formed, the results are normalized such that the fraction of H_3 in high-n states is of the order of 10^{-3}. If the H_3^+ counting rate at electric field $\mathcal{E}_n$ was compared to the counting rate of H_3 as detected by the neutral-particle counter then the fraction $H_3(n \geq 11)/H_3(\text{total})$ was approximately 1. Obviously, most of the H_3^+ capture collisions were into repulsive states of H_3, such that the neutral particles did not arrive at the energy-sensitive detector.

The probability that a HD^+ could be contaminating the H_3^+ prevents one from concluding absolutely that excited states of H_3 exists. Both HD and H_3 exctied states would behave similarily in the electrostatic-stripping field. Several precautions were taken to minimize any contamination of the H_3^+ beam by HD^+. An ion source was used that had not been used previously with deuterium gas such that the only source of HD came from the natural abundance of D_2 in H_2. Also, the ion-source pressure was maintained at a high value to enhance the reaction $H_2^+ + H_2 \rightarrow H_3^+ + H$. Pulse-height analysis of the neutral beam by the silicon-barrier detector indicated only a small flux of particles (HD and H_3) with full acceleration energy. The pressure in the hydrogen collision cell was increased to several microns such that the pulse-height peak at E_0 disappeared first, and then at higher values the pulse-height peak at $\frac{2}{3} E_0$ disappeared indicating that all the diatomic and triatomic particles were dissociated in the gas cell. The same disappearance of particles was observed when the charged-particle detector was set to receive only particles at $\frac{2}{3} E_0$. If a measurable quantity of D or HD was contributing to the signal then the pulse height at $\frac{2}{3} E_0$ would not have disappeared with increased H_2 pressure. These precautions and the results obtained demonstrate with a high degree of confidence that the H_3^+ signal obtained as a function of $\mathcal{E}$ was not HD^+.

†Research sponsored by the U. S. Atomic Energy Commission under contract with the Union Carbide Corp.

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PHYSICAL REVIEW A VOLUME 5, NUMBER 5 MAY 1972

e-H Scattering by the Faddeev Approach

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(Received 22 June 1971)

1*s*-1*s* elastic and 1*s*-2*s* inelastic total cross sections for *e*-H collision have been calculated with and without exchange effects using the Faddeev formalism as developed by Sloan and Moore. We have considered the effect of coupling to 1*s* and 2*s* intermediate states. Our theoretical results have been compared with the existing experimental findings and other theoretical calculations. In the intermediate-energy region, our results for the inelastic process are found to be in close agreement with the experimental observations. Our results for both systems indicate that coupling to states other than the initial and final ones causes a reduction in the cross sections, and even up to 500 eV the effect of exchange is not negligible.

INTRODUCTION

In the theoretical study of electron-atom collision problems, the *e*-H scattering process has enjoyed the widest investigation for its simplicity. But it is still not possible to find any approximation that gives uniformly good results for all energies. The close-coupling (cc) method,[1,2] is based on an expansion of the wave function for the system into the infinite set of eigenstates of the target atom, though only a few eigenstates are considered in a practical calculation and as such the effects of higher bound and continuum states are neglected. Recently Burke *et al.*[3] have suggested a modification of the cc formalism in which the effect of the higher bound and the continuum states are included by a pseudostate expansion. Holt and Moiseiwitsch[4] have introduced a simplified second Born approximation where the coupling effects due to the higher states have been approximated by a

closure relation. In addition to these methods some other simple approaches such as Born, Vainshtein,[5] Ochkur[6,7] polarized orbital,[8] Glauber,[9,10] and many others have been developed and have given more satisfactory agreement with experimental findings over certain energy regions.

Since the pioneering work of Faddeev,[11] his formalism has been widely applied to the three-body collision problems by different workers such as Lovelace,[12] Ahmadzadeh and Tjon,[12] Alt *et al.*,[14] and many others. Chen and his collaborators[15,16] and Sloan and Moore[17] have applied Faddeev equations to electron-atom collision problems. The approximate form of the Faddeev equation due to Sloan and Moore takes account of the exchange effect and preserves unitarity but excludes the virtual excitation and strong distortion effects. This model is rather suitable in the high-energy region. It differs from the unitarized Born approximation[18] (UBA) by the fact that it includes explicitly the couplings between all possible physical states, whereas the UBA takes into account the coupling between the same state only. Moreover the UBA neglects the exchange effect. It has been shown by Sloan and Moore that there is a very close relation between their formulation and the cc approximation. However, in view of the high-energy consideration, this formalism yields a set of coupled algebraic equations which are less laborious to solve than the complicated coupled integrodifferential equations of the cc method. Sloan and Moore have applied this formalism to calculate the elastic scattering cross sections for e-H collision, neglecting the effect of couplings to excited states.

