the order of (radiative wavelength)$^{-3}$, which is typically about 10^{13} cm^{-3}. Resonant broadening effects typically become significant at active-atom densities of 10^{15} atoms/cm^3. If the density of "foreign-gas" perturbers is much greater than that of "resonant" perturbers, the resonant broadening effects may still be negligible by comparison.

[8] We are, in effect, assuming that the atomic system is in equilibrium before the external fields are "turned on" and that the presence of the fields cannot alter the velocity distribution of the active atoms to an extent where they, in turn, can modify the perturber velocity distribution. To allow for changes in the perturber velocity distribution, one would have to consider the density matrix for the total system of active atoms plus perturbers and obtain a Boltzmann equation for its time development. Reduced density matrices for either the active atoms or perturbers are then obtained by appropriate traces of the solutions to this equation.

[9] For example, in many laser problems, one considers a two-level problem with both levels representing excited states. This system is not closed and allowance is made for excitation to and decay from this subsystem.

[10] Note that this is a much stronger condition than that given in Appendix C of QMTE-I for the neglect of velocity-changing collisions. There are really two considerations here. Equation (10) is valid provided velocity-changing collisions have no significant effect on the output of the atomic system. However, the value of $T_{\alpha\beta}^{\alpha'\beta'}(\vec{v})$ to be derived will agree with semiclassical calculations only if the stronger condition $\theta < \theta_c$ is satisfied; in all other cases $T_{\alpha\beta}^{\alpha'\beta'}(\vec{v})$ should be computed from Eq. (5).

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[17] Attempts to include radiation trapping {M. I. D'Yakonov and V. I. Perel, Zh. Eksperim. i Teor. Fiz. 47, 1483 (1964) [Sov. Phys. JETP 20, 997 (1965)]}, photon recoil {A. P. Kol'chenko, S. G. Rautian, and R. I. Sokolovskii, *ibid.* 55, 1864 (1968) [*ibid.* 28, 986 (1961)]}, and resonant broadening {E. G. Pestov and S. G. Rautian, *ibid.* 56, 902 (1969) [*ibid.* 29, 458 (1969)]} effects in transport equations have already been made in various approximations.

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Inelastic *S*-Wave Positron-Hydrogen Scattering

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The variational methods of Kohn and Hulthén are used to calculate the scattering parameters of the positron-hydrogen rearrangement collision. The R-matrix elements are computed for positron energies 0–0.33 a.u. with accuracy of (1–10)%. It is also shown that a good approximation to the diagonal elements of the R matrix can be obtained by ignoring the coupling between the channels.

I. INTRODUCTION

The problem of low-energy scattering of positrons by hydrogen atoms has attracted many researchers by its simple structure and because of the hope that its solution might lead to the development of approximate methods for solving more complex scattering problems. The main difficulty encountered by the theoreticians considering this problem is the lack of experimental data by which the theoretical calculations could be checked. Various approximations were used for calculating the elastic S-wave phase shifts below the positronium formation threshold,[1-6] giving different results. There was, however, no criterion for preferring one result over another.

The "experimental data" for this problem were provided in 1961 by Schwartz,[7] who calculated these phase shifts accurately using Kohn's variational method and the Hylleraas-type wave function. A similar difficulty is encountered in the calculation of the S-wave parameters above the positronium formation threshold. Calculations were recently published by several authors,[8-13] with different results, and again no experimental data are available to which these calculations could be compared.

In the present work we have tried to extend Schwartz's calculation beyond the positronium formation threshold, in order to supply accurate values for the rearrangement collision parameters. The scattering parameters were calculated for positron energies from 0 to 0.33 a.u. to precision of a few percent. In Sec. II we describe the wave functions used and the method of calculation. The results are summarized in Table I, and are discussed in Sec. III.

II. METHOD OF CALCULATION

A. Wave Function

The wave function chosen was comprised of a Hylleraas-type core plus tail:

$$\psi = \psi_H + a\psi_{T_1} + b\psi_{T_2} + c\psi_{T_3} + d\psi_{T_4}\,, \tag{1}$$

$$\psi_H = \sum_{nlm} a_{nlm}\, r_1^n r_2^l r_{12}^m \exp(-b_1 r_1 - b_2 r_2 - b_3 r_{12})\,, \tag{2}$$

$$\psi_{T_1} = \pi^{-1/2} e^{-r_1} (\sin k r_2)/r_2\,, \tag{3}$$

$$\psi_{T_2} = \pi^{-1/2} e^{-r_1} (\cos k r_2 - e^{-\alpha r_2})/r_2\,, \tag{4}$$

