

Multistate Impact-Parameter Calculation of Atom-Atom Excitation Cross Sections: Excitation of H(1s) by He(1¹S)

Hiram Levy II

Smithsonian Astrophysical Observatory, Cambridge, Massachusetts 02138

(Received 24 June 1969)

A general method of calculating the time-dependent matrix elements needed for multistate impact-parameter calculations of atom-atom inelastic cross sections is presented and applied to the collision processes $H(1s) + He(1^1S) \rightarrow H(2s, 2p_m) + He(1^1S)$. Cross sections calculated in the distorted Born, two-state, and four-state impact-parameter approximations over the incident energy range $1.0 \text{ keV} \leq E \leq 200.0 \text{ keV}$ are compared with previous experimental results and first Born-wave calculations. The first Born-wave calculations are in better agreement with the experimental measurements than are the distorted Born, two-state, and four-state impact-parameter calculations, but the fact that the corrections to the first Born become significant for $v \leq 1.0 \text{ a.u.}$ suggests that the good agreement may be accidental. Polarization fractions are calculated, and good agreement is shown with experiment for $v \leq 0.8 \text{ a.u.}$

I. INTRODUCTION

Inelastic atom-atom collision cross sections are of great importance to the study of excitation and ionization in meteor trails, auroras, and other atmospheric phenomena. They have usually been calculated by the first Born-wave approximation, and Levy^{1,2} has presented a general first Born-wave treatment involving the use of elastic and inelastic x-ray form factors, which is easily applied to a wide range of atoms.

However, the first Born-wave approximation becomes inaccurate at intermediate incident velocities owing to the effects of distortion, coupling to other states, and electron exchanges between the target and projectile. Improved calculations can be performed by the use of the multistate impact-parameter approximation in which the scattering solution is represented by a product of atomic wave functions without electron exchange, and the heavy-particle relative motion is described classically.

The impact-parameter approach requires the calculation of time-dependent matrix elements involving integrals over the electronic wave functions of the projectile and target. Flannery and Levy³ have developed a general analytic method for evaluating these matrix elements, which they have employed in H-H excitation cross-section calculations.⁴⁻⁶ Extension of these techniques to more complicated atoms is possible when analytic wave functions are available, but it becomes exceedingly laborious. A method of evaluating these time-dependent matrix elements by the use of generalized oscillator strengths, elastic x-ray form factors, other generalized Born matrix ele-

ments, and a simple numerical integration is proposed. The method can be applied to any atom for which analytical or numerical wave functions are available.

II. THEORY

We assume that the projectile atom travels with a constant velocity v in a straight line at a distance ρ , the impact parameter, from the Z axis, the axis of quantization for both atoms, of a fixed cylindrical coordinate system with the target atom at the origin. The analysis that follows is independent of the time-dependent behavior of the internuclear separation $R(t)$, so a straight-line trajectory, which is accurate in atom-atom collisions down to very low velocities,⁷ is assumed. The electronic part of the scattering solution is described by a time-dependent wave function,

$$\Psi(\vec{r}_A, \vec{r}_B, t) = \sum_m a_m(t) \psi_m(\vec{r}_A, \vec{r}_B) e^{iE_m t}, \quad (1)$$

where ψ_m is a product of the projectile wave function $\phi_i(\vec{r}_A)$ with Z_A electrons and energy ϵ_i^A and the target wave function $\phi_u(\vec{r}_B)$ with Z_B electrons and energy ϵ_u^B , and $E_m = \epsilon_i^A + \epsilon_u^B$.

The electrostatic interaction between the two atoms is given by

$$V[\vec{r}_A, \vec{r}_B, \vec{R}(t)] = \frac{Z_A Z_B}{R(t)} + \sum_{i=1}^{Z_A} \sum_{j=1}^{Z_B} (|\vec{R}(t) + \vec{r}_{Bj} - \vec{r}_{Ai}|)^{-1}$$

$$- \sum_{i=1}^{Z_A} \frac{Z_B}{|\vec{R}(t) - \vec{r}_{Ai}|} - \sum_{j=1}^{Z_B} \frac{Z_A}{|\vec{R}(t) + \vec{r}_{Bj}|} , \quad (2)$$

where $\vec{R}(t)$ is a vector from the center of atom A to the center of atom B , $\vec{r}_{Ai}$ is a vector from the center of A to its i th electron, and $\vec{r}_{Bj}$ is a vector from the center of B to its j th electron. If we adopt V as the time-dependent perturbation, we obtain the infinite set of coupled equations

$$i \dot{a}_n(t) = \sum_m a_m(t) V_{nm}[\vec{R}(t)] e^{iE_{nm}t} , \quad (3)$$

where $E_{nm} = E_n - E_m$,

$$\text{and} \quad V_{nm}[\vec{R}(t)] = \int d\vec{r}_A \int d\vec{r}_B \phi_i^{A*} \phi_u^{B*} \times V[\vec{r}_A, \vec{r}_B, \vec{R}(t)] \phi_j^A \phi_v^B \quad (4)$$

