

CALCULATION OF COMPLEX ANGULAR MOMENTUM POLES AND RESIDUES IN MULTICHANNEL PROBLEMS

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A method for calculation of complex angular momentum poles and residues of the S -matrix is described for multichannel scattering problems. The generalization of the WKB method for the logarithmic derivative of the multichannel wave function is also given. The method is applied to two examples.

1. Introduction

Study of the long-lived states and resonances in collisions is very convenient using the method of complex angular momentum poles of the S -matrix (often referred to as the Regge poles). The convenience of this approach stems from the fact that the scattering amplitude can be represented in the form^{1,2)}

$$f(\theta) = -\frac{i\pi}{k} \sum_n \frac{\lambda_n \beta_n}{\cos(\pi\lambda_n)} P_{\lambda_n - 1/2}(-\cos\theta) + \frac{1}{k_0} \int_0^\infty d\lambda \lambda S(\lambda) e^{-i\pi\lambda} P_{\lambda - 1/2}(-\cos\theta) \quad (1)$$

which is entirely equivalent to the partial wave decomposition. λ_n is the n -th pole and β_n is the appropriate residue of the S -matrix and they are both functions of energy. It can be shown that the poles for atomic and molecular collisions are found only in the first and the third quadrant of the complex λ plane. However, only the poles from the first quadrant are physically significant. P_x is the Legendre function, and the »angular momentum« λ in (1) refers to the variable $\lambda = l + 1/2$.

The sum over the poles represents contribution of the resonances and the long lived states in the scattering amplitude, while the integral represents contribution of the direct reflection. It is the purpose of this paper to show how the

poles and the residues for the inelastic (multichannel) collisions are calculated. However, before doing this it is necessary to review the methods of calculation for single channel problems and in what way the methods described in here supplement the existing ones. Despite the effort put into understanding the single channel problems, using the complex angular momenta, similar analysis of the multichannel problems has not been done. There are some specific features of the atomic and molecular collisions which in the single channel problems have been quite successfully overcome. One is that the wave function is a rapidly oscillating function of the interatomic separation and the second, the interatomic potential is slowly going to zero for large separations. Both these problems have been overcome by using the WKB method in one or the other form. The poles have been calculated either by making analytic continuation of the WKB method into the complex coordinate plane^{3,4,5}), or the numerical integration methods have been used which are based on this method⁶). Both of these approaches are not feasible for the multichannel problems and so a compromise is necessary. In addition to the problems mentioned, there is another one which is specific to the multichannel problems. In the interaction region the numerical instability may arise because some channels are locally open and some are closed. Since the channel wave numbers are typically large in atomic and molecular collision processes, the part of the wave function which corresponds to the closed channels is a rapidly increasing function of the coordinate while the part which corresponds to the open ones is a bounded function. When the two components mix in the equations, the close channel part will start dominating the solution, and thus completely overshadow the open ones. It is thus proposed that the logarithmic derivative method⁷) is used for integrating the multichannel equations until the point where there are no turning points in the channels, which usually happens at relatively short distances, and then use generalization of the WKB method for the multichannel equations in order to propagate the solution to large distances. Generalization of the WKB method for the multichannel logarithmic derivative is described here.

From the study of the energy dependence of the poles alone one can learn about some general features of resonances and long lived states. Each pole λ_n describes a family of resonances⁸). Whenever its real part is half integer, and its imaginary part small, the denominator in the sum (1) is small, and hence the module of the scattering amplitude f is large. A way from this energy the amplitude is small. This change in the scattering amplitude (and hence in the cross section) is interpreted as a resonance in the partial wave $l = \text{Re}(\lambda_n) - 1/2$. The energy width of this resonance can be calculated from the poles. In the vicinity of E_0 the poles are extrapolated by

$$\lambda_n = \lambda_n^0 + \frac{d\lambda_n}{dE}(E - E_0). \quad (2)$$

For a complex energy E the extrapolation (2) can be used to make λ_n real and half integer, in which case l is an integer. The complex E thus obtained represents the resonance energy in the partial wave l . If $\text{Re}(\lambda_n^0) = l + 1/2$ then E is

$$E = E_0 - i \frac{\text{Im}(\lambda_n^0)}{d\lambda_n/dE} \quad (3)$$

from where the width of resonance is obtained.

