar^2k^2/2\mu$, and angular-momentum quantum number ℓ, is

$$-\frac{\hbar^2}{2\mu}\frac{d^2\psi}{dr^2}+\left(V(r)+\frac{\hbar^2\ell(\ell+1)}{2\mu r^2}\right)\psi=E\psi, \tag{1}$$

where the isotropic singular potential is defined by

$$V(r)=\sum_{s\geqslant S}\tilde{v}_s r^s=\frac{\hbar^2}{2\mu}\sum_{s\geqslant S}v_s r^s. \tag{2}$$

The lower limit is $S<-2$ for singular potentials. For example, $S=-12$ for Lennard-Jones and $S=-4$ for the polarization potential. Also, in this paper it is assumed that for large r the potential $V(r)\to 0$. The procedure presented below can be extended for more general cases.

Equation (1) describes an eigenvalue problem in energy, for a given angular momentum, when the wave function ψ is ''regular'' (vanishes at the origin) and decays to zero for $r\to\infty$. When Im $k>0$, there are special values of the angular-momentum quantum number ℓ, in general complex numbers, which define the Regge poles [14] if the wave function is an outgoing plane wave for large r ($\psi\sim e^{ikr}$). This is a generalization of the usual bound-state problem.

Both the origin ($r=0$) and infinity ($r=\infty$) are irregular singular points (not of the Fuchs type [15]) for the differential equation (1). An analytical approach toward solving this problem is very hard, if not impossible. However, the Langer transformation

$$r=e^z, \quad \psi=e^{z/2}\Phi$$

maps the two singular points into one singularity ($z=\infty$), and the problem becomes analytically tractable because all the solutions are entire functions (with no singularities in the open complex z plane). The Schrödinger equation (1) is now an explicit eigenvalue problem for the angular-momentum quantum number, when the energy (or the wave number k) is given as

$$-\frac{d^2\Phi}{dz^2}+\left[\sum_{s\geqslant S}v_s e^{(s+2)z}-k^2e^{2z}\right]\Phi=-(\ell+1/2)^2\Phi. \tag{3}$$

The boundary conditions for this equation are now $\Phi\to 0$ for $z\to\pm\infty$, and they correspond to a regular (at origin) and outgoing [for $\mathrm{Im}(k)>0$] wave function in the r variable. This problem has a discrete set of eigenvalues (Regge poles) $\ell_n(k)$, $n=0,1,2,\ldots$, which depend continuously on the wave number k.

Equation (3) is a one-dimensional scattering problem. When k is a pure imaginary number ($k=i\gamma$, $\gamma>0$), the new ''potential,''

$$U(z)=\sum_s v_s e^{(s+2)z}-k^2e^{2z}=r^2(V(r)-k^2)\big|_{r=e^z},$$

which depends parametrically on k, goes to infinity like e^{2z} for $z\to\infty$ and like $e^{(S+2)z}$ for $z\to-\infty$, and therefore has a global minimum for some value z_m. A solution for general k (with Im $k>0$) is then obtained from the solution of this restricted problem by analytical continuation. Expanding the potential U around the minimum z_m

$$U(z)=U(z_m)+\frac{1}{2}(z-z_m)^2U''(z_m)+U_R(z)$$

and defining the new independent variable ζ by $(z-z_m)=\alpha\zeta$ and the parameter α by $\alpha^4U''(z_m)=2$, Eq. (3) becomes the equation of the perturbed harmonic oscillator

$$-\frac{1}{2}\frac{d^2\Phi}{d\zeta^2}+\frac{\zeta^2}{2}\Phi+\frac{\alpha^2}{2}U_R(z_m+\alpha\zeta)\Phi$$
$$=-\frac{\alpha^2}{2}[(\ell+1/2)^2+U(z_m)]\Phi. \tag{4}$$

The unperturbed Hamiltonian $\mathcal{H}_0=(-d^2/d\zeta^2+\zeta^2)/2$ has eigenvalues $\mathcal{E}(0)=n+1/2$ for $n=0,1,2,\ldots$, and its eigenfunctions are

$$\varphi_n(\zeta)=\pi^{-1/4}e^{-\zeta^2/2}H_n(\zeta),$$

where H_n are the Hermite polynomials. The perturbation is represented by

$$V_I(\zeta)=\frac{\alpha^2}{2}U_R(z_m+\alpha\zeta)=\frac{\alpha^2}{2}U(z_m+\alpha\zeta)-\frac{\alpha^2}{2}U(z_m)-\frac{\zeta^2}{2}. \tag{5}$$

By denoting $R=e^{z_m}$, the corresponding position of the minimum of the potential $U(z)$ in r space, the potential (5) can be written as

$$V_I(\zeta)=\sum_s\frac{\alpha^2}{2}v_sR^{s+2}[e^{\alpha(s+2)\zeta}+s/2-e^{2\alpha\zeta}(1+s/2)]-\frac{\zeta^2}{2} \tag{6}$$

in terms of the Taylor coefficients of the original potential $V(r)$ and the parameter α. The proof of Eq. (6) follows from the identity

$$k^2=\sum_s(s/2+1)v_sR^s, \tag{7}$$

which is a translation in r space of the minimum condition $U'(z_m)=0$. When the energy is given, this equation is solved for R by choosing that solution that gives a Regge pole obeying the general constraint (see [14] for details), $\mathrm{Im}(\ell+1/2)^2>0$.