$$\psi_{T_3} = (8\pi)^{-1/2} e^{-r_{12}/2} (\sin qR)/R\,, \tag{5}$$

$$\psi_{T_4} = (8\pi)^{-1/2} e^{-r_{12}/2} (\cos qR - e^{-\beta R})/R\,, \tag{6}$$

where $\vec{r}_1$ is the position vector of the electron and $\vec{r}_2$ is the position vector of the positron,

$$r_1 = |\vec{r}_1|,\quad r_2 = |\vec{r}_2|,\quad r_{12} = |\vec{r}_2 - \vec{r}_1|,\quad R = \tfrac{1}{2}|\vec{r}_1 + \vec{r}_2|\,,$$
$$k^2 = 2E_p,\quad q^2 = 4(E_p - 0.5)\,, \tag{7}$$

and E_p is the free positron energy in a.u. ψ_{T_1} and ψ_{T_2} describe the asymptotic form of ψ with error of the order $O(r_2^{-4})$. ψ_{T_3} and ψ_{T_4} describe the asymptotic form of ψ with error of the order $O(R^{-4})$.

In order to be able to calculate the matrix elements $(\psi|H - E|\psi)$ analytically, we had to choose another set of tail functions[7,14] T_1, T_2, T_3, T_4. This new set[15] was obtained from the previous one by the following transformation (using Hylleraas coordinates):

$$r_1 = \tfrac{1}{2}(s - t),\quad r_2 = \tfrac{1}{2}(s + t),\quad r_{12} = u\,, \tag{8}$$

$$\begin{aligned} r_2^{-1} &= 2/(s + t) = s^{-1}/[1 - (s - t)/2s] \\ &= 7/4s - t/s^2 + t^2/4s^3 + O(s^{-4})\,, \end{aligned} \tag{9}$$

$$\begin{aligned} R &= \tfrac{1}{2}s[1 - (u^2 - t^2)/s^2]^{1/2} \\ &\doteq \tfrac{1}{2}s - (u^2 - t^2)/4s - (u^2 - t^2)^2/16s^3 + O(s^{-5})\,, \end{aligned} \tag{10}$$

$$R^{-1} = 2/s + (u^2 - t^2)/s^3 + O(s^{-5})\,. \tag{11}$$

Therefore, we have

$$\begin{aligned} T_1 = \pi^{-1/2} e^{-(s-t)/2} &\sin\tfrac{1}{2}k(s + t) \\ &\times (7/4s - t/s^2 + t^2/4s^3)\,, \end{aligned} \tag{12}$$

$$\begin{aligned} T_2 = \pi^{-1/2} e^{-(s-t)/2} &[\cos\tfrac{1}{2}k(s + t) - e^{-\alpha(s+t)/2}] \\ &\times (7/4s - t/s^2 + t^2/4s^3)\,, \end{aligned} \tag{13}$$

$$\begin{aligned} T_3 = (8\pi)^{-1/2} e^{-(1/2)u} \\ \times \{[2/s + (u^2 - t^2)/s^3 + q^2(u^2 - t^2)^2/16s^3] \\ \times \sin(\tfrac{1}{2}qs) - [q(u^2 - t^2)/2s^2]\cos(\tfrac{1}{2}qs)\}, \end{aligned} \tag{14}$$

$$\begin{aligned} T_4 = (8\pi)^{-1/2} e^{-(1/2)u} \\ \times \{[2/s + (u^2 - t^2)/s^3][\cos(\tfrac{1}{2}qs) - e^{-\beta s/2}] \end{aligned}$$

TABLE I. R-matrix elements for the e^+-H inelastic scattering above positronium threshold.

E_p (a.u.)	k	q	Coupled channels[a] R_{11}	R_{12}	R_{22}	Uncoupled R_{11}	Dirks and Hahn[b] R_{11}	R_{12}	R_{22}
0.26	0.721	0.200	−0.066	−0.022	−0.01	−0.064			
0.27	0.735	0.283	−0.074	−0.024	−0.28	−0.070	−0.124	−0.0016	
0.28	0.748	0.346	−0.079	−0.027	−0.53	−0.079	−0.132	−0.0025	
0.29	0.762	0.400	−0.085	−0.032	−0.75	−0.085	−0.139	−0.0044	
0.30	0.775	0.447	−0.090	−0.037	−1.00	−0.091	−0.146	−0.0063	−1.43
0.31	0.787	0.490	−0.100	−0.045	−1.30	−0.098	−0.153	−0.0075	
0.32	0.800	0.529	−0.105	−0.050	−1.50	−0.103	−0.159	−0.0087	−2.448
0.33	0.812	0.566	−0.110	−0.060	−1.90	−0.108	−0.165		

[a] Estimated error within 10%.

