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COMPLEX-ENERGY METHOD FOR ELASTIC e-H SCATTERING ABOVE THE IONIZATION THRESHOLD*

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It is demonstrated that the amplitude for elastic electron–hydrogen atom scattering above ionization threshold can be calculated by using a variational method at several complex energies and continuing into the physical region numerically.

In this Letter we propose a method for calculating the amplitude for the elastic scattering of an electron from a hydrogen atom in its ground state at an incident energy which may be above that required to ionize the atom. The principle of the method also applies to the amplitudes for excitation but for ionization significant changes are needed which are not discussed here. We demonstrate the feasibility of the method by calculating values for the singlet and triplet S-wave elastic scattering amplitudes at $k=1.103$ (the electron's momentum in units with $\hbar=2m=e^2/2=1$; we use the notation of Schwartz[1]). The singlet amplitude is probably correct to within 5% and the error on the triplet amplitude is less.

Our scheme is a generalization of the method of continuation from negative energies proposed by Schlessinger and Schwartz,[2] and applied by Schlessinger[3] to three-particle scattering at energies where only the elastic channel is open. We use a variational principle to estimate the scattering amplitude at several complex values of E, as near as possible to the physical value $E_0=k^2-1$, and extrapolate these values to the real E_0 numerically.

Define the amplitude $T(p)$ by

$$T(p)=\langle Q\varphi_0|QV\varphi_0\rangle+\langle QV\varphi_0|(E-H)^{-1}|QV\varphi_0\rangle,$$

where

$$\varphi_0=\frac{e^{-r_2}\sin kr_1}{2\pi kr_1},\quad V=-\frac{2}{r_1}+\frac{2}{r_3},\quad Q=\frac{1\pm P_{12}}{\sqrt{2}},$$

and $E=p^2-1$ with p complex. $T(p)$ is calculated to second order from the variational principle given by Schlessinger[3]:

$$[T]=\langle Q\varphi_0|QV\varphi_0\rangle+\langle\chi_t'|QV\varphi_0\rangle+\langle QV\varphi_0|\chi_t\rangle-\langle\chi_t'|(E-H)|\chi_t\rangle,$$

where χ_t and χ_t' are to be varied and will actually be related by $\chi_t'=\chi_t^*$. The exact χ is given by $\chi=(E-H)^{-1}|QV\varphi_0\rangle$, and for E in the upper half-plane χ will fall off exponentially for large distances, so that it should be possible to represent χ quite well by a linear combination of normalizable functions. We use the same set as Schwartz,[1] and write

$$\chi_t=(4\pi)^{-1}Q\sum_{l+m+n=M}C_{lmn}e^{-(\kappa/2)(r_1+r_2)}\times r_{12}{}^l r_1{}^m r_2{}^n$$

and vary the N linear parameters C_{lmn} and the nonlinear parameter κ. If p is not too close to the real axis, this procedure leads to a reasonable rate of convergence as N increases. But in order to obtain accurate values of $T(p)$ for p near to $k=1.103$, we found that it helped greatly to in-

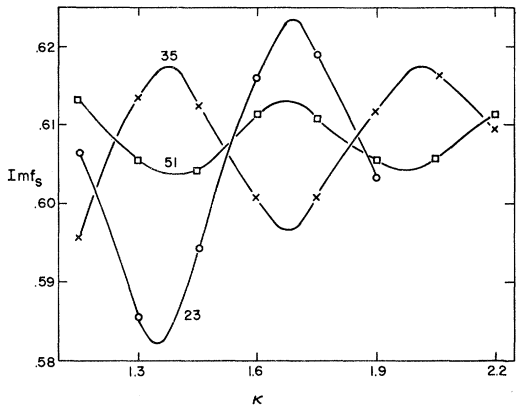

FIG. 1. The dependence of $\mathrm{Im}\, f_S(1.103+0.2i)$ on the nonlinear parameter κ for varying numbers of trial functions.

Table I. Calculated values of $f_S(p)$ for $k=1.103$ and $\mathrm{Re}p=1.103$, for several different values of $\mathrm{Im}p$. The numbers in brackets indicate the uncertainty in the last figure. For $\mathrm{Im}p \leq 0.3$, up to 51 trial functions were used; for $\mathrm{Im}p > 0.3$, up to 23.

$\mathrm{Im}p$	$\mathrm{Re}f_S(p)$	$\mathrm{Im}f_S(p)$
0.1	0.478(5)	0.541(5)
0.15	0.529(3)	0.578(3)
0.2	0.5800(15)	0.6080(15)
0.25	0.6303(10)	0.6325(10)
0.3	0.6798(5)	0.6518(5)
0.35	0.726(5)	0.663(5)
0.4	0.774(2)	0.670(2)
0.45	0.820(2)	0.674(2)
0.5	0.863(2)	0.673(2)

clude an additional trial function in χ_t. This is θ, where

$$\theta = Qe^{-r_2}e^{ipr_1}[1-e^{-(\kappa r_1/2)}]/r_1,$$

which represents asymptotically the contribution to χ of the scattered wave in the lowest channel (threshold $E=-1$). It is this contribution which falls off most slowly at large distances, and its inclusion allows us to improve substantially the accuracy of our results for energies not too far above $E=0$.

