Collisions between ions or atoms and atomic hydrogen

Victor Franco
Physics Department, Brooklyn College of the City University of New York, Brooklyn, New York 11210
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A theory describing collisions between arbitrary atoms or ions and atomic hydrogen is developed. Results are obtained in terms of amplitudes for electron-hydrogen and proton-hydrogen collisions and the arbitrary atom or ion transition form factor. No recourse to scattering by fictitious electron-plus-proton atoms is necessary. Applications are made to the differential and total cross sections for $He^+(1s) + H(1s) \rightarrow He^+(1s) + H(n=2)$. Agreement with recent measurements is obtained. A simple approximation to the results, $\sigma \approx \sigma_{pH}(1s \rightarrow n=2) + 8\sigma_{pH}(1s \rightarrow 2s)$, is obtained and is in fair agreement with recent data.

I. INTRODUCTION

I have recently[1,2] developed a theory for describing collisons between arbitrary atomic systems in which one or both systems make transitions to excited states. It was shown that the interaction potential between the incident atom or ion and the target may be expressed in terms of a net point Coulomb interaction if neither system is neutral, plus the remaining interaction which has the following property. It may be written in terms of interactions between electrons or protons and simple fictitious atoms. Each of these "atoms" consists simply of an electron-proton pair with a transition density matrix equal to that of either the target or projectile, depending on of which one the "atom" is a constituent. We then derived an approximate expression for the scattering amplitude, in terms of the Glauber approximation amplitudes for collisions between a proton or electron and the fictitious electron-plus-proton atoms, which are obtained analytically. To illustrate the theory, we applied it to collisions between helium ions and hydrogen atoms.[3]

In the present work we show that in the special case where the projectile or target is a hydrogen atom, a theory may be formulated without any recourse to the fictitious electron-plus-proton atoms since the interaction between the projectile and target can indeed be expressed in terms of interactions between protons or electrons and a real hydrogen atom. The hydrogen atom, which is a *real* electron-plus-proton atom, obviates the need for any *fictitious* electron-plus-proton atom. Consequently, we obtain an expression for the scattering amplitude directly in terms of Glauber approximation electron-hydrogen (e-H) and proton-hydrogen (p-H) scattering amplitudes, which are known analytically. We apply these results to the differential and total cross sections for the excitation process

$$He^+(1s) + H(1s) \rightarrow He^+(1s) + H(n=2) \qquad (1)$$

and compare the results with other calculations and recent measurements.

In Sec. II we formulate the theory for collisions between arbitrary atomic systems and hydrogen atoms. In Sec. III we apply the theory to process (1) and compare the results with other theories and recent data.

II. COLLISIONS BETWEEN ARBITRARY ATOMIC SYSTEMS AND HYDROGEN ATOMS

In this section we obtain an expression for the amplitude for arbitrary ion-hydrogen or atom-hydrogen collisions in which the hydrogen atom (called target, T) undergoes a transition from initial state i_T to final state f_T and the arbitrary ion or atom (called projectile, P) undergoes a transition from state i_P to state f_P.

Let Z be the atomic number of the arbitrary ion or atom and N the number of bound electrons. Let $\vec{R}$ be the position of the nucleus of the ion or atom relative to the hydrogen nucleus. Let $\vec{r}$ denote the position of the electron in hydrogen relative to its nucleus and $\{\vec{r}_j'\}$ the positions of the N electrons of the ion or atom relative to its nucleus. The Coulomb interaction between the arbitrary ion or atom and the hydrogen atom may be written

$$V(\vec{R}, \{\vec{r}_j'\}, \vec{r}) = Ze^2\left(\frac{1}{R} - \frac{1}{|\vec{R}-\vec{r}|}\right) + e^2\sum_{j=1}^{N}\left(\frac{1}{|\vec{R}+\vec{r}_j'-\vec{r}|} - \frac{1}{|\vec{R}+\vec{r}_j'|}\right). \qquad (2)$$

The first term represents the interaction of the Z protons in the nucleus of the atom (ion) with the entire hydrogen atom. The second term represents the interaction of the N electrons of the atom (ion) with the entire hydrogen atom.

