Simultaneous Ionization and Excitation of Helium by Protons

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

(Received June 21, 1957)

Born's approximation is used to calculate the cross sections for ionization and simultaneous ionization and excitation of helium by collision with protons.

SIMULTANEOUS excitation and ionization of atoms by collisions with protons appears not to have been treated previously. This process, apart from possessing interest itself, is important for the description of auroral and other upper atmospheric phenomena. The simplest case to consider is the collision of protons with helium atoms, and this is the program of this paper.

The nonrelativistic Schrödinger equation for the problem is

$$(H_0+H_i)\psi=E\psi. \tag{1a}$$

$$H_0=-\frac{\hbar^2}{2\mu_2}\nabla_{\gamma_2}{}^2-\frac{\hbar^2}{2\mu_1}(\nabla_{\gamma_3}{}^2+\nabla_{\gamma_4}{}^2)-\frac{\hbar^2}{M_N}\nabla_{\gamma_3}\cdot\nabla_{\gamma_4}$$
$$-\frac{2e^2}{|\gamma_3|}-\frac{2e^2}{|\gamma_4|}+\frac{e^2}{|\gamma_3-\gamma_4|}. \tag{1b}$$

$$H_i=-\frac{e^2}{|\gamma_2-(M_1/M_2)\gamma_3+(m/M_2)\gamma_4|}$$
$$-\frac{e^2}{|\gamma_2+(m/M_2)\gamma_3-(M_1/M_2)\gamma_4|}$$
$$+\frac{2e^2}{|\gamma_2+(m/M_2)(\gamma_3+\gamma_4)|}. \tag{1c}$$

Here the masses are: m—electron; M—proton; M_N—helium nucleus, $M_1=M_N+m$, $M_2=M_N+2m$, $\mu_1=mM_N/M_1$, $\mu_2=MM_2/(M+M_2)$. The laboratory coordinates are: $\mathbf{r}_1$, $\mathbf{r}_2$—electrons; $\mathbf{r}_N$—helium nucleus; $\mathbf{R}$—proton.

$$\gamma_2=\mathbf{R}-[M_N\mathbf{r}_N+m(\mathbf{r}_1+\mathbf{r}_2)]/M_2,$$
$$\gamma_3=\mathbf{r}_1-\mathbf{r}_N,$$
$$\gamma_4=\mathbf{r}_2-\mathbf{r}_N.$$

e=electron charge, and $\hbar$=Planck's constant$\div 2\pi$.

Since the center-of-mass coordinate has been eliminated, E is the energy of relative motion in Eq. (1a).

The Born amplitude can now be obtained by any of the standard methods and is

$$f_0{}^{n,k}=-\frac{\mu_2}{2\pi\hbar^2}\int d\gamma_2 d\gamma_3 d\gamma_4$$
$$\times\exp(i\mathbf{A}\cdot\gamma_2)\psi_{k,n}(\gamma_3,\gamma_4)H_i\psi_0(\gamma_3,\gamma_4). \tag{2}$$

Bethe's formula,[1]

$$\frac{4\pi}{A^2}\exp(i\mathbf{A}\cdot\mathbf{r})=\int\frac{\exp(i\mathbf{A}\cdot\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}',$$

is employed to reduce Eq. (2) to

$$f_0{}^{n,k}=\frac{2\mu_2e^2}{\hbar^2}\int d\gamma_3 d\gamma_4\psi_{k,n}{}^*(\gamma_3,\gamma_4)[\exp i(\mathbf{A}_1\cdot\gamma_3-\mathbf{A}_2\cdot\gamma_4)$$
$$+\exp i(\mathbf{A}_1\cdot\gamma_4-\mathbf{A}_2\cdot\gamma_3)$$
$$-2\exp i\mathbf{A}_2\cdot(\gamma_3+\gamma_4)]\psi_0(\gamma_3,\gamma_4). \tag{2a}$$

Here K_0, K_n are the initial and final wave vectors of relative motion, respectively; k, n label the positive energy electron and bound electron of the final state, respectively, and 0 labels the singlet ground state of the helium atom.

$$\mathbf{A}=\mathbf{K}_0-\mathbf{K}_n,\quad \mathbf{A}_1=\frac{M_1}{M_2}\mathbf{A},\quad A_2=\frac{m}{M_2}\mathbf{A}.$$

