Production of $H^-(1s^2)$ by Hydrogen Atom Collisions

ROBERT A. MAPLETON
Geophysics Research Directorate, Air Force Cambridge Research Center, Air Research and Development Command, L. G. Hanscom Field, Bedford, Massachusetts

(Received February 2, 1959; revised manuscript received September 22, 1959)

The post matrix element form of Born's approximation is used to calculate the cross section for $H^-(1s^2)$ production in hydrogen atom collisions. The Coulomb wave function is approximated by a plane wave, and two different wave functions derived by Chandrasekhar, one of which contains the inter-electron distance, are used for the H^- state. The value of the cross section obtained with the wave function containing the interelectron distance term is roughly 25% larger than the other cross section. Since the direct and exchange charge transfer amplitudes, $f_s(\theta)$ and $f_s(\pi-\theta)$, are sharply peaked about $\theta=0$ and $\theta=\pi$, respectively, the interference terms are negligible. Thus, only $f_s(\theta)$ has to be calculated to obtain the cross section.

THE charge exchange cross section for the collision of neutral atoms of the same species is difficult to calculate and in many cases nearly impossible to measure within the framework of present experimental methods. Nevertheless, it is becoming increasingly important to know the values of these cross sections for the current problems of the upper atmosphere. The simplest cross section of this class to evaluate is the hydrogen atom case, and this paper presents the formulation and calculation of reaction (A) in Born approximation.

$$\mathrm{H}(1s)+\mathrm{H}(1s)\rightarrow \mathrm{H}^-(1s^2)+\mathrm{H}^+. \tag{A}$$

In the center-of-mass system, and with the neglect of spin-dependent forces, the nonrelativistic equation for this process is given by

$$(H_0'-e^2V')\Psi=(H_0-e^2V)\Psi=E\Psi, \tag{1a}$$

$$H_0'=-\frac{\hbar^2}{2\mu_1}\nabla_{\mathbf{R}'}{}^2-\frac{\hbar^2}{2\mu}(\nabla_{\mathbf{x}_1'}{}^2+\nabla_{\mathbf{x}_2'}{}^2)-\frac{e^2}{|\mathbf{x}_1'|}-\frac{e^2}{|\mathbf{x}_2'|}, \tag{1b}$$

$$\begin{aligned}V'=&\frac{1}{|\mathbf{R}'+(\mu/m)\mathbf{x}_1'+(\mu/M)\mathbf{x}_2'|}\\&+\frac{1}{|-\mathbf{R}'+(\mu/M)\mathbf{x}_1'+(\mu/m)\mathbf{x}_2'|}\\&-\frac{1}{|-\mathbf{R}'-(\mu/m)\mathbf{x}_1'+(\mu/m)\mathbf{x}_2'|}\\&-\frac{1}{|-\mathbf{R}'+(\mu/M)\mathbf{x}_1'-(\mu/M)\mathbf{x}_2'|},\end{aligned} \tag{1c}$$

$$\begin{aligned}H_0=&-\frac{\hbar^2}{2\mu_2}\nabla_{\mathbf{R}}{}^2-\frac{\hbar^2}{2\mu}(\nabla_{\mathbf{x}_1}{}^2+\nabla_{\mathbf{x}_2}{}^2)-\frac{\hbar^2}{M}\nabla_{\mathbf{x}_1}\cdot\nabla_{\mathbf{x}_2}\\&-\frac{e^2}{|\mathbf{x}_1|}-\frac{e^2}{|\mathbf{x}_2|}+\frac{e^2}{|-\mathbf{x}_1+\mathbf{x}_2|}-\frac{e^2}{|\mathbf{R}|},\end{aligned} \tag{1d}$$

$$\begin{aligned}V=&\frac{1}{|\mathbf{R}+(M_1/M_2)\mathbf{x}_1-(m/M_2)\mathbf{x}_2|}\\&+\frac{1}{|\mathbf{R}-(m/M_2)\mathbf{x}_1+(M_1/M_2)\mathbf{x}_2|}\\&-\frac{1}{|-\mathbf{R}+(m/M_2)(\mathbf{x}_1+\mathbf{x}_2)|}-\frac{1}{|\mathbf{R}|}.\end{aligned} \tag{1e}$$

In the laboratory system, $\mathbf{r}_1$, $\mathbf{r}_2$ are the proton coordinates, and $\mathbf{r}_3$, $\mathbf{r}_4$ are the electron coordinates. e is the electron charge; $\hbar$ is Planck's constant divided by 2π, and the particle masses are as follows: m=electron, M=proton, $M_1=M+m$, $M_2=M+2m$, $\mu_1=M_1/2$, $\mu=mM/M_1$, $\mu_2=MM_2/2M_1$. The relative coordinates for the prior system (primed) are

$$\mathbf{x}_1'=\mathbf{r}_3-\mathbf{r}_1,\quad \mathbf{x}_2'=\mathbf{r}_4-\mathbf{r}_2,\quad \mathbf{R}'=\frac{M\mathbf{r}_1+m\mathbf{r}_3}{M_1}-\frac{M\mathbf{r}_2+m\mathbf{r}_4}{M_1},$$

and the relative coordinates for the post system (unprimed) are

$$x_1=\mathbf{r}_3-\mathbf{r}_1,\quad \mathbf{x}_2=\mathbf{r}_4-\mathbf{r}_1,\quad \mathbf{R}=\frac{M\mathbf{r}_1+m(\mathbf{r}_3+\mathbf{r}_4)}{M_2}-\mathbf{r}_2.$$

Conservation of energy is given by

$$\frac{\hbar^2K_0^2}{2\mu_1}-2\epsilon_0=\frac{\hbar^2K_n^2}{2\mu_2}-\epsilon_n. \tag{2a}$$

In (2a), K_0, K_n are the magnitudes of initial and final wave vectors of relative motion, respectively, while ϵ_0, ϵ_n are the binding energies of $H(1s)$ and $H^-(1s^2)$, respectively.