[b] Interpolated values from Ref. 11.

TABLE II. Elastic and inelastic cross sections for S-wave positron-hydrogen and positronium-proton scattering. (Subscript 1 denotes the positron-hydrogen channel and subscript 2 denotes the positronium-proton channel.)

E_p	k	q	σ_{11}	σ_{21}	σ_{12}	σ_{22}
0.26	0.721	0.200	0.10	0.011	0.15	0.025
0.27	0.735	0.283	0.13	0.012	0.08	12
0.28	0.748	0.346	0.14	0.013	0.06	23
0.29	0.762	0.400	0.15	0.014	0.05	28
0.30	0.775	0.447	0.17	0.014	0.04	31
0.31	0.787	0.490	0.20	0.015	0.04	33
0.32	0.800	0.529	0.21	0.015	0.03	31
0.33	0.812	0.566	0.22	0.015	0.03	31

$$-[(u^2-t^2)^2/16s^3][q^2\cos(\tfrac{1}{2}qs)+\beta^2e^{-\beta s/2}]$$

$$+[(u^2-t^2)/2s^2][q\sin(\tfrac{1}{2}qs)-\beta e^{-\beta s/2}]\}\,; \qquad (15)$$

we also have

$$\psi_H^{(N)}=\sum_{n+l+m\leq N}h_{nlm}s^nt^lu^me^{-\lambda s-\mu t-\nu u}\,. \qquad (16)$$

These four functions represent the four tail functions with about the same formal accuracy as ψ_{T_1}, ψ_{T_2}, ψ_{T_3}, and ψ_{T_4}, respectively. The effect of the transformation on the results was tested by replacing ψ_{T_1} and ψ_{T_2} by T_1 and T_2 in the calculation of the elastic phase shifts below the positronium threshold. The convergence with T_1 and T_2 is slower than with ψ_{T_1} and ψ_{T_2}, but we still get two significant digits with sixth-order Hylleraas functions.

Using these functions we define the channel wave functions in the usual way:

$$\psi_1=\psi_H+k^{-1/2}(T_1+R_{11}T_2)+(\tfrac{1}{2}q)^{-1/2}R_{21}T_4$$

$$\text{(positron hydrogen)}, \qquad (17)$$

$$\psi_2=\psi_H+(\tfrac{1}{2}q)^{-1/2}(T_3+R_{22}T_4)+k^{-1/2}R_{12}T_4$$

$$\text{(positronium proton)}, \qquad (18)$$

where R_{ij} are the elements of the R matrix.

B. Variational Calculation

After choosing the wave functions, we tried to calculate the R matrix by Kohn's variational method. Following the idea of Schwartz,[7] we plotted the R-matrix elements as a function of the nonlinear parameter λ in ψ_H looking for "flat" parts of the graph. As was to be expected, we found too many pseudoresonances, and so had to smooth the graph using Nesbet's idea of combining several variational methods together.[16] The variational methods employed were those of Kohn, Hulthén and inverse Kohn.

The Kohn and inverse-Kohn variational procedures for inelastic collisions were discussed in detail in Ref. 16. Here we show briefly how we used the three variational methods for our rearrangement collision, where the incoming particle has mass m_1 and the outgoing particle has mass m_2.

Following Refs. 16 and 17 let us define Z_k:

$$Z_k=T_k+\sum_{n+l+m\leq N}a^k_{nlm}s^nt^lu^me^{-\lambda s-\mu t-\nu u}\,,$$

$$k=1,\cdots,4 \qquad (19)$$

so that

$$(s^nt^lu^me^{-\lambda s-\mu t-\nu u}|H-E|Z_k)=0$$

$$(\text{for all } n+l+m\leq N). \qquad (20)$$

Let us now define $S_1=Z_1$, $C_1=Z_2$, $S_2=Z_3$, $C_2=Z_4$. Then the Kohn wave functions are

$$\psi_1^K=(k/m_1)^{-1/2}(S_1+R_{11}C_1)+(q/m_2)^{-1/2}R_{21}C_2\,, \qquad (21)$$

$$\psi_2^K=(q/m_2)^{-1/2}(S_2+R_{22}C_2)+(k/m_1)^{-1/2}R_{12}C_1\,. \qquad (22)$$