For inelastic collisions of protons with hydrogen, one can easily demonstrate that it is permissible to neglect m as compared to M with little error in the results. In this problem such an approximation is equivalent to putting $A_2=0$, $A_1=A$, $\mu_1=m$, and $\mu_2=MM_N/(M+M_N)$. Then Eq. (2a) becomes

$$f_0{}^{n,k}=\frac{2\mu_2e^2}{\hbar^2A^2}\int d\gamma_3 d\gamma_4\psi_{k,n}{}^*(\gamma_3,\gamma_4)[\exp(i\mathbf{A}\cdot\gamma_3)$$
$$+\exp(i\mathbf{A}\cdot\gamma_4)]\psi_0(\gamma_3,\gamma_4), \tag{2b}$$

in which reduction the orthogonality relation $(\psi_{k,n},\psi_0)=0$ is invoked. The expression given by Eq. (2b) could have been obtained directly by the use of the relative coordinate $\gamma_2'=\mathbf{R}-\mathbf{r}_N$; however, H_i would have contained a term $(\hbar^2/M_N)\nabla_{\gamma_2'}\cdot(\nabla_{\gamma_3}+\nabla_{\gamma_4})$. Thus, the neglect of m as compared to M and M_N is equivalent to replacing γ_2 by γ_2' and dropping the term $\nabla_{\gamma_2'}\cdot(\nabla_{\gamma_3}+\nabla_{\gamma_4})$.

The helium wave functions are approximated by products of normalized hydrogen wave functions. Thus, $\psi_{(1s)^2}=\psi_0=\phi_0(Z_1|\gamma_3)\phi_0(Z_1|\gamma_4)$ with $Z_1=1.6875$, and

[1] H. Bethe, Ann. Physik 5, 325 (1930).

where ϕ_0 is the ground state wave function.

$$\psi_{k,n}(\gamma_3,\gamma_4)=\frac{1}{\sqrt{2}}[\phi_k(Z_3|\gamma_3)\phi_n(Z_2|\gamma_4)+\phi_k(Z_3|\gamma_4)\phi_n(Z_2|\gamma_3)], \quad (2c)$$

ϕ_k being the positive energy function for a Coulomb field of charge $(-Z_3e)$ and ϕ_n the bound state case for a field of charge $(-Z_2e)$. Of course, only singlet excitation need be considered since only electrostatic interaction terms are included. Atomic units are now introduced and the symmetry properties are used to reduce Eq. (2b) to

$$f_{(1s)^2n,k}=\frac{2\sqrt{2}\mu_2 Z_1^3 a_0}{\pi m A^2}\int d\gamma_3 d\gamma_4[\phi_k^*(Z_3|\gamma_3)\phi_n^*(Z_2|\gamma_4)+\phi_k^*(Z_3|\gamma_4)\phi_n^*(Z_2|\gamma_3)]\times\exp[i\mathbf{A}\cdot\gamma_3-Z_1(\gamma_3+\gamma_4)], \quad (2d)$$

in which relation a_0 is the Bohr radius, and ϵ_0 is 13.61 ev.

The cross section, Q, is given by $Q_0^{n,k}=\int d\mathbf{k}d\Omega|f_0^{n,k}|^2$, with $d\mathbf{k}$ the volume element in the space of the wave vector of the ejected electron, and with $d\Omega$ the solid angle of the scattered protons. If ϵ_0 and ϵ_n are the binding energies of the initial and final atomic states, respectively, conservation of energy requires that

$$\frac{\hbar^2K_0^2}{2\mu_2}-\epsilon_0=\frac{\hbar^2K_n^2}{2\mu_2}+\frac{\hbar^2k^2}{2m}-\epsilon_n=E,$$

with ϵ_0 and ϵ_n positive. It is convenient to introduce the momentum-change variables in place of $d\Omega$,[2] $d\Omega=2\pi AdA/(K_0K_n)$, and to use spherical coordinates in $\mathbf{k}$-space, $d\mathbf{k}=k^2dkd\Omega_k$.