In practice, the summation in Eq. (3) is truncated, and the finite set of N coupled equations is solved for a particular trajectory to find the probability of transition from the initial state 1 to a final state n , $P_{1n}^N(\rho\phi) = |a_n(+\infty)|^2$. Integration of the transition probability over all possible trajectories for a particular v gives the cross section for the transition

$$Q^N(1, n) = \int_0^\infty \rho d\rho \int_0^{2\pi} d\phi P_{1n}^N(\rho, \phi) . \quad (5)$$

The solution of the truncated subset of Eq. (3) and the evaluation of the resulting cross sections are straightforward.⁸ The difficulty for collisions involving many-electron atoms lies in the accurate evaluation of the interaction matrix elements [Eq. (4)].

Applying the Fourier-transform method³ to Eq. (4), we find

$$V_{nm}[\vec{R}(t)] = \frac{Z_A Z_B}{2\pi^2} \int \frac{e^{i\vec{q} \cdot \vec{R}(t)}}{q^2} [\delta_{ij} \delta_{uv} + I_{ij}^-(\vec{q}) I_{uv}^+(\vec{q}) - I_{ij}^-(\vec{q}) \delta_{uv} - I_{uv}^+(\vec{q}) \delta_{ij}] d\vec{q} , \quad (6)$$

where the generalized Born matrix element is

$$I_{nm}^+(\vec{q}) = \left(\sum_{i=1}^Z \int \phi_n^* \phi_m e^{\pm i\vec{q} \cdot \vec{r}_i} d\vec{r} \right) / Z . \quad (7)$$

If desirable, Z_A and Z_B in Eq. (6) can be replaced by the velocity-dependent scaling factors $\eta_A(v)$ and

$\eta_B(v)$.¹

If $n = m = 0$ represent the ground state of the atom, $I_{0,0}^\pm(q)$ is just the elastic x-ray form factor $F(q)$, which has been accurately tabulated for many atoms. If n and m represent singly excited-state wave functions obtained with the frozen-core approximation,

$$I_{nm}^\pm(\vec{q}) = \sum_L D(l_n l_m L, m_n m_m M) Y_{LM}(\hat{q}) T_{nm}^\pm(L|q) , \quad (8)$$

where the angular D coefficients are products of Clebsch-Gordan coefficients.³ If n is the ground s state, then $T_{0m}^\pm(L|q)$ is directly related to $f(0 - m|q)$,⁹ the generalized oscillator strength, which has been either calculated theoretically or determined experimentally for a number of atoms.

The angular integration in Eq. (6) is then performed analytically, leaving a single numerical integration over q .

There are many collision problems for which the generalized Born matrix elements or, more specifically, the scalar quantities $T_{nm}^\pm(L|q)$ are not available, but their tabulation requires no technique not already used in the calculation of x-ray form factors or generalized oscillator strengths.

Since the distorted Born and two-state impact-parameter formulations have been discussed by Levy,⁶ they will not be presented here.

The five-state approximation involving a_n ($n = 1 - 5$) for, respectively, $1s1^1S$, $2p_01^1S$, $2p_{+1}1^1S$, $2p_{-1}1^1S$, and $2s1^1S$ states of the scattering system has been discussed by Flannery⁵ for H-H single-excitation collisions, and the form of the coupled equations is independent of the target atom. By use of appropriate phase factors for a_3 and a_4 , it is possible to reduce the five coupled equations to four. It should be noted that the $a_4(+\infty)$ of Eq. (9) of Flannery⁵ leads to the cross section

$$Q^4(1, 4) = Q^4(1s, 2p_+) + Q^4(1s, 2p_-) . \quad (9)$$

The necessary matrix elements are listed below:

$$V_{1s2s}[\vec{R}(t)] = Z_{\text{He}} V_{1s2s}^0(R) ,$$

$$V_{1s2p_0}[\vec{R}(t)] = Z_{\text{He}} Y_{10}(\hat{R}) V_{1s2p}^1(R) ,$$

$$V_{1s2p_{-}}[\vec{R}(t)] = Z_{\text{He}} Y_{1-1}(\hat{R}) V_{1s2p}^1(R) ,$$

$$V_{2p_02s}[\vec{R}(t)] = Z_{\text{He}} \left(\frac{4}{3}\pi\right)^{1/2} Y_{10}(\hat{R}) V_{2p2s}^1(R) ,$$