The "inverse-Kohn" wave functions are

$$\psi_1^I=(k/m_1)^{1/2}(C_1+U_{11}S_1)+(q/m_2)^{-1/2}U_{21}S_2\,, \qquad (23)$$

$$\psi_2^I=(q/m_2)^{-1/2}(C_2+U_{22}S_2)+(k/m_1)^{-1/2}U_{12}S_1\,. \qquad (24)$$

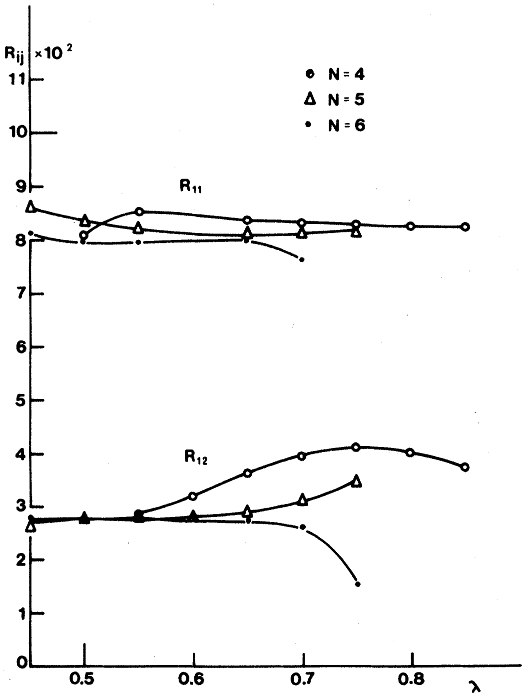

FIG. 1. Smoothed R_{11} and R_{12} as functions of the nonlinear parameter λ. $E_p=0.28$ a.u.

TABLE III. Phase shifts for elastic S-wave e^+-H scattering (a.u.).

k	Schwartz[a]	Bhatia *et al.*[b]	Houston and Drachman[c]	Present work
0.1	0.151	0.1483	0.149	0.148
0.2	0.188	0.1877	0.189	0.187
0.3	0.168	0.1677	0.169	0.167
0.4	0.120	0.1201	0.123	0.120
0.5	0.062	0.0624	0.065	0.062
0.6	0.007	0.0039	0.008	0.0033
0.7	−0.054	−0.0512	−0.049	−0.0515

[a] Reference 7. [b] Reference 18. [c] Reference 19.

In the Kohn variational calculation we solved the four linear equations

$$(C_i|H-E|\psi_j^K)=0\,, \quad i,j=1,2 \tag{25}$$

for the values R_{ij}^0, and then

$$R_{ij}=R_{ij}^0-2\,(\psi_i^K|H-E|\psi_j^K)\,, \quad i,j=1,2\,. \tag{26}$$

In the inverse-Kohn variational calculation we solved the equations

$$(S_i|H-E|\psi_j^I)=0\,, \quad i,j=1,2 \tag{27}$$

for the values U_{ij}^0, and then

$$(R^{-1})_{ij}=U_{ij}=U_{ij}^0+2(\psi_i^I|H-E|\psi_j^I), \quad i,j=1,2\,. \tag{28}$$

In the Hulthén variational calculation we solved the four nonlinear equations

$$(\psi_i^K|H-E|\psi_j^K)=0, \quad i,j=1,2 \tag{29}$$

for the R_{ij}, by using the Newton-Raphson method, starting from the values obtained from the Kohn variational calculation.

In all cases we solved the four equations using the symmetry of the R matrix as a check for the results.

Except near the singular points of the Kohn and inverse-Kohn methods, all three methods yield practically the same results. Around the singular points of one of the methods, the results from the two other methods did not differ significantly. Thus, by choosing the nonsingular values, we obtained smooth graphs for the R-matrix elements as functions of the nonlinear parameter λ. An example of such a smoothed curve is given in Fig. 1.

For each value of E_p the R-matrix elements were calculated using Hylleraas functions with $N=4$ (35×35 matrix), $N=5$ (56×56), and $N=6$ (84×84). As can be seen from Fig. 1, actual convergence begins only for $N=5$, making error estimation a difficult task.

The computed R-matrix elements are given in Table I. The partial cross sections for elastic and inelastic scattering are shown in Table II.