Energy dependence of residues is deduced from the parametrization of the scattering matrix

$$S(\lambda) = \prod_n \frac{\lambda^2 - \lambda_n^{*2}}{\lambda^2 - \lambda_n^2} e^{i\pi\lambda + i\delta} \tag{4}$$

δ is the background phase which is an even function of λ , and it is very well approximated by the expansion $\delta \approx \delta^0 + \delta''\lambda^2/2$ in a relatively large neighbourhood of $\lambda = 0$. Therefore the energy dependence of the phase of residue is essentially determined by the energy dependence of λ_n and δ . It is easily shown from (4) that the n -th residue is proportional to the imaginary part of the n -th pole, when this imaginary part is small.

2. The theory

The multichannel equations for spherically symmetric potential are

$$\frac{d^2\psi}{dr^2} = \left[V(r) + \frac{\lambda^2 - 1/4}{r^2} - K^2 \right] \psi = F\psi \tag{5}$$

where $V(r)$ is the potential matrix and $\lambda = l + 1/2$, where l is the angular momentum. K^2 is diagonal matrix of the channel energies. The set of equations (5) is typical of electronic excitation problems in collisions of atoms. The regular solution of Eq. (5), which is defined with the initial conditions $\psi(r_0) = 0$ and $\psi'(r_0) = I$, where r_0 is taken from the vicinity of the origin, is a linear combination of the form

$$\psi = f^+ J^+ + f^- J^- \tag{6}$$

where J^\pm are the Jost functions (matrices), and f^\pm are the two irregular solutions of (5) which are defined by the asymptotic form $f^\pm = \exp(\pm iKr)$ for large r . It can be shown that the Jost functions are explicitly given in terms of the regular solution as

$$J^\pm = \mp (2iK)^{-1} \hat{f}^\mp (q^\mp - X) \psi \tag{7}$$

where $X = \psi'/\psi$, which is called the log-derivative of ψ . Similarly $q^\pm = f^{\pm'}/f^\pm$. It should be pointed out that ψ is an $N \times N$ matrix, rather than a single column one. The n -th column corresponds to the n -th linearly independent solution.

The S -matrix is given by

$$S = K^{1/2} J^+ (J^-)^{-1} K^{-1/2} e^{i(\lambda + 1/2)} \tag{8}$$

so that the poles of the S -matrix are solutions of the equation

$$\text{Det}(J^-) = 0. \tag{9}$$

In almost all applications the roots of Eq. (9) are nondegenerate and simple and therefore from now on we do not have to take care of the problems which might arise if they are otherwise.

In particular, the complex angular momentum poles are the roots of Eq. (9) in λ and they are functions of K^2 . If λ_0 is one pole of the S -matrix then the appropriate residue is

$$\beta = \lim_{\lambda \rightarrow \lambda_0} (\lambda - \lambda_0) S(\lambda). \quad (10)$$

In theory the poles are obtained by solving the set of equations (5) for a complex λ and then by finding the roots of the Eq. (9). When the pole is found the residue is calculated from (10). However, in practice there are several obstacles to this straightforward procedure. One is that the numerical solution of (5) is very often an unstable procedure, due to the mixing of two components which have vastly different orders of magnitude. This happens when for a particular r at least one diagonal term on the right-hand side is positive. The problem is remedied by solving the equations for the log-derivative X

$$X' = P - X^2 \quad (11)$$

which is a stable numerical procedure⁷⁾. Since the log-derivative does not give the wave function explicitly, the equations for the poles and residues must be related to this quantity. From the Eqs. (7) and (9) one obtains the equation for the poles in the form $\text{Det}(X - iK) = 0$, because $\text{Det}(\varphi) \neq 0$ for all λ . Likewise, it can be shown that

$$S = -iK^{-1/2} \hat{f}^- (q^- - X) (q^+ - X)^{-1} (\hat{f}^+)^{-1} K^{1/2} e^{i\pi\lambda} \quad (12)$$

which is also given in terms of X and the irregular solution.