$$\begin{aligned}
V_{2p-2s}[\vec{R}(t)] &= Z_{\text{He}} \left(\frac{4}{3}\pi\right)^{1/2} Y_{1-1}(\hat{\vec{R}}) V_{2p2s}^1(\vec{R}), & V_{2p_0 2p_0}[\vec{R}(t)] - V_{1s1s}[\vec{R}(t)] \\
V_{2p_0 2p_-}[\vec{R}(t)] &= Z_{\text{He}} \left(\frac{8}{15}\pi\right)^{1/2} Y_{2-1}(\hat{\vec{R}}) V_{2p2p}^2(R), & = Z_{\text{He}} [\mathfrak{U}_{2p2p}^0(R) + Y_{20}(\hat{\vec{R}}) \mathfrak{U}_{2p2p}^2(R)], \\
V_{2p_+ 2p_-}[\vec{R}(t)] &= -Z_{\text{He}} \left(\frac{16}{15}\pi\right)^{1/2} Y_{2-2}(\hat{\vec{R}}) V_{2p2p}^2(R), & V_{2p_- 2p_-}[\vec{R}(t)] - V_{1s1s}[\vec{R}(t)] \\
V_{2s2s}[\vec{R}(t)] - V_{1s1s}[\vec{R}(t)] &= Z_{\text{He}} \mathfrak{U}_{2s2s}^0(R), & = Z_{\text{He}} [\mathfrak{U}_{2p2p}^0(R) - \frac{1}{2} Y_{20}(\hat{\vec{R}}) \mathfrak{U}_{2p2p}^2(R)]. \quad (10)
\end{aligned}$$

TABLE I. Interaction matrix elements for $\text{H}(1s) + \text{He}(1^1S) \rightarrow \text{H}(2s, 2p_0, 2p_{\pm}) + \text{He}(1^1S)$. The exponent on the numerical value gives the power of ten by which the entry must be multiplied.

