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Differential and integrated cross sections for the elastic process $H^+ + H(1s) \rightarrow H^+ + H(1s)$ were calculated with the use of results of coupled-state calculations in the energy range 15–200 keV. Results are presented and, at 60 keV, compared favorably with preliminary experimental data. The asymptotic form of the elastic amplitude for $b >> a_0$ (where $b$ is the impact parameter) is derived for the two cases $\lambda << 1$ and $\lambda >> 1$, where $\lambda$ is the ratio of the collision duration to the orbital period. The asymptotic form for $\lambda >> 1$ provides a useful test on the numerical accuracy of the amplitudes.

The main purpose of this Brief Report is to present theoretical estimates of the differential and integrated cross sections for the elastic scattering of protons from hydrogen atoms, in their ground state, in the (laboratory) energy range 15–200 keV. This report was stimulated by the recent acquisition of relevant experimental data by Park and co-workers.[1]

Our results were obtained by using the amplitudes previously calculated[2] by approximately solving the time-dependent impact parameter Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}\Psi(t) = H(t)\Psi(t) \ , \tag{1a}$$

$$H(t) = -\frac{\hbar^2}{2m}\nabla^2_{\vec{r}} - \frac{e^2}{r} - \frac{e^2}{|\vec{r}-\vec{R}(t)|} + \frac{e^2}{R(t)} \ , \tag{1b}$$

$$\vec{R}(t) = \vec{b} + \vec{v}t \ , \tag{1c}$$

where, in the laboratory frame, $\vec{r}$ is the position vector of the electron relative to the target proton, and $\vec{b}$ and $\vec{v}$ are the impact parameter and (constant) velocity of the projectile proton. Equation (1a) was approximately solved[2] by replacing the electron wave function $\Psi(t)$ by a linear combination of 68 basis functions (34 centered about each proton) with time-dependent coefficients determined from the numerical integration of the standard coupled-state equations. The basis functions were formed from scaled hydrogenic functions. For enhanced numerical accuracy, the coupled-state equations were integrated with a modified Hamiltonian $H_{\rm mod}(t)$ which differs from $H(t)$ by the term $(-e^2/R)\exp(-R/a_0)$, with $R = R(t)$; note that $H_{\rm mod}(t)$ does not diverge at $R = 0$. If $A(b)$ and $A_{\rm mod}(b)$, respectively, denote the amplitudes when the Hamiltonians $H(t)$ and $H_{\rm mod}(t)$ are used, we have

$$A(b) = \exp[-i\alpha(b)]A_{\rm mod}(b) \ , \tag{2a}$$

$$\alpha(b) = \frac{1}{\hbar}\int_{-\infty}^{\infty} dt \frac{e^2}{R}\exp\left(\frac{-R}{a_0}\right) = 2\left(\frac{e^2}{\hbar v}\right)K_0\left(\frac{b}{a_0}\right) \ , \tag{2b}$$

where $K_0(x)$ is the modified Bessel function of order zero. With it understood that $A(b)$ denotes the amplitude for the *elastic* channel, the integrated elastic cross section is

$$\sigma = \int_0^{\infty} 2\pi b \, db \, |A(b) - 1|^2 \ . \tag{3}$$

The differential elastic cross section, for scattering through an angle $\theta$ in the *center-of-mass* frame, is[3]

$$\frac{d\sigma}{d\Omega} = \left(\frac{\overline{M}}{2\pi\hbar^2}\right)^2 |T(\theta)|^2 \ , \tag{4a}$$

$$T(\theta) = 2\pi\hbar v \int_0^{\infty} b \, db \, [A(b) - 1] J_0\left(\frac{b\overline{M}v}{\hbar}\sin\theta\right) \ , \tag{4b}$$