With the assumption that $\Psi=\sum_m g_m(\mathbf{R})\psi_m(\mathbf{x}_1,\mathbf{x}_2)$ is a permissible representation for the wave function, $\psi_m(\mathbf{x}_1,\mathbf{x}_2)$ being a member of a complete orthogonal set of H^- wave functions, one readily obtains the equation

for $g_n(\mathbf{R})$ as given by

$$\left[\nabla_R^2+\frac{2\mu_2 e^2}{\hbar^2|\mathbf{R}|}+K_n^2\right]g_n(\mathbf{R})$$
$$=-\frac{2\mu_2 e^2}{\hbar^2}\int\psi_n^*(\mathbf{x}_1,\mathbf{x}_2)V(\mathbf{R},\mathbf{x}_1,\mathbf{x}_2)$$
$$\times\Psi(\mathbf{R},\mathbf{x}_1,\mathbf{x}_2)d\mathbf{x}_1 d\mathbf{x}_2. \quad (2b)$$

The inclusion of the R^{-1} term in V of (1e) causes V to decrease faster than R^{-1} for large R, and the inclusion of this term in H_0 of (1d) causes H_0 to assume the true unperturbed value of (H_0-e^2V) for large R. The Born approximation consists of the replacement of $\Psi(\mathbf{R},\mathbf{x}_1,\mathbf{x}_2)$ in (2b) by

$$\Psi=\exp(i\mathbf{K}_0\cdot\mathbf{R}')\phi_0(\mathbf{x}_1')\phi_0(\mathbf{x}_2'),$$

in which relation ϕ_0 is the normalized hydrogen wave function for the 1s-state. Equation (2b) is solved subject to the restriction that $g_n(\mathbf{R})$ is outgoing for large R and is finite at the origin.[1] The approximate solution of (2b) subject to these boundary conditions is readily obtained by using the Green's function as given by

$$G(\mathbf{R},\mathbf{R}'')=\frac{K_n}{4\pi}\sum_{l=0}^{\infty}(2l+1)P_l(\cos\Theta)$$
$$\times\begin{cases}L_l(R)H_l(R''), & R<R''\\ L_l(R'')H_l(R), & R>R''.\end{cases} \quad (2c)$$

Let $W_{1,2}$ represent the two solutions of the confluent hypergeometric equation, F the confluent hypergeometric function, P_l the Legendre polynomial, Γ, the gamma function, and $a_0=\hbar^2/me^2$, $\alpha=-\mu_2/mK_n a_0$,

$$\eta_l=\arg\Gamma(l+1+i\alpha),$$
$$\cos\Theta=\cos\theta\cos\theta''+\sin\theta\sin\theta''\cos(\phi-\phi'').$$

Then the quantities L_l and H_l of (2c) are defined as follows[2]:

$$F(l+1+i\alpha;2l+2;-i2K_nR)=W_1+W_2,\quad H_l=K_l+iL_l,$$
$$L_l=\frac{\exp(-\pi\alpha/2)|\Gamma(l+1+i\alpha)|(2K_nR)^l\exp(iK_nR)}{(2l+1)!}$$
$$\times(W_1+W_2),$$
$$K_l=\frac{i\exp(-\pi\alpha/2)|\Gamma(l+1+i\alpha)|(2K_nR)^l\exp(iK_nR)}{(2l+1)!}$$
$$\times(W_1-W_2).$$

[1] W. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Oxford University Press, New York, 1949), second edition, p. 112.
[2] Reference 1, pp. 52, 53.

For large R, L_l and H_l become

$$L_l\sim\frac{\sin[K_nR-(l\pi/2)+\eta_l-\alpha\ln(2K_nR)]}{K_nR},$$
$$H_l\sim\frac{\exp i[K_nR-(l\pi/2)+\eta_l-\alpha\ln(2K_nR)]}{K_nR},$$

and $G(\mathbf{R},\mathbf{R}'')$ reduces to

$$G\sim\frac{\exp i[K_nR-\alpha\ln(2K_nR)]}{4\pi R}$$
$$\times\sum_{l=0}^{\infty}(2l+1)i^l\exp(i\eta_l)L_l(R)P_l[\cos(\pi-\Theta)].$$

Thus, the asymptotic form of the Green's function can be written as[3]

$$G\sim\frac{\exp i[K_nR-\alpha\ln(2K_nR)]}{4\pi R}\exp(-\pi\alpha/2)\Gamma(1+i\alpha)$$
$$\times\exp i[K_nR''\cos(\pi-\Theta)]F(a;c;z),$$

with $a=-i\alpha$, $c=1$, and $z=iK_nR''[1-\cos(\pi-\Theta)]$. The solution of (2b) is given by

$$g_n(\mathbf{R})=-(2\mu_2e^2/\hbar^2)\int G(\mathbf{R},\mathbf{R}'')\psi_n^*(\mathbf{x}_1,\mathbf{x}_2)V(\mathbf{R}'',\mathbf{x}_1,\mathbf{x}_2)$$
$$\times\exp(i\mathbf{K}_0\cdot\mathbf{R}')\phi_0(\mathbf{x}_1')\phi_0(\mathbf{x}_2')d\mathbf{x}_1d\mathbf{x}_2d\mathbf{R}'', \quad (2d)$$

and the amplitude for scattering, by

$$f_n(\theta)=-\frac{\mu_2e^2}{2\pi\hbar^2}\exp(-\pi\alpha/2)$$
$$\times\Gamma(1+i\alpha)\int\exp i[K_nR\cos(\pi-\Theta)]$$
$$\times F(a;c;z)\psi_n^*(\mathbf{x}_1,\mathbf{x}_2)V(\mathbf{R},\mathbf{x}_1,\mathbf{x}_2)$$
$$\times\exp(i\mathbf{K}_0\cdot\mathbf{R}')\phi_0(\mathbf{x}_1')\phi_0(\mathbf{x}_2')d\mathbf{x}_1d\mathbf{x}_2d\mathbf{R}. \quad (2e)$$

