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# $s$-Wave Elastic Positron-Hydrogen Scattering in the Ionization Region

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The method of extrapolating the $t$ matrix from complex energies to real energies is tested on the positron-hydrogen $s$-wave amplitude at 29 energies in the elastic and inelastic regions, including 10 energies in the ionization region. The error in the extrapolated $t$ matrix is not expected to be more than 10% in the ionization region.

## I. INTRODUCTION

Recently a method has been proposed for computing scattering amplitudes at energies allowing final states for three charged particles.[1] In this paper we report the results of an $s$-wave study of this complex-energy extrapolation method applied to positron-hydrogen scattering. This method is of interest because it is the only mathematically sound and practical procedure that has been proposed to describe the scattering of three charged particles above the ionization threshold.

The first step in this method is to calculate variationally the scattering amplitude at complex energies where the calculation is known to converge. As a variational technique, we use the inhomogeneous Rayleigh-Ritz method. The results of this paper show, as expected, that the convergence rate of the variational method increases with increasing imaginary part of energy. In the case treated here, however, it is possible, even in the ionization region, to obtain good convergence surprisingly close to the real axis in energy.

It has been determined[2] that in this case the amplitude has a singularity, as the complex momentum $p$ approaches its real physical value $k$, of the form $C_0 + C_1 q + C_2 q^2 + D_3 q^3 \ln q + C_4 q^3 \cdots$, where $q = p - k$. This singularity is so weak that it appears that the extrapolation from the calculated values of the amplitude to the point $p = k$ should not be too difficult, provided we keep away from thresholds and resonances. The accuracy of the extrapolation procedure might be improved by fitting the calculated amplitude with a function containing the singularity above, but we have not attempted to do this here.

First, describing our procedure in more detail, we present numerical results in the elastic and inelastic regions.

## II. PROCEDURE

We use the inhomogeneous Rayleigh-Ritz variational principle given by McDonald and Nuttall[1] as follows:

$$[T(p)] = \langle \phi | V\phi \rangle + \langle \chi_t | V\phi \rangle + \langle V\phi | \chi_t \rangle - \langle \chi_t | (E - H)\chi_t \rangle ,$$

where

$$\phi = \frac{1}{2\pi} e^{-r_1} \frac{\sin kr_2}{kr_2}$$

and $E = p^2 - 1$, $k = \mathrm{Re}p$. Here, $H$ is the Hamiltonian and $V$ is the potential for $e^+$-$H$ elastic scattering. The trial function $\chi_t$ is taken to be a sum of the form

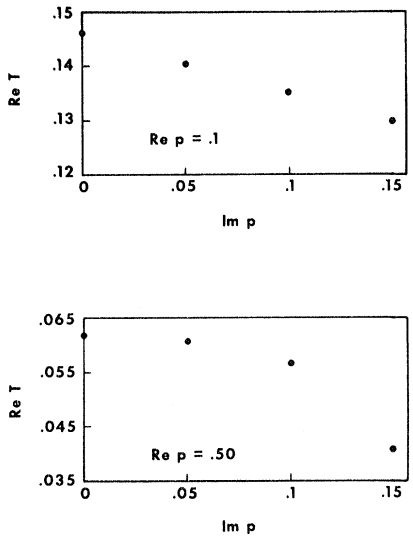


FIG. 1. Re$T$ as a function of the imaginary part of the momentum $p$ for Re$p$ = 0.1 and 0.5.

$$\chi_t = \sum_{L,M,N=0}^{L+M+N=\Omega} a_{LMN}\, e^{-\lambda(r_1+r_2)/2}\, r_1^L r_2^M r_3^N \,, \qquad (1)$$

where the $a$'s are linear variational parameters and $\lambda$ is the nonlinear parameter. The calculation was done using values of $\Omega$ as large as 7 (120 trial functions). We also included a trial function of the form

$$\Theta = \frac{1}{4\pi}\, e^{-r_1}\, \frac{e^{ipr_2}}{r_2}\, (1 - e^{-\lambda r_2/2})$$

to obtain the correct asymptotic behavior in the elastic region. Consequently, our calculation converged on the real axis in the elastic region where we were able to obtain results which agree to three figures with the recent precise bound calculation of Bhatia *et al.*[3] and with the less restrictive bounds of Kleinman, Hahn, and Spruch.[4]

