

Calculation of Some Three-Body Scattering Amplitudes*

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Using a method based on numerical analytic continuation, *S*-wave, three-body, bound-state, elastic scattering amplitudes are calculated for both Coulomb (electron-hydrogen) and short-range potentials. In the calculations one particle is taken to be infinitely heavy, and only the spherically symmetric portion of the *S*-wave amplitude is considered.

I. INTRODUCTION

IN a previous paper¹ we discussed a method which uses the analytic properties of the nonrelativistic scattering amplitude $T(W)$ as a function of the complex energy variable W to calculate scattering phase shifts. The method consists of finding the values of the off-energy-shell scattering amplitude $T(W)$ for several values of W for fixed and physical values of the external momenta in an energy region where these calculations are easiest. These numerical values are then analytically continued to the physical energy to obtain scattering amplitudes. Because the values of the amplitude are obtained in an unphysical energy region, the first step in the calculation is considerably easier than the direct solution of the Schrödinger equation. The second step in the calculation is accomplished by using a rational-fraction approximation similar to the Padé method.

Here we apply this method to the calculation of some three-body, bound state, elastic scattering amplitudes including *S*-wave electron-hydrogen scattering and scattering by short-range or Yukawa potentials. We also present a brief discussion of the problems involved in the application of this method to the calculation of breakup amplitudes.

II. FORMALISM AND GENERAL METHOD

We consider the nonrelativistic scattering of three particles with masses m_1, m_2, m_3 and coordinates r_1, r_2, r_3 interacting through the pair potentials $V_{ij}(|r_i - r_j|)$, $i, j = 1, 2, 3$. The total Hamiltonian H is given as

$$H = H_0 + V_{12} + V_{13} + V_{23} = H_0 + V,$$

where H_0 is the free Hamiltonian and we define $V_0 \equiv 0$ for completeness. Although we are mainly concerned with bound-state elastic scattering, we discuss the formalism for any type of three-particle process. The scattering operator $T(W)$ for a transition from the state α to the state β has been given by Lovelace² as a

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¹ L. Schlessinger, Phys. Rev. **167**, 1411 (1968).

² C. Lovelace, in *Strong Interactions and High Energy Physics*, edited by R. G. Moorhouse (Oliver and Boyd, London, 1964).

function of the complex energy variable W as

$$T_{\beta\alpha}(W) = \hat{V}_\beta + \hat{V}_\beta(W - H)^{-1} \hat{V}_\alpha, \quad (2.1)$$

where, in our notation, α, β label the two-body bound pair in the asymptotic state ($\alpha, \beta = 12, 13, 23$, or 0 ; 0 corresponds to three free particles), and

$$\hat{V}_\alpha = V - V_\alpha.$$

The on-shell scattering amplitude is obtained as the matrix element of $T_{\beta\alpha}(W)$ between the physical or energy-shell eigenstates of H_β and H_α , where

$$H_\alpha = H_0 + V_\alpha$$

as W approaches the physical energy E in the complex plane. That is,

$$T(\beta, \alpha, E) = \lim_{W \rightarrow E + i\epsilon} (\varphi_\beta, T_{\beta\alpha}(W) \varphi_\alpha). \quad (2.2)$$

The asymptotic wave functions φ_α satisfy the equation

$$(E - H_0 - V_\alpha) \varphi_\alpha = 0. \quad (2.3)$$

Knowing the spectrum of the operator H , we conclude that T has poles at negative real values of W corresponding to three-particle bound states of H , a line of singularities beginning at negative real values of W associated with the two-body bound states of H , and a line of singularities beginning at $W = 0$ corresponding to the continuum of three-free-particle scattering states of H . T has simple square-root branch points at the two-body bound-state energies E_α since the physical process involved at those points is two-body scattering although one of the particles is composite. These results have been proven in a more formal way by Lovelace,² who also shows that the T matrix behaves as $W^2 \ln W$ at the three-particle threshold. In the complex plane, T has the structure shown in Fig. 1 and is analytic everywhere else on the first sheet of the W plane.