where $\overline{M}$ is the reduced mass ($=\frac{1}{2}$ proton mass) and $J_0(x)$ is the Bessel function of order zero. Up to a correction of the order of the square of $(m/\overline{M}) \times (e^2/\hbar v)$, where $m$ is the electron mass, the value of $\sigma$ obtained by integrating $d\sigma/d\Omega$ over the full solid angle using Eqs. (4a) and (4b) is the same as the value of $\sigma$ obtained from Eq. (3); this provides a check on the numerical integration of Eq. (4b). In the Appendix, for added interest, we sketch a derivation of the analytic form of $A(b)$ when $b >> a_0$ for the two cases $\lambda << 1$ and $\lambda >> 1$ where $\lambda = (b/a_0)(e^2/\hbar v)$. Equation (A14), which is applicable when $b >> a_0$ and $\lambda >> 1$, provides a useful test on the numerical accuracy of any calculation of $A(b)$. The values of $A(b)$ from Ref. 2 converge

 

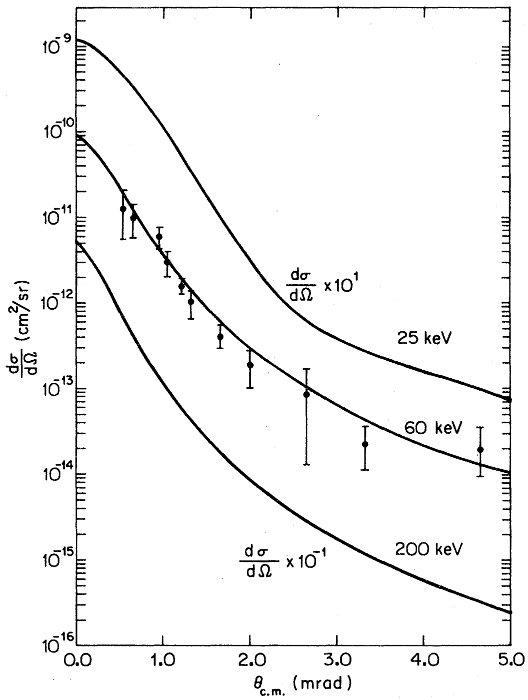


FIG. 1. Differential cross section for elastic proton-hydrogen atom scattering. Experimental data of Ref. 1: ●; present theoretical results: ——.

well with increasing $b$ to the right-hand side of Eq. (A14), giving us added confidence in these results. Equation (A14) may also be used to simply estimate $A(b)$ for $b >> a_0$. (The contribution to $\sigma$ from, say, the region $b > 8a_0$ is small, but the contribution from this region to $d\sigma/d\Omega$ is appreciable at very small angles—about 10% at $\theta=0$.) Equation (A6a) provides a test and an estimate of $A(b)$ when the conditions $b >> a_0$ and $\lambda << 1$ are simultaneously satisfied; these conditions are not satisfied over the energy range considered here, and we have included our analysis of the case $\lambda << 1$ only for added interest.

In Fig. 1 we plot our results for $d\sigma/d\Omega$ at some representative energies.[4] [We have not plotted $d\sigma/d\Omega$ at the lowest energy, 15 keV, since at this energy $A(b)$ exhibits an oscillation over the range $0 \leq b \leq a_0$, and we did not have sufficient data from Ref. 2 to accurately interpolate $A(b)$ over this range of $b$. Consequently, our results for $d\sigma/d\Omega$ at 15 keV are of doubtful accuracy for $\theta \geq 2$ mrad. We are more confident in the accuracy of $\sigma$ at 15 keV since the integrand of Eq. (3) is non-negative and the contribution from the region $b < a_0$ is fairly small.] The only existing experimental data are the preliminary data of Park[1] and co-workers at the single energy of 60 keV, which are also plotted in Fig. 1. The agreement is good. In Table I we present our results for $\sigma$, along with results obtained from the first Born approximation. The first Born estimates of $\sigma$ converge to our estimates as the incident energy increases; the discrepancy is about 7% at 200 keV. Our estimates of $d\sigma/d\Omega$ and $\sigma$ will provide a standard of comparison for results of future calculations.