The evaluation of $f_n(\theta)$ is still prohibitively difficult, but the next approximation reduces this difficulty to a tolerable level. One of the criteria for the validity of the Born approximation is that

$$\frac{e^2}{\hbar v_0}=\frac{\mu_1}{mK_0a_0}\doteq\frac{\mu_2}{mK_na_0}=|\alpha|\ll1.$$

With this condition $\exp(-\pi\alpha/2)\Gamma(1+i\alpha)F(a;c;z)$ is nearly unity; consequently, the approximate Born

[3] Reference 1, p. 46.

amplitude reduces to the form

$$f_n(\theta)=-(\mu_2e^2/2\pi\hbar^2)\int \exp(-i\mathbf{K}_n\cdot\mathbf{R}) \times\psi_n^*(\mathbf{x}_1,\mathbf{x}_2)V(\mathbf{R},\mathbf{x}_1,\mathbf{x}_2) \times\exp(i\mathbf{K}_0\cdot\mathbf{R}')\phi_0(\mathbf{x}_1')\phi_0(\mathbf{x}_2')d\mathbf{x}_1d\mathbf{x}_2d\mathbf{R}_2. \quad (3a)$$

The calculation of $f_n(\theta)$ can be simplified by the introduction of the coordinates $(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3=\mathbf{x}_2')$ as independent variables. With this change of variables, $f_n(\theta)$ and $V(\mathbf{R},\mathbf{x}_1,\mathbf{x}_2)$ are given by

$$f_n(\theta)=-\frac{\mu_2e^2}{2\pi\hbar^2}\int \exp[i(\mathbf{A}_1\cdot\mathbf{x}_1-\mathbf{A}_2\cdot\mathbf{x}_2+\mathbf{A}_3\cdot\mathbf{x}_3)] \times\psi_n^*(\mathbf{x}_1,\mathbf{x}_2)V(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3) \times\phi_0(\mathbf{x}_1)\phi_0(\mathbf{x}_3)d\mathbf{x}_1d\mathbf{x}_2d\mathbf{x}_3,$$

$$V(\mathbf{R},\mathbf{x}_1,\mathbf{x}_2)=V(\mathbf{x}_1,\mathbf{x}_2\mathbf{x}_3)=|\mathbf{x}_1-\mathbf{x}_2+\mathbf{x}_3|^{-1} +|\mathbf{x}_3|^{-1}-|\mathbf{x}_2-\mathbf{x}_3|^{-1} -|(M_1/M_2)\mathbf{x}_2-\mathbf{x}_3-(m/M_1)\mathbf{x}_1|^{-1}, \quad (3b)$$

$$\mathbf{A}_1=(m/M_1)\mathbf{A}_2,\quad \mathbf{A}_2=\mathbf{K}_0-(M_1/M_2)\mathbf{K}_n,\quad \mathbf{A}_3=(M/M_1)\mathbf{K}_0-\mathbf{K}_n.$$

It is easily shown that the effect of the last term of V in (3b) is, to a very good approximation, $|\mathbf{x}_2-\mathbf{x}_3|^{-1}$; thus, the working formula for $f_n(\theta)$ is given by (3b) with the last term of V replaced by $|\mathbf{x}_2-\mathbf{x}_3|^{-1}$. This amplitude is the approximate Born-post matrix element. The exact matrix element given in (2e) is equal to the prior matrix element, with interaction given in (1c), provided that exact H^- wave functions are used.[4] The calculation of the prior matrix element with the plane wave approximation and the same H^- wave functions serves as a test of these approximations. The author will present the results of this task in a future paper.[5]

The details of the calculation are deferred until the effects of particle identity are discussed. In the formulation that has been presented, the approximate solution has been obtained for an incoming state $\Phi_1=\Phi(1234)=\exp(i\mathbf{K}_0\cdot\mathbf{R}_1')\phi_0(\mathbf{x}_{11}')\phi_0(\mathbf{x}_{21}')$ which is a solution of $H_{01}'\Phi_1=E\Phi_1$. (Here $\mathbf{R}_1'=\mathbf{R}'$, $\mathbf{x}_{11}'=\mathbf{x}_1'$, $\mathbf{x}_{21}'=\mathbf{x}_2'$.) By permutation of the laboratory particle coordinates, three other systems of prior relative coordinates are derived, the effect being to change the ordering of the particles in the incident state, Φ_i, $(i=1, 2, 3, 4)$. The normalized singlet and triplet states (of the electron coordinates without the spin functions) are $\Phi_{s,t}(12)=2^{-\frac{1}{2}}[\Phi(1234)\pm\Phi(1243)]$ and $\Phi_{s,t}(21)=2^{-\frac{1}{2}}[\Phi(2134)\pm\Phi(2143)]$, in which relations the subscripts, s and t, refer to the upper and lower signs, respectively. Since $\psi_n(\mathbf{x}_1,\mathbf{x}_2)$ is a normalized singlet state in the electron coordinates, the singlet amplitude, $f_s(\theta)$, is calculated with a normalized singlet incoming state. [The subscript n is now dropped. $\psi_n(\mathbf{x}_1,\mathbf{x}_2)=\psi(\mathbf{x}_1,\mathbf{x}_2)$, $\mathbf{K}_n=\mathbf{K}$.] For a given post relative coordinate, R, $\Phi_s(12)$ and $\Phi_s(21)$ are used in (3b) to obtain the singlet direct and exchange amplitude, respectively. Equation (4a) is presented for clarification to the reader. The initial states

