Regge poles as complex eigenvalues

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Abstract.   We report a new direct method for calculating Regge pole positions and residues. Upon introduction of an absorbing optical potential sufficiently far in the asymptotic region, the problem reduces to several iterative diagonalizations of a symmetric complex matrix. The method is tested on well-studied cases of potential scattering.

1. Introduction

There has been recent interest in the complex angular momentum (CAM) techniques in the theory of chemical reactions [1]. If an atom–diatom system possesses a transition state resonance, collision partners form a long-lived triatomic complex whose rotation and eventual decay lead to specific structures in the observable angular distributions [1]. Quantally, the angular velocity and angular lifetime of the complex are determined by the position λ_{res} of the (Regge) pole of the S-matrix element in the CAM plane, while the corresponding residue r_{res} defines the magnitude of the resonance contribution to the differential cross section [2]. It is useful, therefore, to devise a method for calculating these quantities for an arbitrary atom–diatom system. Various methods developed for calculation of λ_{res} and r_{res} in potential scattering include integration of the Schrödinger equation in the CAM-plane [3–5], the use of a generalized variational principle [6], semiclassical quantization techniques [7] and, more recently, the dimensional perturbation theory [8]. Although quite accurate, these methods often require cumbersome procedures, such as root searching in the complex plane [3–5] or are difficult to extend beyond one dimension [7]. In this paper we introduce a simple direct approach which can be adapted to multichannel systems and does not invoke semiclassical quantization rules. In order to do so we shall follow the ideas already used in direct calculations of the complex energy poles [9] and introduce an imaginary potential capable of absorbing the outgoing wave in each channel. We shall demonstrate the applicability of the method in the case of elastic scattering and defer detailed analysis of the multichannel systems to further publications.

2. Regge states

Consider the radial Schrödinger equation for a single particle with angular momentum ℓ and energy $E = \hbar^2 k^2/2m$ scattered by a short-ranged central field (for convenience we replace ℓ by $\lambda - \frac{1}{2}$)

$$\frac{\mathrm{d}^2\Psi}{\mathrm{d}r^2} + \left[k^2 - U(r) - \frac{(\lambda^2 - \frac{1}{4})}{r^2} \right] \Psi = 0. \tag{1}$$

The physical scattering solution $\Psi(r)$ vanishes at the origin,

$$\Psi(r = 0) = 0 \tag{2}$$

and as $r \to \infty$ has the asymptotic form

$$\Psi(r) \approx \exp(-\mathrm{i}kr + \mathrm{i}\lambda\pi/2 - \mathrm{i}\pi/4) + S(\lambda)\exp(\mathrm{i}kr - \mathrm{i}\lambda\pi/2 + \mathrm{i}\pi/4) \tag{3}$$

where $S(\lambda)$ is the S-matrix. For real (half-integer) values of λ conservation of particle forces $|S(\lambda)| = 1$ but if $\Psi(r)$ is analytically continued into the complex λ-plane, $S(\lambda)$ may diverge near, say, $\lambda_n, n = 1, 2, 3\ldots$ so that as $\lambda \to \lambda_n$

$$S(\lambda) = \frac{r_n}{\lambda - \lambda_n} + S_{\mathrm{reg}}(\lambda) \qquad n = 1, 2, 3 \tag{4}$$

where $S_{\mathrm{reg}}(\lambda)$ denotes the regular part of the S-matrix. Physically, equation (4) indicates that at $\lambda = \lambda_n$ equation (1) has a solution which, while regular at the origin, contains, as $r \to \infty$, only an outgoing wave produced by the emitting centrifugal potential $(\lambda_n^2 - \frac{1}{4})/r^2$. Indeed, dividing equation (3) by $S(\lambda)$ and choosing appropriate normalization yields, as $\lambda \to \lambda_n$ a Regge state $\Psi_{\lambda_n}(r)$ such that

$$\Psi_{\lambda_n}(r) \approx \exp(\mathrm{i}kr) \qquad r \to \infty. \tag{5}$$

Our aim is to calculate both the Regge pole position λ_n and the value of the corresponding residue $r_n, n = 1, 2, 3\ldots$ for a given value of k.