Using a new set of parameters

$$u_s=\alpha^4 v_s R^{s+2}, \tag{8}$$

the potential (6) has a simpler form:

$$V_I(\zeta)=\sum_s \frac{u_s}{2\alpha^2}[e^{\alpha(s+2)\zeta}+s/2-e^{2\alpha\zeta}(1+s/2)]-\frac{\zeta^2}{2}.$$

Also, the relation that defines α, $\alpha^4 U''(z_m)/2=1$, becomes

$$\alpha^4\sum_s s(1+s/2)v_s R^{s+2}=\sum_s s(1+s/2)u_s=1. \tag{9}$$

The original set of parameters, $(\{\tilde{v}_s\},E)$ or $(\{v_s\},\gamma)$, defining the eigenvalue problem Eqs. (1) or (3) is replaced by a new set $(\{u_s\},\alpha)$ appropriate for a perturbative solution of Eq. (4). It is worth noting that the new parameters are dimensionless, $\alpha^2\sim\hbar/\sqrt{2\mu}$ and α vanishes in the limit of high energy. These suggest that a perturbative solution (with α as the perturbation parameter) of Eq. (4) could be valuable both in the $E\to\infty$ and $\hbar/\sqrt{2\mu}\to 0$ limit. An $\hbar$ expansion is thus utilized for the calculation of Regge poles, since the parameters u_s carry no $\hbar$ dependence. Because of Eq. (9), not all u_s parameters are independent. This is explained by the fact that Eq. (1) is invariant on the scaling $r\to\chi r$ and $v_s\to\chi^{s+2}v_s$, $\gamma\to\chi\gamma$. Thus when the energy E and N coefficients $\tilde{v}_s$ are specified, the angular-momentum quantum number ℓ corresponding to the Regge pole depends only on N parameters, instead of $N+1$ parameters. For examples presented in Sec. III, ℓ depends on only one parameter (α) for the polarization potential and on two parameters (α and β) for the Lennard-Jones potential.

For small α or ζ, the perturbation potential (6) is

$$V_I(\zeta)\approx\frac{\alpha\zeta^3}{12}\sum_s s(s+2)(s+4)u_s, \tag{10}$$

which proves that V_I represents a singular perturbation and the perturbed eigenvalue of Eq. (4) can be expanded (at least formally) in a series of powers of the perturbation parameter α:

$$\mathcal{E}(\alpha)=-\frac{\alpha^2}{2}[(\ell+1/2)^2+U(z_m)]=\sum_{i=0}^{\infty}Q_i\alpha^i. \tag{11}$$

The nth Regge pole will then be derived from the nth perturbed harmonic-oscillator eigenvalue $\mathcal{E}^{(n)}(\alpha)$. For example, the zero-order Regge pole of order n is

$$\ell^{(n)}=-1/2\pm i\sqrt{\frac{2n+1}{\alpha^2}+U(z_m)}. \tag{12}$$

Equations (11) and (12) can be written explicitly in terms of α and u_s because

$$U(z_m)=-\frac{1}{2\alpha^4}\sum_s s u_s.$$

The coefficients Q_i are obtained recursively by using perturbation theory. The perturbed eigenfunction Φ is expanded in terms of unperturbed wave functions

$$\Phi(\zeta)=\sum_{m=0}^{\infty}F_m(\alpha)\varphi_m(\zeta),$$

so that $\mathcal{E}$ is obtained as an eigenvalue of the system of equations

$$[E_p-\mathcal{E}(\alpha)]F_p(\alpha)+\sum_{m=0}^{\infty}F_m(\alpha)V_{mp}(\alpha)=0, \tag{13}$$

where E_p is the energy corresponding to the unperturbed wave function φ_p and the matrix elements V_{mp} defined by

$$\varphi_m(\zeta)V_I(\zeta)=\sum_{p=0}^{\infty}V_{mp}(\alpha)\varphi_p(\zeta)$$

are

$$V_{mp}(\alpha)=\frac{1}{2\alpha^2}\sum_s u_s\left[W_{mp}((s+2)\alpha)-\left(1+\frac{s}{2}\right)W_{mp}(2\alpha)\right]+\frac{1}{4\alpha^4}\sum_s s u_s-\left(\frac{\zeta^2}{2}\right)_{mp}.$$