The method now consists of the same two steps used for two-body scattering. First we calculate the values of the matrix elements of $T_{\beta\alpha}(W)$ for several values of W less than E_0 , the lowest two-body bound-state energy. Then we analytically continue these numerical results to $W = E + i\epsilon$, as shown in Fig. 1, to obtain the scattering amplitude.

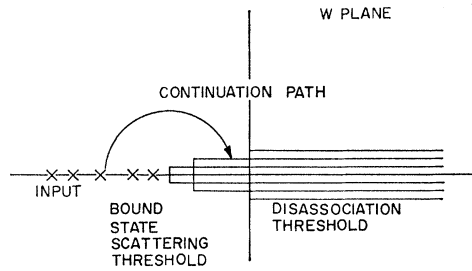


Fig. 1. Analytic structure of the three-body scattering amplitude in the complex energy plane.

III. METHODS OF CALCULATION

The first step in the calculation is done using a Kohn-type variational principle. We write the T matrix in the form

$$(\varphi_\beta, T_{\beta\alpha}(W) \varphi_\alpha) = (\varphi_\beta, \hat{V}_\beta \psi_\alpha(W)) = (\psi_\beta(W), \hat{V}_\alpha \varphi_\alpha), \quad (3.1)$$

where

$$(W - H)\psi_\alpha(W) = (W - H_\alpha)\varphi_\alpha \quad (3.2)$$

and α labels the asymptotic state. Representing $\psi_\alpha(W)$ as

$$\psi_\alpha(W) = \varphi_\alpha + \chi_\alpha(W),$$

(3.2) becomes

$$(W - H)\chi_\alpha(W) = \hat{V}_\alpha \varphi_\alpha. \quad (3.3)$$

For $W < E_0$, the lowest two-body bound-state energy, the asymptotic behavior of $\chi_\alpha(W)$ for bound-state elastic scattering processes (one particle scattering from a bound state of the other two) is that of a decaying exponential in all directions in coordinate space.³ Solving (3.3) for these unphysical energies eliminates the complicated asymptotic terms usually necessary in the Kohn principle and the calculation is simplified considerably. The variational principle used is

$$[(\varphi_\beta, T_{\beta\alpha}(W) \varphi_\alpha)] = (\varphi_\beta, \hat{V}_\beta \varphi_\alpha) + (\varphi_\beta, \hat{V}_\beta \chi_\alpha(W)) + (\chi_\beta(W), \hat{V}_\alpha \varphi_\alpha) + (\chi_\beta(W), [W - H]\chi_\alpha(W)). \quad (3.4)$$

The left-hand side of (3.4) is equal to the matrix element of $T_{\beta\alpha}(W)$ when χ_α, χ_β satisfy (3.3) and it is stationary under small variations of χ_α and χ_β about those values. The details of this part of the calculation are discussed in Sec. IV.

To analytically continue these numerical results past a single two-body scattering threshold we represent the amplitude as a ratio of polynomials in the variable $(-W + E_\alpha)^{1/2}$, where E_α is the two-body bound-state energy. Evaluating the rational fraction thus obtained at the physical energy yields scattering phase shifts and amplitudes. To continue past two such thresholds we use the uniformization procedure discussed for two-

³ The wave function $\chi_\alpha(W)$ falls off at large distances at least as fast as the potential. In our approximation of the interelectron potential this is an exponential decay, but for the full Coulomb potential this is not true.

channel scattering and represent the amplitude as the ratio of polynomials in the variable

$$\left[\frac{(-W + E_\alpha)^{1/2} + i(E_\beta - E_\alpha)^{1/2}}{(-W + E_\beta)^{1/2} - i(E_\beta - E_\alpha)^{1/2}} \right]^{1/2},$$

where E_β is the energy of the second two-body bound state.⁴ For more than two such thresholds one could perhaps approximate the amplitude as the sum of rational fractions in the variables $(-W + E_{\alpha_i})^{1/2}$, one rational fraction for each bound state of energy E_{α_i} . We have not tried the latter representation since, in these examples, we do not continue past more than two such thresholds.⁵ We tried various methods to include the three-body logarithmic singularity in the continuation but none of these techniques yielded satisfactory (convergent) results. Thus the breakup threshold was ignored in the continuation of the bound-state amplitudes.