The residue (10) of the S -matrix is calculated from (12), but making first a suitable transformation. If a matrix U is defined with the property

$$U^{-1} (q^+ - X) U = j \quad (13)$$

where j diagonal, then the S -matrix becomes

$$S = -iK^{-1/2} \hat{f}^- (q^- - q^+ + q^+ - X) U j^{-1} U^{-1} (\hat{f}^+)^{-1} K^{1/2} e^{i\pi\lambda}. \quad (14)$$

If λ_0 is the first order root of Eq. (9) then only one eigenvalue j_n is zero for this root. Let the N -th eigenvalue is zero, in which case in the vicinity of λ_0 the S -matrix (14) is dominated by the term j_N . The residue is therefore

$$\beta_{m,n} = - \frac{2(K_m K_n)^{1/2}}{f_m^+ f_n^-} \frac{U_{m,N} U_{n,N}}{[U^{-1} (\hat{q}^+ - X) U]_{N,N}} e^{i\pi\lambda_0} \quad (15)$$

where the dot designates derivative with respect to λ . It should be noted that only the diagonal elements of the residue matrix are independent. The off-diagonal elements are the geometric mean of the appropriate diagonal ones²¹.

Another disadvantage of the suggested procedure for calculating poles and residues is encountered when calculating the irregular solution in (15). It is tacitly assumed that the point where the matching to the irregular solution is done is in the region where the potential and the centrifugal term are negligible. In this way f^\pm is replaced by $\exp(\pm iKr)$. However, in practice the integration of X into this region is very time consuming and therefore it would be of advantage if it is carried out much closer to the origin. In such a case, though, one would have to find a way of calculating the irregular solutions and corresponding log-derivatives analytically. This is described in the next section.

3. Multichannel WKB expansion

It was shown that in the calculation of the poles and residues one needs the log-derivatives q^\pm of the irregular solutions of (5). The equation for q^\pm is

$$q^{\pm'} = P - q^{\pm 2} \tag{16}$$

where P is of the order \hbar^{-2} while q (the superscript \pm is omitted from now on) is of the order \hbar^{-1} . Therefore, we can write expansion

$$q = \hbar^{-1}q_{-1} + \hbar^0q_0 + \hbar^1q_1 + \hbar^2q_2 + \dots \tag{17}$$

and if it is introduced in (16) then the following set of equations for the coefficients q_n is obtained

$$q_{-1}^2 = P$$

$$q_{-1}' = -q_{-1}q_0 - q_0q_{-1} \tag{18}$$

$$\begin{aligned} q_0' &= -q_0^2 - q_{-1}q_1 - q_1q_{-1} \\ &\vdots \end{aligned} \tag{19}$$

The set can be solved by defining a unitary matrix T which diagonalizes F . If $p = \hat{T}PT$, and if a matrix η is defined by $T' = T\eta$, then the set (18) becomes

$$Q_{-1} = p^{1/2}$$

$$\eta Q_{-1} - Q_{-1}\eta + Q_{-1}' = -p^{1/2}Q_0 - Q_0p^{1/2} \tag{20}$$

$$\begin{aligned} \eta Q_0 - Q_0\eta + Q_0' &= -Q^2 - p^{1/2}Q_1 - Q_1p^{1/2} \\ &\vdots \end{aligned} \tag{21}$$

where $Q_n = \hat{T}q_n T$ and $Q'_n = \hat{T}q'_n T$. The set (20) has solution

$$Q_{0;i,j} = - \frac{1}{p_i^{1/2} + p_j^{1/2}} [Q'_{-1;i,j} + (\eta Q_{-1})_{i,j} - (Q_{-1}\eta)_{i,j}] \quad (22)$$

$$Q_{1;i,j} = - \frac{1}{p_i^{1/2} + p_j^{1/2}} [(Q_0^2)_{i,j} + Q'_{0;i,j} + (\eta Q_0)_{i,j} - (Q_0\eta)_{i,j}] \quad (23)$$

⋮

It can be shown that

$$\eta_{i,j} = \frac{[\tilde{T}F'T]_{i,j}}{p_j - p_i} \quad (24)$$

The matrix q is obtained by the inverse transform of Q .