## III. ELASTIC REGION

We used the techniques described above to compute the scattering amplitude for 14 values of the real part ranging from 0.05 to 0.7 and for four values of the imaginary part of $p$ ranging from 0 to 0.15. We find that the answers for real energies have converged to about four places to the right of the decimal point for the real part of the amplitude and five places for the imaginary part. These results are shown in Table I. The phase shifts given in this table were computed using the real part and unitarity.

To check the accuracy of the complex-energy extrapolation, we extrapolate the off-axis values to get the real part of $T$ using a simple quadratic fit to the three off-axis values. These extrapolated values are given in Table I. As can be seen, the results are accurate to three figures. Two of these curves are plotted in Fig. 1 to illustrate the typical dependence of Re$T$ on the imaginary part of $p$.

In this region, we tried adding another trial function to reproduce the asymptotic form at the positronium channel:

$$\Theta' = e^{-r_3/2}\, \frac{e^{ip(r_1+r_2)/2}}{r_1}\, (1 - e^{-r_1}) \,.$$

We found that the computer time necessary to include this function was more profitably used to increase $\Omega$ in Eq. (1).

Recently, Bhatia *et al.*[3] performed a bound calculation in this elastic region at seven values of the momentum. Their phase shifts are included in Table I. Our phase shifts agree with theirs to an

TABLE I. Real and imaginary parts of the $e^+$-H amplitude in the elastic region. Extrapolated values were calculated using a quadratic fit to three off-axis values.

| Re$p$ | Re$T$ | Im$T$ | $\delta$ | Extrapolated Re$T$ | $\delta$ of Bhatia *et al.* |
|---|---|---|---|---|---|
| 0.05 | 0.0895 | 0.008 10 | 0.0900 | 0.0886 | 0.1483 |
| 0.10 | 0.1460 | 0.021 55 | 0.1481 | 0.1461 | 0.1483 |
| 0.15 | 0.1741 | 0.031 25 | 0.1779 | 0.1732 | |
| 0.20 | 0.1832 | 0.034 80 | 0.1876 | 0.1841 | 0.1877 |
| 0.25 | 0.1785 | 0.032 87 | 0.1826 | 0.1795 | |
| 0.30 | 0.1640 | 0.027 67 | 0.1671 | 0.1648 | 0.1677 |
| 0.35 | 0.1436 | 0.021 10 | 0.1457 | 0.1432 | |
| 0.40 | 0.1187 | 0.014 30 | 0.1199 | 0.1190 | 0.1201 |
| 0.45 | 0.0912 | 0.008 40 | 0.0917 | 0.0915 | |
| 0.50 | 0.0621 | 0.003 89 | 0.0623 | 0.0625 | 0.0624 |
| 0.55 | 0.0325 | 0.001 03 | 0.0325 | 0.0333 | |
| 0.60 | 0.0034 | $\lvert\ \rvert < 0.000\,01$ | 0.0034 | 0.0049 | 0.0039 |
| 0.65 | −0.0247 | 0.000 62 | −0.024 | −0.0247 | |
| 0.70 | −0.0515 | 0.002 65 | −0.051 | −0.0504 | −0.0512 |