Let $\vec{v}$ be the velocity of the projectile relative to the target, and let the components of $\vec{r}_j'(\vec{r})$ parallel and perpendicular, respectively, to $\vec{v}$ be $\vec{z}_j'$ and $\vec{s}_j'$ ($\vec{z}$ and $\vec{s}$). Similarly, let $\vec{R} = \vec{b} + \vec{\zeta}$, where

$\vec{b}$ and $\vec{\xi}$ are, respectively, perpendicular and parallel to $\vec{v}$. Define the phase shift function

$$\chi(\vec{b},\{\vec{s}_j'\},\vec{s}) = -\frac{1}{\hbar v}\int_{-\infty}^{\infty} V(\vec{R},\{\vec{r}_j'\},\vec{r})\,d\xi\,. \tag{3}$$

The corresponding function $\chi_{pH}(\vec{b},\vec{b}-\vec{s})$ for collisions between a proton (p) and neutral hydrogen (H) is[4]

$$\chi_{pH}(\vec{b},\vec{b}-\vec{s}) = (-2e^2/\hbar v)\ln(|\vec{b}-\vec{s}|/b) \tag{4}$$

with a similar expression, differing by a sign, for χ_{eH} for e-H collisions. It follows from Eqs. (2) and (3) that χ for collisions between arbitrary atoms or ions and atomic hydrogen may be expressed entirely in terms of χ_{pH} and χ_{eH} for collisions of protons and electrons with hydrogen atoms. The result is simply

$$\chi(\vec{b},\{\vec{s}_j'\},\vec{s}) = Z\chi_{pH}(\vec{b},\vec{b}-\vec{s}) + \sum_{j=1}^{N}\chi_{eH}(\vec{b}+\vec{s}_j',\vec{b}+\vec{s}_j'-\vec{s})\,. \tag{5}$$

The amplitude $F_{fi}(\vec{q},k)$ for collisions in which a composite, incident with momentum $\hbar k$, transfers momentum $\hbar\vec{q}$ to another composite and the entire system makes a transition from initial state i to final state f is given, in the Glauber approximation, by[5,6]

$$F_{fi}(\vec{q},k) = \frac{ik}{2\pi}\int e^{i\vec{q}\cdot\vec{b}}\langle f|\,1-\exp[i\chi(\vec{b},\{\vec{s}_j'\},\vec{s})]\,|i\rangle\,d^2b\,, \tag{6}$$

$$= \frac{ik}{2\pi}\int e^{i\vec{q}\cdot\vec{b}}\Gamma_{fi}(\vec{b})\,d^2b\,, \tag{7}$$

where Eqs. (6) and (7) define a profile function $\Gamma_{fi}(\vec{b})$. Consequently,

$$\Gamma_{fi}(\vec{b}) = \delta_{fi} - \langle f|\,\exp[i\chi(\vec{b},\{\vec{s}_j'\},\vec{s})]\,|i\rangle\,. \tag{8}$$

Once $\Gamma_{fi}(\vec{b})$ is obtained, the scattering amplitude F_{fi} may be calculated from Eq. (7).

The profile function, Γ_{xH}, for x-H collisions is[4]

$$\Gamma_{xH}(\vec{b},\vec{b}-\vec{s}) = 1-\exp[i\chi_{xH}(\vec{b},\vec{b}-\vec{s})]\,. \tag{9}$$

We expand Γ_{fi} of Eq. (8) in terms of Γ_{pH} and Γ_{eH} by means of Eqs. (5) and (9). The first-order expansion retains in Γ_{fi} both the pH and eH profile function to first order. This procedure still accounts for some multiple collisions since the Glauber approximation for particle-hydrogen atom scattering takes double scattering into account.[4,7] The result is

$$\Gamma_{fi} = \Gamma_{fi}^{(1)} + \ldots\,, \tag{10}$$

where the first-order profile function $\Gamma_{fi}^{(1)}$ is given by

$$\Gamma_{fi}^{(1)} = \langle f|\,\Gamma^{(1)}\,|i\rangle, \tag{11}$$

$$\Gamma^{(1)} = Z\Gamma_{pH}(\vec{b},\vec{b}-\vec{s}) + \sum_{j=1}^{N}\Gamma_{eH}(\vec{b}+\vec{s}_j',\vec{b}+\vec{s}_j'-\vec{s})\,. \tag{12}$$

We note in passing that since $\Gamma_{eH}(\vec{b}+\vec{s}_j',\vec{b}+\vec{s}_j'-\vec{s})$ is a single-particle operator as far as the electrons in the atom (ion) are concerned, its matrix element vanishes if, in the final state f, more than one electron in the atom (ion) is excited.