The expansion is rapidly convergent, however, it has only meaning if r is greater than the largest turning point of all f 's. Continuation of the solution through one of the turning points of f 's is not straightforward and will not be treated here. In many instances of interest the turning points are well inside the region of potential which is sufficient to apply the technique and not to integrate the log-derivative equation. The sign of $f^{1/2}$ is determined according to the choice of the irregular solution. For q^+ the value is $p^{1/2} = i |p|^{1/2}$.

It remains now to calculate the irregular solutions of (5) which are required in (15). From the definition of the log-derivative the wave function is solution of

$$\psi' = q\psi \quad (25)$$

and if the wave function is transformed into $\varphi = \hat{T}\psi$, the equation for φ is

$$\varphi' = (Q - \eta)\varphi \quad (26)$$

In the region where the irregular solutions are required the elements of the matrix η are small. They are large in the vicinity of the crossing points between channels, but in this region it is assumed that the log-derivative equations are integrated numerically. Therefore, Eq. (26) is parametrized as

$$\varphi' - Q_0\varphi = (Q_1 - \eta)\varphi \quad (27)$$

where Q_0 contains the diagonal elements of Q . The Eq. (27) has solution

$$\varphi = e^\Phi + e^\Phi \int_{\infty}^r dr' e^{-\Phi} (Q_1 - \eta)\varphi \quad (28)$$

which can be solved by iteration. The phase Φ is defined as $\Phi = \int dr' Q_0$, where the lower limit is undefined and depends on where the initial conditions are taken.

For the irregular solutions the initial conditions are taken at infinity, hence the phase Φ is

$$\Phi = iKr + \int_{\infty}^r dr' (Q_0 - iK) \quad (29)$$

where it was assumed that ψ^+ solution is required.

The first iteration of Eq. (28) produces approximate solution

$$\varphi = e^{\Phi} + e^{\Phi} \int_{\infty}^r dr' e^{-\Phi} (Q_1 - \eta) e^{\Phi} \quad (30)$$

and similarly for the second iteration. One way of calculating the integral in Eq. (30) is by the asymptotic techniques. Both Q_1 and η are monotonic functions and the phase difference $\Phi_m - \Phi_n$ is assumed to be large, so that the integral is approximately

$$\varphi_{m,n} \approx \frac{(Q_1 - \eta)_{m,n}}{Q_{0;n} - Q_{0;m}} e^{\Phi_m - \Phi_n}. \quad (31)$$

In this way we have demonstrated how to calculate the log-derivatives q^{\pm} and the appropriate irregular solutions f^{\pm} analytically. The only restriction is that the turning points of p_n are not encountered.

4. Two examples and discussion

In order to illustrate the method two examples were investigated. In one a model potential was used which, in many respects, is typical of the atom-atom collision processes with two channels^{9,10}. One channel corresponds to the ionic electronic state and the other to the covalent. The potential is

$$V_{1,1} = 1051 e^{-0.664r}$$

$$V_{2,2} = 500 e^{-r+2} (e^{-r+2} - 2) + 200 \quad (32)$$

$$V_{1,2} = V_{2,1} = \varepsilon V_{1,1}$$

where r is in the units of 10^{-10} m. Since we use a model potential, the units for it are arbitrary, and for convenience the potential is measured in 10^{20} m (wave number squared). The collision energy is also measured in these units. ε is a dimensionless parameter which was varied from zero to some arbitrary value. The potential does not include the long range part of the form r^{-n} but this does not alter the main conclusions. Fig. 1 shows the diagonal potentials of (32), together with the appropriate diabatic potentials (broken line).

Typical behaviour of the poles for collision energy $E = 10^{-10}$ m when ε is increased from $\varepsilon = 0$ is shown in Fig. 2. The dots designate separation in units of $\varepsilon = 0.01$. Their indices correspond to the quantum number of the bound states which they represent (the potential $V_{2,2}$ supports 22 bound states). These indices