R (a_0)	V_{1s2s}^0	V_{1s2p}^1	V_{2p2s}^1	V_{2p2p}^2	$\mathfrak{U}_{2s2s}^0$	$\mathfrak{U}_{2p2p}^0$	$\mathfrak{U}_{2p2p}^2$
0.0	-7.842 ⁻²	0.0	0.0	0.0	2.081 ⁻¹	2.324 ⁻¹	0.0
0.1	...	-7.934 ⁻³	-1.203 ⁻³	-5.898 ⁻⁵	2.045 ⁻¹	2.283 ⁻¹	-8.816 ⁻⁵
0.2	-7.291 ⁻²	-1.535 ⁻²	-2.310 ⁻³	-2.315 ⁻⁴	1.949 ⁻¹	2.173 ⁻¹	-3.460 ⁻⁴
0.4	-6.105 ⁻²	-2.746 ⁻²	-4.022 ⁻³	-8.666 ⁻⁴	1.667 ⁻¹	1.846 ⁻¹	-1.295 ⁻³
0.6	-4.782 ⁻²	-3.533 ⁻²	-4.945 ⁻³	-1.776 ⁻³	1.353 ⁻¹	1.480 ⁻¹	-2.655 ⁻³
0.8	-3.562 ⁻²	-3.928 ⁻²	-5.135 ⁻³	-2.819 ⁻³	1.061 ⁻¹	1.412 ⁻¹	-4.214 ⁻³
1.0	-2.540 ⁻²	-4.010 ⁻²	-4.478 ⁻³	-3.877 ⁻³	8.119 ⁻²	8.547 ⁻²	-5.794 ⁻³
1.2	-1.734 ⁻²	-3.868 ⁻²	-3.964 ⁻³	-4.856 ⁻³	6.104 ⁻²	6.237 ⁻²	-7.259 ⁻³
1.4	-1.127 ⁻²	-3.585 ⁻²	-2.954 ⁻³	-5.700 ⁻³	4.524 ⁻²	4.447 ⁻²	-8.519 ⁻³
1.6	-6.866 ⁻³	-3.223 ⁻²	-1.852 ⁻³	-6.374 ⁻³	3.310 ⁻²	3.094 ⁻²	-9.527 ⁻³
1.8	-3.784 ⁻³	-2.830 ⁻²	-7.614 ⁻⁴	-6.866 ⁻³	2.391 ⁻²	2.095 ⁻²	-1.026 ⁻²
2.0	-1.707 ⁻³	-2.438 ⁻²	2.485 ⁻⁴	-7.179 ⁻³	1.702 ⁻²	1.368 ⁻²	-1.073 ⁻²
2.2	-3.663 ⁻³	-2.069 ⁻²	1.135 ⁻³	-7.329 ⁻³	1.190 ⁻²	8.488 ⁻³	-1.095 ⁻²
2.4	4.503 ⁻⁴	-1.733 ⁻²	1.878 ⁻³	-7.333 ⁻³	8.101 ⁻³	4.835 ⁻³	-1.096 ⁻²
2.6	9.052 ⁻⁴	-1.437 ⁻²	2.469 ⁻³	-7.216 ⁻³	5.303 ⁻³	2.312 ⁻³	-1.079 ⁻²
2.8	1.118 ⁻³	-1.180 ⁻²	2.915 ⁻³	-7.000 ⁻³	3.250 ⁻³	6.063 ⁻⁴	-1.046 ⁻²
3.0	1.175 ⁻³	-9.617 ⁻³	3.228 ⁻³	-6.707 ⁻³	1.754 ⁻³	-5.141 ⁻⁴	-1.002 ⁻²
3.2	1.138 ⁻³	-7.777 ⁻³	3.421 ⁻³	-6.358 ⁻³	6.726 ⁻⁴	-1.220 ⁻³	-9.503 ⁻³
3.4	1.049 ⁻³	-6.257 ⁻³	3.514 ⁻³	-5.970 ⁻³	-9.839 ⁻⁵	-1.635 ⁻³	-8.924 ⁻³
3.6	9.339 ⁻⁴	-5.006 ⁻³	3.522 ⁻³	-5.560 ⁻³	-6.464 ⁻⁴	-1.850 ⁻³	-8.311 ⁻³
3.8	8.111 ⁻⁴	-3.985 ⁻³	3.463 ⁻³	-5.140 ⁻³	-1.004 ⁻³	-1.928 ⁻³	-7.683 ⁻³
4.0	6.916 ⁻⁴	-3.159 ⁻³	3.352 ⁻³	-4.720 ⁻³	-1.241 ⁻³	-1.916 ⁻³	-7.055 ⁻³
4.4	4.820 ⁻⁴	-1.961 ⁻³	3.025 ⁻³	-3.911 ⁻³	-1.447 ⁻³	-1.738 ⁻³	-5.845 ⁻³
4.8	3.227 ⁻⁴	-1.202 ⁻³	2.626 ⁻³	-3.178 ⁻³	-1.437 ⁻³	-1.477 ⁻³	-4.750 ⁻³
5.2	2.095 ⁻⁴	-7.270 ⁻⁴	2.212 ⁻³	-2.540 ⁻³	-1.317 ⁻³	-1.207 ⁻³	-3.797 ⁻³
5.6	1.329 ⁻⁴	-4.350 ⁻⁴	1.821 ⁻³	-2.001 ⁻³	-1.149 ⁻³	-9.601 ⁻⁴	-2.991 ⁻³
6.0	8.235 ⁻⁵	-2.580 ⁻⁴	1.470 ⁻³	-1.558 ⁻³	-9.676 ⁻⁴	-7.494 ⁻⁴	-2.329 ⁻³
6.4	4.994 ⁻⁵	-1.521 ⁻⁴	1.168 ⁻³	-1.200 ⁻³	-7.946 ⁻⁴	-5.764 ⁻⁴	-1.794 ⁻³
6.8	2.973 ⁻⁵	-8.991 ⁻⁵	9.159 ⁻⁴	-9.169 ⁻⁴	-6.398 ⁻⁴	-4.385 ⁻⁴	-1.370 ⁻³
7.2	1.764 ⁻⁵	-5.341 ⁻⁵	7.098 ⁻⁴	-6.949 ⁻⁴	-5.079 ⁻⁴	-3.315 ⁻⁴	-1.038 ⁻³
7.6	1.077 ⁻⁵	-3.192 ⁻⁵	5.450 ⁻⁴	-5.225 ⁻⁴	-3.987 ⁻⁴	-2.499 ⁻⁴	-7.810 ⁻⁴
8.0	7.038 ⁻⁶	-1.880 ⁻⁵	4.149 ⁻⁴	-3.907 ⁻⁴	-3.101 ⁻⁴	-1.881 ⁻⁴	-5.840 ⁻⁴
8.4	4.866 ⁻⁶	-1.040 ⁻⁵	3.137 ⁻⁴	-2.904 ⁻⁴	-2.388 ⁻⁴	-1.409 ⁻⁴	-4.340 ⁻⁴
8.8	3.269 ⁻⁶	-5.000 ⁻⁶	2.360 ⁻⁴	-2.145 ⁻⁴	-1.816 ⁻⁴	-1.042 ⁻⁴	-3.207 ⁻⁴
9.2	1.876 ⁻⁶	...	1.766 ⁻⁴	-1.575 ⁻⁴	-1.358 ⁻⁴	-7.542 ⁻⁵	-2.354 ⁻⁴
9.6	...	...	1.317 ⁻⁴	-1.150 ⁻⁴	-9.994 ⁻⁵	-5.325 ⁻⁵	-1.718 ⁻⁴
10.0	...	...	9.782 ⁻⁵	-8.345 ⁻⁵	-7.249 ⁻⁵	-3.681 ⁻⁵	-1.247 ⁻⁴
10.4	...	...	7.251 ⁻⁵	-6.030 ⁻⁵	-5.222 ⁻⁵	-2.528 ⁻⁵	-9.013 ⁻⁵
10.8	...	...	5.381 ⁻⁵	-4.350 ⁻⁵	-3.770 ⁻⁵	-1.763 ⁻⁵	-6.502 ⁻⁵
11.2	...	...	4.006 ⁻⁵	-3.136 ⁻⁵	-2.736 ⁻⁵	-1.262 ⁻⁵	-4.687 ⁻⁵
11.6	...	...	3.005 ⁻⁵	-2.261 ⁻⁵	-1.985 ⁻⁵	-9.146 ⁻⁶	-3.380 ⁻⁵
12.0	...	...	2.280 ⁻⁵	-1.633 ⁻⁵	-1.425 ⁻⁵	-6.526 ⁻⁶	-2.440 ⁻⁵