The elementary matrix elements W_{mp} defined for any β by

$$e^{\beta\zeta}\varphi_m(\zeta)=\sum_{p=0}^{\infty}W_{mp}(\beta)\varphi_p(\zeta)$$

are potential independent. The detailed calculation of these matrix elements is presented in Appendix A. However, two important properties are noted here: (i) the Taylor series of W_{mp} starts with $\beta^{|m-p|}$ and (ii) the Taylor series of W_{mp} has only even or odd powers in β, the same parity as the first power $|m-p|$ in the series. The W_{mp} matrix elements have then the power expansion

$$W_{mp}(\beta)=\sum_{t=|m-p|,|m-p|+2,\ldots}^{\infty}W_{mpt}\beta^t.$$

The matrix elements for the perturbation potential have the power expansion $V_{mp}=\Sigma_t V_{mpt}\alpha^t$ where

$$V_{mpt}=W_{mp,t+2}2^{t+1}\sum_s u_s\left(1+\frac{s}{2}\right)\left[\left(1+\frac{s}{2}\right)^{t+1}-1\right],$$

and the summation index t starts with $|m-p|-2$ when $|m-p|>2$, with 2 when $|m-p|=2$ or 0, and with 1 when $|m-p|=1$. Also, this expansion has only even or odd pow-

ers provided $|m-p|$ is even or odd. This is in agreement with expansion (10), such that, for any m and p, $V_{mp0}=0$. Furthermore, the matrix elements V_{mpt} can be written as a product of a potential independent factor (W_{mnt}) and a potential dependent factor ($\mathcal{V}_t$):

$$V_{mpt}=2^{t+1}W_{mp,t+2}\mathcal{V}_t,$$

where the set $\mathcal{V}_t$ with $t=1,2,3,\ldots$ is defined by

$$\mathcal{V}_t=\sum_s u_s\left(1+\frac{s}{2}\right)\left[\left(1+\frac{s}{2}\right)^{t+1}-1\right]. \tag{14}$$

Expanding F_m in powers of α as $F_m=\Sigma_{t=0}^{\infty}F_{mt}\alpha^t$ and using it in Eq. (13) together with expansion (11), one gets (for any positive p)

$$E_pF_{pt}-\sum_{i=0}^{t}Q_iF_{p,t-i}+\sum_{i=0}^{t}\sum_{m=0}^{\infty}F_{m,t-i}V_{mpi}=0 \tag{15}$$

after equating the coefficients of like powers of α. Because of the above-mentioned properties of the matrix elements V_{mpt}, the m summation in the last term of Eq. (15) is in fact restricted to a finite range around the (given) value of the index p. This essential feature allows a recursive solution of the Eqs. (15) to find the Taylor coefficients Q_i. For $t=0$, the infinite system of equations (15) reduces to $(E_p-Q_0)F_{p0}=0$, which shows that when $Q_0=n+1/2$ then $F_{p0}=\delta_{pn}$. For $t=1$, Eq. (15) gives $Q_1=0$ when $p=n$, $F_{n\pm1,1}=\mp V_{n,n\pm1,1}$ when $p=n\pm1$, and $F_{p1}=0$ for any other value of p. For any $t>2$ and $p=n$ a new coefficient Q_t can be generated if all other Q coefficients of smaller index are known by using the following recurrence relations:

$$Q_t=V_{nnt}+\sum_{i=1}^{t-1}\sum_{m=n-i-2}^{n+i+2}V_{mni}F_{m,t-i} \tag{16}$$

and

$$F_{pt}=\left(V_{npt}-\sum_{i=1}^{t-1}Q_iF_{p,t-i}+\sum_{i=1}^{t-1}\sum_{m=p-i-2}^{p+i+2}\times V_{mpi}F_{m,t-i}\right)\Big/(n-p). \tag{17}$$

Also, because of the special properties of the matrix elements V_{mpt}, it can be shown that all odd index coefficients Q_i are zero, leading to an α^2, rather than an α, expansion. This means that the result is obtained in the form of an $\hbar$ expansion.

In this way, any desired number of terms in the series (11) can be calculated. For example, the exact expressions for the first six coefficients for arbitrary order n and for any potential, are

$$Q_0^{(n)}=n+1/2,$$

$$Q_1^{(n)}=0,$$

$$Q_2^{(n)}=-\frac{1}{18}[11+30n(1+n)]\mathcal{V}_1^2+\frac{1}{4}[1+2n(1+n)]\mathcal{V}_2,$$

$$Q_3^{(n)}=0,$$

$$Q_4^{(n)}=\frac{(1+2n)}{216}\{-20[31+47n(1+n)]\mathcal{V}_1^4+36[19+25n(1+n)]\mathcal{V}_1^2\mathcal{V}_2-3[21+17n(1+n)]\mathcal{V}_2^2$$
$$-12[13+14n(1+n)]\mathcal{V}_1\mathcal{V}_3+6[3+2n(1+n)]\mathcal{V}_4\},$$