To obtain an approximate result for F_{fi}, we use Eqs. (11) and (12) for Γ_{fi} in Eq. (7) and find

$$F_{fi}(\vec{q},k) = Z\frac{ik}{2\pi}\int e^{i\vec{q}\cdot\vec{b}}\langle f|\,\Gamma_{pH}(\vec{b},\vec{b}-\vec{s})\,|i\rangle\,d^2b + \frac{ik}{2\pi}\sum_{j=1}^{N}\langle f|\int e^{i\vec{q}\cdot\vec{b}}\Gamma_{eH}(\vec{b}+\vec{s}_j',\vec{b}+\vec{s}_j'-\vec{s})d^2b\,|i\rangle\,. \tag{13}$$

The first integral is precisely the form taken by the p-H scattering amplitude in the Glauber approximation.[4] Furthermore, since $\vec{s}$ corresponds to the electron in the hydrogen atom, the integral indeed represents the p-H scattering amplitude in the Glauber approximation. There is consequently no need to introduce any fictitious electron-plus-proton atom since the target is a real electron-plus-proton atom. Thus we have

$$\frac{ik_p}{2\pi}\int e^{i\vec{q}\cdot\vec{b}}\langle f|\,\Gamma_{pH}(\vec{b},\vec{b}-\vec{s})\,|i\rangle d^2b$$

$$= \delta_{f_P i_P} f_{pH}(\vec{q},k_p;i_T\to f_T)\,, \tag{14}$$

where $\hbar k_p$ is the momentum of a proton with relative velocity v and $f_{pH}(\vec{q},k_p;i_T\to f_T)$ is the Glauber approximation amplitude for p-H collisions in which the hydrogen atom makes a transition from initial state i_T to final state f_T. The second integral may be evaluated similarly after shifting the origin in the integration to yield

$$\frac{ik_e}{2\pi}\langle f|\int e^{i\vec{q}\cdot\vec{b}}\Gamma_{eH}(\vec{b}+\vec{s}_j',\vec{b}+\vec{s}_j'-\vec{s})d^2b\,|i\rangle$$

$$= \frac{ik_e}{2\pi}\langle f|\int \exp[i\vec{q}\cdot(\vec{b}-\vec{s}_j')]\Gamma_{eH}(\vec{b},\vec{b}-\vec{s})\,|i\rangle \tag{15}$$

$$= S_{f_P i_P}^{P}(-\vec{q})f_{eH}(\vec{q},k_e;\,i_T\to f_T)\,, \tag{16}$$

where S is the transition form factor for the projectile,

$$S^P_{f_P i_P}(\vec{q}) \equiv \int e^{i\vec{q}\cdot\vec{r}}\, \rho^P_{f_P i_P}(\vec{r})\, d^3r, \tag{17}$$

in which $\rho^P_{f_P i_P}(\vec{r})$ is the one-particle transition density matrix for the projectile. The quantity f_{eH} is the scattering amplitude for e-H collisions in the Glauber approximation and $\hbar k_e$ is the momentum of an electron with relative velocity v. Combining Eqs. (13), (14), and (16), we obtain the result

$$F_{fi}(\vec{q}, k) = k[Z\delta_{f_P i_P} f_{pH}(\vec{q}, k_p; i_T \to f_T)/k_p + NS^P_{f_P i_P}(-\vec{q}) f_{eH}(\vec{q}, k_e; i_T \to f_T)/k_e]. \tag{18}$$

The atom (ion)-hydrogen scattering amplitude is thereby simply related to the e-H and p-H amplitudes and the transition form factor of the atom (ion).