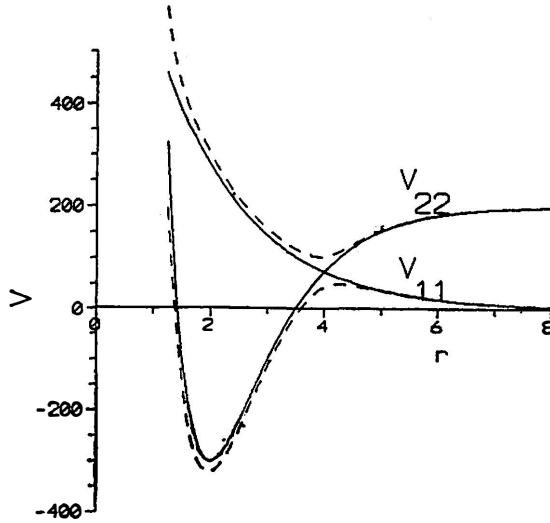


Fig. 1. Diabatic (solid line) and adiabatic (broken line) model potentials for a two channel problem. The adiabatic potentials were obtained for $\varepsilon = 0.4$.

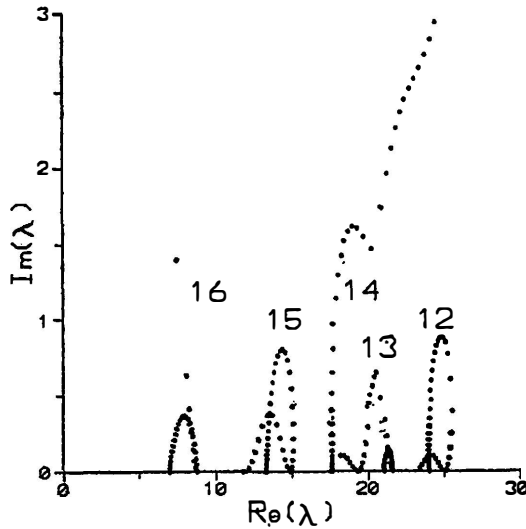


Fig. 2. Various complex angular momentum poles which correspond to the potentials in Fig. 1., for varying coupling strength.

are determined for $\varepsilon = 0$ and then continually kept as ε and E is varied. For example λ_{16} has the value ≈ 7 for $\varepsilon = 0$, meaning that the bound state $n = 16$ of $V_{2,2}$ has binding energy $E = 10^{-10}$ m (measured from the zero point energy defined in Fig. 1) for this angular momentum.

The ε dependence of poles is rather complicated. The poles move away from the real axis according to the estimate of the perturbation theory. Already at $\varepsilon = 0.1$ there is deviation from this approximation and some of the poles start returning towards the real axis, however some continue to increase their imaginary part (e. g. the pole λ_{14}). The latter will eventually become poles which can be traced to the adiabatic potential v_1 for large values of ε . Those poles which return towards the real axis at some point will touch it and their imaginary part will be zero. If at that point the real part of the pole is half integer then according to Eq. (3) the appropriate resonance appears with zero width, like a bound state. One then talks about a bound state imbedded into the continuum. However, such events are rare and in fact they are of zero measure. Among the poles which return some remain close to the real axis and are traced to the bound states of the adiabatic potential v_2 .

TABLE 1.

r (10^{-10}m)	V_{11} (eV)	V_{22} (eV)	V_{12} (eV)
1.587	17.0070	13.6726	-3.0449
2.116	11.9868	5.5354	-2.8203
2.645	9.6532	1.6968	-2.0051
2.909	8.9555	.8178	-1.5094
3.174	8.3835	.3261	-1.0671
3.438	7.8817	.0639	-.7132
3.703	7.4250	-.0633	-.4549
3.967	6.9997	-.1097	-.2835
4.232	6.6067	-.1168	-.1791
4.496	6.2453	-.1037	-.1136
4.761	5.9175	-.0870	-.0716
5.290	5.3505	-.0585	-.0283
5.819	4.8797	-.0396	-.0115
6.877	4.1445	-.0201	-.0024
7.935	3.6109	-.0118	-.0012
8.993	3.2096	-.0075	-.0010
10.051	2.8633	-.0048	-.0008
11.109	2.5750	-.0035	-.0008
12.167	2.3474	-.0026	-.0006
13.225	2.1624	-.0020	-.0005
15.870	1.8088	-.0013	-.0003

 Potential matrix for $\text{Al}^{2+} + \text{H}^+$ system.