TABLE I. Elastic cross sections, $\sigma_{\text{Born}}$ and $\sigma$, obtained from the first Born and coupled-state approximations, respectively, vs the laboratory energy $E$ of the incident proton. $\sigma_{\text{Born}} = \frac{7}{3}(e^2/\hbar v)^2(\pi a_0^2)$.

| $E$ (keV) | $\sigma_{\text{Born}}(\pi a_0^2)$ | $\sigma(\pi a_0^2)$ |
|---|---|---|
| 15 | 3.89 | 3.06 |
| 25 | 2.33 | 1.66 |
| 40 | 1.46 | 1.07 |
| 50 | 1.17 | 0.877 |
| 60 | 0.972 | 0.752 |
| 75 | 0.778 | 0.639 |
| 145 | 0.402 | 0.378 |
| 200 | 0.292 | 0.272 |

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## APPENDIX: ASYMPTOTIC FORM OF $A(b)$ FOR $b >> a_0$

In the elastic channel, the target hydrogen atom is subject to the perturbation

$$V(t) \equiv -\frac{e^2}{|\vec{r}-\vec{R}(t)|}+\frac{e^2}{R(t)} \quad . \tag{A1}$$

For $R >> r$ we have the multipole expansion

$$V(t) = -e^2\frac{(\vec{r}\cdot\hat{R})}{R^2}-\frac{e^2}{2R^3}[3(\vec{r}\cdot\hat{R})^2-r^2]+O\left(\frac{1}{R^4}\right), \tag{A2}$$

where $\hat{R}=\hat{R}(t)=\vec{R}(t)/R(t)$. We now assume that $b >> a_0$. It follows that $R >> a_0$, the characteristic value of $r$, so that expansion (A2) may be used. Furthermore, the perturbation $V(t)$ is weak so that the elastic amplitude $A(b)$ may be calculated within time-dependent second-order perturbation theory:

$$A(b) \approx 1-\frac{i}{\hbar}\int_{-\infty}^{\infty}dt\langle 0|V(t)|0\rangle-\frac{1}{\hbar^2}\int_{-\infty}^{\infty}dt_1\int_{-\infty}^{t_1}dt_2\langle 0|V(t_1)\exp[-i(H_0-\epsilon_0)(t_1-t_2)/\hbar]V(t_2)|0\rangle \quad , \tag{A3}$$

where $H_0$ is the Hamiltonian of the target hydrogen atom and $|0\rangle$ is the ground-state eigenvector of $H_0$ with eigenvalue $\epsilon_0$. Since the ground-state expectation values of all multipoles vanish, the ground-state expectation value of $V(t)$ of Eq. (A1) decreases exponentially with increasing $R$ and is therefore very small, and so the second term on the right-hand side of Eq. (A3) will hereafter be neglected. The collision duration is roughly $\tau_{\rm coll} \equiv b/v$, whereas the orbital period of the electron in the ground state of the target atom is roughly $\tau_{\rm orb} \equiv \hbar a_0/e^2$. Defining $\lambda \equiv \tau_{\rm coll}/\tau_{\rm orb}$, we now consider the two cases (i) $\lambda << 1$ and (ii) $\lambda >> 1$.