We have carried out the calculation with $\mathrm{Re}p = 1.103$ and a number of different values for $\mathrm{Im}p$, using in some cases up to 51 trial functions and varying the nonlinear parameter. (The computer program was checked by applying it to $k=0.4$, studied by Schwartz.[1]) The results for a typical case, $p=1.103+0.2i$, are shown in Fig. 1. We plot $\mathrm{Im}f(p)$, where $f(p)=-kT(p)$, so that in the elastic region $f(p)$ would be $e^{i\delta}\sin\delta$. We show the singlet amplitude, where convergence is slower than for the triplet. As $\mathrm{Im}p$ increases, the convergence rate improves rapidly. In Table I, we give the results for $f(p)$ in the singlet case, with the numbers in parentheses indicating the uncertainty in the last figure. These values were all obtained from plots like Fig. 1.

We have tried to continue to real p by fitting the values in Table I to a rational fraction, but do not regard the values produced as any more accurate than can be obtained by eye. For the singlet amplitude f_S at $k=1.103$ we estimate the value $f_S=0.365(15)+0.44(2)i$. For the triplet, the same technique gives $f_T=0.237(4)+0.932(4)i$.

This case, corresponding to an energy of 16.55 eV, was studied in order to compare with a calculation of Burke,[4] using the close-coupling method, which is not in principle valid in this region. For the singlet and triplet S-wave partial cross sections in the $1s$-$2s$-$2p$-$3s$-$3p$ approximation, Burke finds 0.1911 and 2.301. Our values are 0.27 and 2.3. The triplet agrees very well but there appears to be a significant discrepancy in the singlet case. The reason for this must lie in the symmetry of the wave functions; in the triplet case the electron appears to interact little with the atom. This is borne out by the inelastic cross section predicted by our f_T, which could be zero and is certainly small. It is not surprising that the close-coupling method gives good results in this situation. In the singlet case, however, inelastic processes are more important, and, if our results are to be believed, the close-coupling method involves sizable errors.

The same program may be used to perform calculations in the excitation region, and we have determined f_T at $k=0.9$, obtaining an answer that agrees with Burke, Ormonde, and Whitaker.[5]

The method seems to have considerable promise and we are extending our efforts to excitation cross sections in the ionization region. There is room for improvement in the continuation procedure. With 51 trial functions we have not yet reached the limits of the capability of the computer, and if necessary more functions could be used. The scheme can probably be generalized to ionization processes, and may also have important applications to problems with short-range forces involving three or more particles.

The computations were carried out on the CDC-6600 computer at the University of Texas Computation Center, whose help we gratefully acknowledge.

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CHARGE-EXCHANGE EXCITATION AND cw OSCILLATION IN THE ZINC-ION LASER*

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We have investigated the afterglow decay rates of the Zn II laser lines in spontaneous emission. Measurements indicate that the dominant mechanism for excitation of these lines is thermal-energy charge-transfer collisions between zinc atoms and both atomic and molecular ions of helium.

We have previously proposed[1,2] that thermal-energy charge-transfer collisions involving the helium ion and ground-state zinc atoms of the type

$$He^+ + Zn \rightarrow He + (Zn^+)^* \qquad (a)$$

could be used to obtain cw oscillation in the zinc-ion laser and that such collisions in fact constituted the dominant mechanism for excitation of the upper levels in its earlier pulsed form.[3] Our subsequent investigations have given support to this proposal.

Relatively little work has been done at low energies involving inelastic processes such as Reaction (a). Lipeles, Novick, and Tolk[4] have reported charge transfer with simultaneous excitation in He^+-Ar reactions at beam energies as low as 10 eV with cross sections of about 10^{-16} cm^2. As discussed by Dworetsky et al.,[5] appreciable cross sections for this type of reaction may be expected since the levels of the temporary molecule formed during the collisions are grossly different from the levels of the isolated particles. Thus, for example, excitation can occur nonadiabatically through "curve crossings" between the different intermolecular potentials describing the molecule formed during the collision.

There is even less quantitative information available regarding inelastic charge-transfer reactions at thermal energies, and the experimental situation regarding optical excitation through thermal-energy charge-exchange reactions has not changed greatly since the qualitative review given sometime ago by Meyerott.[6]

During preliminary work with the zinc-ion laser, we observed the decay rates of the laser transitions in spontaneous emission in the afterglow of a pulsed discharge.[1] These decay rates were rather slow ($\simeq 10^4$ sec^{-1}) and increased linearly with zinc partial pressure. This was in sharp contrast to transitions whose upper states were slightly above the energy of the helium ion. The decay rates of the latter transitions were fast and did not change with zinc density. It was thus apparent that the upper laser states were being populated in the afterglow by inelastic collisions involving some long-lived carrier of excitation (see Fig. 1).

In a simplified model of the discharge afterglow, the carrier density will vary roughly as

$$N = N_0 \exp(-\gamma t), \qquad (1)$$

where

$$\gamma = D/\Lambda^2 + n\bar{v}\bar{\sigma}. \qquad (2)$$

The first term in γ represents diffusion to the walls with subsequent de-excitation; the second term represents a volume loss due to collisions with ground-state zinc atoms of density n. $\bar{v}$ is the mean relative thermal velocity between the carrier and the zinc atoms, $\bar{\sigma}$ is the total velocity-averaged cross section for destruction of the carrier, and Λ is the characteristic diffusion length of the container. To the extent that impurity ions excited by collisions such as those of Reaction (a) decay in a time short compared with $1/\gamma$, the light emitted by the impurity states would also be expected to vary as the carrier density. The above model assumes that only the dominant diffusion mode is excited, and that effects such as three-body collisions, collisions