IV. EXAMPLES

The first example we consider is S -wave electron-hydrogen scattering. We assume that the proton is infinitely heavy and use $a_0 = \hbar^2/m_e^2$ as the unit of length. The coordinates used are r_1 (the coordinate of electron 1), r_2 (the coordinate of electron 2), and $r_{12} = r_1 - r_2$ (the relative coordinate of the two electrons). The total Hamiltonian with these conventions is

$$H = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 + 1/r_1 + 1/r_2 - 1/r_{12}. \quad (4.1)$$

To simplify the numerical computations we only allowed the electrons to interact through S waves in their relative coordinates. More precisely, we represent the two-electron wave function as

$$\psi(r_1, r_2) = \sum_l \psi_l(r_1, r_2) P_l(\cos\theta_{12}), \quad (4.2)$$

where θ_{12} is the angle between r_1 and r_2 , and keep only the first term ($l=0$) in the expansion. This is not an essential limitation since the other coordinate may be included in the wave functions in a straightforward (but tedious) way. Projecting out the relative S -wave part of the Hamiltonian, (4.1) becomes

$$H = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 + 1/r_1 + 1/r_2 - 1/r_>, \quad (4.3)$$

where $r_>$ is the greater of r_1 and r_2 .

⁴ Branch points corresponding to all the closed thresholds should also be included in the continuation. For Coulomb scattering, there are an infinite number of thresholds below the breakup threshold which cannot be included in the continuation. Our numerical results for two-channel problems where both thresholds could be correctly included in the continuation were relatively insensitive to the inclusion of the closed thresholds. For this reason and because of the difficulties associated with the inclusion of more than two thresholds exactly, we keep, whenever possible, only the open thresholds in the continuation.

⁵ We have not found a way to include exactly more than two thresholds in the continuation. The procedure described here is merely suggested as a possible approximation to the effect of several branch points.

The fact that the electrons are identical particles is taken into account by symmetrization of the wave functions φ_α and $\chi_\alpha(W)$. For S -wave scattering the spatial wave functions may be symmetric (singlet) or antisymmetric (triplet) under the exchange $r_1 \leftrightarrow r_2$, and because the Hamiltonian is symmetric under this interchange the states do not mix.

The procedure used to solve (3.4) for the elastic amplitude is similar to that used in the two-body case. We first represent $\chi_\alpha(W)$ as the sum of a complete set of functions

$$U_i(r_1, r_2), \quad i=1 \cdots$$

as

$$\chi_\alpha(W) = \sum_{i=1}^{\infty} A_i(W) U_i(r_1, r_2), \quad (4.3)$$

and form a matrix representation of (3.4) in that basis, keeping only the first N terms in the expansion (4.3). Variation of the parameters A_i leads to the set of linear equations

$$\begin{aligned} H_{ij} A_j &= D_i, \quad i, j=1 \cdots N \\ H_{ij} &= (U_i, (W-H) U_j), \\ D_i &= (U_i, \hat{V}_\alpha \varphi_\alpha), \end{aligned}$$

and the N th approximation to T is obtained as

$$(\varphi_\alpha, T_{\alpha\alpha}(W) \varphi_\alpha)^{(N)} = (\varphi_\alpha, \hat{V}_\alpha \varphi_\alpha) + \sum_{i,j=1}^N D_i H_{ij}^{-1} D_j.$$