$$Q_5^{(n)}=0,$$

$$Q_6^{(n)}=-\frac{1}{1458}\{39709+15n(1+n)[10827+7717n(1+n)]\}\mathcal{V}_1^6+\frac{1}{324}\{15169+15n(1+n)[3959+2585n(1+n)]\}\mathcal{V}_1^4\mathcal{V}_2$$
$$-\frac{1}{648}\{11827+3n(1+n)[14493+8315n(1+n)]\}\mathcal{V}_1^2\mathcal{V}_2^2+\frac{1}{144}\{111+n(1+n)[347+125n(1+n)]\}\mathcal{V}_2^3$$
$$-\frac{1}{405}\{4517+15n(1+n)[1121+651n(1+n)]\}\mathcal{V}_1^3\mathcal{V}_3+\frac{1}{90}\{474+5n(1+n)[325+161n(1+n)]\}\mathcal{V}_1\mathcal{V}_2\mathcal{V}_3$$
$$-\frac{1}{1800}\{449+70n(1+n)[20+9n(1+n)]\}\mathcal{V}_3^2+\frac{1}{162}\{323+3n(1+n)[375+181n(1+n)]\}\mathcal{V}_1^2\mathcal{V}_4$$

$$-\frac{1}{36}\{12+n(1+n)[35+11n(1+n)]\}\mathcal{V}_2\mathcal{V}_4-\frac{1}{18}\{5+2n(1+n)[8+3n(1+n)]\}\mathcal{V}_1\mathcal{V}_5$$
$$+\frac{1}{144}\{3+2n(1+n)[4+n+n^2)]\mathcal{V}_6\}. \tag{18}$$

Because the unperturbed wave functions φ_p do not have the right asymptotic behavior (they do not decay fast enough), the formal expansions (11) have a zero radius of convergence. Still, it is useful in the asymptotic regime or if a convergence accelerator, like Padé approximations, is used. Finally, by analytical continuation, the nth Regge pole is calculated for any k (Im $k>0$), not only for $k=i\gamma$ ($\gamma>0$), as

$$\mathcal{E}^{(n)}=-\frac{1}{2}\pm i\left(\frac{2}{\alpha^2}\sum_i{}' \; Q_i^{(n)}(\{u_s\})\alpha^i-\frac{1}{2\alpha^4}\sum_s su_s\right)^{1/2}, \tag{19}$$

where the symbol Σ' can be any approximation of the formal Taylor expansion of the perturbed eigenvalue $\mathcal{E}$, which can give a meaningful numerical sense for it. The sections that follow will prove that even a simple truncation of the above formal series can give accurate results in certain regimes like high energy or semiclassical.

To summarize, the following steps lead to a fully analytic solution for the Regge trajectory for any singular potential:

(i) A particle with mass μ and energy E moves in a singular potential defined by the set of coefficients $\{\tilde{v}_s\}$ given by Eq. (2).

(ii) The position z_m (or R) of the minimum of the potential $U(z)$ is determined by solving Eq. (7).

(iii) The parameter α results from Eq. (9) and the set u_s from Eq. (8). With them, $\mathcal{V}_t$ and the matrix elements V_{mpt} are constructed by using Eq. (14).

(iv) Using the recursion relations (16) and (17), any number of coefficients Q_i can be calculated.

(v) The Regge trajectory is then defined by Eq. (19) where a convergence accelerator is eventually used to calculate the $\mathcal{E}$ series from Eq. (11). The result can be analytically continued in the upper half of the complex k plane.

III. SPECIFIC POTENTIAL RESULTS

A. Polarization potential

The polarization potential $V(r)=a^2/r^4$ is important in the electron-atom scattering. For this potential, then,

$$v_{-4}=\frac{2\mu}{\hbar^2}a^2 \quad \text{and} \quad v_s=0 \quad \text{for } s\neq -4.$$

Solving Eq. (7), one gets

$$R=\left(\frac{2\mu}{\hbar^2}\frac{a^2}{-k^2}\right)^{1/4}.$$

From Eq. (9) we have

$$\alpha=\left(\frac{1}{4x}\right)^{1/4}, \quad \text{where } x=a\sqrt{\frac{-2\mu k^2}{\hbar^2}},$$

and from Eq. (8) $u_{-4}=1/4$. With $\mathcal{V}_t=[1-(-1)^{t+1}]/4$, the first Q coefficients are

$$Q_0^{(n)}=n+\frac{1}{2},$$

$$Q_2^{(n)}=\frac{1}{8}(1+2n+2n^2),$$

$$Q_4^{(n)}=-\frac{2n+1}{32}(1+n+n^2),$$

$$Q_6^{(n)}=\frac{1}{128}(3+11n+16n^2+10n^3+5n^4).$$

The nth Regge pole is then

$$\mathcal{E}^{(n)}=-\frac{1}{2}\pm i\left[2x+4\sqrt{x}\left(Q_0^{(n)}+\frac{Q_2^{(n)}}{2\sqrt{x}}+\frac{Q_4^{(n)}}{4x}+\ldots\right)\right]^{1/2}.$$

This result is in agreement with [16] and [17], which give a limited number of terms in the $\mathcal{E}$ expansion. In the present approach, a large number of terms can be calculated. Three Regge trajectories are presented in Fig. 1. For these trajectories, 40 analytic terms are calculated in the $\mathcal{E}$ series. The convergence is improved by using the Jacobi continued fraction [18] associated with the Taylor series,

$$\mathcal{E}=n+\frac{1}{2}+\cfrac{C_1\alpha^2}{D_1+\alpha^2-\cfrac{C_2\alpha^2}{D_2+\alpha^2-\ldots}},$$

where coefficients C_i and D_i are derived recursively from the Taylor coefficients Q_i.