$$\begin{aligned} &i=1\cdots4, \quad H_{0i}'\Phi_i=E\Phi_i, \quad \Phi_1=\Phi(1234),\\ &\Phi_2=\Phi(1243), \quad \Phi_3=\Phi(2134), \quad \Phi_4=\Phi(2143),\\ &\Phi_i=\exp(i\mathbf{K}_0\cdot\mathbf{R}_i')\phi_0(\mathbf{x}_{1i}')\phi_0(\mathbf{x}_{2i}'),\\ &\mathbf{x}_{13}'=\mathbf{x}_{22}', \quad \mathbf{x}_{23}'=\mathbf{x}_{12}', \quad \mathbf{R}_3'=-\mathbf{R}_2',\\ &\mathbf{x}_{14}'=\mathbf{x}_{21}', \quad \mathbf{x}_{24}'=\mathbf{x}_{11}', \quad \mathbf{R}_4'=-\mathbf{R}_1', \end{aligned} \quad (4a)$$

$$\psi(12)\sim\Phi_s(12)+Sf_s(\theta),$$

$$\psi(21)\sim\Phi_s(21)+Sf_s(\pi-\theta),$$

$$S=R^{-1}\exp\{i[KR-\alpha\ln(2KR)]\}\psi(\mathbf{x}_1,\mathbf{x}_2),$$

$$f_s(\theta)=\sqrt{2}f(\theta),$$

are retained in the expressions for the asymptotic form of the wave functions in (4a) to show the relation between the amplitudes and the initial states; however, they vanish since initial and final bound states are in different channels.[4] Let $\chi_p{}^t$, $\chi_p{}^s$ represent the triplet and singlet proton spin functions, respectively, and $\chi_l{}^t$, $\chi_l{}^s$, the corresponding electron spin functions. The antisymmetrical initial state, Φ, is given by (4b). The probability

$$\Phi=\{[\Phi_t(12)-\Phi_t(21)]\chi_p{}^t+[\Phi_t(12)+\Phi_t(21)]\chi_p{}^s\}\chi_l{}^t +\{[\Phi_s(12)-\Phi_s(21)]\chi_p{}^t +[\Phi_s(12)+\Phi_s(21)]\chi_p{}^s\}\chi_l{}^s \quad (4b)$$

density of this incoming state is

$$P=\tfrac{1}{16}\sum_{\text{spin}}\int d\mathbf{x}_1'd\mathbf{x}_2'|\Phi|^2,$$

with P normalized to the number of spin states. This value is $P=1+\frac{1}{4}\cos(2\mathbf{K}_0\cdot\mathbf{R}_1')$, and its average value is $\bar{P}=1$.[6]

The antisymmetical singlet amplitude and the differ-

[4] E. Gerjuoy, Ann. Phys. **5**, 58 (1958); Phys. Rev. **109**, 1806 (1958). (These two articles contain an extensive bibliography of the theory of rearrangement collisions.)

[5] The author has calculated both post and prior cross sections (unpublished) for the reaction $p+\text{He}(1s^2)\rightarrow\text{H}(1s)+\text{He}^+(1s)$ (as well as for other final states) and found substantial agreement. Of course, only the wave function of $\text{He}(1s^2)$ is approximated for this reaction, since there are no Coulomb functions.

[6] In the evaluation of $\bar{P}$ only the contribution from $R_1'\rightarrow\infty$ is included, for with $\mathbf{R}_1'$ large the bound state part of Φ that contains R_2'' vanishes. If both parts are added, $\bar{P}=2$. This situation is analogous to $e-e$ Coulomb scattering in which case, with a value of $\bar{P}=2$, the calculated cross section is a measure of all electrons scattered, directs and recoils. Since the cross sections of this paper are for the total production of H^- ions, the analogy is apparent.

ential cross section are given by

$$F=\{[f_s(\theta)-f_s(\pi-\theta)]\chi_p{}'+[f_s(\theta)+f_s(\pi-\theta)]\chi_p{}^s\}\chi_i{}^s,$$
$$\sigma=\tfrac{1}{16}(v_f/v_i)\sum_{\text{spin}}|F|^2$$
$$=(v_f/v_i)[\tfrac{3}{16}|f_s(\theta)-f_s(\pi-\theta)|^2+\tfrac{1}{16}|f_s(\theta)+f_s(\pi-\theta)|^2], \quad (4c)$$
$$v_i=\hbar K_0/\mu_1, \quad v_f=\hbar K/\mu_2'.$$

As the calculation shows, the interference terms in (4c) are negligible for the energy range investigated. Thus, the total cross section, Q, is given by

$$Q=\frac{\pi v_f}{v_i}\int_0^\pi d\theta\,\sin\theta|f_s(\theta)|^2=\frac{2\pi v_f}{v_i}\int_0^\pi d\theta\,\sin\theta|f(\theta)|^2. \quad (4d)$$

It is emphasized that the omission of the interference terms is a numerical approximation, and does not mean that the identical particles are treated as distinguishable. If triplet H^- states exist, the differential cross section is given by (4e) in which formula the notation is obvious.

$$\sigma_t=(v_f(t)/v_i)[\tfrac{9}{16}|f_t(\theta)-f_t(\pi-\theta)|^2+\tfrac{3}{16}|f_t(\theta)+f_t(\pi-\theta)|^2]. \quad (4e)$$

The wave functions used to represent the H^- state are those derived by Chandrasekhar,[7] while Heinrich's[8] calculated value of 0.747 ev is employed for the electron affinity of H^-. The calculations are presented under Cases I and II.

