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Small-angle scattering of ions or atoms by atomic hydrogen

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A theory for small-angle scattering of arbitrary medium- or high-energy atoms or ions by atomic hydrogen is described. Results are obtained in terms of the known closed-form and easily calculable Glauber-approximation scattering amplitudes for electron-hydrogen collisions and for collisions between the nucleus (treated as one charged particle) of the ion or atom and the hydrogen atom, and in terms of the transition form factor of the arbitrary ion or atom. Applications are made to the angular differential cross sections for the excitation of atomic hydrogen to its $n=2$ states by singly charged ground-state helium ions having velocities of roughly between $\frac{1}{2}$ and 1 a.u. The differential cross sections are obtained in terms of electron-hydrogen amplitudes and the known He^+ ground-state form factor. Comparisons are made with other calculations and with recent measurements. The results are in good agreement with the data. It is seen that the effect of the He^+ electron is to produce significant constructive interference at most energies.

I. INTRODUCTION

Angular distributions for the excitation of atomic hydrogen to its $n=2$ states by medium-energy ($v \gtrsim \frac{1}{2}$ a.u.) helium ions were recently measured for the first time.[1] The collision studied,

$$\mathrm{He}^+(1s)+\mathrm{H}(1s)\rightarrow\mathrm{He}^+(1s,\theta)+\mathrm{H}^*(n=2)\ , \tag{1}$$

is perhaps the most basic type of ion-atom collision in which both the projectile and the target contain structure. It is a particularly interesting reaction since the wave functions of both composite systems are known exactly, and therefore it can provide a stringent test of any scattering theory that attempts to describe collisions between composite atomic systems. In this energy region the greater theoretical significance of angular distributions, compared to integrated (i.e., total) cross sections, is clear since the differential cross sections are strongly peaked in the forward direction[1] and consequently the integrated cross sections are predominantly determined by only one or two measurement points.[1] Furthermore, a theory may predict an excellent total cross section obtained from a completely erroneous angular distribution, since the total cross section is just the integral of the angular distribution. Hence, whenever possible, theoretical studies of collision processes should include calculations of angular distributions.

We have shown[2] that medium- and high-energy ion-atom or atom-atom collisions involving atomic hydrogen as target or projectile may for small scattering angles be approximately described in terms of electron-hydrogen (eH) and proton-hydrogen (pH) collisions. In obtaining such a simplified representation for the collision process, it was necessary to consider the interaction between the nucleus of the arbitrary ion or atom of atomic number Z and the hydrogen atom as resulting from the separate interactions of the Z individual protons in the nucleus of the atom or ion with the hydrogen atom, and to expand the profile function for the collision process in terms of the proton-hydrogen profile function. Although this procedure leads to rather simple results in terms of eH and pH collisions, it is perhaps somewhat artificial. It would be more natural to consider the nucleus of the arbitrary ion or atom as a single entity of charge Ze, despite the fact that such a procedure precludes the possibility of describing the collision in terms of the more accessible eH and pH collisions. That is the purpose of the present work. Although our results will no longer be amenable to the *additional* small-angle approximations that led to approximate simple formulas for cross sections between atoms or ions and hydrogen atoms in terms of only pH cross sections, they are as easy to use as earlier results[2] which were expressed in terms of eH and pH scattering amplitudes. Now, however, they will be expressed in terms of eH amplitudes and amplitudes for collisions between a particle of charge Ze and hydrogen.

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 the recent data.

II. COLLISIONS WITH 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 vector 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

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

$$=V_{ZH}(\vec{R},|\vec{R}-\vec{r}|)+\sum_{j=i}^{N}V_{eH}(|\vec{R}+\vec{r}'_j|,|\vec{R}+\vec{r}'_j-\vec{r}|)\ . \tag{3}$$

The first term represents the interaction of the nucleus of the atom or ion with the entire hydrogen atom. The second term represents the interaction of the N electrons of the atom or ion with the entire hydrogen atom.