The fictitious electron-proton atom which appeared[1,2] in the treatment of collisions between arbitrary targets and projectiles does not appear in the present treatment since the target is a hydrogen atom and, therefore, it is unnecessary to "decompose" it into fictitious atoms made up of electron-proton pairs. The entire target is an actual atom made up of an electron-proton pair.

III. COLLISIONS BETWEEN He^+ IONS AND HYDROGEN ATOMS

If the projectile, say, is He^+ we have $Z=2, N=1$, and

$$F_{fi}(\vec{q}, k) = k[2\delta_{f_P i_P} f_{pH}(\vec{q}, k_p; i_T \to f_T)/k_p + S^P_{f_P i_P}(-\vec{q}) f_{eH}(\vec{q}, k_e; i_T \to f_T)/k_e]. \tag{19}$$

We apply this result to the excitation process

$$He^+(1s) + H(1s) \to He^+(1s) + H(n=2).$$

For this case $i_T = f_P = i_P = 1s$ and Eq. (19) becomes

$$F_{fi}(\vec{q}, k) = 2k f_{pH}(\vec{q}, k; 1s \to f_T)/k_p + kS^{He^+}_{1s1s}(q) f_{eH}(\vec{q}, k_e; 1s \to f_T)/k_e. \tag{20}$$

The elastic form factor is a simple analytic function, and the Glauber scattering amplitudes are given[8] in closed form in terms of hypergeometric functions. The differential cross section for (1) is given by

$$\frac{d\sigma}{d\Omega}(q, k) = \frac{k'}{k}[\,|F_{fi}(q, k; f_T = 2s)|^2 + \Sigma_m |F_{fi}(\vec{q}, k; f_T = 2p_m)|^2], \tag{21}$$

where $\hbar k'$ is the final momentum of the projectile. The total cross section is given by

$$\sigma = \frac{2\pi}{kk'} \int_{q_{min}}^{q_{max}} \frac{d\sigma}{d\Omega}\, q\, dq, \tag{22}$$

where $\hbar q_{min}$ and $\hbar q_{max}$ are the minimum and maximum allowable momentum transfers.

In Fig. 1 we present the results obtained from Eqs. (20)–(22) (solid curve) for the total cross section for process (1) together with the Born-approximation results,[9,10] the four-state impact-parameter calculation,[9] and the calculation involving the fictitious electron-proton atom.[3] There is little difference among the Born, four-state impact-parameter, and present results for incident He^+ energies above ~250 keV. At lower energies all calculations exhibit a broad maximum, but they occur at different energies and are of different magnitudes. The maximum near 200 keV in the present calculation is traceable to the maxima in the Glauber approximation proton-hydrogen $1s \to 2s$ and $1s \to 2p$ cross sections near ~55–60 keV,[11] which corresponds to approximately the same relative speed as that of a 200-keV ^4He ion. Our results also exhibit a very shallow minimum near 50 keV and a maximum near 38 keV. This is traceable to the minimum and maximum in the Glauber-approximation proton-hydrogen $1s \to 2s$ cross section near ~15 keV and ~8 keV, respectively.

The present calculation is in good agreement with the recent preliminary measurements which

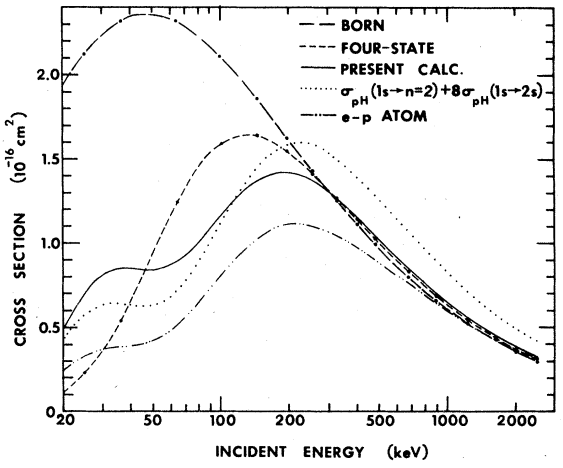

FIG. 1. Total cross section for excitation of atomic hydrogen to the $n=2$ state by He^+. The solid curve is the present calculation. The dotted curve is the approximation Eq. (25). The two dashed curves are the Born approximation and four-state impact-parameter calculations of Ref. 9; the solid circles represent the values actually calculated in Ref. 9. The dash-dot-dot curve is the calculation involving the fictitious electron-proton atom of Ref. 3.