Case I

$$\psi_1=N_1[\exp(-ax_1-bx_2)+\exp(-ax_2-bx_1)],$$
$$a=1.03925, \quad b=0.28309,$$
$$N_1=\frac{1}{4\pi}\left[\frac{8a^3b^3(a+b)^6}{(a+b)^6+64a^3b^3}\right]^{\frac{1}{2}}.$$

In all that follows, the unit of length is the Bohr radius and the unit of energy is the binding energy of $H(1s)$. The methods of integration are amply illustrated in other papers.[9]

$$f(\theta)=(128\mu_2N_1'a_0/m)[b(1+a)(I_1{}^0+I_2{}^0-2I_3{}^0)+a(1+b)(I_4{}^0+I_5{}^0-2I_6{}^0)]. \quad (5a)$$

In (5a) $N_1'=\pi N_1=9.8781\times10^{-2}$, and the other symbols are defined below.

$$I_1{}^0(a,b)=\int_0^1 dx\,x(1-x)^3\int_0^1 dy\,y(1-y)\times\left(\frac{\partial}{\partial u_1}+\frac{\partial}{\partial v_1}\right)^4\frac{1}{u_1v_1{}^{\frac{1}{2}}},$$
$$I_4{}^0(a,b)=I_1{}^0(b,a),$$
$$u_1=(1-x)(1-y)(b^2+A_2{}^2)+x(1+A_3{}^2)+y(1-x)[(1+a)^2+A_1{}^2], \quad (5b)$$
$$v_1=(1-x)(1-y)b^2+x+y(1-x)(1+a)^2+x(1-x)|\mathbf{A}_2-\mathbf{A}_3|^2+y(1-x)\times[1-y(1-x)]|\mathbf{A}_1-\mathbf{A}_2|^2+2xy(1-x)\times(\mathbf{A}_3-\mathbf{A}_2)\cdot(\mathbf{A}_2-\mathbf{A}_1).$$
$$I_2{}^0(a,b)=[(1+a)^2+A_1{}^2]^{-2}(b^2+A_2{}^2)^{-2}(1+A_3{}^2)^{-1}, \quad (5c)$$
$$I_5{}^0(a,b)=I_2{}^0(b,a).$$
$$I_3{}^0(a,b)=[(1+a)^2+A_1{}^2]^{-2}\int_0^1 dx\,x(1-x)\times\left(\frac{\partial}{\partial u_3}+\frac{\partial}{\partial v_3}\right)^2\frac{1}{u_3v_3{}^{\frac{1}{2}}}, \quad (5d)$$
$$I_6{}^0(a,b)=I_3{}^0(b,a),$$
$$u_3=(1-x)(b^2+A_2{}^2)+x(1+A_3{}^2),$$
$$v_3=x+(1-x)b^2+x(1-x)|\mathbf{A}_3-\mathbf{A}_2|^2.$$

Case II

$$\psi_2(\mathbf{x}_1,\mathbf{x}_2)=N_2[\exp(-ax_1-bx_2)+\exp(-ax_2-bx_1)]\times[1+c|\mathbf{x}_1-\mathbf{x}_2|],$$
$$a=1.07478, \quad b=0.47758, \quad c=0.31214,$$
$$2\pi^2N_2{}^2\{[(a+b)^6+64a^3b^3]a^{-3}b^{-3}(a+b)^{-6}+c[ab(a^2-b^2)^{-3}(7a^{-3}-7b^{-3}+3a^2b^{-5}-3b^2a^{-5})+560(a+b)^{-7}]+c^2[3(a^{-5}b^{-3}+a^{-3}b^{-5})+1536(a+b)^{-8}]\}=1, \quad (6a)$$
$$N_2'=\pi N_2=9.8093\times10^{-2},$$
$$f(\theta)=(128\mu_2N_2'a_0/m)[b(1+a)(I_1{}^0+I_2{}^0-2I_3{}^0)+a(1+b)(I_4{}^0+I_5{}^0-2I_6{}^0)+bc(1+a)(I_1'+I_2'-2I_3')+ac(1+b)(I_4'+I_5'-2I_6')].$$

In (6a) $I_1{}^0$ through $I_6{}^0$ are formally the same as presented under Case I. In order to reduce the integrals of (3b) that contain the term $|\mathbf{x}_1-\mathbf{x}_2|/|\mathbf{x}_2-\mathbf{x}_3|$ as a factor of the integrand, the approximation $A_1=0$ was used.[10] Without this simplification, I_3' and I_6' reduce to triple integrals, and the numerical evaluation of these integrals is prohibitively complicated. Since this approximation limits the accuracy to which $f(\theta)$ can be calculated, this approximation is also used to derive the terms I_2'

[7] S. Chandrasekhar, Astrophys. J. **100**, 176 (1944).
[8] L. R. Heinrich, Astrophys. J. **99**, 59 (1943).
[9] J. D. Jackson and H. Schiff, Phys. Rev. **89**, 359 (1953); E. Corinaldesi and L. Trainor, Nuovo cimento **9**, 940 (1952).
[10] Bransden, Dalgarno, and King, Proc. Phys. Soc. (London) **A67**, 1075 (1954).

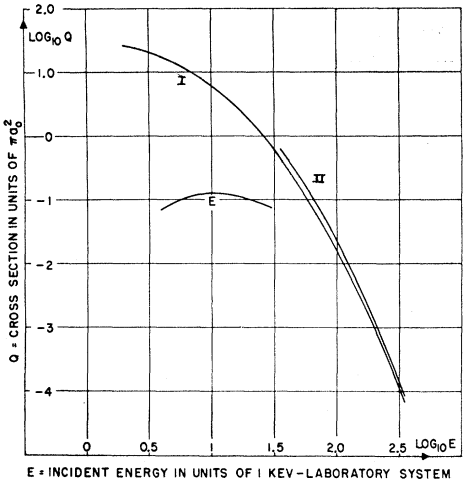

FIG. 1. Cross sections for *capture* (see text for explanation of curves I, II, and E).

and I_5'. I_1' and I_4' are derived without this approximation since little simplification is obtained.