Let $\vec{v}$ be the velocity of the projectile relative to the target, and let the componenet 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 $\vec{\zeta}$ are, respectively, perpendicular and parallel to $\vec{v}$. Define the phase-shift function

$$\chi(\vec{b},\{\vec{s}'_j\},\vec{s},v)\equiv-\frac{1}{\hbar v}\int_{-\infty}^{\infty}V(\vec{R},\{\vec{r}'_j\},\vec{r})d\zeta\ . \tag{4}$$

The corresponding function $\chi_{eH}(\vec{b},\vec{b}-\vec{s},v)$ for collisions between an electron (e) and neutral hydrogen (H) is[3]

$$\chi_{eH}(\vec{b},\vec{b}-\vec{s},v)=(2e^2/\hbar v)\ln(|\vec{b}-\vec{s}|/b)\ , \tag{5}$$

and the corresponding function $\chi_{ZH}(\vec{b},\vec{b}-\vec{s},v)$ for collisions between a nucleus of charge Ze and hydrogen is

$$\chi_{ZH}(\vec{b},\vec{b}-\vec{s},v)=(-2Ze^2/\hbar v)\ln(|\vec{b}-\vec{s}|/b)\ . \tag{6}$$

It follows from Eqs. (3) and (4) that the phase-shift function χ for collisions between arbitrary atoms or ions and atomic hydrogen may be expressed entirely in terms of χ_{eH} and χ_{ZH} for collisions of electrons and positively charged particles (nuclei) with hydrogen atoms. The result is simply

$$\chi(\vec{b},\{\vec{s}'_j\}\vec{s},v)=\chi_{ZH}(\vec{b},\vec{b}-\vec{s},v)+\sum_{j=i}^{N}\chi_{eH}(\vec{b}+\vec{s}'_j,\vec{b}+\vec{s}'_j-\vec{s},v)\ . \tag{7}$$

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 an initial state i to a final state f is given, in the Glauber approximation, by[4,5]

$$F_{fi}(\vec{q},k)=\tfrac{1}{2}ik\pi^{-1}\int e^{i\vec{q}\cdot\vec{b}}\langle f|1-\exp[i\chi(\vec{b},\{\vec{s}'_j\},\vec{s},v)]|i\rangle d_2b \tag{8}$$

$$=\tfrac{1}{2}ik\pi^{-1}\int e^{i\vec{q}\cdot\vec{b}}\Gamma_{fi}(\vec{b},v)d^2b\ , \tag{9}$$

where Eqs. (8) and (9) define the profile function $\Gamma_{fi}(\vec{b},v)$. (This approximation is expected to be valid at small scattering angles and medium- or high-incident energies.) From Eqs. (8) and (9) we may write

$$\Gamma_{fi}(\vec{b},v)=\delta_{fi}-\langle f|\exp[i\chi(\vec{b},\{\vec{s}'_j\},\vec{s},v)]|i\rangle\ . \tag{10}$$

Once Γ_{fi} is obtained, the scattering amplitude F_{fi} may be calculated from Eq. (9).

The profile function, $\Gamma_{x\mathrm{H}}$, for x-H collisions is[3]

$$\Gamma_{x\mathrm{H}}(\vec{b},\vec{b}-\vec{s},v)=1-\exp[i\chi_{x\mathrm{H}}(\vec{b},\vec{b}-\vec{s},v)]\ . \qquad (11)$$

We expand Γ_{fi} of Eq. (9) in terms of $\Gamma_{e\mathrm{H}}$ and $\Gamma_{Z\mathrm{H}}$ by means of Eqs. (7) and (11). The first-order expansion retains in Γ_{fi} both the eH and ZH profile functions to first order. This procedure will account for a class of multiple collisions since the Glauber approximation for particle-hydrogen atom scattering takes double scattering into account.[3,6] Furthermore, it should be an improvement over an earlier procedure[2] in which the contribution to the amplitude arising from the nucleus-H atom interaction was approximated by Z times the proton-hydrogen scattering amplitude, since now the nucleus is left intact, i.e., is being treated as a single entity. Its effect is represented by a nucleus-H atom scattering amplitude, rather than by the sum of Z proton-hydrogen atom scattering amplitudes. The result is

$$\Gamma_{fi}=\Gamma_{fi}^{(1)}+\cdots\ , \qquad (12)$$

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

$$\Gamma_{fi}^{(1)}=\langle f\,|\,\Gamma^{(1)}\,|\,i\rangle\ , \qquad (13)$$

$$\Gamma^{(1)}=\Gamma_{Z\mathrm{H}}(\vec{b},\vec{b}-\vec{s},v)+\sum_{j=1}^{N}\Gamma_{e\mathrm{H}}(\vec{b}+\vec{s}\,'_j,\vec{b}+\vec{s}\,'_j-\vec{s},v)\ . \qquad (14)$$