TABLE II. Cross sections for $H(1s) + He(1^1S) \rightarrow H(2s) + He(1^1S)$. The exponent on the numerical values give the power of ten by which the entry must be multiplied.

v (a. u.)	$Q^4(2s)$ (a_0^2)	$Q^2(2s)$ (a_0^2)	$\sigma_{DB}(2s)$ (a_0^2)	$\sigma_B(2s)$ (a_0^2)
2.0	2.36^{-2}	2.34^{-2}	2.35^{-2}	2.36^{-2}
1.4	4.76^{-2}	4.68^{-2}	4.71^{-2}	4.85^{-2}
1.0	9.05^{-2}	8.79^{-2}	8.88^{-2}	9.49^{-2}
0.8	1.35^{-1}	1.29^{-1}	1.31^{-1}	1.47^{-1}
0.6	2.09^{-1}	1.95^{-1}	2.01^{-1}	2.52^{-1}
0.5	2.50^{-1}	2.30^{-1}	2.40^{-1}	3.43^{-1}
0.4	2.59^{-1}	2.33^{-1}	2.48^{-1}	4.60^{-1}
0.3	1.56^{-1}	1.37^{-1}	1.53^{-1}	5.38^{-1}
0.2	1.27^{-2}	1.07^{-2}	1.18^{-2}	3.42^{-1}

We note that the initial-state diagonal matrix element $V_{1s,1s}(\vec{R})$ has been subtracted from all four diagonal elements in Eq. (9) of Flannery⁵ to simplify their evaluation.

The scalar quantities $V_{ij}^L(R)$ and $U_{ij}^L(R)$ listed in Table I were calculated by using the He elastic x-ray form factors of Kim and Inokuti,¹⁰ the generalized Born matrix elements for H calculated analytically with Eq. (13) of Levy and Flannery,³ and a Simpson's rule numerical integration over q .

The subscript reference to the ground state of the helium target atom is now omitted. Previous work¹ has shown that velocity-dependent scaling is not necessary for helium.

III. RESULTS AND DISCUSSION

Excitation cross sections for the collisions $H(1s) + He(1^1S) \rightarrow H(2s, 2p_0, 2p_{\pm}) + He(1^1S)$ have been calculated with an error $< 1.0\%$ in the distorted Born, two-state, and four-state impact-parameter approximations; and the effects of distortion, coupling to the initial state, coupling between $2s$ and $2p$, and coupling between magnetic substates have been examined.

The results for excitation of $H(1s)$ to $H(2s)$ are presented in Table II, and those for excitation of $H(1s)$ to $H(2p_m)$ in Table III.

Over-all, the corrections to the first Born-wave approximation affect the $2s$ cross sections more than they do those for the $2p$ because the $2p_0$ and $2p_{\pm}$ cross sections behave in an opposite manner, and their sum tends to cancel.

Back coupling and coupling between the $2s$ and $2p_m$ states have opposite effects on the $2s$ cross section and tend to cancel. Back coupling does not change the $2p$ cross section significantly for $v \geq 0.5$ a. u. The combined effect on the $2p$ cross section of coupling to the $2s$ state and coupling between magnetic substates is small at all velocities studied.