The asymptotic wave function used for S -wave scattering from the hydrogen atom in its ground state is

$$\varphi_\alpha = \varphi_{2s} = \frac{2}{\sqrt{2}} \left[\frac{\sin p r_1}{p r_1} e^{-r_2} \pm \frac{\sin p r_2}{p r_2} e^{-r_1} \right],$$

where $2e^{-r}$ is, in these units, the S -wave ground-state wave function for hydrogen and p is the momentum of the incident electron. The trial functions $U_i(r_1, r_2)$ used in (4.4) are chosen to best represent the actual solution of (3.3). To match the behavior of the potential at $r_1=r_2$ we took as our set

$$U_i(r_1, r_2) = r_{<}^k r_{>}^l e^{-\alpha r_{<}} e^{-\beta r_{>}}$$

for the singlet and

$$U_i(r_1, r_2) = (r_1 - r_2) [r_{<}^k r_{>}^l e^{-\alpha r_{<}} e^{-\beta r_{>}}]$$

for the triplet, where $r_{>}$ ($r_{<}$) is the greater (lesser) value of r_1 and r_2 , α and β are adjustable parameters, and i is assigned a value depending on k and l . In our case $i = \frac{1}{2}(k+l-1)(k+l) + l + 1$.

The other example we study is S -wave scattering of three particles interacting through short-range Yukawa potentials. We consider one particle scattering elastically from a bound state of the other two and make the same approximations as in the electron-hydrogen problem; that is, particle 3 is infinitely heavy and only S -wave interactions are considered between the other

TABLE I. Values of $(\tan\delta)/pa_0$ for singlet S -wave elastic ($1s \rightarrow 1s$) e -H scattering.

pa_0	$(\tan\delta)/pa_0$ (continuation)	$(\tan\delta)/pa_0^a$
0.0	-7.842	-7.815
0.2	-14.64	-14.77
0.4	7.98	8.048
0.6	2.15	2.147
0.8	1.11	1.110

^a See Ref. 7.

two particles which have the same mass⁶ but are not identical. Specifically, the potentials used are

$$\begin{aligned} V_{13}(r_1) &= \lambda_1 e^{-\mu_1 r_1} / r_1, \\ V_{23}(r_2) &= \lambda_2 e^{-\mu_2 r_2} / r_2, \\ V_{12}(r_1, r_2) &= \frac{\lambda_3 \sinh(\mu_3 r_{<}) e^{-\mu_3 r_{>}}}{\mu_3} \frac{1}{r_{<} r_{>}}, \end{aligned}$$

where V_{12} is the relative S -wave projection of

$$\lambda_3 e^{-\mu_3 r_{12}} / r_{12}$$

and in this case we take

$$H_0 = -\nabla_1^2 - \nabla_2^2.$$

The ranges μ_1, μ_2, μ_3 as well as the coupling constants $\lambda_1, \lambda_2, \lambda_3$ are parameters which can be varied. We chose the coupling constants so there was a two-body bound state in the 2-3 system and the two-body bound-state wave function was calculated using the Rayleigh-Ritz variational principle. In practice we picked the two-body bound-state energy and the Rayleigh variational principle supplied the appropriate coupling constant and the bound-state wave function. We used the same trial functions as for the e -H problem but we included both the symmetric and antisymmetric functions for each calculation. The results of both the above calculations are presented in Sec. V.

Since we could obtain a small number of two-body bound states with these short-range potentials, we also attempted to calculate the amplitude for the breakup process, that is, the transition from an initial

TABLE II. Values of $(\tan\delta)/pa_0$ for triplet S -wave elastic ($1s \rightarrow 1s$) e -H scattering.

pa_0	$(\tan\delta)/pa_0$ (continuation)	$(\tan\delta)pa_0^a$
0.0	-2.348	-2.3482
0.2	-2.4909	-2.4908
0.4	-3.0467	-3.0467
0.6	-4.8486	-4.8486
0.8	-27.00	-27.24

^a See Ref. 7.

⁶ For short-range potentials we solve the Schrödinger equation with $\hbar^2 = 2m = 1$.

TABLE III. Successive approximations to $(\tan\delta)/pa_0$ and the unitarity condition for triplet elastic e -H scattering at $pa_0=0.1$.