In this paper, using their method, we have calculated the total cross sections with and without exchange effect for the elastic $1s$-$1s$ and inelastic $1s$-$2s$ scattering of hydrogen atom by electron. We have considered the effect of couplings to $1s$ and $2s$ states only and neglected higher s-state couplings, since their contributions are negligible in comparison to the $2s$ states. In order to avoid enormous analytical complications, we have further neglected the effect of couplings due to higher l values for the equation.

THEORY

Following Sloan and Moore, we write the three-body scattering amplitude for the electron-hydrogen system as (notations are the same as used by Sloan and Moore)

$$\langle \vec{K}'n' | Y | \vec{K}n\rangle = \langle \vec{K}'n' | Y^{(1)\pm} | \vec{K}n\rangle + \sum_{n''=1}^{N} \int \frac{d\vec{K}'' \langle \vec{K}'n' | Y^{(1)\pm} | \vec{K}''n''\rangle \langle \vec{K}''n'' | Y^{\pm} | \vec{K}n\rangle}{S - E''} . \tag{1}$$

Y and $Y^{(1)}$ denote the three- and two-body operators where $\langle \vec{K}'n' | Y^{\pm} | \vec{K}n\rangle$ are the three-body singlet and triplet amplitudes and $\langle \vec{K}'n' | Y^{(1)\pm} | \vec{K}n\rangle$ are the two-body singlet and triplet amplitudes.

Now the pole term in (1) may be expressed as

$$\frac{1}{E + i\epsilon - E''} = -i\pi\delta(E - E'') + \frac{P}{E - E''} .$$

The pole term is then approximated[17] for the high energies by taking only the δ function and Eq. (1) becomes

$$\langle \vec{K}'n' | Y^{\pm} | \vec{K}n\rangle = \langle \vec{K}'n' | Y^{(1)\pm} | \vec{K}n\rangle - i\pi \sum_{n''=1}^{N} \int d\vec{K}'' \langle \vec{K}'n' | Y^{(1)\pm} | \vec{K}''n''\rangle \times \delta(E - E'') \langle \vec{K}''n'' | Y^{\pm} | \vec{K}n\rangle . \tag{2}$$

Moreover neglecting the multiple-scattering terms, the two-body operators have been expressed (Sloan and Moore) as

$$Y_{11}^{(1)} \simeq V_{13} + V_{12}, \qquad Y_{21}^{(1)} \simeq V_{23} + V_{12} .$$

We have retained the $1s$ and $2s$ states in the summation in (2) and obtained a pair of coupled equations for the $1s$-$1s$ and $1s$-$2s$ transitions

$$\begin{aligned}
\langle \vec{K}'1s | Y^{\pm} | \vec{K}1s\rangle &= \langle \vec{K}'1s | Y^{(1)\pm} | \vec{K}1s\rangle - i\pi \int d\vec{K}'' \langle \vec{K}'1s | Y^{(1)\pm} | \vec{K}''1s\rangle \, \delta(E - E'') \langle \vec{K}''1s | Y^{\pm} | \vec{K}1s\rangle \\
&\quad - i\pi \int d\vec{K}'' \langle \vec{K}'1s | Y^{(1)\pm} | \vec{K}''2s\rangle \, \delta(E - E'') \langle \vec{K}''2s | Y^{\pm} | \vec{K}1s\rangle , \\
\langle \vec{K}_1'2s | Y^{\pm} | \vec{K}1s\rangle &= \langle \vec{K}_1'2s | Y^{(1)\pm} | \vec{K}1s\rangle - i\pi \int d\vec{K}_1'' \langle \vec{K}_1'2s | Y^{(1)\pm} | \vec{K}_1''1s\rangle \delta(E - E_1'') \langle \vec{K}_1''1s | Y^{\pm} | \vec{K}1s\rangle \\
&\quad - i\pi \int d\vec{K}_1'' \langle \vec{K}_1'2s | Y^{(1)\pm} | \vec{K}_1''2s\rangle \delta(E - E_1'') \langle \vec{K}_1''2s | Y^{\pm} | \vec{K}1s\rangle .
\end{aligned} \tag{3}$$