A general feature of these results is the major correction to the first Born-wave cross section that comes from the inclusion of distortion, and the minor changes that occur when all the other couplings are included. The results are quite similar to those of Flannery^{4,5} for two- and four-state impact-parameter calculations of H-H single-excitation collisions.

Total cross sections for excitation of $H(1s)$ to

TABLE III. Cross section for $H(1s) + He(1^1S) \rightarrow H(2p_0, 2p_{\pm}) + He(1^1S)$. The exponent on the numerical value gives the power of ten by which the entry must be multiplied.

v (a. u.)	$Q^4(2p_0)$ (a_0^2)	$Q^4(2p_{\pm})$ (a_0^2)	$Q^2(2p_0)$ (a_0^2)	$Q^2(2p_{\pm})$ (a_0^2)	$\sigma_{DB}(2p_0)$ (a_0^2)	$\sigma_{DB}(2p_{\pm})$ (a_0^2)	$\sigma_B(2p)$ (a_0^2)
2.0	5.05^{-3}	2.20^{-2}	4.91^{-3}	2.21^{-2}	4.91^{-3}	2.21^{-2}	4.82^{-2}
1.4	1.87^{-2}	4.08^{-2}	1.82^{-2}	4.09^{-2}	1.83^{-2}	4.10^{-2}	9.75^{-2}
1.0	5.81^{-2}	6.65^{-2}	5.67^{-2}	6.72^{-2}	5.68^{-2}	6.73^{-1}	1.85^{-1}
0.8	1.11^{-1}	8.45^{-2}	1.09^{-1}	8.59^{-2}	1.09^{-1}	8.61^{-2}	2.75^{-1}
0.6	2.09^{-1}	9.70^{-2}	2.06^{-1}	1.00^{-1}	2.08^{-1}	1.00^{-1}	4.22^{-1}
0.5	2.61^{-1}	9.10^{-2}	2.59^{-1}	9.53^{-2}	2.62^{-1}	9.59^{-2}	5.10^{-1}
0.4	2.57^{-1}	6.55^{-2}	2.58^{-1}	7.16^{-2}	2.62^{-1}	7.23^{-2}	5.61^{-1}
0.3	1.25^{-1}	2.38^{-2}	1.26^{-1}	2.87^{-2}	1.29^{-1}	2.93^{-2}	4.61^{-1}
0.2	8.89^{-3}	9.85^{-4}	8.27^{-3}	1.67^{-3}	8.52^{-3}	1.76^{-3}	1.55^{-1}

$H(2s)[\sigma^4(2s) = Q^4(2s) + \sigma_I(2s)]$, $H(2p)[\sigma^4(2p) = Q^4(2p) + \sigma_I(2p)]$ and both $[\sigma^4(2s) + \sigma^4(2p)]$ are compared in Figs. 1–3 with earlier first Born-wave results¹ and with the experimental data of Dose *et al.*¹¹ and Ankudinov *et al.*¹² The cross sections $\sigma_I(2s)$ and $\sigma_I(2p)$ are first Born-wave calculations¹ for all collisions that excite both the projectile and the target, and they use the closure approximation.

The four-state calculations do not agree so well as do the first Born-wave calculations with the two cross sections measured, $\sigma_{\text{expt}}(2p)$ and $\sigma_{\text{expt}}(2p) + \sigma_{\text{expt}}(2s)$. The four state does show better agreement with $\sigma_{\text{expt}}(2s)$. It is possible that neglect of electron exchange and cascade effects is responsible for the discrepancy between theory and experiment, but further experimental work would be of interest.

The polarization fractions for the $2p_m$ excitation, $P_N(2p)$, calculated using the formula of Percival and Seaton,¹³

$$P_N(2p) = 300 \frac{Q^N(2p_0) - Q^N(2p_{\pm})}{7Q^N(2p_0) + 11Q^N(2p_{\pm})}, \quad (11)$$

are presented in Table IV. Here again, back coupling has a very small effect, while the combination of coupling to the $2s$ state and coupling between magnetic substates causes significant changes at low energy.

The polarization fractions calculated in the four-state impact-parameter approximation show good agreement with the experimental results of Dose *et al.*¹⁴ for $v \leq 0.8$ a.u. For higher velocities, the calculated fractions become negative while the experimental results remain positive, probably owing to contributions from collisions that excite both the projectile and the target. This effect has already been observed theoretically by Levy⁶ for H-H collisions, and H-He collisions should display similar behavior.