To obtain the corresponding result for the scattering amplitude F_{fi}, we use Eqs. (13) and (14) for Γ_{fi} in Eq. (9) and find

$$F_{fi}(\vec{q},k)=\tfrac{1}{2}ik\pi^{-1}\int e^{i\vec{q}\cdot\vec{b}}\langle f\,|\,\Gamma_{Z\mathrm{H}}(\vec{b},\vec{b}-\vec{s},v)\,|\,i\rangle d^2b+\tfrac{1}{2}ik\pi^{-1}\sum_{j=1}^{N}\langle f\,|\int e^{i\vec{q}\cdot\vec{b}}\Gamma_{e\mathrm{H}}(\vec{b}+\vec{s}\,'_j,\vec{b}+\vec{s}\,'_j-\vec{s},v)d^2b\,|\,i\rangle\ . \qquad (15)$$

The first integral is precisely the form taken by the Glauber approximation for the scattering amplitude for collisions between a particle of charge Ze and atomic hydrogen.[3] Thus we have

$$\tfrac{1}{2}ik\pi^{-1}\int e^{i\vec{q}\cdot\vec{b}}\langle f\,|\,\Gamma_{Z\mathrm{H}}(\vec{b},\vec{b}-\vec{s},v)\,|\,i\rangle d^2b=k\delta_{f_Pi_P}f_{Z\mathrm{H}}(\vec{q},k_Z;i_T\rightarrow f_T)/k_Z\ , \qquad (16)$$

where $\hbar k_Z$ is the momentum of the nucleus with relative velocity v and $f_{Z\mathrm{H}}(\vec{q},k_Z;i_T\rightarrow f_T)$ is the Glauber approximation for collisions between the nucleus and the H atom in which the H atom makes a transition from initial state i_T to final state f_T. The second integral in Eq. (15) may be evaluated similarly to yield

$$\tfrac{1}{2}ik\pi^{-1}\langle f\,|\int e^{i\vec{q}\cdot\vec{b}}\Gamma_{e\mathrm{H}}(\vec{b}+\vec{s}\,'_j,\vec{b}+\vec{s}\,'_j-\vec{s},v)d^2b\,|\,i\rangle=kS^P_{f_Pi_P}(-\vec{q})f_{e\mathrm{H}}(\vec{q},k_e;i_T\rightarrow f_T)/k_e\ , \qquad (17)$$

where S is the transition form factor for the projectile,

$$S^P_{f_Pi_P}(\vec{q})\equiv\int e^{i\vec{q}\cdot\vec{r}}\rho^P_{f_Pi_P}(\vec{r})d^3r\ , \qquad (18)$$

in which $\rho^P_{f_Pi_P}(\vec{r})$ is the one-particle transition density matrix for the projectile. The quantity $f_{e\mathrm{H}}$ 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. (15)–(17), we obtain the result

$$F_{fi}(\vec{q},k)=k\,[\delta_{f_Pi_P}f_{Z\mathrm{H}}(\vec{q},k_Z;i_T\rightarrow f_T)/k_Z+NS^P_{f_Pi_P}(-\vec{q})f_{e\mathrm{H}}(\vec{q},k_e;i_T\rightarrow f_T)/k_e]\ . \qquad (19)$$

The atom(ion)-hydrogen scattering amplitude is thereby simply related to the electron-hydrogen atom and nucleus-hydrogen atom amplitudes and the transition form factor of the atom(ion). These particle-hydrogen atom scattering amplitudes are given in closed form in the Glauber approximation for arbitrary final states[7] and are easily calculable.