yield a cross section which is approximately $(0.65 \pm 0.25) \times 10^{-16}$ cm^2 at 20 keV, remains essentially constant for energies ≤ 60 keV, and then rises to approximately $(0.9 \pm 0.2) \times 10^{-16}$ cm^2 at 200 keV.[12] We also note that the four-state impact-parameter method yields a rather marked improvement in the cross section over that obtained from the Born approximation.

Replacing He^+ by a proton with relative velocity v is a poor approximation to our results for energies below ~600 keV. However, Eq. (20) does lead to a simple approximate formula for the cross section for (1) in terms of p-H cross sections. Since most of the scattering occurs at small momentum transfers, the amplitudes in Eq. (20) might be approximated by their small-q limits. In this limit Eq. (20) becomes

$$F_{fi}(\vec{q}, k) \underset{q \to 0}{\sim} 2k f_{pH}(\vec{q}, k_p; 1s \to f_T)/k_p + k f_{eH}(\vec{q}, k_e; 1s \to f_T)/k_e . \quad (23)$$

Using the small-q results for the $1s \to 2s$ and $1s \to 2p$ Glauber amplitudes,[8] we find that for small q, $d\sigma/d\Omega$ for (1) is given approximately by

$$\frac{d\sigma}{d\Omega}(1s \to n=2, v; q) \approx \left(\frac{8}{5}\right)^2 \left(\frac{d\sigma_{pH}}{d\Omega}(1s \to n=2, v; q) + 8\frac{d\sigma_{pH}}{d\Omega}(1s \to 2s, v; q)\right), \quad (24)$$

and the total cross section is given approximately by the simple formula

$$\sigma(1s \to n=2, v) \approx \sigma_{pH}(1s \to n=2, v) + 8\sigma_{pH}(1s \to 2s, v), \quad (25)$$

where the cross sections $d\sigma_{pH}/d\Omega$ and σ_{pH} are Glauber approximation proton-hydrogen cross sections at relative velocity v. Approximation (25) is shown by the dotted curve in Fig. 1. It gives results qualitatively similar to the full calculation (solid curve).

In obtain approximations (24) and (25), we used some properties of the Glauber amplitudes f_{pH} and f_{eH}. However, approximations (24) and (25) may be more generally valid. Consequently, Eq. (25) could be a useful phenomenological relationship between the cross section for (1) and the p-H

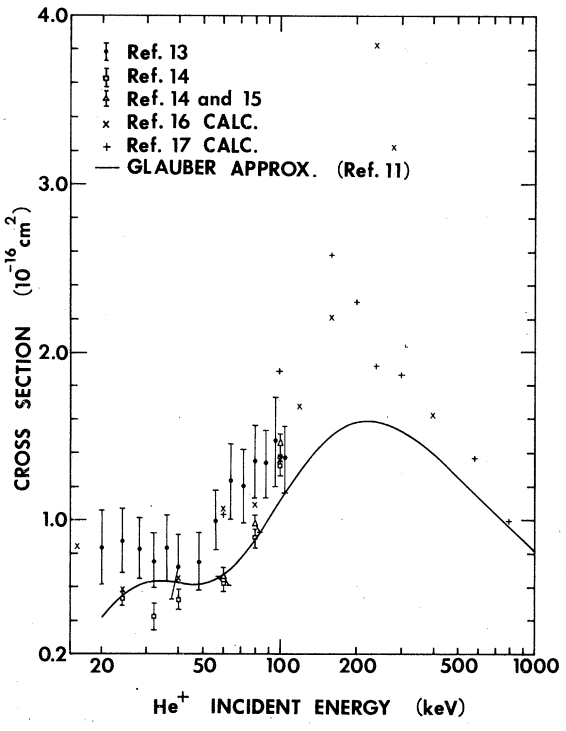

FIG. 2. Combination $\sigma_{pH}(1s \to n=2, v) + 8\sigma_{pH}(1s \to 2s, v)$. The pH measurements (data points) are from Refs. 13–15. The crosses (× and +) represent the pH calculations of Refs. 16 and 17, respectively The curve is the Glauber approximation of Ref. 11.