$$I_2'(a,b)=b^{-1}(1+A_3^2)^{-1}\{(3b^2-A_2^2)(a+1)^{-4}\times(b^2+A_2^2)^{-3}+2(a+1)^{-6}(b^2+A_2^2)^{-1}-2(a+1)^{-6}[(a+b+1)^2+A_2^2]^{-1}-(a+b+1)(a+1)^{-5}[(a+b+1)^2+A_2^2]^{-2}\},\tag{6b}$$

$$I_5'(a,b)=I_2'(b,a),$$

$$I_3'(a,b)=2b(a+1)^{-4}I_{31}-b^{-1}(a+1)^{-4}I_{32}+2b^{-1}(a+1)^{-6}I_{33}-2b^{-1}(a+1)^{-6}I_{34}-(a+b+1)b^{-1}(a+1)^{-5}I_{35},$$

$$I_6'(a,b)=I_3'(b,a),$$

$$I_{31}=-\int_0^1 dx\,x(1-x)^2\left(\frac{\partial}{\partial u_1}+\frac{\partial}{\partial v_1}\right)^3\frac{1}{u_1v_1^{\frac{1}{2}}},$$

$$I_{32}=\int_0^1 dx\,x(1-x)\left(\frac{\partial}{\partial u_1}+\frac{\partial}{\partial v_1}\right)^2\frac{1}{u_1v_1^{\frac{1}{2}}},$$

$$I_{33}=-\int_0^1 dx\,x\left(\frac{\partial}{\partial u_1}+\frac{\partial}{\partial v_1}\right)\frac{1}{u_1v_1^{\frac{1}{2}}},\tag{6c}$$

$$I_{34}=-\int_0^1 dx\,x\left(\frac{\partial}{\partial u_2}+\frac{\partial}{\partial v_2}\right)\frac{1}{u_2v_2^{\frac{1}{2}}},$$

$$I_{35}=\int_0^1 dx\,x(1-x)\left(\frac{\partial}{\partial u_2}+\frac{\partial}{\partial v_2}\right)^2\frac{1}{u_2v_2^{\frac{1}{2}}},$$

$$u_1=(1-x)(b^2+A_2^2)+x(1+A_3^2),$$

$$v_1=x+(1-x)b^2+x(1-x)|\mathbf{A}_2-\mathbf{A}_3|^2,$$

$$u_2=(1-x)[(1+a+b)^2+A_2^2]+x(1+A_3^2),$$

$$v_2=x+(1-x)(1+a+b)^2+x(1-x)|\mathbf{A}_2-\mathbf{A}_3|^2,$$

$$I_1'(a,b)=\int_0^1 dx\,x(1-x)\chi_1^{-\frac{1}{2}}\int_0^1 dy\,y(1-y)\times\Bigg(\Bigg\{3y^2\left(\frac{\partial}{\partial u_1}+\frac{\partial}{\partial v_1}\right)^2-3y\chi_1^{-1}\left(\frac{\partial}{\partial u_1}+\frac{\partial}{\partial v_1}\right)+(9/4)\chi_1^{-2}+\left[R^2\left(\frac{\partial}{\partial u_1}+\frac{\partial}{\partial v_1}\right)-2(yR^2+\mathbf{R}\cdot\mathbf{S})\frac{\partial}{\partial v_1}\right]\times\left[2y^3\left(\frac{\partial}{\partial u_1}+\frac{\partial}{\partial v_1}\right)^2-2y^2\chi_1^{-1}\left(\frac{\partial}{\partial u_1}+\frac{\partial}{\partial v_1}\right)+\tfrac{3}{2}y\chi_1^{-2}\right]\Bigg\}\left(\frac{\partial}{\partial u_1}+\frac{\partial}{\partial v_1}\right)^2u_1v_1^{-\frac{1}{2}}-(945/16)y^3v_1^{-11/2}-(105/8)y^2v_1^{-9/2}\chi_1^{-1}-(45/16)v_1^{-7/2}\chi_1^{-2}\Bigg),\tag{6d}$$

$$I_4'(a,b)=I_1'(b,a),$$

$$\chi_1=x(1+a)^2+(1-x)b^2+x(1-x)|\mathbf{A}_1-\mathbf{A}_2|^2,$$

$$u_1=(1-y)(1+A_3^2)+y(1-x)(b^2+A_2^2)+xy[(1+a)^2+A_1^2],$$

$$v_1=(1-y)+y(1-x)b^2+xy(1+a)^2+y(1-y)|\mathbf{A}_2-\mathbf{A}_3|^2,$$

$$R^2=|\mathbf{A}_2+x(\mathbf{A}_1-\mathbf{A}_2)|^2,$$

$$\mathbf{R}\cdot\mathbf{S}=(1-y)\mathbf{A}_3\cdot[\mathbf{A}_2+x(\mathbf{A}_1-\mathbf{A}_2)].$$

A discussion of the derivation of these integrals is presented in the Appendix.

The results of the calculations are presented in Table I and Fig. 1. The curves labelled I and II correspond, respectively, to Cases I and II. Also plotted in Fig. 1 are the experimental results (labelled E) for the cross section per gas atom of reaction (B).[11]

$$H+H_2\rightarrow H^-+H_2^+.\tag{B}$$

A basis for the comparison of the measured values of (B) (curve E in Fig. 1) with the calculated cross sections of (A) is that H_2 behaves like two isolated H atoms in the charge transfer process. Unfortunately, the approximations of this paper are not valid over the energy range for which these measured values exist; consequently, no conclusions can be formed from this comparison. However, there is some evidence that tends to refute the concept that H_2 can be treated as two isolated H atoms.

[11] S. K. Allison, Revs. Modern Phys. **30**, 1137 (1958).

TABLE I. Table of cross sections. Q=cross section in units of $\pi a_0^2=8.79\cdot10^{-17}$ cm^2; E=incident energy of H atom in units of kev—laboratory system.