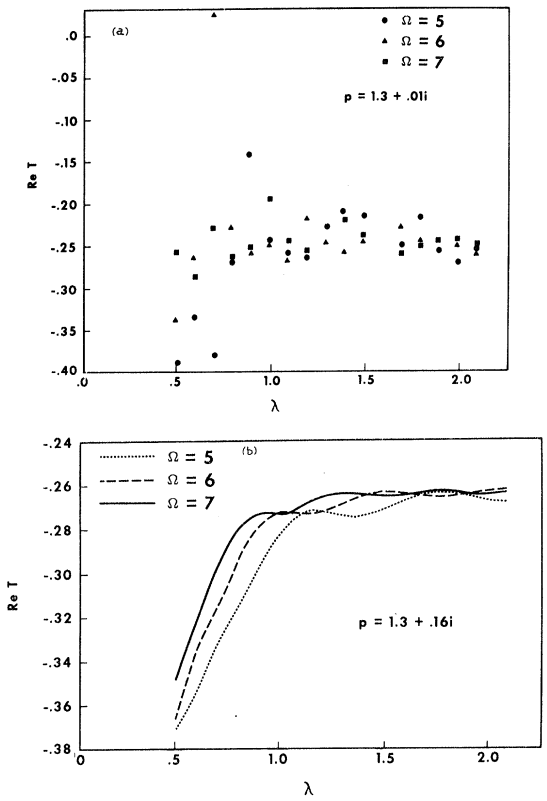


FIG. 2. (a) Re$T$ versus nonlinear parameter for 56, 85, and 120 terms in the trial function, corresponding to $\Omega = 5$, 6, and 7. The convergence is poor because $p = 1.3 + 0.01i$, which is quite near the real axis. It is reasonable to estimate that $\mathrm{Re}T \approx -0.25 \pm 0.03$ from this graph. (b) Re$T$ versus nonlinear parameter for $\Omega = 5$, 6, and 7. The convergence is improved so that it is reasonable to estimate $\mathrm{Re}T \approx -0.263 \pm 0.002$ from this graph.

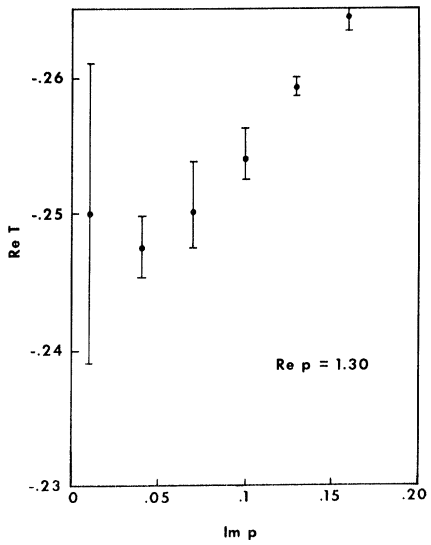


FIG. 3. Re$T$ as a function of the imaginary part of the momentum for Re$p = 1.3$.

accuracy of a few parts in the fourth figure to the right of the decimal. Both calculations differ slightly, however, from the previous calculation by Schwartz[5] at three values of the momentum.

## IV. INELASTIC REGION

We calculated the $t$ matrix for 15 values of the real part of $p$ ranging from 0.8 to 1.5 and for six values of the imaginary part of $p$ ranging from 0.01 to 0.16. The convergence rate improved as the distance from the real axis increased. Figure 2(a) shows a graph of the real part of $T$ for several values of the nonlinear parameter $\lambda$ at $p = 1.3 + 0.01i$. Figure 2(b) shows the same curve for $p = 1.3 + 0.16i$. For values of Re$p > 1$, there was poor convergence for Im$p = 0.01$. For Im$p = 0.16$, $T$ converged to three figures for all the values of Re$p$ tried. The extrapolated numbers are presented in Table II. The uncertainty in Re$T$ and Im$T$ causes an anticipated error of a few percent in $\eta$ and $\delta$.

Figure 3 illustrates the usefulness of a complex-energy extrapolation. The real part of $T$ is plotted against the imaginary part of the momentum. The error bars represent the maximum error we expect in the variational calculation. We do not expect the error to exceed 10% of the extrapolated value in the ionization region.

Previous calculations in the inelastic region have been carried out.[6-8] At $p = 0.8$, our phase shift, $-0.140$, is consistent with Dirks and Hahn's lower bound of $-0.158$. At this same momentum Fels and Mittleman obtain $-0.177$ for the $s$-wave phase shift, whereas Bransden and Jundi obtain $-0.082$.