The limits of integration for dA, in atomic units, are

$$A_{\min}=K_0-K_n\doteq\frac{1}{2}\left[\frac{\mu_2\epsilon_0}{mE_0}\right]^{\frac{1}{2}}\frac{\Delta E}{\epsilon_0}\left[1+\frac{\Delta E}{4E_0}\right], \quad E_0=\frac{\hbar^2K_0^2}{2\mu_2};$$

$$A_{\max}=K_0+K_n\doteq 2K_0,$$

provided that $\Delta E\ll E_0$, with $\Delta\epsilon=\epsilon_k+(\epsilon_0-\epsilon_n)$, and ϵ_k is the energy of the ejected electron. $A_{\max}$ can be set equal to infinity, since in the cases considered the integrands, as a function of A, decrease to negligibly small values for $A<A_{\max}$. The limit of integration for dk is $k=0$ to $k=k_{\max}$, $k_{\max}$ being derived from the energy relations, *viz.*,

$$k_{\max}=\left[\frac{m}{\mu_2}K_0^2-\frac{2m}{\hbar^2}(\epsilon_0-\epsilon_n)\right]^{\frac{1}{2}}, \quad K_n=0.$$

The first cases considered are excitation to states in which He^+ is in a $n\,^2S_{\frac{1}{2}}$ state.

[2] W. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Oxford University Press, New York, 1949), second edition, Chap. XI.

Case I. $Z_3=1$, $Z_2=2$

There is clearly a violation of orthogonality between initial and final atomic states for this choice of Z_3 and Z_2. Moreover, the violation of orthogonality arises from the S-wave part of ϕ_k. With this type of final-state wave function for single excitation of helium to the bound states $n\,^1P$, $n\,^1D$, and $n\,^1F$ by electron impact, and with the same initial state as ψ_0 in this paper, Massey and Mohr[3] obtained cross sections in fair agreement with experiment. However, to obtain cross sections to bound states of the $n\,^1S$-type, more elaborate final state functions were required to insure orthogonality and reasonable bound-state energy values. Since the final state wave function for ionization is a mixture of states $n\,^1S$, $n\,^1P$, $n\,^1D$, $\cdots$, only one being an $n\,^1S$-type (n now labels the overlapping discrete and continuous spectra), this type of final state function was tried, although others[4] have cautioned that the violation of orthogonality is likely to give absurd results for the cross-section–energy dependence.

The function ϕ_k is given by[5]

$$\phi_k(Z_3|\gamma)=\frac{1}{2\pi}\left[\frac{in}{1-\exp(-i2\pi n)}\right]^{\frac{1}{2}}\frac{\exp(ik\gamma)}{\Gamma(1+n)}\times\int_0^\infty duu^nJ_0[2(iku\eta)^{\frac{1}{2}}]\exp(-u)$$

$$=\frac{1}{2\pi\Gamma(1+n)}\left(\frac{in}{1-\exp(-i2\pi n)}\right)^{\frac{1}{2}}\exp(ik\gamma)\times\sum_{l=0}^{\infty}\frac{i^l\Gamma(l+1+n)(2k\gamma)^l}{(2l)!}P_l(\cos\theta)\times F(l+1+n,\,2l+2,\,-i2k\gamma), \quad (3a)$$

with $n=Z_3/ik$ and $\eta=\gamma(1-\cos\theta)$, θ being the angle between γ and the direction of ejection.

For spherical coordinates in $\mathbf{k}$-space, ϕ_k is normalized so that

$$\int\phi^*_{k_2}(\gamma)\phi_{k_1}(\gamma)d\gamma=\frac{\delta(k_1-k_2)\delta(\theta_1-\theta_2)}{2\pi k_1^2\sin^2\theta_1}. \quad (3b)$$

That this is correct can be seen from the series representation of ϕ_k for large k (small n),

$$\lim_{n\to 0}\phi_k=\left(\frac{1}{2\pi}\right)^{\frac{3}{2}}\sum_{l=0}^{\infty}(2l+1)i^lP_l(\cos\theta)\frac{\sin(k\gamma-\frac{1}{2}l\pi)}{k\gamma}=(2\pi)^{-\frac{3}{2}}\exp(i\mathbf{k}\cdot\gamma),$$

a normalized plane wave.[6]

[3] H. S. W. Massey and C. B. O. Mohr, Proc. Roy. Soc. (London) **140**, 613 (1933).

[4] Bates, Fundaminsky, and Massey, Trans. Roy. Soc. (London) **A243**, 93 (1950).

[5] A. Sommerfeld, Ann. Physik **11**, 257 (1951); also see Chap. III of reference 2.

[6] See p. 49 of reference 2.