Another example is collision of ions Al^{2+} and H^+ going into $\text{Al}^{3+} + \text{H}$. Table gives the numerical values of the potential¹¹⁾ which was used in the calculation of the ε dependence of the pole at the collision energy $E = 8.09$ eV. The dissociation limit of the nonionic potential is $E_{diss} = 8.170419$ eV. Fig. 3. shows the ionic potential (broken line) and the nonionic (solid line). The latter has a shallow minimum, thus supporting a bound state.

The ε dependence of the pole between 0 (the circle on the far right) and 1.02 is shown in Fig. 4. It has rather oscillatory structure, and its imaginary part is very small. Oscillations of the imaginary part indicate strong interaction even for very small values of ε (circles indicate separation in units of $\varepsilon = 0.02$, except between the third and the fourth circle from the right where there is a jump from

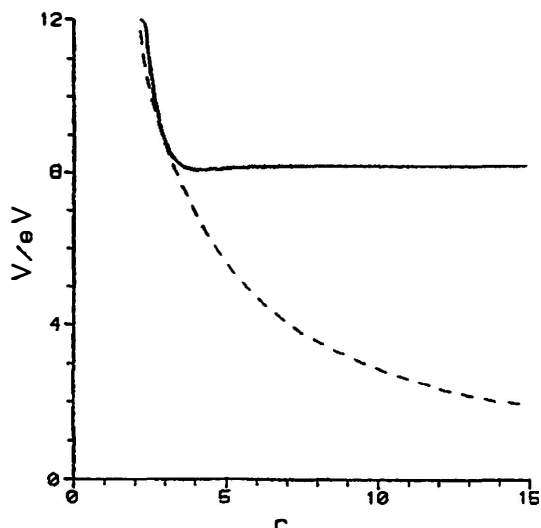


Fig. 3. Diabatic potentials for the system $\text{Al}^{3+} + \text{H}$ (solid line) and $\text{Al}^{2+} + \text{h}^+$ (broken line).

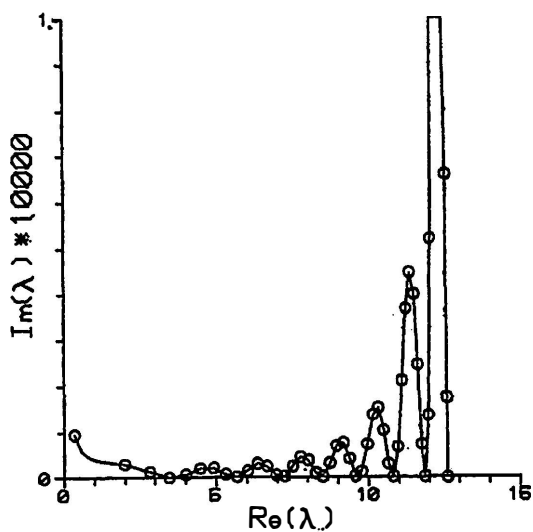


Fig. 4. The pole for potentials in Fig. 3. as function of the coupling strength.

$\varepsilon = 0.04$ to $\varepsilon = 0.22$). The weak interaction limit applies only in the very small neighbourhood of $\varepsilon=0$. A number of states with the zero width are noticed, even when the real part of the pole is half-integer.

These two examples show that with the method it is possible to calculate the poles and residues of the S -matrix, even when the imaginary part of the poles is very small (the second example). It should be noted, though, that the Eq. (9) does not produce any result if the integration limit for the logarithmic derivative X is in the far away regions. The integration limit should be suitable chosen somewhere in the interaction region (in the first example that was $r = 4 \cdot 10^{-10}$ m and in the second $r = 4.2 \cdot 10^{-10}$ m), and then numerically integrate the equation for q^\pm . This procedure is quite stable and efficient because the starting point for integration of q^\pm can be chosen relatively close to the matching point by using the WKB expansion of the logarithmic derivative.

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RAČUNANJE POLOVA I REZIDUA KOMPLEKSNE KUTNE KOLIČINE GIBANJA U VIŠEKANALNIM PROBLEMIMA

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Opisana je metoda računanja polova i rezidua kompleksne kutne količine gibanja S -matrice u višekanalnim problemima. Dano je poopćenje WKB metode za log-derivaciju višekanalne valne funkcije. Metoda je primijenjena na dva primjera.