3. Regge pole positions

Equation (5) suggests that we can restrict the problem to a finite r-range by introducing at $r = R$ sufficiently far in the asymptotic region an infinite hard wall augmented by a complex-valued potential $W_{\mathrm{opt}}(r), \mathrm{Im}\,W_{\mathrm{opt}} < 0$, capable of absorbing (without reflection) the outgoing wave $\exp(\mathrm{i}kr)$ (figure 1). Indeed, let $W_{\mathrm{opt}}(r)$ be confined to $[R_{\mathrm{opt}}, R]$. Then, for $\lambda = \lambda_n$ we have a square integrable solution $\Phi_n(r)$ which vanishes at the origin, contains only an outgoing wave for large $r < R_{\mathrm{opt}}$ and then vanishes again at $r = R$ as this wave is absorbed by $W_{\mathrm{opt}}(r)$. In general, there may be many Regge poles λ_n and (integrable) Regge states $\Phi_n(r), n = 1, 2, 3\ldots$. Introducing

$$\varphi_n(r) \equiv \Phi_n(r)/r \qquad n = 1, 2, 3\ldots \tag{6}$$

and multiplying the Schrödinger equation by r we see that $\varphi_n(r)$ are the eigenfunctions of an operator $\hat{\mathcal{L}}$,

$$\begin{aligned} \hat{\mathcal{L}}\varphi_n &= \Lambda_n\varphi_n \qquad n = 1, 2, 3\ldots \\ \varphi_n(0) &= \varphi_n(R) = 0 \end{aligned} \tag{7}$$

where

$$\hat{\mathcal{L}} \equiv \left\{ r\frac{\mathrm{d}^2}{\mathrm{d}r^2}r + r^2[k^2 - U(r) - W_{\mathrm{opt}}(r)] \right\} \tag{8}$$

and the pole positions λ_n are related to discrete eigenvalues Λ_n as

$$\lambda_n = (\Lambda_n + \tfrac{1}{4})^{1/2} \qquad n = 1, 2, 3\ldots. \tag{9}$$

Note that due to the presence of the absorbing potential $W_{\mathrm{opt}}(r)$, $\hat{\mathcal{L}}$ is non-Hermitian and, therefore, both Λ_n and λ_n are complex valued. For a suitable set of basis functions $\{\varphi_m\}$, $\varphi_m(0) = \varphi_m(R) = 0, m = 1, 2, 3\ldots M$, solving equation (7) now reduces to diagonalization of an $M \times M$ symmetric complex matrix $\mathcal{L}_{mm'} \equiv \langle\varphi_m|\hat{\mathcal{L}}|\varphi_{m'}\rangle$. A concrete choice of $W_{\mathrm{opt}}(r)$
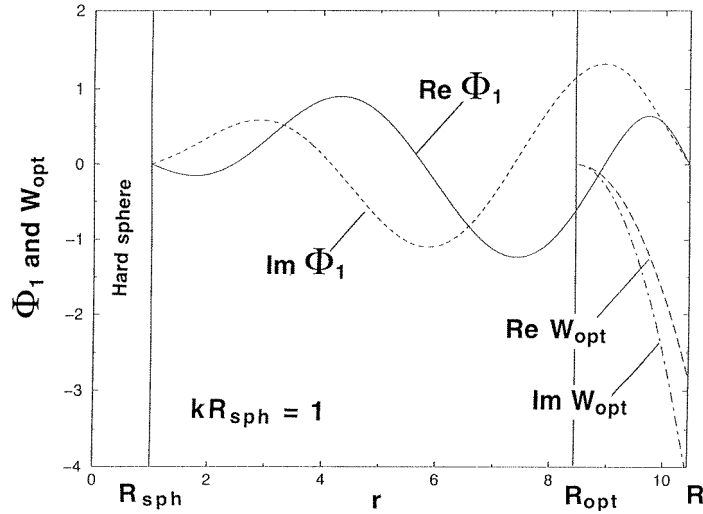
Figure 1. Real (full) and imaginary (broken) parts of the (unnormalized) first Regge state Φ_1 for a hard sphere potential plotted versus r (arbitrary units), for $k \equiv (2mE)^{1/2}/\hbar = 1$. The sphere radius R_{sph} is chosen so that $kR_{sph} = 1$, and the absorbing potential $W_{opt}(r) = W_0(r - R_{opt})^2$ is confined to $R_{opt} < r < R$. Re W_{opt} and Im W_{opt} are shown by the long broken and chain curves, respectively.