The integrations over coordinate space and the solid angle of **k**-space are performed to give the following results, in which Q is in units of πa_0^2, and E_0 is in units of kev.

$$(1s)^2 \rightarrow 1s, k$$

$$U=\frac{Z_3}{2k}\ln\left[\frac{(A+k)^2+Z_1^2}{(A-k)^2+Z_1^2}\right],$$

$$I_{D^2}=k\{3[(Z_1+Z_3)A^2+(Z_1-Z_3)(Z_1^2+k^2)]^2+4Z_1^2A^2(Z_3^2+k^2)\}$$

$$\times\frac{\exp\left\{-\frac{2Z_3}{k}\left[\frac{\pi}{2}-\tan^{-1}\left(\frac{A^2-k^2+Z_1^2}{2Z_1k}\right)\right]\right\}}{[1-\exp(-i2\pi n)]A^3[(A-k)^2+Z_1^2]^3[(A+k)^2+Z_1^2]^3},$$

$$I_{B^2}=\frac{k\exp\left[-\frac{4Z_3}{k}\tan^{-1}\left(\frac{k}{Z_1}\right)\right]}{[1-\exp(-i2\pi n)]A^3(Z_1^2+k^2)^4}, \tag{4a}$$

$$I_{BD}=\frac{2k[(A^2-k^2-Z_1^2)\sin U+2Z_1A\cos U]\exp\left\{-\frac{2Z_3}{k}\tan^{-1}\left(\frac{k}{Z_1}\right)-\frac{Z_3}{k}\left[\frac{\pi}{2}-\tan^{-1}\left(\frac{A^2-k^2+Z_1^2}{2Z_1k}\right)\right]\right\}}{[1-\exp(-i2\pi n)]A^4(k^2+Z_1^2)^2},$$

$$p_1=Z_1+Z_2, \quad n=Z_3/ik, \quad \Delta E=\epsilon_k+24.463 \text{ ev}, \quad y=(A^2+p_1^2)^{-2}.$$

$$Q=\frac{1}{E_0}\int_0^{k_{\max}}dk\int_{A_{\min}}^{\infty}dA[3.205\times10^4I_{D^2}+1.554\times10^9y^2I_{B^2}+6.112\times10^6yI_{BD}].$$

$$(1s)^2 \rightarrow 2s, k$$

The previous remarks relevant to the final atomic states do not apply here, since this is simultaneous excitation and ionization. This will be discussed at an appropriate place.

$$\Delta E=\epsilon_k+65.293 \text{ ev}, \quad p_2=Z_1+\tfrac{1}{2}Z_2,$$

$$y=[(Z_1+Z_2)A^2+(Z_1-Z_2)p_2^2][A^2+p_2^2]^{-3},$$

$$Q=\frac{1}{E_0}\int_0^{k_{\max}}dk\int_{A_{\min}}^{\infty}dA[3.615\times10^2I_{D^2}+1.428\times10^7y^2I_{B^2}-6.233\times10^4yI_{BD}]. \tag{4b}$$

$$(1s)^2 \rightarrow 3s, k$$

$$\Delta E=\epsilon_k+72.854 \text{ ev}, \quad p_3=Z_1+\tfrac{1}{3}Z_2,$$

$$y=[9p_3+6Z_2(A^2-3p_3^2)(A^2+p_3^2)^{-1}-8Z_2^2p_3(A^2-p_3^2)(A^2+p_3^2)^{-2}][A^2+p_3^2]^{-2}, \tag{4c}$$

$$Q=\frac{1}{E_0}\int_0^{k_{\max}}dk\int_{A_{\min}}^{\infty}dA[5.810\times10I_{D^2}+5.225\times10^4y^2I_{B^2}-1.509\times10^3yI_{BD}].$$

The cross sections are presented in Figs. 1, 2, and 3, and are labeled "I."

Case II. $Z_3=Z_1$, $Z_2=2$, $n=Z_1/(ik)$

Apart from the fact that $Z_2=2$, this is the case treated by Massey and Mohr[7] for electron impact, neglecting exchange. Consequently, attention is directed to the fact that in the approximation used in this paper, the Born amplitude for electron impact, as given by Massey and Mohr (see reference 7), is obtained

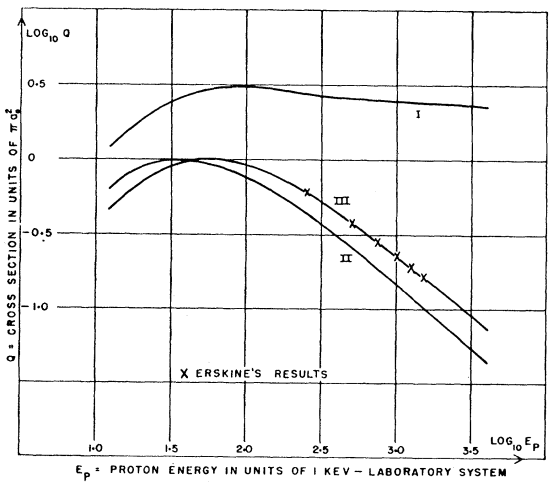

FIG. 1. Cross sections for ionization. (See text for explanation of curves I, II, and III.)