E	2	3.56	6.32	11.2	20	35.6	63.2	112	200	356
Q(I)	25.8	19.1	11.7	5.60	1.92	$4.94\cdot10^{-1}$	$9.00\cdot10^{-2}$	$1.15\cdot10^{-2}$	$1.05\cdot10^{-3}$	$6.95\cdot10^{-5}$
Q(II)						$6.5\cdot10^{-1}$	$1.2\cdot10^{-1}$	$1.5\cdot10^{-2}$	$1.3\cdot10^{-3}$	$8.5\cdot10^{-5}$

The preliminary theoretical work of Gerjuoy and Tuan[12] shows that no simple relation exists between the cross sections for reactions (C) and (D),

$$H^+ + H \rightarrow H + H^+, \quad \text{(C)}$$

$$H^+ + H_2 \rightarrow H + H_2^+, \quad \text{(D)}$$

although the calculated values of (C) agree very well with the measured values of (D).[13] Thus, any conclusions concerning the validity of the approximations of this paper will have to await the support of future measurements of (A).

ACKNOWLEDGMENTS

In conclusion the author wishes to express his gratitude to Dr. A. Dalgarno of the Queen's University of Belfast for several instructive conversations relevant to this work, and particularly to Dr. F. R. Innes, of this laboratory, for his painstaking criticism of the application of the Pauli Exclusion Principle to problems of this type.

All numerical calculations were performed on the IBM-704 by the New York Data Processing Center of the Service Bureau Corporation.

APPENDIX

The procedure for deriving the integral I' of Case II illustrates the methods of integration used in this paper. Consider the integral given by

$$I=\int d\mathbf{x}_1 d\mathbf{x}_2 d\mathbf{x}_3 \frac{|\mathbf{x}_1-\mathbf{x}_2|}{|\mathbf{x}_3+\mathbf{x}_1-\mathbf{x}_2|}\exp[i(\mathbf{A}_1\cdot\mathbf{x}_1-\mathbf{A}_2\cdot\mathbf{x}_2+\mathbf{A}_3\cdot\mathbf{x}_3)-(a+1)x_1-bx_2-x_3]. \quad \text{(A1a)}$$

The following two integral representations are introduced to facilitate the integrations over the nine-dimensional configuration space:

$$|\mathbf{x}_1-\mathbf{x}_2|=\frac{1}{2\pi^2}\lim_{\alpha\rightarrow0}\frac{\partial^2}{\partial\alpha^2}\int\frac{d\mathbf{K}_2}{K_2^2+\alpha^2}\exp[i\mathbf{K}_2\cdot(\mathbf{x}_1-\mathbf{x}_2)],$$

$$|\mathbf{x}_3+\mathbf{x}_1-\mathbf{x}_2|^{-1}=\frac{1}{2\pi^2}\lim_{\epsilon\rightarrow0}\times\int\frac{d\mathbf{K}_1}{K_1^2+\epsilon^2}\exp[i\mathbf{K}_1\cdot(\mathbf{x}_3+\mathbf{x}_1-\mathbf{x}_2)].$$

With these representations inserted into (A1a) the coordinate integrations are performed to get (A1b).

$$I=\frac{(8\pi)^3b(1+a)}{4\pi^4}\int\frac{d\mathbf{K}_1}{K_1^2+\epsilon^2}\frac{\partial^2}{\partial\alpha^2}\int\frac{d\mathbf{K}_2}{K_2^2+\alpha^2}\times[(1+a)^2+|\mathbf{A}_1+\mathbf{K}_1+\mathbf{K}_2|^2]^{-2}\times[b^2+|\mathbf{A}_2+\mathbf{K}_1+\mathbf{K}_2|^2]^{-2}[1+|\mathbf{A}_3+\mathbf{K}_1|^2]^{-2}. \quad \text{(A1b)}$$

In writing (A1b) and all following relations, the limit operations are understood. The Feynman integral representation

$$(ab)^{-2}=b\int_0^1 dx\, x(1-x)[b+(a-b)x]^{-4}$$

(see reference 9) is used for the relevant factors of the integrand so that the $\mathbf{K}_2$-integration can be performed. The $\mathbf{K}_2$-integration is then done and the operation $\lim_{\alpha\rightarrow0}\partial^2/\partial\alpha^2$ is performed so that (A1b) is reduced to

$$I=\frac{(8\pi)^3b(1+a)}{2\pi^2}\int\frac{d\mathbf{K}_1}{K_1^2+\epsilon^2}[1+|\mathbf{A}_3+\mathbf{K}_1|^2]^{-2}\times\int_0^1 dx\, x(1-x)[18\Delta_1^{-4}\chi_1^{-\frac{1}{2}}+6\Delta_1^{-3}\chi_1^{-\frac{3}{2}}+(9/4)\Delta_1^{-2}\chi_1^{-\frac{5}{2}}-48Q^2\Delta_1^{-5}\chi_1^{-\frac{1}{2}}-12Q^2\Delta_1^{-4}\chi_1^{-\frac{3}{2}}-3Q^2\Delta_1^{-3}\chi_1^{-\frac{5}{2}}], \quad \text{(A1c)}$$

$$Q^2=|\mathbf{A}_2+x(\mathbf{A}_1-\mathbf{A}_2)+\mathbf{K}_1|^2,$$

$$\Delta_1=(1-x)(b^2+A_2^2)+x[(1+a)^2+A_1^2]+K_1^2+2[\mathbf{A}_2+x(\mathbf{A}_1-\mathbf{A}_2)]\cdot\mathbf{K}_1,$$

$$\chi_1=(1-x)b^2+x(1+a)^2+x(1-x)|\mathbf{A}_1-\mathbf{A}_2|^2.$$

The integration of (A1c) over $\mathbf{K}_1$-space is simplified by the introduction of the Feynman representations for the terms $\Delta_1^{-n}[1+|\mathbf{A}_3+\mathbf{K}_1|^2]^{-2}$ with $n=2, 3, 4, 5$. These

[12] T. F. Tuan and E. Gerjuoy, Bull. Am. Phys. Soc. **3**, 171 (1958).