A second pair of similar equations can be obtained for $2s$-$1s$ and $2s$-$2s$ transitions. Now the matrix elements of two-body operators have been expressed as

$$\langle \vec{K}'n' | Y^{(1)\pm} | \vec{K}n\rangle = -(1/4\pi) f_{n'n}^{B\pm}(\vec{K}' \cdot \vec{K}) ,$$

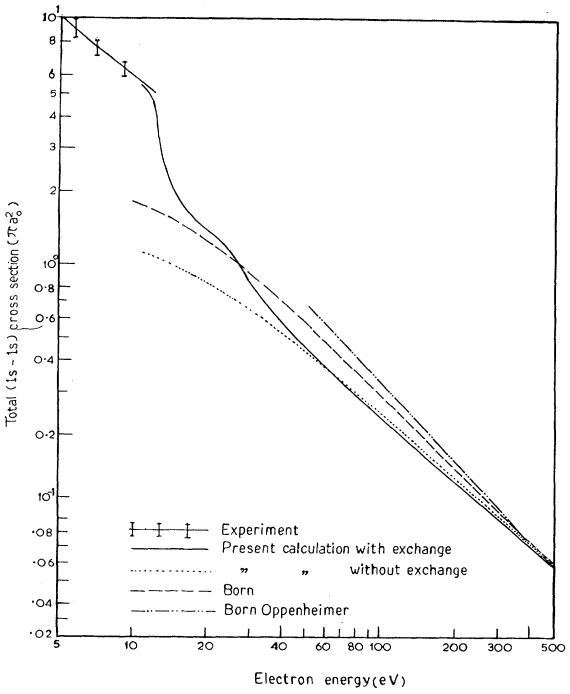

FIG. 1. 1s-1s elastic total cross sections for electron-hydrogen scattering.

with

$$f^{B\pm} = f^{B} \pm g^{BO} ,$$

where f^B and g^{BO} are the FBA and Born-Oppenheimer (BO) scattering amplitudes. Similar expressions have been used for the three-body amplitudes

$$\langle \vec{K}' n' | Y^{\pm} | \vec{K} n \rangle = -(1/4\pi^2) f^{\pm}_{n'n}(\vec{K}' \cdot \vec{K}) .$$

We have written the partial-wave form for $f^{B\pm}_{n'n}(\vec{K}' \cdot \vec{K})$ as

$$f^{B\pm}_{n'n}(\vec{K}' \cdot \vec{K}) = \frac{1}{K} \sum_{l=0}^{\infty} (2l+1) T^{B\pm}_{l}(n'n) P_l(\vec{K}' \cdot \vec{K}) ,$$

and similar expressions have been used for $f^{B\pm}_{n'n}(\vec{K}' \cdot \vec{K})$. Substituting these expressions in (3) we have obtained a set of coupled algebraic equations

$$T^{\pm}_{l}(11) = \frac{T^{B\pm}_{l}(11)}{1 - iT^{B\pm}_{l}(11)} + i \frac{T^{B\pm}_{l}(21) T^{\pm}_{l}(21)}{1 - iT^{B\pm}_{l}(11)} ,$$

$$T^{\pm}_{l}(21) = \frac{T^{B\pm}_{l}(21)}{1 - iT^{B\pm}_{l}(22)} + i \frac{T^{B\pm}_{l}(21) T^{\pm}_{l}(11)}{1 - iT^{B\pm}_{l}(22)} .$$

It should be noted that with the help of a second pair of coupled equations, we will obtain similar relations for $T^{\pm}_{l}(12)$ and $T^{\pm}_{l}(22)$. Expressing $T^{\pm}_{l}$'S in terms of $T^{B\pm}_{l}$'s we find that $T^{\pm}_{l}(21) = T^{\pm}_{l}(12)$. We have converted the BO amplitudes to partial-wave form as given in the Appendix.

RESULTS AND DISCUSSION

Total cross sections for the elastic scattering and 1s-2s excitation in e-H collisions have been calculated for the range of incident electron energies 10.6 to 500 eV. We have further obtained both these cross sections neglecting exchange effect. The two-body BO partial amplitudes required as the input have been reduced to one-dimensional integrals (see the Appendix) which have been integrated numerically by using 12-point Gaussian quadrature. At the highest energy, i.e., 500 eV, we have calculated the partial amplitudes up to 30 l values.