*Case (i):* $\lambda << 1$. Since

$$(H_0-\epsilon_0)(t_1-t_2)/\hbar \sim (-2\epsilon_0/\hbar)\tau_{\rm coll} = \lambda << 1$$

we may set the propagator equal to the identity operator in the third term on the right of Eq. (A3), to obtain

$$A(b) \approx 1 - \frac{1}{\hbar^2}\int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{t_1} dt_2 \langle 0|V(t_1)V(t_2)|0\rangle \ . \tag{A4}$$

Retaining only the dipole term in the expansion (A2), we have

$$\langle 0|V(t_1)V(t_2)|0\rangle \approx \frac{e^4 I}{R^3(t_1)R^3(t_2)} \ , \tag{A5a}$$

$$I = \langle 0|(\vec{r}\cdot\vec{A})(\vec{r}\cdot\vec{B})|0\rangle \ , \tag{A5b}$$

where $\vec{A} = \vec{R}(t_1)$ and $\vec{B} = \vec{R}(t_2)$. Now, since $I$ is a scalar and is linear in $\vec{A}$ and $\vec{B}$, we must have $I = (\vec{A}\cdot\vec{B})J$ where $J$ is independent of $\vec{A}$ and $\vec{B}$. If we set $\vec{A} = \vec{B}$ we obtain

$$A^2 J = \langle 0|(\vec{r}\cdot\vec{A})^2|0\rangle = A^2 a_0^2 \ .$$

Therefore $J = a_0^2$ and $I = a_0^2 \vec{R}(t_1)\cdot\vec{R}(t_2)$ so that

$$A(b) \approx 1 - \frac{e^4 a_0^2}{\hbar^2}\int_{-\infty}^{\infty} dt_1 \frac{\vec{R}(t_1)}{R^3(t_1)} \int_{-\infty}^{t_1} dt_2 \frac{\vec{R}(t_2)}{R^3(t_2)}$$

$$= 1 - \frac{e^4 a_0^2}{2\hbar^2}\left(\int_{-\infty}^{\infty} dt \frac{\vec{R}(t)}{R^3(t)}\right)^2$$

$$= 1 - 2(e^2/\hbar v)^2 (a_0/b)^2 \tag{A6a}$$

$$= 1 - 2(a_0/b)^4 \lambda^2 \ . \tag{A6b}$$

Since both $(a_0/b) << 1$ and $\lambda << 1$, $A(b)$ differs from unity by a very small correction. This correction represents a loss of flux from the elastic channel (into the excited-state channels) which may be simulated by a purely imaginary one-body optical potential $v(R)$:

$$v(R) = -i\left(\frac{e^2}{\hbar v}\right)\left(\frac{e^2 a_0^2}{R^3}\right) \tag{A7}$$

which, in the eikonal approximation[5] for potential scattering, yields the amplitude

$$A(b) \approx \exp\left(-\frac{i}{\hbar}\int_{-\infty}^{\infty} dt\, v(R)\right) \ , \tag{A8}$$

in agreement with Eq. (A6a). This optical potential appears, in the context of elastic electron scattering from hydrogen, in the second edition of Mott and Massey[6] [see Sec. 7, Chap. X; in particular, Eq. (36) on p. 222], but it seems to have been omitted from the third edition (perhaps because the correction is so small when both $a_0/R << 1$ and $\lambda << 1$).

*Case (ii)* $\lambda >> 1$. Since, now,

$$(H_0-\epsilon_0)(t_1-t_2)/\hbar \sim \lambda >> 1 \ ,$$

the integral over $t_2$ in Eq. (A3) may be expanded, effectively in powers of $\lambda^{-1}$, by a successive integration by parts:

$$\int_{-\infty}^{t_1} dt_2 \exp[-i(H_0-\epsilon_0)(t_1-t_2)/\hbar]V(t_2)|0\rangle \approx i\hbar G_0(\epsilon_0)V(t_1)|0\rangle + \hbar^2 G_0^2(\epsilon_0)\frac{dV}{dt_1}(t_1)|0\rangle \ , \tag{A9}$$

where $G_0(\epsilon_0) = (\epsilon_0 - H_0)^{-1}$. The second term on the right of Eq. (A9) is smaller than the first term by a factor of the order of $\lambda^{-1}$. It follows from Eqs. (A3) and (A9) that

$$A(b) \approx 1 - \frac{i}{\hbar}\int_{-\infty}^{\infty} dt[v_1(R) + v_2(R)] \ , \tag{A10}$$

where

$$v_1(R) = \langle 0|V(t)G_0(\epsilon_0)V(t)|0\rangle \ , \tag{A11a}$$

$$v_2(R) = -i\hbar\langle 0|V(t)G_0^2(\epsilon_0)\frac{dV}{dt}(t)|0\rangle = -\frac{i\hbar}{2}\frac{d}{dt}\langle 0|V(t)G_0^2(\epsilon_0)V(t)|0\rangle \ . \tag{A11b}$$