ACKNOWLEDGMENTS

The author wishes to thank Professor A. Dalgarno for his advice and comments regarding

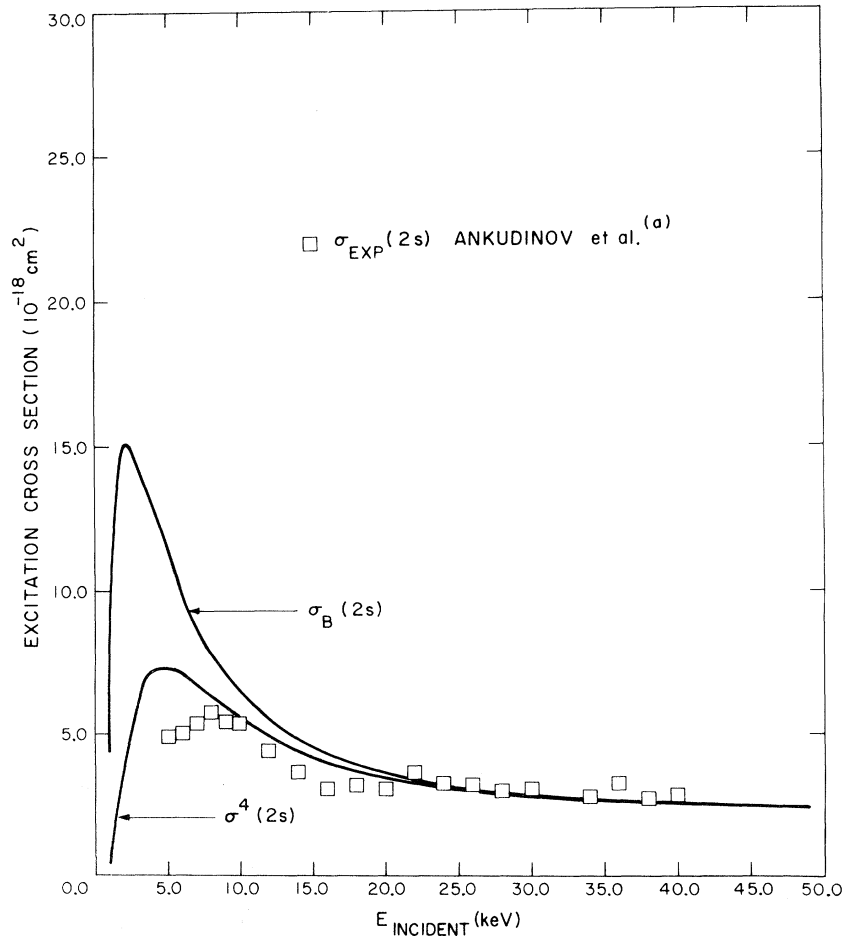


FIG. 1. Excitation cross sections for $H(1s) + He(1^1S) \rightarrow H(2s) + He(1^1S)$: (a) see Ref. 12.

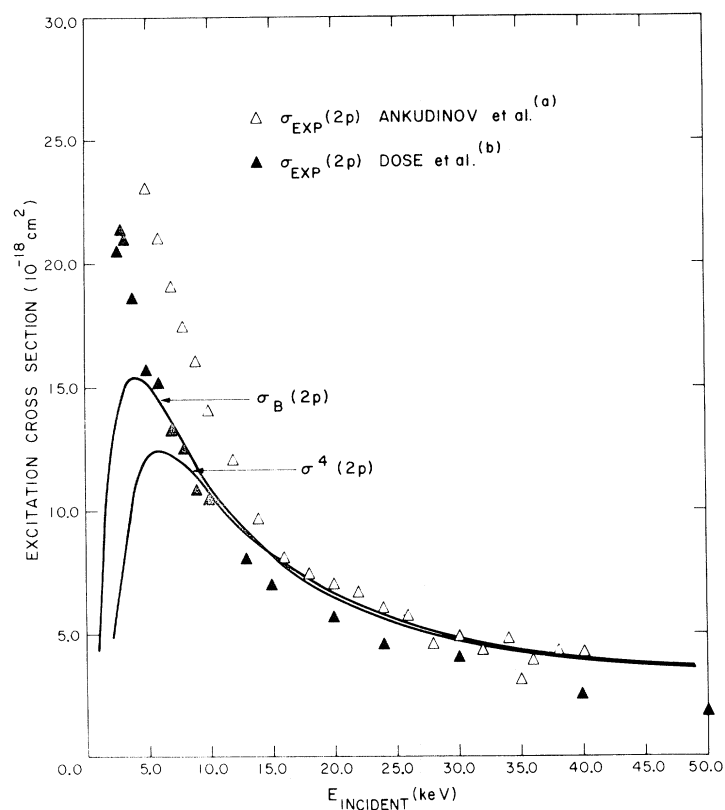


FIG. 2. Excitation cross sections for $\text{H}(1s) + \text{He}(1^1S) \rightarrow \text{H}(2p) + \text{He}(1^1S)$: (a) see Ref. 12, (b) see Ref. 11.