[7] See reference 3, and reference 2, Chap. XI, Sec. 2.2.

from Eq. (2d) with the replacement of μ_2 by m.

$$I_{D^2}=\frac{4Z_1^2k[3A^2+Z_1^2+k^2]\exp\left\{-\frac{2Z_1}{k}\left[\frac{\pi}{2}-\tan^{-1}\frac{A^2-k^2+Z_1^2}{2Z_1k}\right]\right\}}{[1-\exp(-i2\pi n)]A[(A-k)^2+Z_1^2]^3[(A+k)^2+Z_1^2]^3},\quad n=Z_1/ik. \tag{5a}$$

$$(1s)^2\rightarrow 1s,\ k$$

$$Q=\frac{5.409\times10^4}{E_0}\int_0^{k_{\max}}dk\int_{A_{\min}}^{\infty}dAI_{D^2}. \tag{5b}$$

$$(1s)^2\rightarrow 2s,\ k$$

$$Q=\frac{6.100\times10^2}{E_0}\int_0^{k_{\max}}dk\int_{A_{\min}}^{\infty}dAI_{D^2}. \tag{5c}$$

$$(1s)^2\rightarrow 3s,\ k$$

$$Q=\frac{9.804\times10}{E_0}\int_0^{k_{\max}}dk\int_{A_{\min}}^{\infty}dAI_{D^2}. \tag{5d}$$

These results are labeled "II," in Figs. 1, 2, and 3.

Case III

In this case $Z_3=Z_1$ for the $l=0$ term of ϕ_k, and $Z_3=1$ for $l>0$. This insures orthogonality of the atomic states considered. Thus, the continuum part of the wave function is

$$\psi_k=\phi_k(1|\mathbf{r})-\phi_k^0(1|\mathbf{r})+\phi_k^0(Z_1|\mathbf{r}),$$

with $\phi_k(1|\mathbf{r})$ as before, and ϕ_k^0 the $l=0$ part of ϕ_k. A calculation shows that

$$\int\psi_{k_2}^*(r)\psi_{k_1}(r)dr=\frac{\delta(k_2-k_1)\delta(\theta_2-\theta_1)}{2\pi k_1^2\sin\theta_1},$$

as in Eq. (3b), so that the normalization is unchanged.

$$n_1=\frac{Z_1}{ik},\quad n_2=\frac{1}{ik},\quad U_1=\frac{Z_1}{2k}\ln\left[\frac{(A+k)^2+Z_1^2}{(A-k)^2+Z_1^2}\right],$$

$$U_2=\frac{1}{2k}\ln\left[\frac{(A+k)^2+Z_1^2}{(A-k)^2+Z_1^2}\right],$$

I_{D^2} is the same as in Eq. (4a) with $Z_3=1$.

$$I_1=\frac{3Z_1k[(A^2-k^2-Z_1^2)\sin U_1+2Z_1A\cos U_1]^2\exp\left\{-\frac{2Z_1}{k}\left[\frac{\pi}{2}-\tan^{-1}\left(\frac{A^2-k^2+Z_1^2}{2Z_1k}\right)\right]\right\}}{4[1-\exp(-i2\pi n_1)]A^5[(A-k)^2+Z_1^2]^2[(A+k)^2+Z_1^2]^2},$$

$$I_2=\frac{3k[(A^2-k^2-Z_1^2)\sin U_2+2Z_1A\cos U_2]^2\exp\left\{-\frac{2}{k}\left[\frac{\pi}{2}-\tan^{-1}\left(\frac{A^2-k^2+Z_1^2}{2Z_1k}\right)\right]\right\}}{4[1-\exp(-i2\pi n_2)]A^5[(A-k)^2+Z_1^2]^2[(A+k)^2+Z_1^2]^2}, \tag{6a}$$