In Fig. 1, we have plotted our results for the total elastic cross sections with and without exchange and compared them with FBA and BO findings. In Fig. 2, we have given two curves representing our results for the total inelastic 1s-2s excitation cross sections. For comparison we have shown, in the same figure, the mean experimental curve[19] of Stebbings *et al.* along with the results of other theoretical calculations. We have further tabulated the singlet and triplet cross sections for the both of the systems in Table I. From Fig. 1, it is apparent that our curves with and without exchange pass below the BO and FBA curves, respectively. Moreover our curve with exchange also passes below FBA except in the low-energy region. These features have also been noticed by Sloan and Moore. But in our case, differences between the FBA and our curves are slightly greater than that observed by Sloan and Moore.[17] At incident energy $E \lesssim 30$, where the present method is not expected to give good results, our curve including exchange rises suddenly with the decrease of incident energy in surprisingly close agreement with the experimental

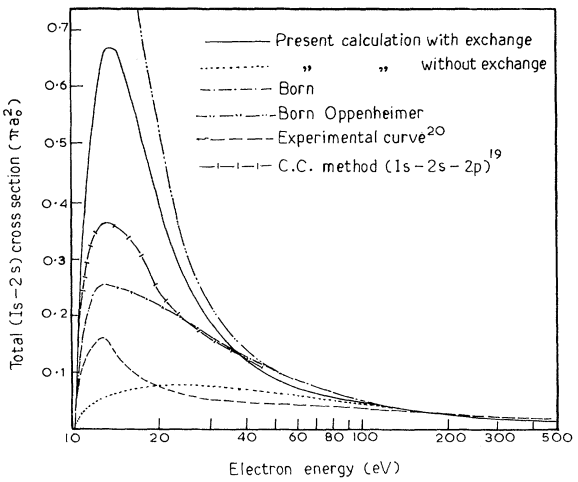

FIG. 2. 1s-2s inelastic total cross sections for electron-hydrogen scattering.

TABLE I. Calculated total cross sections for elastic and 1s-2s inelastic e-H scattering including electron exchange.

Electron energy (eV)	$Q^+(1s)$ (in units[a] πa_0^2)	$Q^-(1s)$	$Q^+(2s)$ (in units[a] πa_0^2)	$Q^-(2s)$
100	3.001 (−1)	2.101 (−1)	4.829 (−2)	5.230 (−2)
200	1.629 (−1)	1.138 (−1)	2.644 (−2)	2.767 (−2)
300	1.104 (−1)	8.087 (−2)	1.664 (−2)	1.882 (−2)
400	8.324 (−2)	6.324 (−2)	1.309 (−2)	1.428 (−2)
500	6.668 (−2)	5.230 (−2)	1.079 (−2)	1.151 (−2)

[a]The number in parentheses in each entry is the power of 10 by which the cross-section value should be multiplied.

findings.[20]

For the case of inelastic 1s-2s excitation also, our curve with exchange lies below the corresponding BO curve and our curve without exchange lies below the corresponding FBA curve. At incident energy $E \gtrsim 200$ eV, all theoretical curves almost coincide with the experimental one. As is evident from Fig. 2, our curves with and without exchange are in better agreement with the experiment than the corresponding BO and FBA curves. However, in the intermediate-energy region our curves give better agreement with the experimental findings than the other theoretical curves given in Fig. 2. At incident energy above 40 eV, our results including exchange effects are in reasonably good agreement with those calculated by cc method.[21] From Fig. 2 it appears that our result for the total inelastic cross section including exchange effects gives a maxima nearly in the same energy region as that of the experimental findings, although we obtain a much more pronounced peak as compared with the experiment. However our calculation without exchange effect does not produce any such peak. Very high peak values[22] have also been obtained by the calculation of BO as well as by the distorted wave approximations[23] which are considered to be the modifications of FBA. Even the most refined cc method gives the peak value higher than FBA.

For both processes, our results indicate that coupling to states other than the initial and final ones causes a reduction in the cross sections. This feature has also been pointed out by Moiseiwitsch and Smith.[24] Moreover, from Table I, this feature indicates that the exchange effect for both the processes is of considerable importance even up to 500 eV. This behavior has also been noticed by Sloan and Moore.[17]

Sloan and Moore[17] have omitted the principal part from the original three-body Green's function. This is equivalent to neglecting virtual excitation and other strong distortion effects. Further, in their formalism multiple scattering has been neglected by keeping only the first term of the $Y^{(1)}$ matrix, and the two-body input amplitudes are taken to be FBA and BO amplitudes.[25] All these factors may be responsible for the discrepancy in our results at the low-energy region.