III. COLLISIONS BETWEEN He^+ IONS AND HYDROGEN ATOMS

If the projectile, for example, is He^+ we have $N=1$ and the nucleus of the projectile is an alpha particle (α). Equation (19) reduces, in this case, to

$$F_{fi}(\vec{q},k)=k[\delta_{f_p i_p} f_{\alpha H}(\vec{q},k_\alpha;i_T\rightarrow f_T)/k_\alpha+S^P_{f_p i_p}(-\vec{q})f_{eH}(\vec{q},k_e;i_T\rightarrow f_T)/k_e] . \tag{20}$$

We apply this result to the excitation process

$$He^+(1s)+H(1s)\rightarrow He^+(1s)+H(n=2). \tag{21}$$

For this case $i_T=i_P=f_P=1s$ and Eq. (20) becomes

$$F_{fi}(\vec{q},k)=kf_{\alpha H}(\vec{q},k_\alpha;1s\rightarrow n=2,l'_T,m'_T)/k_\alpha+kS^{He^+}_{1s\,1s}(q)f_{eH}(\vec{q},k_e;1s\rightarrow n=2,l'_T,m'_T)/k_e . \tag{22}$$

The ground-state form factor S is a simple analytic function, and the $n=2$, l'_T, m'_T Glauber scattering amplitudes are given[8] in closed form in terms of hypergeometric functions. The differential cross section for (21) is given by a sum over final $n=2$, l'_T, m'_T states of hydrogen,

$$\left[\frac{d\sigma}{d\Omega}\right]_{\text{c.m.}}=\frac{k'}{k}\sum_{l'_T,m'_T}|F_{fi}(\vec{q},k;n'_T=2,l'_T,m'_T)|^2 , \tag{23}$$

where $\hbar k'$ is the final momentum of the projectile.

It is interesting to note that since the αH and eH contributions to the scattering amplitudes are coherent, the possibility for the appearance of structure in the differential cross sections is enhanced. From Eq. (22) we see that the eH contribution contains the ground-state form factor $S^{He^+}_{1s\,1s}$ of He$^+$ as a multiplicative factor. Since this form factor decreases rapidly with increasing momentum transfer q, the appearance of sharp structure such as minima in the differential cross section is most likely at small q. Since, for inelastic collisions, the smallest values of q occur at small angles and *high* energies, such structure is less likely at lower energies than at medium or high energies.

In Figs. 1–3 we compare our results with those of the Born approximation, a four-state impact parameter calculation[9,10] at 100 keV, the approximation in terms of pH and eH amplitudes[2] at 100 and 50 keV, and the data.[1] To our knowledge there are no other medium-energy differential cross section calculations in the literature, although a recent result for the integrated cross sections using the approximation of Vainshtein, Presnyakov, and Sobel'man exists.[11] We also show the effect of ignoring the electron of He$^+$ in our calculation; that is, we also calculate the cross section for αH collisions, obtained from the first term in Eq. (22). In all figures the data of Ref. 1 have been renormalized by the factor[12] 0.9218 which represents the ratio of the Glauber to Born cross sections at 200 keV for excitation of H to $n=2$ by proton impact since the data were originally[1] normalized using that Born approximation result at 200 keV.

In Fig. 1 we present the results for the different cross section in the center-of-mass system for 100-keV ^{4}He$^+$ ions, as a function of the scattering angle in the c.m. system. The four-state impact parameter calculation[10] (FS) and the approximation