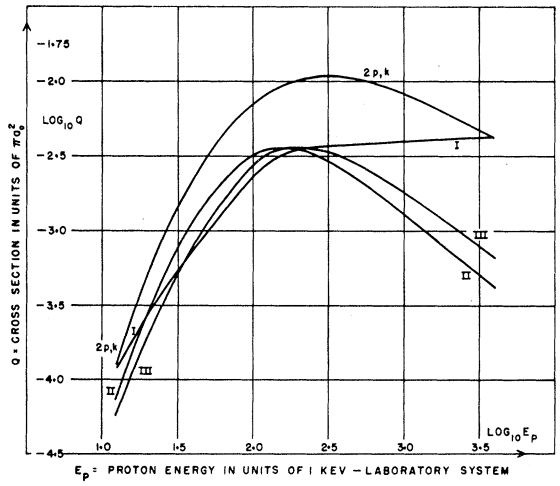

FIG. 2. Cross sections for simultaneous excitation and ionization to the states $2p,\ k$ and $2s,\ k$. (See text for explanation of I, II, and III.)

$$(1s)^2\rightarrow 1s,\ k$$

$$Q=\frac{3.205\times10^4}{E_0}\int_0^{k_{\max}}dk\int_{A_{\min}}^{\infty}dA[I_{D^2}+I_1-I_2]. \tag{6b}$$

$$(1s)^2\rightarrow 2s,\ k$$

$$Q=\frac{3.615\times10^2}{E_0}\int_0^{k_{\max}}dk\int_{A_{\min}}^{\infty}dA[I_{D^2}+I_1-I_2]. \tag{6c}$$

$$(1s)^2\rightarrow 3s,\ k$$

$$Q=\frac{5.810\times10}{E_0}\int_0^{k_{\max}}dk\int_{A_{\min}}^{\infty}dA[I_{D^2}+I_1-I_2]. \tag{6d}$$

These cross sections are labeled "III" in curves 1, 2, and 3.

For the configurations $2p,\ k$, $3p,\ k$, and $3d,\ k$ of helium, the final state wave functions with $Z_3=1$, $Z_2=2$ are orthogonal to the ground state function.

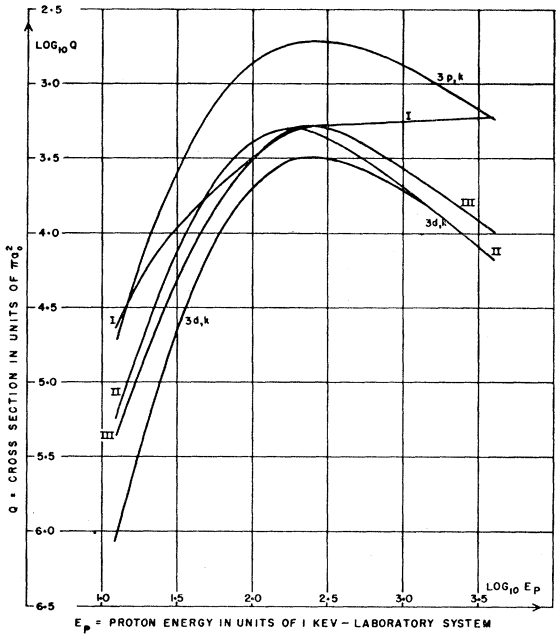

FIG. 3. Cross sections for simultaneous excitation and ionization to the states $3s, k$; $3p, k$; and $3d, k$. (See text for explanation of curves I, II, and III.)

Let

$$I=\frac{k\exp[-(4Z_3/k)\tan^{-1}(k/Z_1)]}{[1-\exp(-i2\pi n)](k^2+Z_1^2)^4}.$$

$$(1s)^2\rightarrow 2p, k$$

In this case p_2 and ΔE are the same as in Eq. (4b).

$$Q=\frac{1.651\times 10^9}{E_0}\int_0^{k_{\max}}dk\int_{A_{\min}}^{\infty}dA\frac{I}{A(A^2+p_2^2)^6}. \quad (7a)$$

$$(1s)^2\rightarrow k, 3p$$

In this case p_3 and ΔE are the same as in Eq. (4c).

$$Q=\frac{1.236\times 10^7}{E_0}\int_0^{k_{\max}}dk\,I\int_{A_{\min}}^{\infty}\frac{dA}{A(A^2+p_3^2)^6}\times\left[6+\frac{Z_2}{p_3}\left(\frac{A^2-5p_3^2}{A^2+p_3^2}\right)\right]^2. \quad (7b)$$

$$(1s)^2\rightarrow 3d, k.$$

In this case p_3 and ΔE are the same as in Eq. (4c).

$$Q=\frac{4.236\times 10^7}{E_0}\int_0^{k_{\max}}dk\,I\times\left[\frac{1}{(A_{\min}^2+p_3^2)^7}-\frac{1}{(A_{\max}^2+p_3^2)^7}\right]. \quad (7c)$$

These cross sections are displayed in Figs. 2 and 3.