and $\{\varphi_m\}$ will be given below. Note that the use of absorbing potentials for finding poles in the CAM plane is simpler than for finding complex energy eigenvalues [9]. Indeed, to obtain complex energies one requires an optical potential acting as a (nearly) perfect absorber for a wide range of energies. The task of finding such a potential is quite difficult [10]. In the case of Regge poles, the energy E is fixed, while the asymptotic form (5) applies to all (not too large) values of λ. We therefore only require a potential $W_{opt}(r)$ capable of absorbing a single plane wave $\exp(ikr)$ with $E = \hbar^2 k^2/2m$, which is easy to construct.

4. The residues

In the case of a single-channel system, the nth residue of the S-matrix, r_n, can be found by a simple quadrature, provided $\Psi_{\lambda_n}(r)$ in equation (5) is known. This can be obtained by analysing the behaviour of the coefficient multiplying an incoming wave in equation (3) in the vicinity of λ_n. Indeed, a small shift of λ away from λ_n, $\lambda_n \to \lambda_n + \delta\lambda$, produces a small change $\delta V_{cent}(r)$ in the centrifugal term in equation (1),

$$\delta V_{cent}(r) = 2\lambda_n \delta\lambda / r^2. \tag{10}$$

The large r asymptote of the solution regular at the origin contains, at $\lambda = \lambda_n + \delta\lambda$, a small incoming wave

$$\Psi_{\lambda_n+\delta\lambda}(r) \approx \exp(ikr) + \delta D \exp(-ikr) \qquad r \to \infty. \tag{11}$$

Calculating δD with the help of perturbation theory [11] to the first order in δV_{cent}, dividing equation (11) by δD and comparing with equation (4) yields [12]

$$r_n = \left\{ -ik^{-1}\lambda_n \int_0^\infty \Psi_{\lambda_n}^2(r)r^{-2}\,dr \right\}^{-1} \qquad n = 1, 2, 3\ldots. \tag{12}$$

Finally, we note that the integral in equation (12) converges due to the presence of r^{-2}. This suggests that for a finite-range calculation with sufficiently large R_{opt}, $\Psi_{\lambda_n}^2(r)r^{-2}$ in equation (12) may be replaced by $\varphi_n^2(r)$ defined in equation (6).

5. Calculations and results

To demonstrate applicability of the method, we analyse the cases of potential scattering by a hard sphere and by a Yukawa potential [3, 4]. In the hard sphere case, the analytical continuation of the S-matrix into the complex λ-plane is readily available in terms of the Hankel functions [13], which provides a straightforward test for the accuracy of our method. Regge poles for Yukawa potentials have been studied earlier by Burke and co-workers [3, 4]. Several comments are in order. It would follow from the discussion at the end of section 3 that a $W_{\text{opt}}(r)$ independent of λ and located far enough into the asymptotic region should give good estimates for a number of Regge poles closest to the origin. The use of equation (5) requires, however, that the centrifugal term $(\lambda_n^2 - \frac{1}{4})/r^2$ is negligible inside $[R_{\text{opt}}, R]$, so that as $|\lambda_n|$ increases the method will become increasingly less accurate. In practice, slow convergence of $\Psi_{\lambda_n}(r)$ to its asymptotic value (5) requires very large values of R if $\lambda_n \cong 1$ and, therefore, large basis sets are needed to span the interval $[0, R]$. The difficulty can be overcome by using smaller values of R and an iterative procedure to converge the pole positions. For R_{opt} large enough to neglect the short-range $U(r)$ in equation (1), the potential inside $[R_{\text{opt}}, R]$ is $W_{\text{opt}}(r) - (\lambda_n^2 - \frac{1}{4})/r^2$ and the solution of equation (1) to the left of R_{opt} is of the form