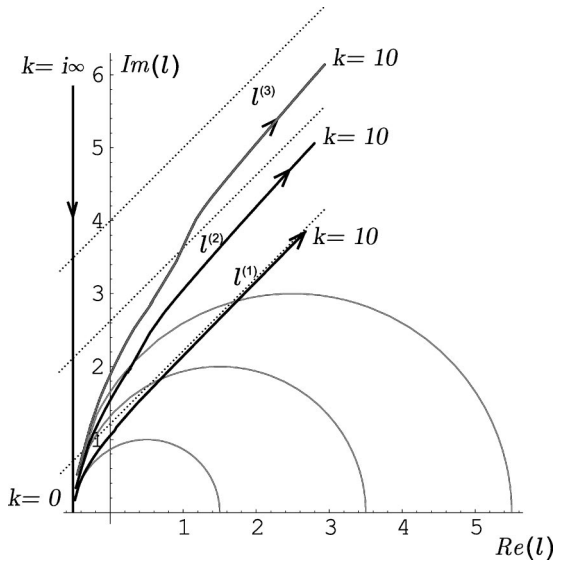

FIG. 1. The first three Regge trajectories in the CAM plane for the $1/r^4$ potential.

In the high-energy limit, the Regge trajectories approach some parallel asymptotic lines (dotted lines in figure). At low, but still positive energy, the Regge trajectories converge to the -0.5 angular momentum. For negative energy, $(\ell+1/2)^2$ is a negative number and all Regge trajectories melt into the vertical line $\mathrm{Re}(\ell)=-1/2$.

B. Lennard-Jones potential

The Lennard-Jones (12,6) potential is considered in this section:

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

for which

s:	-12	-6,
$\tilde{v}_s$:	$4\epsilon\sigma^{12}$	$-4\epsilon\sigma^{6}$,
v_s:	$\frac{4A^2}{K}\sigma^{10}$	$-\frac{4A^2}{K}\sigma^{4}$,
u_s:	$\beta/12$	$(1-5\beta)/12$,

where the parameters $A^2=2\mu\sigma^2E/\hbar^2$ and $K=E/\epsilon$ are common in the literature. Parameter β is defined below. The value of R is obtained from Eq. (7):

$$R=\sigma\left(\frac{10}{2+\delta}\right)^{1/6},$$

where $\delta=\pm\sqrt{4-5K}$, and the sign is chosen to select the branch of the Regge trajectory of interest. For instance, choosing the negative sign, one obtains Regge poles with $\mathrm{Re}(\ell+1/2)>0$ and $\mathrm{Im}(\ell+1/2)>0$.

The identity given by Eq. (9) yields, for the specific potential considered here,

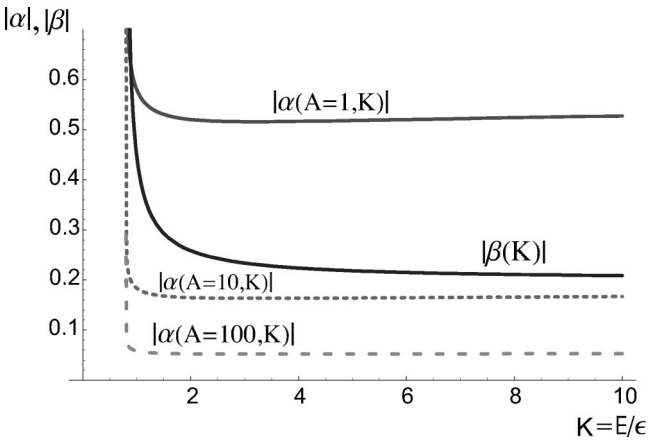

FIG. 2. Absolute values of parameters β and α (for A = 1, 10, and 100) as functions of K.

$$\alpha^4\frac{48A^2}{K}\left[5\left(\frac{\sigma}{R}\right)^{10}-\left(\frac{\sigma}{R}\right)^{4}\right]=1,$$

which defines the expansion parameter α as

$$\alpha=\left[\frac{(2-\delta)(2+\delta)^{1/3}}{12\times10^{1/3}A^2\delta}\right]^{1/4}.$$

The coefficients u_{-12} and u_{-6} presented in the table above follow from Eq. (8). The new parameter β is introduced for convenience:

$$\beta=\frac{1}{5}\left(1+\frac{2}{\delta}\right),$$

allowing for a direct comparison with previously published results [19]. Figure 2 shows the absolute values of α and β as functions of the reduced energy $K>4/5$. Three values are taken for $A=1,10,100$. When A and K are large, the perturbation parameter is small. For very large values of A the corrections due to the perturbation are expected to be small even for moderate values of K.

After using Eqs. (14) and (19), the analytic expression for the Regge-pole positions is

$$\ell^{(n)}=-\frac{1}{2}\pm i\left(\frac{1-3\beta}{4\alpha^4}+\frac{2}{\alpha^2}\sum_i{}'\,Q_i^{(n)}(\{u_s\})\alpha^i\right)^{1/2},$$

where the meaning of Σ' can be a simple truncation of the summation Σ_0^N up to some order N or some other convergence accelerator.