Because of the known resonances and thresholds

TABLE II. Real and imaginary values for the $e^+$-H amplitude in the inelastic region, obtained by extrapolating from complex values. $\delta$ and $\eta$ are solutions to $T = \eta e^{i\delta} \sin\delta$.

| Re$p$ | Re$T$ | Im$T$ | $\delta$ | $\eta$ |
|---|---|---|---|---|
| 0.8 | −0.098 | 0.014 | −0.14 | 0.7 |
| 0.85 | −0.122 | 0.018 | −0.14 | 0.8 |
| 0.9 | −0.143 | 0.020 | −0.14 | 1.0 |
| 0.95 | −0.162 | 0.027 | −0.16 | 1.0 |
| 1.00 | −0.174 | 0.03 | −0.17 | 1.0 |
| 1.05 | −0.190 | 0.05 | −0.25 | 0.8 |
| 1.10 | −0.201 | 0.05 | −0.25 | 0.8 |
| 1.15 | −0.22 | 0.06 | −0.27 | 0.8 |
| 1.20 | −0.22 | 0.07 | −0.3 | 0.8 |
| 1.25 | −0.23 | 0.08 | −0.3 | 0.7 |
| 1.30 | −0.240 | 0.09 | −0.35 | 0.7 |
| 1.35 | −0.246 | 0.10 | −0.4 | 0.7 |
| 1.40 | −0.25 | 0.10 | −0.4 | 0.7 |
| 1.45 | −0.27 | 0.11 | −0.4 | 0.8 |
| 1.50 | −0.28 | 0.12 | −0.4 | 0.8 |

in the inelastic region below ionization, we expect that our extrapolation may not be as accurate there as in the region above the ionization threshold.

## V. CONCLUSION

On the basis of this calculation, it is reasonable to expect that a complex-energy extrapolation will yield approximately two-figure accuracy for the elastic-scattering amplitude above ionization threshold. We obtained approximately three-figure accuracy for complex energies sufficiently far from the real-energy axis. The limits of error increased rapidly as the real axis was approached.

## ACKNOWLEDGMENTS

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†National Research Council, Resident Research Associate.

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# Collisional Excitation of the $4\,^2F$ Levels in Lithiumlike Ne VIII†

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Collisional excitation rates from the ground state to the $4f$ levels in lithiumlike Ne VIII have been derived from the absolute intensity of the $3\,^2D$-$4\,^2F$ radiative transition. At temperatures of the order of the excitation energy and within the ~30% relative accuracy, the magnitude of these $\Delta l = 3$ rates is equal to that for the corresponding $\Delta l = 1$ dipole rates to the $4p$ levels. For the purpose of these measurements the Ne VIII $3\,^2D$-$4\,^2F$ doublet has been identified.

## INTRODUCTION

Theoretical excitation rate coefficients for lithiumlike ions[1-4] have been verified only recently by laboratory measurements.[5,6] In Ref. 6 the measurements were made for excitation to all $n = 3$ levels as well as to the $4s$, $4p$, and $4d$ levels. At present, neither theoretical nor experimental values are available for excitation from the ground state to the $4f$ levels, which corresponds to a $\Delta l = 3$ collisional transition. The knowledge of the corresponding rate coefficient is not only of interest *per se* but is also of importance when interpreting absolute line intensities in laboratory and solar plasmas originating from the $3d$ levels in lithiumlike ions. Besides the resonance transition $2p \rightarrow 2s$, the $3d \rightarrow 2p$ radiative transitions give rise to the strongest lines in the spectrum of lithiumlike ions, and at low electron densities this is because the $2s \rightarrow 3d$ collisional excitation rate is larger than the rates leading to $3s$ and $3p$. (At higher electron densities, where the $2p$ levels become populated considerably, the $2p \rightarrow 3d$ collisional excitation rate becomes important, so that the $3d \rightarrow 2p$ line remains strong.) Moreover, since at low electron densities the $4f$ level can decay only by a radiative transition to the $3d$ level, the $3d \rightarrow 2p$ line intensity is further increased relative to lines originating from $3s$ or $3p$.

## THEORETICAL CONSIDERATIONS

The principle of the measurement is described in Ref. 6 and will therefore not be discussed in detail. Atoms of interest are introduced into a well-diagnosed plasma produced in a $\theta$-pinch device where they are ionized to the lithiumlike ionization stage. Appropriate line intensities are measured absolutely and are finally interpreted in