$$\Psi(r) = r^{1/2} H_\lambda^{(1)}(kr) + A(W_{\text{opt}}, \lambda) r^{1/2} H_\lambda^{(2)}(kr) \tag{13}$$

where $H_\lambda^{(1)}(kr)$ and $H_\lambda^{(2)}(kr)$ are the Hankel functions of the first and second kind, respectively. In the first iteration we replace $r^{1/2} H_\lambda^{(1)}(kr)$ and $r^{1/2} H_\lambda^{(2)}(kr)$ in equation (13) by their asymptotic values $C^{(1)} \exp(\mathrm{i}kr)$ and $C^{(2)} \exp(-\mathrm{i}kr)$ and obtain, therefore, W_{opt} which absorbs the plane wave $\exp(\mathrm{i}kr)$. This W_{opt} is then substituted into equation (8) and the values of λ_n, $n = 1, 2, 3 \ldots$ are calculated as discussed in section 3. Then a chosen value λ_j is used to recalculate W_{opt} in equation (13) using this time exact values of the Hankel functions. The modified W_{opt} is then substituted back into equation (8) and the procedure is repeated until a converged value of λ_j is obtained. Note that after the first iteration the modified W_{opt} becomes dependent on the choice of λ_j so that only one pole at a time can be converged iteratively. The simplest choice of W_{opt} is a complex-valued δ-potential $W_{\text{opt}}(r) = W_0 \delta(r - R_{\text{opt}})$ for which W_0 can be obtained analytically. For the same basis set the accuracy can, however, be increased by choosing a smooth absorbing potential $(W_0 = W_1 + \mathrm{i}W_2)$, $W_{\text{opt}}(r) = W_0(r - R_{\text{opt}})^N$, $R_{\text{opt}} < r < R$, and 0 otherwise, so that $\Phi_n(r)$ in equation (6) has a discontinuity in the N-th derivative at $r = R_{\text{opt}}$.

Finally, to calculate the residue r_j we use the accurate eigenfunction Φ_j of equation (6) normalized according to equation (5). To speed up the convergence, we integrate $\varphi_j^2(r) = \Phi_j^2(r)/r^2$ numerically to some cut-off value R_C sufficiently large for Φ_j to have the asymptotic form $\Phi_j \approx r^{1/2} H_{\lambda_j}^{(1)}(kr)$. The rest of the integral in equation (14) is calculated numerically along a contour transformed from the real to the imaginary r-axis where $H_{\lambda_j}^{(1)}(kr)$ decays exponentially.

For a hard sphere potential of radius R_{sph}

$$U(r) = \begin{cases} \infty & 0 < r < R_{\text{sph}} \\ 0 & \text{otherwise} \end{cases} \tag{14}$$

Table 1. Positions λ_1 and residues r_1 of the first ($n = 1$) Regge pole as a function of kR_{sph} for the hard sphere potential (14). Also given are their exact values calculated independently.