N (order of approximation)	$(\tan\delta)/pa_0$	Unitarity
1	2.377	1.28
2	2.3818	0.995
3	2.3822	0.9993
4	2.3822	0.9980
5	2.3824	1.0002

state of one particle incident upon a bound state of the other two to a final state of three free particles. By modifying Eq. (3.3) to include two-body scattering wave functions below threshold we obtain equations similar to (3.3) and (3.4) for the wave function $\chi_0(W)$ and the breakup amplitude $T_{0\alpha}(W)$. Furthermore, the parts of $\chi_0(W)$ to be calculated are exponentially decaying in coordinate space for $W < E_0$. Using these equations we calculated convergent values for $T_{0\alpha}(W)$. We have not, however, been successful in continuing these amplitudes above the three-particle threshold. We believe that this failure is probably caused by our inability to include the three-body logarithmic singularity in the continuation in a satisfactory way, although other nearby singularities on the second sheet of the W plane cannot be ruled out as a possible cause of the poor continuation. The results for the elastic amplitude, however, are very nicely convergent, as we show in Sec. V.

V. RESULTS

A. Electron-Hydrogen Scattering

Tables I and II show a comparison between the values of $(\tan\delta)/p$ obtained using our method and those obtained in other ways⁷ for singlet and triplet S -wave e -H scattering with the approximations previously discussed. In all cases the agreement is quite good. Our triplet results are more precise than the singlet results because the input to the continuation was more accurate for the triplet (five to eight decimal places) than for the singlet (four to seven decimal places). To obtain these results we used 11 input points distributed along the negative W axis from $W = -E_0$ to $W \rightarrow -\infty$ as described for two-body scattering. An example of the convergence of our results for $(\tan\delta)/p$ and the

TABLE IV. The spherically symmetric ($l=0$) portion of the ($1s \rightarrow 1s$) elastic cross section for the triplet scattering of electrons by atomic hydrogen in units of πa_0^2 (a statistical factor of $\frac{3}{4}$ is included in σ).

pa_0	σ (continuation)	σ^a
0.88	3.860	3.864
0.89	3.768	3.773
0.90	3.672	3.684
0.92	3.507	...
0.94	3.345	3.349

^a See Ref. 8.

⁷ C. Schwartz, Phys. Rev. **126**, 1015 (1962).

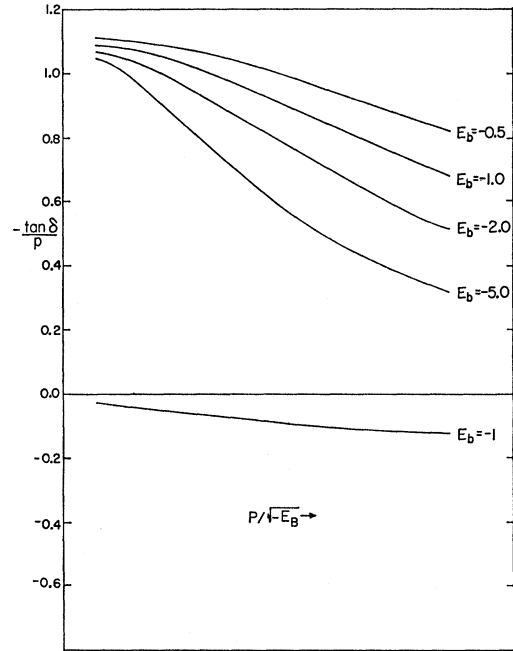


FIG. 2. $(\tan\delta)/p$ versus $p/\sqrt{-E_b}$ for the spherically symmetric part of S -wave bound-state elastic scattering for $\lambda_1=1$, $\lambda_3=1$; bottom curve is for $\lambda_1=-1$, $\lambda_3=1$. E_b is the binding energy of the two-body bound state.

unitarity condition, $\text{Im}(T^{-1})/p=1$, which holds below the first inelastic threshold is given in Table III for the triplet state at $pa_0=0.1$.