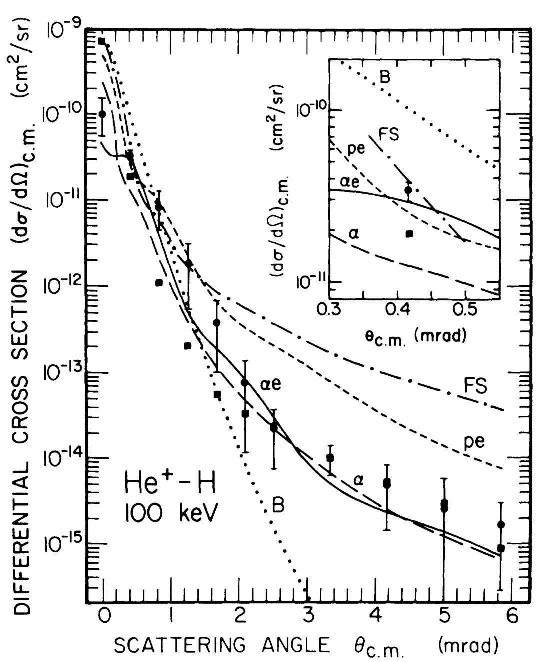

FIG. 1. Differential cross section for He$^+$(1s)+H(1s)$\rightarrow$He$^+$(1s)+H*($n=2$) at 100-keV incident He$^+$ kinetic energy. The solid circles with error bars and the solid squares are measurements (Ref. 1). The dotted (· · · ·) curve, B, is the first Born approximation. The dot-dashed (—·—·—·) curve, FS, is a four-state impact-parameter calculation taken from Ref. 10, Figs. 2 and 3 and, for $\theta_{\text{c.m.}}>1.6$ mrad, taken from Ref. 1, Fig. 2. The short-dashed (— — —) curve, pe, is the two-proton plus electron approximation of Ref. 2. The long-dashed (——— ———) curve, α, is the present calculation with the He$^+$ electron ignored. The solid (——) curve, αe, is the present full calculation. The inset shows the region $0.3\leq\theta_{\text{c.m.}}\leq0.55$ mrad enlarged for greater clarity.

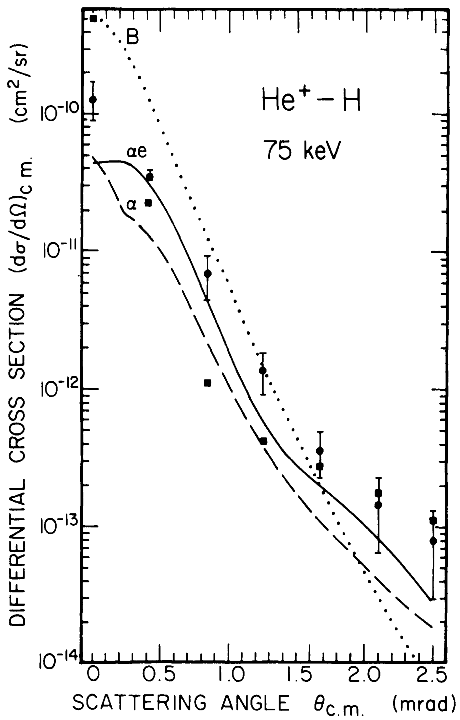

FIG. 2. Same as Fig. 1, for 75-keV incident He$^+$ kinetic energy.

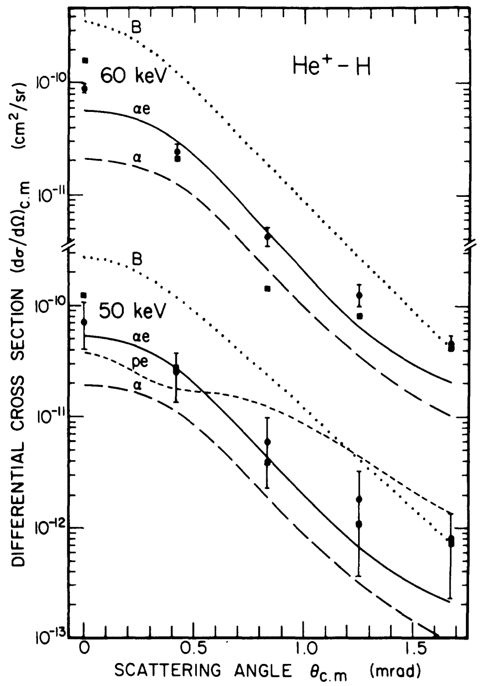

FIG. 3. Same as Fig. 1, for 60- and 50-keV incident He$^+$ kinetic energies.