ACKNOWLEDGMENT

We are thankful to P. Sinha for helping us in calculating the two-body BO scattering amplitudes.

APPENDIX

Our aim is to reduce the BO partial-wave amplitudes to a suitable analytical form for numerical calculations. The BO amplitudes are being multiplied by $P_l(\vec{p}\cdot\vec{q})\,d(\vec{p}\cdot\vec{q})$ and after performing the integrations we are left with one-dimensional integrals which have been evaluated numerically. For the calculation of 1s-1s elastic BO scattering amplitudes, one has to solve the following type of integration (notations used here are same as those of Corinaldesi and Trainor[26]): Using the parametrization method, A can be written as

$$A = 4\,\frac{\partial}{\partial\alpha}\,\frac{\partial}{\partial\beta}\int_{-1}^{1} dz \int \frac{d\vec{K}}{K^2[(\vec{K}-\vec{\rho})^2+\lambda^2]^2}\ ,$$

where

$$\vec{\rho} = \vec{p}\cdot\tfrac{1}{2}(1-z) - \vec{q}\circ\tfrac{1}{2}(1+z)$$

and

$$\lambda^2 = M + Nt\,,$$

with

$$M = \tfrac{1}{4}(p^2+q^2)(1-z^2) + \tfrac{1}{2}(\alpha^2+\beta^2)z + \tfrac{1}{2}(\alpha^2+\beta^2)\,,$$

$$N = \tfrac{1}{2}p\,q\,(1-z^2) \quad \text{and} \quad t = \cos(\vec{p}\cdot\vec{q})\,.$$

Performing integration[27] with respect to $\vec{K}$, we have

$$A = 4\pi^2\,\frac{\partial}{\partial\alpha}\,\frac{\partial}{\partial\beta}\int_{-1}^{1}\frac{dz}{(M+Nt)^{1/2}(D+Ez)}\ ,$$

where

$$D = p^2+q^2+\alpha^2+\beta^2\,,$$

$$E = q^2+\alpha^2-p^2-\beta^2\,.$$

Multiplying both sides by $P_l(t)$ and integrating with respect to dt, the range of integration being $(-1, 1)$, we have

$$\int_{-1}^{1} A\,P_l(t)\,dt = 4\pi^2\,\frac{\partial}{\partial\alpha}\,\frac{\partial}{\partial\beta}\sum_{l=0}^{\infty}\frac{2}{2l+1}\int_{-1}^{1}\frac{h^l\,dz}{D+Ez}\ ,$$

where

$$h = (M-N)^{1/2} - 1\,.$$

Now one can easily get the required BO partial-wave amplitudes for different values of l, α, and β for the other elastic and inelastic processes.

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PHYSICAL REVIEW A VOLUME 5, NUMBER 5 MAY 1972

Impact-Parameter Dependence of X-Ray Production in Collisions between Energetic Heavy Ions and Atoms

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(Received 13 December 1971)

18- to 46-MeV $_{53}$I ions were scattered by thin $_{52}$Te targets. The L x rays produced in the nearly identical particles $_{53}$I and $_{52}$Te were measured in coincidence with the scattered I ions. The differential cross section for L x-ray emission shows a maximum at impact parameters comparable to the L-shell radii. For the ion energies E investigated, the total cross section for L x-ray emission in I and Te was found to be proportional to $E^{0.8}$. The results are discussed and compared with theoretical models for inner-shell excitation.

I. INTRODUCTION

In collisions between swift charged particles (electrons, protons, α particles, heavy ions) and atoms vacancies in inner electron shells may be produced. These vacancies are filled by electrons from higher shells via radiative or nonradiative (Auger) transitions. The fraction of radiative transitions is given by the fluorescence yield ω. The corresponding transition probability is strongly dependent on the nuclear charge Z, and dominates in inner shells of heavy atoms.

Atomic collisions can be characterized by a parameter $\eta = (v/u)^2$, where v is the relative velocity of the collision partners and u the orbital velocity of the electrons in the shell being excited.[1] In the high-velocity limit, $\eta \gg 1$, the excitation and ionization cross section can be calculated by a simple perturbation treatment (e.g., Born approximation, cf. Refs. 1 and 2). In contrast to electron scattering, excitation and ionization in collisions between atomic particles are still possible in the "quasiadiabatic" velocity region, $\eta < 1$. Here, the calculation is generally more difficult. Under certain conditions, a simple perturbation treatment as in the high velocity limit is sufficient: if $Z_1 \ll Z_2$,