The $Q_{2p}^{(n)}$ are polynomials of degree $2p$ in β, and the first six of them are obtained directly from Eq. (18) as

$$Q_0^{(n)} = n + 1/2,$$

$$Q_2^{(n)} = \frac{1}{9}(2+3n+3n^2) + \frac{10}{3}(2+3n+3n^2)\beta - \frac{25}{8}(11+30n+30n^2)\beta^2, \tag{20}$$

$$Q_4^{(n)} = (1+2n)\left[\frac{5}{54}(-1+n+n^2) + \frac{10}{9}(22+5n+5n^2)\beta - \frac{25}{4}(134+85n+85n^2)\beta^2 + \frac{125}{4}(179+220n+220n^2)\beta^3 - \frac{9375}{32}(31+47n+47n^2)\beta^4\right], \tag{21}$$

$$Q_6^{(n)} = \frac{1}{1458}(161-135n-1680n^2-3090n^3-1545n^4) + \frac{5}{81}(539+513n+588n^2+150n^3+75n^4)\beta - \frac{1}{216}(1\,778\,513+4\,019\,625\,n+4\,600\,560\,n^2+1\,161\,870\,n^3+580\,935\,n^4)\beta^2 + \frac{625}{27}(8683+25\,785n+33\,684n^2 + 15\,798n^3+7899\,n^4)\beta^3 - \frac{125}{96}(1\,203\,331+4\,201\,335n+6\,299\,880n^2+4\,197\,090n^3+2\,098\,545n^4)\beta^4 + \frac{3125}{16}(24\,203+93\,015n+151\,320n^2+116\,610n^3+58\,305n^4)\beta^5 - \frac{15625}{128}(39\,709+162\,405n + 278\,160n^2+231\,510n^3+115\,755n^4)\beta^6. \tag{22}$$

Next, the theory presented above is compared with state of the art numerical calculation of the Regge pole [11]. A common benchmark for Lennard-Jones calculations is the potential with parameters $A=141.425$ and $K=5$. Zero-order approximation, where only Q_0 is retained in the $\mathcal{E}$ series, already gives about three digits of precision.

Another approximation uses the first four terms in the formal series (11) to give a [1/1] Padé approximation for $\mathcal{E}$, in the variable α^2:

$$\left(l_n^{(1)} + \frac{1}{2}\right)^2 = \frac{3\beta-1}{4(\alpha^2)^2} - \frac{2}{\alpha^2}\left[n + \frac{1}{2} + \frac{[Q_2^{(n)}]^2\alpha^2}{Q_2^{(n)} - Q_4^{(n)}\alpha^2}\right]. \tag{23}$$

With this simple formula,which uses only elementary functions, three to four more digits of precision are gained for both real and imaginary parts of the Regge pole [19].

Even more precise results can be obtained if more terms are considered in the $\mathcal{E}$ expansion. Using a truncated series with 12 terms as the next approximation significantly improves the precision of the results. Because the series (11) is Borel summable, its convergence is accelerated by constructing a Borel-Padé approximation [20] from the first 12 terms. This method gives the best results, up to 14 digits of precision for the Regge pole. The formulas for this approximation are still analytic, but they involve transcendental Γ-incomplete functions. A detailed presentation of this method is given in Appendix B.

Table I presents a summary of these results for the benchmark Lennard-Jones potential considered. The relative errors for the various methods to improve the convergence are calculated with respect to the highly accurate quantum results of [11]. Even a low-order approximation, with a modest numbers of terms, gives excellent results, which can be obtained by using only a pocket calculator. Higher poles, with higher index n, have less precision due to the perturbative nature of the method presented. However, more and more terms can be easily calculated by using reccurence relations (16) and (17) until the desired accuracy is obtained.

Another common Lennard-Jones potential is defined by the set of parameters $A=15$ and $K=1.8$. A comparison between semiclassical and quantal results for this potential is discussed in [1]. Because both A and K have smaller values, the accuracy of the present method is low (three to four significant digits) for a reduced number of terms in $\mathcal{E}$ expansion (12 in the example presented). Still, this is comparable with the accuracy of [1]. Of course, more terms added to the series of $\mathcal{E}$ contribute to an increased precision in the results. Figure 3 shows some ''snapshots'' of the first six Regge trajectories taken for $K=1.0,1.5,2.0,2.5,$ and 3.0 in the CAM space.