in terms of pH and eH amplitudes[2] (pe), although not in good agreement with the measurements for $\theta \gtrsim 2$ mrad, represent rather marked improvements over the Born approximation (B) which is in poor agreement with the data. The calculation (α) obtained from only the first term of Eq. (22), thereby neglecting the effects of the electron in He$^+$, is in excellent agreement with the data for $\theta \gtrsim 1.5$ mrad, but fails for the smaller angles. Our full calculation (αe), obtained from Eq. (22) which includes the effects of the He$^+$ electron, improves the results significantly so that there is excellent agreement with the measurements throughout the entire angular range. In this angular range the measured differential cross section decreases by some five orders of magnitude. We note the appearance of a very shallow minimum near the forward direction which results from destructive interference between calculted eH and αH amplitudes.

As the incident energy is decreased, the angular range over which the approximation is expected to be valid will tend to decrease. For 75-keV He$^+$ we present, in Fig. 2, the results for $0 \le \theta \le 2.5$ mrad. There are no previously published calculations at this energy, to our knowledge. The Born approximation (B) again fails, being too high near the forward direction, and decreasing too rapidly so that it is too low at the larger angles. The αH approximation (α) is generally too low. The full calculation (αe), on the other hand, yields rather larger cross sections and is in good agreement with the data, except at 0° as a result of destructive interference near the forward direction which produces a very shallow minimum.

In Fig. 3 we show results for 60 and 50 keV for angles $0 \le \theta \le 1.7$ mrad. The Born approximation (B) is too high at the smaller angles and decreases too rapidly, fortuitously agreeing with the data at $\theta = 1.67$ mrad. The approximation in terms of pH and eH amplitudes[2] (pe) is in moderate agreement with the data at 50 keV. The αH approximation (α) is too low for both energies. The inclusion of the He$^+$ effects (αe) leads to a large increase in the cross section, to significantly improved results at 60 keV, and to excellent agreement with the 50-keV data.

We have also calculated the differential cross sections for $0 \le \theta \le 0.84$ mrad at five incident energies between 45 and 20 keV. In all cases the full calculation (αe), which includes the effect of the He$^+$ electron, substantially increases the cross sections, leading to excellent agreement with the measurements at all energies except 45 keV where the measurements at the two smallest angles (0 and 0.4 mrad) are $\sim 40\%$ below the theoretical predictions. We do not present these results in detail, however, since the competing charge-transfer process $He^+(1s)+H(1s)\rightarrow He(2^1S,2^1P)+H^+$ is near resonance with the direct excitation process (1) and may significantly influence the cross section for (1) at those lower energies.[13]

The general increase in the differential cross sections below 100 keV that occurs when the effects of the He^+ electron is taken into account is due in essence to constructive interference between one or more αH amplitudes and the corresponding eH amplitudes. Such constructive interference is not possible in a calculation such as the Born approximation. There the effect of the electron is, in essence, merely to multiply the differential cross section by $[1-\frac{1}{2}S_{1s1s}^{He^+}(q)]^2 \geq \frac{1}{4}$ which results in a relatively weak, partial destructive interference. However, since the Glauber approximation leads to the correct modulus *and* (to within an insignificant constant) phase of the two-body Coulomb scattering amplitude, the αH and eH amplitudes possess much richer structure in the complex plane and afford considerable possibilities for constructive interference, particularly at energies below ~ 80 keV. In addition, it occasionally happens that the contribution to the full scattering amplitude coming from the electron exceeds that from the nucleus, particularly at very small angles.

Although the results we have presented are generally in good agreement with the data, as the incident energy decreases below 100 keV, the angular range for which our results remain valid decreases. Thus for energies ≤ 75 keV there exist data[1] at angles larger than those shown in Figs. 2 and 3. If Eq. (22) were used to calculate the differential cross sections for these angles the results would not be in agreement with the data; they would be too low in general. In order to successfully describe cross sections in this energy and angular range it may be necessary to consider higher-order multiple collisions of the rather complex type in which, for example, the He^+ nucleus excites (or is elastically scattered by) the H atom and the He^+ electron deexcites (or excites) it to the $n=2$ state.

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