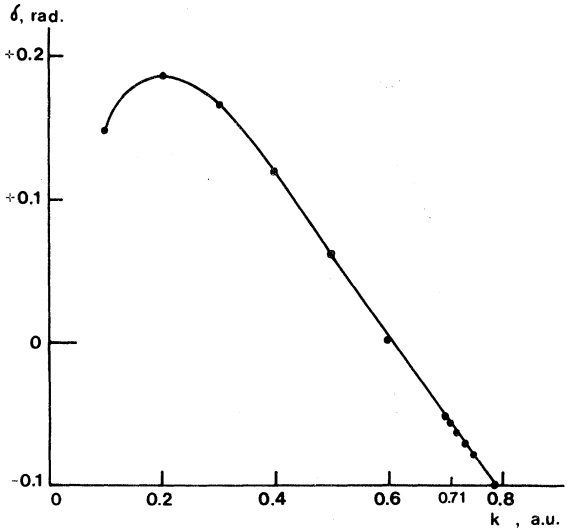

FIG. 2. Elastic S-wave positron-hydrogen phase shift as a function of k. The curve is almost continuous at the positronium threshold ($k=0.71$). (Above the threshold $\delta=\tan^{-1}R_{11}$.)

C. Calculation with Decoupled Channels

The main difficulty in this calculation was the "mixing" of two types of coordinates: in the positron channel, the natural coordinates are r_1 and r_2, while in the positronium channel they are r_{12} and R. Knowing, from the present and previous calculations, that the coupling between the channels is weak, we repeated our calculation for the elastic phase shift ignoring the coupling between the channels. The results, shown in Table I, differ from the full calculation by less than 6%.

III. DISCUSSION

Below the positronium threshold the values of the R-matrix elements are within 1% of the correct ones. The phase shifts are compared with those of Schwartz,[7] Bhatia *et al.*,[18] and Houston and Drachman[19] in Table III. It is estimated that above the threshold the values are within 10% of the correct ones. In Fig. 2 we plotted the elastic phase shift as a function of k. Because of the weakness of the coupling between the channels the curve is almost continuous through the threshold. Dirks and Hahn[11] calculated lower bounds to the values of R_{11} and R_{22}. The values as computed here are indeed higher (Table I).

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Electron-Impact Excitation and Ionization of Atomic Oxygen*

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We utilize the analytic atomic independent-particle model (IPM) of Green, Sellin, and Zachor to calculate generalized oscillator strengths (GOS) and total cross sections for excitation and ionization of atomic oxygen. First we average over the experimental energy levels within a multiplet to arrive at single-particle levels. Then we adjust the two parameters of the IPM potential so that it accurately characterizes the ground state and 15 lowest excited states. Using the wave functions so obtained, and assuming the Born approximation and the *LS*-coupling scheme, we calculate absolute GOS and cross sections for excitation to these levels, and for ionization with incident energies up to 1000 eV and secondary electron energy up to 200 eV. We obtain an analytic representation of the excitation GOS as a function of the momentum transfer. We also obtain an analytic representation of the energy differential cross section for ionization as a function of the energies of the incident and secondary electrons. Comparison is made with available experimental data and other calculations.

I. INTRODUCTION

Because of the importance of atomic oxygen in the upper atmosphere (it is the predominant species above 150 km), it is essential for an understanding of aeronomical phenomena to have a reliable characterization of its properties. Of particular interest to the understanding of auroral, dayglow, and ionospheric phenomena are electron-impact cross sections. Unfortunately, because of difficulties in working with atomic oxygen, there is little experimental information available on important cross sections.

From a theoretical point of view, atomic oxygen plus the electron constitutes a nine-electron system. Techniques for treating such systems rigorously have not yet been reduced to practice. For this reason, the present theoretical calculation exploits a realistic independent-particle-model (IPM) description for arriving at approximate electron-impact cross sections in the Born–Bethe approximation.

In comparison to Hartree–Fock–Slater calculations and to experiment, a simple two-parameter IPM potential has been found to provide a good representation of atoms[1] and electron-atom interactions.[2-5] We apply the IPM to the excitation and ionization of oxygen.

II. EXPERIMENTAL LEVELS AND IPM POTENTIAL

The ground state of oxygen has the configuration

$$1s^2 2s^2 2p^4 (^3P_2) \ . \tag{1}$$

From the tables of Moore,[6] it can be seen that of the 44 excited states below the ionization limit which are listed, 40 of them are in the configuration