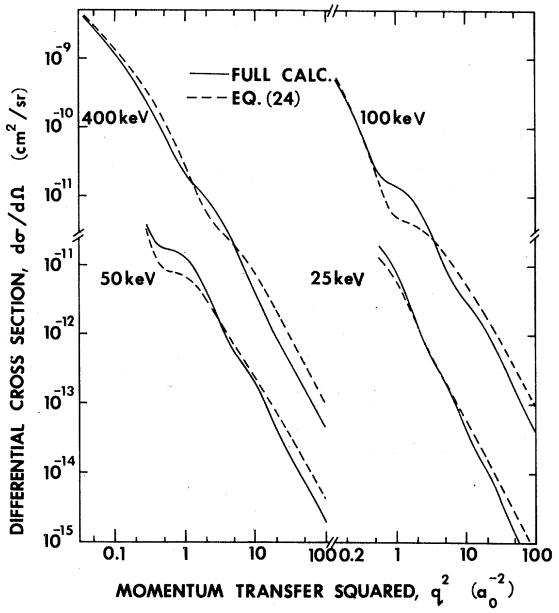

FIG. 3. Center-of-mass differential cross section for excitation of atomic hydrogen to the $n=2$ state by He^+ as a function of the squared momentum transfer q^2, in units of a_0^{-2}. The solid curves represent the present calculation [Eqs. (20) and (21)]. The dashed curves represent the approximation (24) to Eqs. (20) and (21). The upper scale for $d\sigma/d\Omega$ belongs to the 400- and 100-keV curves, the lower to the 50- and 25-keV curves. The scale on the left for q^2 belongs to the 400- and 50-keV curves, that on the right to the 100- and 25-keV curves.

$1s \rightarrow n=2$ and $1s \rightarrow 2s$ cross sections. Reliable calculations or measurements of these p-H cross sections could be used to predict the cross section for process (1). Appropriate proton-hydrogen measurements at velocities corresponding to He^+ energies between 20 and 104 keV do exist.[13-15] We therefore have "deduced" the cross sections for (1) from the right-hand side of Eq. (25) and the p-H data of Refs. 13–15. These deduced cross sections are shown in Fig. 2, where we plot the measured values of $\sigma_{pH}(1s \rightarrow n=2, v) + 8\sigma_{pH}(1s \rightarrow 2s, v)$ as a function of the equivalent He^+ energy. The results are in rather good agreement with the recent He^+-H measurements.[12] We have also used seven-state close-coupling calculations,[16] the Glauber approximation,[11] and elaborate 35-state close-coupling calculations[17] for $\sigma_{pH}(n=2, v)$ and $\sigma_{pH}(1s \rightarrow 2s, v)$ in Eq. (25) for σ; the results are shown by crosses (×), the solid curve, and the crosses (+), respectively. We note that the calculations[11,16,17] are all in reasonably good agreement with p-H data. In addition, the use of the calculations of Refs. 11 and 16 in Eq. (25) yields good agreement with the He^+ data.[12] These results indicate that the simple approximation (25) for process (1) may be generally valid and of considerable utility.

In Fig. 3 we present the differential cross section (solid curves) for process (1) at incident energies of 25, 50, 100, and 400 keV, as a function of q^2. The results are in reasonable agreement with the preliminary measurements except at 100 keV and near the forward direction at 25 keV. The dashed curves represent the approximation (24) to Eqs. (20) and (21) and are seen to give a qualitative representation of the full calculation at small momentum transfers, although there are significant quantitative differences at some energies.

The results we have obtained for the cross section for process (1) represent a substantial improvement over the Born-approximation results and are attained with little more effort than that needed for the Born approximation. The method used is applicable to collisions involving arbitrary ions or atoms and atomic hydrogen. It also leads to simple approximate formulas for the cross section in terms of proton-hydrogen cross sections which may be used to obtain qualitative estimates with great ease.

ACKNOWLEDGMENTS

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