The one-body potential $v_1(R)$ is purely real and describes the static polarization of the target atom by the impinging proton; inserting expansion (A2) into Eq. (A11a) yields

$$v_1(R) \approx -\frac{\alpha_1 e^2}{2R^4} - \frac{\alpha_2 e^2}{2R^6} \ , \tag{A12}$$

where $\alpha_1$ and $\alpha_2$, respectively, are the electric dipole and quadrupole polarizabilities of hydrogen, which have the values[7]

$$\alpha_1 = \tfrac{9}{2}a_0^3 \ , \tag{A13a}$$

$$\alpha_2 = 15 a_0^5 \ . \tag{A13b}$$

The one-body potential $\nu_2(R)$ is purely imaginary and, owing to the presence of the time derivative, would seem to take into account dynamic effects. However, $\nu_2(R)$ does, in fact, give no contribution to $A(b)$ since it is an exact differential, and the integral vanishes at the limits $t=\pm\infty$. This is not surprising since Kleinman *et al.*[8] have shown that the dynamic contribution to the long-range interaction of an (infinitely massive) hydrogen atom with a particle of charge $e'$ and mass $M$ is, to leading order,

$$3\left(\frac{e'}{e}\right)^2\frac{\hbar^2}{M}\frac{\beta_1}{R^6} ,$$

where $\beta_1$ is the dynamic polarizability, with value $\frac{43}{8}a_0^4$. In the present case $M$ is the proton mass, which is regarded as infinite, so that the dynamic contribution to the long-range interaction vanishes through the order considered.[9]

Combining Eqs. (A10) and (A12) and using Eqs. (A13) gives

$$A(b)\approx 1+\frac{i\pi}{16}\left(\frac{e^2}{\hbar v}\right)\left(\frac{4\alpha_1}{b^3}+\frac{3\alpha_2}{b^5}\right)$$

$$=1+i\frac{9\pi}{16}\left(\frac{e^2}{\hbar v}\right)\left(\frac{a_0}{b}\right)^3\left(2+\frac{5a_0^2}{b^2}\right) . \quad \text{(A14)}$$


[1] J. T. Park, in *Proceedings of the Twelfth International Conference on the Physics of Electronic and Atomic Collisions,* edited by S. Datz (North-Holland, Amsterdam, 1982).

[2] R. Shakeshaft, Phys. Rev. A 18, 1930 (1978).

[3] See, e.g., L. Wilets and S. J. Wallace, Phys. Rev. 169, 84 (1969).

[4] The results of an independent calculation by J. Peacher of $d\sigma/d\Omega$ at 60 keV, also based on the results of Ref. 2, were reported in Ref. 1 and are in agreement with our values of $d\sigma/d\Omega$.

[5] R. J. Glauber, *Lectures in Theoretical Physics* (Interscience, New York, 1958), Vol. 1, p. 315.

[6] N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions,* 2nd ed. (Oxford, New York, 1949).

[7] A. Dalgarno, Adv. Phys. 11, 281 (1962).

[8] C. J. Kleinman, Y. Hahn, and L. Spruch, Phys. Rev. 165, 53 (1968).

[9] The dynamic part of the interaction arises from the third term in the expansion (A9) and is of order $\lambda^{-2}(e^2a_0^3/R^4)\sim(\hbar v/e^2)^2(e^2a_0^5/R^6)$.