IV. CONCLUSION AND DISCUSSIONS

A general framework for obtaining analytic results for the Regge poles has been developed within the class of singular potentials. A perturbation expansion, equivalent to an $\hbar$ expansion, has been employed. Even though the resulting formal series is divergent, the results are still useful when a convergence accelerator (such as a Padé approximation) is used. The formulas obtained are simple and give physical insight into the nature and behavior of the Regge poles. Clear

TABLE I. The relative error of Regge poles is given as 10^{-s}. Values for s are calculated in various approximations used in this work; separately for the real and imaginary parts. The reference Regge poles are given in the second column.

n	$\mathscr{l}^{(n)}$ [d]	4 terms [a]		12 terms [b]		12 terms [c]	
		Re	Im	Re	Im	Re	Im
0	180.011 948 024 39+*i* 21.218 915 128 43	8.65	7.39	13.4	12.1	13.5	13.4
1	179.238 987 840 84+*i* 24.034 748 840 56	8.05	7.19	10.9	10.7	13.0	12.4
2	178.522 893 751 20+*i* 26.890 095 347 76	6.63	6.98	9.55	8.75	12.1	11.3
3	177.866 576 996 32+*i* 29.780 188 101 64	5.96	6.75	8.58	7.64	11.7	10.5
4	177.272 390 601 19+*i* 32.700 076 842 78	5.50	6.03	7.84	6.83	12.2	9.36
5	176.742 125 996 15+*i* 35.644 692 524 87	5.14	5.29	7.24	6.18	11.2	8.64

[a]Padé Eq. (23).
[b]Truncated sum.
[c]Borel-Padé.
[d]From Ref. [11].

links between the parameters of the problem (e.g., energy or potential) and the Regge poles are transparent.

The numerical precision achieved is higher or comparable to the published examples. Better results can be obtained for a wide range of energies because the formal series can be easily extended by using powerful recurrence relations. The Regge poles for an even larger class of potentials can be calculated using the procedure presented in this paper. The singular potential problem Eq. (1) is transformed into a regular problem by $r \to 1/r'$ and $\Psi \to \Phi/r'$ transformations. Also, singular potentials that depend on fractional powers of r can be treated directly using the formalism described.

To study or calculate the behavior of the scattering amplitude, not only the precise location of the Regge poles in the complex plane is required but also the values of their *residues*. Let us first briefly outline how the residues are computed. Let λ_0 and k_0 be, respectively, the complex angular momentum and the complex energy of the Regge pole. The corresponding residue is given by [22]

$$R = \frac{e^{i\pi\lambda_0} k_0}{\lambda_0} \frac{1}{\mu_{-2}}, \tag{24}$$

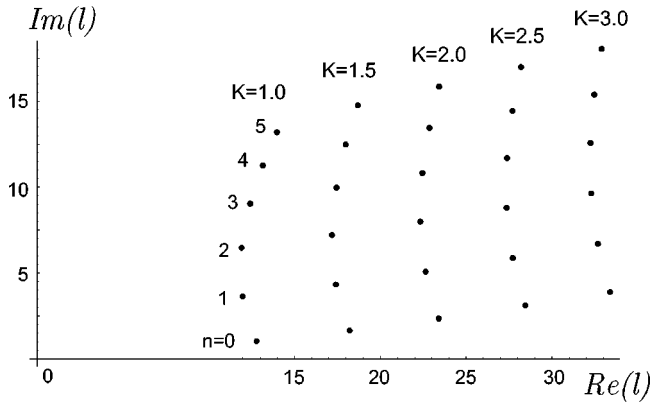

FIG. 3. The first six Regge poles for $K=1.0$, 1.5, 2.0, 2.5, 3.0 in the CAM space for a Lennard-Jones potential with $A=15$ and $K=1.8$.

where

$$\mu_{-2} = \int_0^{+\infty} r^{-2} f_-^2(\lambda_0, k_0, r)\, dr. \tag{25}$$

Here $f_-(\lambda_0, k_0, r)$ is the solution of the Schrödinger equation that behaves at large physical distances as

$$f_-(\lambda_0, k_0, r) \to e^{ik_0 r}, \quad r \to +\infty. \tag{26}$$

Although Eq. (24) has been demonstrated in [21] only for regular potentials, it can be readily extended to singular potentials. It is clear from Eqs. (24), (25), and (26), that an accurate residue calculation requires, in order:

(i) A precise knowledge of the position, in the complex plane, of the Regge pole. This has been the major objective of our paper on singular potentials.

(ii) A correct *normalization* to $e^{ik_0 r}$ of the wave function at large distances.

With the method described in this paper, the *normalization factor* cannot be determined for the following reasons. From examination of Eq. (4), it is seen that the calculation of the Regge trajectories has been transformed into a more classical ''perturbed harmonic oscillator'' eigenvalue computation. Therefore the basis onto which the eigenfunctions are expanded is that of the harmonic oscillator. Consequently, *we cannot normalize correctly the wave function at infinity*. The reason is that the harmonic-oscillator basis involves the *square* of the distance in the exponential, while the normalization condition Eq. (26) requires a *linear* term in the exponential. As far as the computation of the generalized eigenvalues (Regge poles) is concerned, this difference plays no role and our results are among the most precise in the literature. However, this basis is *not suitable* for correctly *normalizing* the wave function at large distances as is required for the residue computation.

The limitation of a method to only the calculation of the Regge poles is not specific and limited to our approach. It is also manifest in the method of Germann and Kais [8], which is suited *only* for the calculation of the Regge poles and not the associated residues. However, since the calculation of the

residues requires the *preliminary* knowledge of the precise location of the Regge poles, any suitable method like that of Sukumar and Bardsley [4] or Connor *et al.* [21] can be used.