[13] See Jackson and Schiff, reference 9.

representations permit (A1c) to be written as

$$I=\frac{(8\pi)^3 b(1+a)}{2\pi^2}\int_0^1 dx\, x(1-x)$$
$$\times\int_0^1 dy\int\frac{d\mathbf{K}_1}{K_1^2+\epsilon^2}\chi_1^{-\frac{1}{2}}\Big\{360y^3(1-y)Z_1^{-6}$$
$$+72y^2(1-y)\chi_1^{-1}Z_1^{-5}+\frac{54}{4}y(1-y)\chi_1^{-2}Z_1^{-4}$$
$$-Q^2[1440y^4(1-y)Z_1^{-7}+240y^3(1-y)\chi_1^{-1}Z_1^{-6}$$
$$+36y^2(1-y)\chi_1^{-2}Z_1^{-5}]\Big\}, \quad \text{(A1d)}$$
$$u_1=(1-y)(1+A_3^2)+y(1-x)(b^2+A_2^2)$$
$$+xy[(1+a)^2+A_1^2],$$
$$\mathbf{R}=\mathbf{A}_2+x(\mathbf{A}_1-\mathbf{A}_2),\quad \mathbf{T}=(1-y)\mathbf{A}_3+y\mathbf{R},$$
$$Q^2=|\mathbf{R}+\mathbf{K}_1|^2,\qquad Z_1=K_1^2+2\mathbf{T}\cdot\mathbf{K}_1+u_1.$$

The following relations are used to perform the $\mathbf{K}_1$-integration:

$$\frac{2\mathbf{K}_1\cdot\mathbf{R}}{Z_1^n}=-\frac{R}{(n-1)y}\frac{\partial}{\partial R}Z_1^{-(n-1)},$$
$$\int\frac{d\mathbf{K}_1}{[K_1^2+\epsilon^2]Z_1^n}=\frac{\pi^2(-1)^n}{(n-1)!}\frac{\partial^{n-2}}{\partial u_1^{n-2}}u_1^{-1}v_1^{-\frac{1}{2}},$$
$$\int\frac{d\mathbf{K}_1K_1^2}{[K_1^2+\epsilon^2]Z_1^n}=\frac{\pi^2(-1)^n}{(n-1)!}\frac{\partial^{n-2}}{\partial u_1^{n-2}}v_1^{-\frac{1}{2}},$$
$$v_1=u_1-T^2,\quad R=|\mathbf{R}|.$$

With the new notation (A1d) reduces to

$$I=\frac{(8\pi)^3 b(1+a)}{2}\int_0^1 dx\, x(1-x)\chi_1^{-\frac{1}{2}}\int_0^1 dy\, y(1-y)$$
$$\times\Big\{\Big[3y^2\frac{\partial^4}{\partial u_1^4}-3y\chi_1^{-1}\frac{\partial^3}{\partial u_1^3}+\frac{9}{4}\chi_1^{-2}\frac{\partial^2}{\partial u_1^2}$$
$$+R^2\Big(2y^3\frac{\partial^5}{\partial u_1^5}-2y^2\chi_1^{-1}\frac{\partial^4}{\partial u_1^4}+\frac{3y}{2}\chi_1^{-2}\frac{\partial^3}{\partial u_1^3}\Big)$$
$$+R\frac{\partial}{\partial R}\Big(2y^3\frac{\partial^4}{\partial u_1^4}-2y^2\chi_1^{-1}\frac{\partial^3}{\partial u_1^3}+\frac{3y}{2}\chi_1^{-2}\frac{\partial^2}{\partial u_1^2}\Big)\Big]u_1^{-1}v_1^{-\frac{1}{2}}$$
$$+\Big[2y^3\frac{\partial^5}{\partial u_1^5}-2y^2\chi_1^{-1}\frac{\partial^4}{\partial u_1^4}+\frac{3y}{2}\chi_1^{-2}\Big]v_1^{-\frac{1}{2}}\Big\}. \quad \text{(A1e)}$$

With the omission of the factor outside the integral sign (A1e) can be written in the form given for I_1' under Case II in the main body of this paper.

PHYSICAL REVIEW VOLUME 117, NUMBER 2 JANUARY 15, 1960

Range Straggling of Charged Particles in Be, C, Al, Cu, Pb, and Air*

R. M. STERNHEIMER
Brookhaven National Laboratory, Upton, New York
(Received August 5, 1959)

The straggling of the range of charged particles due to fluctuations of the ionization loss has been evaluated for six substances (Be, C, Al, Cu, Pb, and air). The calculations extend up to $T/\mu c^2\sim 100$, where T is the kinetic energy and μ is the mass of the incident particle. At high energies ($T/\mu c^2\gtrsim 5$), the integral giving the range straggling becomes somewhat dependent on the ratio μ/m, where m is the electron mass. Two separate calculations have therefore been carried out, which apply to protons and μ mesons, respectively. The results for protons can also be used for π and K mesons in the energy range of interest ($T/\mu c^2\lesssim 5$).

I. INTRODUCTION

RECENTLY tables of the range-energy relations for protons[1] have been obtained for several substances, which are based on accurate values[2] of the mean excitation potential I. These tables were calculated up to a maximum proton energy $T_p=100$ Bev, in order to enable one to obtain ranges of μ mesons up to an energy $T_\mu\sim 10$ Bev. The calculations were carried out for Be, C, Al, Cu, Pb, and air. In connection with these tables, it seemed of interest also to obtain the range straggling due to the fluctuations of the ionization loss process as given by the theory of Bohr.[3] In the present paper, we give the results of these calculations. It may be noted that the range straggling in nuclear emulsion has been previously investigated by Barkas,

* Work performed under the auspices of the U. S. Atomic Energy Commission.
[1] R. M. Sternheimer, Phys. Rev. **115**, 137 (1959). This paper will be referred to as I.
[2] Bichsel, Mozley, and Aron, Phys. Rev. **105**, 1788 (1957); V. C. Burkig and K. R. MacKenzie, Phys. Rev. **106**, 848 (1957); D. O. Caldwell, Phys. Rev. **100**, 291 (1955).
[3] N. Bohr, Phil. Mag. **30**, 581 (1915).