We also calculated the triplet elastic amplitude above the first inelastic threshold. These results, expressed in terms of cross sections for ease in comparison, are given in Table IV along with the results of Temkin and Kyle.⁸ Again our results are in good agreement with those obtained by other techniques.

B. Short-Range Potentials

The results obtained from the calculation of $(\tan\delta)/p$ for S -wave elastic scattering of particle 1 from a bound state of the 2,3 pair of various binding energies E_b and combinations of coupling constants are shown in Fig. 2. For these examples, the range of the potential is

TABLE V. Successive approximations to $(\tan\delta)/p$ and the unitarity condition for short-range potentials. $\lambda_1=1$, $\lambda_2=1$, $\lambda_3=-3.206$, $E_b=-0.5$, $p=0.272$.^a

N (order of approximation)	$(\tan\delta)/p$	Unitarity
1	1.07	1.005
2	1.037	0.995
3	1.050	1.003
4	1.047	1.001
5	1.048	0.9998

^a See Ref. 6.

⁸ H. L. Kyle and A. Temkin, Phys. Rev. **139**, A600 (1964).

taken as unity. As in all the elastic scattering calculations, the unitarity condition is a useful check on the computations. Table V shows the convergence of the results and the unitarity condition for $\lambda_1=1$, $\lambda_2=1$, $\lambda_3=-3.206\cdots$, $E_b=-0.05$, $p=0.272$. From the convergence of the approximations and the accuracy of our input values we estimate the accuracy of the results to be between 1 and 0.1%. All the results reported here concerning short-range potentials were obtained in about 2 min of IBM 360 computer time, where 12 values of $(\tan\delta)/p$ were calculated for each bound-state energy E_b .

VI. CONCLUSIONS

With this method we have been able to obtain precise values for some model three-body scattering phase

shifts and amplitudes in a simple and efficient way. We have not, however, been able to calculate breakup amplitudes, probably because of the neglect of the three-body logarithmic threshold. Despite this failing, we believe that the method employed here can be a useful tool in the solution of a wide variety of scattering problems.

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Embedding of $SU(3)$ in $SU(8)$ *

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The fact that $SU(8)$ symmetry has recently been applied to the nonleptonic decays of baryons, both in a pole model and in a current-algebra model, suggests a closer look at this symmetry. The $SU(8)$ algebra is constructed so that the $SU(3)$ structure is preserved. The possible application of other physical processes is then considered. It is shown that with certain restrictive assumptions, approximate octet dominance follows from a current-current interaction.

I. INTRODUCTION

THE use of $SU(8)$ symmetry in the parity-conserving baryon-pole model by Lee¹ and by Graham, Pakvasa, and Rosen² has supplied the motivation for a more careful look at $SU(8)$. More recently, in fact, $SU(8)$ has been applied to parity-violating baryon decays in the pole model³ and in a current-algebra model.⁴ If one should believe that $SU(3)$ might not be the smallest possible internal symmetry that has relevance to particle physics, then it seems to be important to consider the possibility of a more general application of $SU(8)$.

The $SU(8)$ algebra of Ref. 3 was constructed in terms of the Gell-Mann or Hermitian basis. Here, the algebra will be constructed in terms of the 8×8 traceless matrices A_j^i , $i, j=1, \dots, 8$, which satisfy the commu-

tation relations

$$[A_j^i, A_l^k] = \delta_j^k A_l^i - \delta_l^i A_j^k.$$

As will be shown in Secs. II and III, the actual construction will be a generalization of the Elliott model of $SU(3)$.⁵

The basic requirement for the construction of such a higher symmetry is that the $SU(3)$ structure must be preserved. One example of such a symmetry would be the $SU(4)$ model,⁶ which is described by

$$SU(4) = SU(3) \times U(1).$$

That is, a new quantum number, "supercharge," is added to the $SU(3)$ algebra, enlarging it to $SU(4)$. In the construction of $SU(8)$, however, it will not be necessary to assume the existence of any new quantum numbers since, as mentioned, the structure is simply a generalization of the Elliott model. For this reason, it is useful to describe this model briefly.

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