In conclusion, the motivation of this paper has been the need to provide an accurate and efficient *analytical* method to augment the relatively few existing methods, which are mostly numerical, for calculating Regge-pole positions. Besides the traditional rainbow scattering problem that involves Regge-pole calculations for the singular Lennard-Jones potential, there are other important physical problems that can be treated. Such an example is the Bose-Einstein condensation and superfluidity of ^{4}He at extremely low temperatures. The possibility of forming dimer resonances in the He-He collision problem has been investigated [2] using the two versions of the Aziz potential [23,24]. The problem has been solved within the framework of the singular potential method because of the inadequacy of the regular potentials methods for this case.

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APPENDIX A: MATRIX ELEMENTS FOR $e^{\beta x}$

The eigenfunctions for the harmonic oscillator are

$$u_n(x)=\pi^{-1/4}e^{-x^2/2}H_n(x),$$

where H_n are Hermite polynomial with the generating function

$$e^{2zx-z^2}=\sum_{n=0}^{\infty}\frac{z^n}{n!}H_n x.$$

The goal of this section is to give the expansion in powers of β for the matrix element $W_{nm}(\beta)$ of $e^{\beta x}$:

$$e^{\beta x}u_n(x)=\sum_{m=0}^{\infty}W_{nm}(\beta)u_m(x).$$

The generating function for $e^{\beta x}H_n(x)$,

$$\exp(\beta x+2zx-z^2)=\sum_{n=0}^{\infty}\frac{z^n}{n!}e^{\beta x}H_n x, \tag{A1}$$

can also be written as

$$\exp(\beta^2/4+\beta z)\exp(2(z+\beta/2)x-(z+\beta/2)^2)$$

$$=e^{\beta^2/4}\sum_{m=0}^{\infty}\frac{1}{m!}e^{\beta z}(z+\beta/2)^m H_m(x). \tag{A2}$$

Equating the coefficients of the z powers from Eqs. (A1) and (A2), one gets the following expansion:

$$e^{\beta x}H_n(x)=\sum_{m=0}^{\infty}W_{nm}(\beta)H_m(x),$$

where

$$W_{nm}(\beta)=e^{\beta^2/4}\frac{n!}{2^m}\beta^{n+m}\sum_{k=0}^{\min(m,n)}\left(\frac{2}{\beta^2}\right)^k\frac{1}{k!(n-k)!(m-k)!}.$$

It is easy to see that the function $W_{nm}(\beta)$ is a polynomial in β times the even factor $e^{\beta^2/4}$. The lowest power of β in the polynomial is $|n-m|$ because $m+n-2\min(m,n)=|m-n|$. Also, the polynomial has only even or odd powers of β depending on whether the starting power $|n-m|$ is even or odd, respectively. These properties are inherited by the Taylor expansion of $W_{nm}(\beta)$ since the factor $e^{\beta^2/4}$ is an entire even function in β.

APPENDIX B: PADÉ-BOREL APPROXIMATION

If a function $F(z)$ is defined by its Taylor series and only a finite number of coefficients f_n are known, various approximations are employed to calculate the function. Good results are obtained when the value of z is inside the convergence disk of the associated Taylor series. When little is known about the radius of convergence or this is zero, or z is outside the convergence disk, in general, the simple truncation of the Taylor series does not work very well, and most of the times does not work at all. A way to obtain a better approximation is to use the rational or Padé approximation for the given function. This is done in two steps. In the first step, a continued fraction (of the Stiltjes or more powerful Jacobi type, depending around what point the expansion is known) is constructed from the set of Taylor coefficients. In the second step, a truncation of the infinite continued fraction defines the rational approximtion, as a ratio of two polynomials or using the residue-pole representation

$$F(z)\approx\sum_{k=1}^{N}\frac{\rho_k}{1-a_k z}. \tag{B1}$$

A more refined approximation can be developed by using the Borel Transform [20]. Writing the function as

$$F(z)=\sum_{n=0}^{\infty}\left(\frac{f_n}{n!}\right)n!z^n$$

and the factorial as

$$n!=\int_0^{\infty}t^n e^{-t}dt,$$

the following result is obtained:

$$F(z)=\int_0^{\infty}e^{-t}\hat{F}(tz)dt,$$

where the Borel transformed $\hat{F}$ of the original function F has the Taylor coefficients defined by $\hat{f}_n = f_n/n!$. Writing the rational approximation of the $\hat{F}$ in the residue-pole form (B1), one gets

$$F(z) \approx \sum_{k=1}^{N} \rho_k \mathcal{E}(a_k z),$$

where the function $\mathcal{E}$ is

$$\mathcal{E}(z) = \frac{e^{1/z}}{z} \Gamma\left(0, \frac{1}{z}\right),$$

and the incomplete Γ function has the definition

$$\Gamma(a,z) = \int_z^\infty t^{a-1} e^{-t} dt.$$

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