kR_{sph}	λ_1	λ_1 (exact)	r_1	r_1 (exact)
1.0	(1.88, 1.71)	(1.88, 1.71)	(0.248, −0.119)	(0.248, −0.119)
2.0	(3.13, 2.10)	(3.13, 2.10)	(0.302, −0.153)	(0.302, −0.153)
3.0	(4.30, 2.39)	(4.30, 2.39)	(0.340, −0.177)	(0.340, −0.177)
4.0	(5.44, 2.61)	(5.44, 2.61)	(0.370, −0.196)	(0.370, −0.196)
5.0	(6.56, 2.80)	(6.55, 2.81)	(0.396, −0.212)	(0.396, −0.212)
6.0	(7.66, 2.97)	(7.66, 2.98)	(0.419, −0.226)	(0.419, −0.226)
7.0	(8.74, 3.13)	(8.75, 3.13)	(0.440, −0.238)	(0.440, −0.238)
8.0	(9.83, 3.24)	(9.83, 3.26)	(0.458, −0.250)	(0.459, −0.250)
9.0	(10.9, 3.38)	(10.9, 3.39)	(0.476, −0.261)	(0.476, −0.260)
10.0	(12.0, 3.51)	(12.0, 3.51)	(0.492, −0.270)	(0.492, −0.270)

Table 2. Positions λ_1 and residues r_1 of the first ($n = 1$) Regge pole as a function of k^2 for an attractive Yukawa potential (15). Also given are their values calculated using the computer code described in [4].

k^2	λ_1	λ_1 [4]	r_1	r_1 [4]
0.01	(1.53, 8.77(−2))	(1.53, 8.75(−2))	(8.32(−4), 1.75(−2))	(8.32(−4), 1.74(−2))
0.1	(1.11, 8.30(−3))	(1.11, 8.30(−3))	(2.95(−2), 0.165)	(2.95(−2), 0.165)
0.2	(1.14, 0.156)	(1.14, 0.156)	(7.46(−2), 0.314)	(7.54(−2), 0.314)
0.32589	(1.16, 0.237)	(1.16, 0.237)	(0.139, 0.488)	(0.139, 0.487)
0.505824	(1.17, 0.338)	(1.17, 0.339)	(0.231, 0.723)	(0.232, 0.724)
0.680519	(1.17, 0.424)	(1.17, 0.424)	(0.324, 0.945)	(0.329, 0.942)
0.918214	(1.14, 0.526)	(1.15, 0.526)	(0.448, 1.24)	(0.445, 1.23)
1.1	(1.13, 0.596)	(1.13, 0.595)	(0.533, 1.45)	(0.535, 1.45)
2.06547	(0.989, 0.874)	(0.989, 0.873)	(0.824, 2.35)	(0.895, 2.63)

we have used the simplest basis of sine functions spanning the interval $d \equiv [R_{\mathrm{sph}}, R]$, $\varphi_m(r) = d^{-1/2} \sin[\pi m(r - R_{\mathrm{sph}})d]$, $m = 1, 2, 3, \ldots$ to diagonalize $\mathcal{L}_{mm'}$. The results for the first Regge pole ($j = 1$) are given in table 1, together with the exact values of λ_1 and r_1 for different values of kR_{sph} between 0 and 10. The exact values of pole positions and residues in table 1 were obtained independently with the help of the relation $S(\lambda) = -H_\lambda^{(2)}(kR_{\mathrm{sph}})/H_\lambda^{(1)}(kR_{\mathrm{sph}})$ [13]. Table 2 gives the pole positions and residues for the Yukawa potential

$$U(r) = Ar^{1/2} \exp(-\alpha r) \qquad (15)$$

with $A = -5$ and $\alpha = 1$ studied in [4].

6. Conclusions

We have proposed a simple direct method for calculating the Regge pole parameters by several iterative diagonalizations of a complex symmetric matrix. For a single-channel system, the results are shown to be in good agreement with those in [3, 4]. The method can be extended to multichannel systems by inserting different absorbing potentials into different open channels, provided the total angular momentum enters the coupled equations in a sufficiently simple form, as is the case for atom–diatom collisions [14]. Note, however, that in this case there is no simple relation, similar to equation (12), between the Regge state

and the matrix of residues. Finally, the effort of computing the pole parameters increases with the value of kR_0 (R_0 is the size of the target potential). In general, efficiency of the method can be improved with the help of various numerical techniques available for matrix diagonalization and by a careful choice of the basis functions, e.g. through prediagonalization of a part of the operator in equation (8).

Acknowledgments

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