FIG. 3. Excitation cross sections for $\text{H}(1s)$ excited to $\text{H}(2s)$ or $\text{H}(2p)$ by $\text{He}(1^1S)$: (a) see Ref. 12.

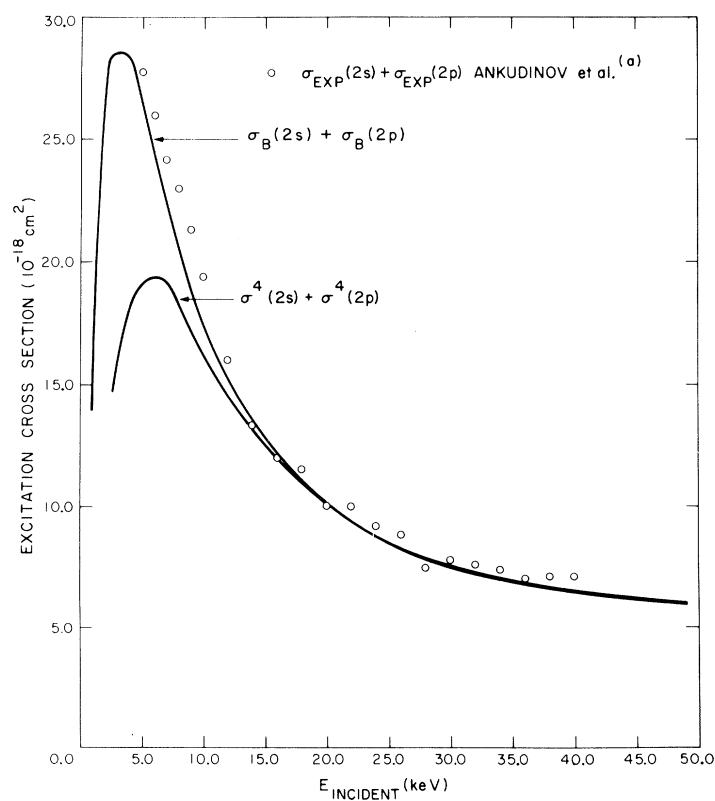


TABLE IV. Polarization fractions for $H(1s) + He(1^1S) \rightarrow H(2p_0, 2p_{\pm}) + He(1^1S)$.

v (a.u.)	$P_4(2p)$	$P_2(2p)$	$P_{DB}(2p)$
2.0	-18.3	-18.6	-18.6
1.4	-11.4	-11.7	-11.8
1.0	-2.2	-2.8	-2.8
0.8	+4.7	+4.1	+4.0
0.6	+13.3	+12.5	+12.7
0.5	+18.0	+17.2	+17.2
0.4	+22.8	+21.6	+21.6
0.3	+26.7	+24.4	+24.4
0.2	+32.5	+26.0	+25.7

this paper. The author also wishes to thank Dr. R. H. G. Reid for providing the computer programs used in these calculations and for many helpful discussions concerning their applications. This work was supported in part by NASA contract NSR 09-015-033.

¹H. Levy II, Phys. Rev. 185, 7 (1969).

²H. Levy II, preceding paper, Phys. Rev. 187, 130 (1969).

³M. R. Flannery and H. Levy II, J. Phys. B2, 314 (1969).

⁴M. R. Flannery, Phys. Rev. 183, 231 (1969).

⁵M. R. Flannery, Phys. Rev. 183, 241 (1969).

⁶H. Levy II, Phys. Rev. 184, 97 (1969).

⁷D. R. Bates and A. H. Boyd, Proc. Phys. Soc. (London) 79, 710 (1962).

⁸D. R. Bates, Quantum Theory, Elements I (Academic Press Inc., New York, 1961), pp. 297-521.

⁹N. F. Mott and H. S. W. Massey, The Theory of Atomic Collisions (Clarendon Press, Oxford, 1965), 3rd ed.,

p. 478.

¹⁰Y.-K. Kim and M. Inokuti, Phys. Rev. 165, 39 (1968).

¹¹V. Dose, R. Gunz, and V. Meyer, Helv. Phys. Acta 41, 269 (1968).

¹²V. A. Ankudinov, E. P. Andrew, and A. L. Orbeli, in Proceedings of the Fifth International Conference on the Physics of Electronic and Atomic Collisions, edited by I. P. Flaks (Publishing House "Nauka," Leningrad, USSR, 1967), p. 312.

¹³I. C. Percival and M. J. Seaton, Phil Trans. Roy. Soc. London, 251A, 113 (1958).

¹⁴V. Dose, R. Gunz, and V. Meyer, Helv. Phys. Acta 41, 264 (1968).