DISCUSSION

In all of the following comparisons with other theoretical calculations, the same initial-state atomic wave function is used. Ionization cross sections for α-particle impact and electron impact neglecting exchange have been performed by Erskine,[8] and his work provides a comparison with the measured cross sections of Smith[9] as well as the calculated cross sections of this paper. Erskine's final-state wave function see [Eq. (2c)] used $Z_2=2$ for $\phi_{1s}(Z_2|\gamma)$ and employed $Z_3=Z_1$ for all $l\neq 1$ in $\phi_k(Z_3|\gamma)$ [see Eq. (3a)]. For $l=1$, the p-wave, the radial function was obtained by integrating the radial wave equation numerically for a positive energy electron moving in the average field of the $1\,^2S_{\frac{1}{2}}$ state of the helium ion. This field, $V(r)$, is given by

$$V(r)=-e^2\left[\frac{1}{r}+\left(\frac{2}{a_0}+\frac{1}{r}\right)\exp\left(-\frac{4r}{a_0}\right)\right].$$

For 6-Mev α particles, his calculations show that about 70% of the total Coulomb cross section comes from the p-wave Coulomb cross section; moreover, for this same energy, the p-wave cross section derived from the field $V(r)$ is roughly twice as large as the corresponding Coulomb p-wave cross section. Since the cross sections for electron impact calculated by Erskine agreed very well with Smith's[9] experimental results for electron energies above 400 ev, and showed a substantial improvement over the previously calculated results of Massey and Mohr,[10] it is believed that the α-particle cross sections likewise are rather accurate.

The ionization cross sections for proton impact are now derived from those of α-particle impact. Let v_0 be the velocity for both particles, μ', E', the reduced mass and energy for α particles; μ_2, E_0, the same quantities for protons. Consequently, the relation for energy is

$$E_0=\tfrac{1}{2}\mu_2 v_0^2=\frac{\mu_2}{\mu'}E',$$

and thus

$$A_{\min}\doteq\frac{1}{2}\left(\frac{\mu_2\epsilon_0}{mE_0}\right)^{\frac{1}{2}}\frac{\Delta E}{\epsilon_0}=\frac{1}{2}\left(\frac{\mu'\epsilon_0}{mE'}\right)^{\frac{1}{2}}\frac{\Delta E}{\epsilon_0},$$

if one neglects the small correction factors $1+\Delta E/4E_0$ and $1+\Delta E/4E'$. Therefore,

$$A_{\min}(p;E,\mu_2)=A_{\min}(\alpha;E',\mu').$$

The cross section for α particles, Q_α, is

$$Q_\alpha=\frac{CZ_\alpha^2\mu'}{mE'}\int_0^{k_{\max}}dk\int_{A_{\min}(\alpha;E',\mu)}^{\infty}dAI(A,k)\doteq\frac{CZ_\alpha^2\mu_2}{mE_0}\int_0^{k_{\max}}dk\int_{A_{\min}(p;E,\mu_2)}^{\infty}dAI(A,k), \quad (8a)$$

[8] G. A. Erskine, Proc. Roy. Soc. (London) **A224**, 362 (1954).
[9] P. T. Smith, Phys. Rev. **36**, 1293 (1930).
[10] See reference 3 and Chap. XI, Sec. 3.3 of reference 2.

TABLE I. Table of cross sections. $Q_0^{n,k}$ = cross section in units of πa_0^2; E_p = proton energy in units of kev—laboratory system.

n, k \ E_p =	12.50	22.29	39.02	71.09	125.0	222.9	390.2	710.9	1250	2229	3902
$3d, k$	8.60×10^{-7}	7.88×10^{-6}	4.07×10^{-5}	1.33×10^{-4}	2.50	3.21	3.11	2.44	1.71	1.10×10^{-4}	6.78×10^{-5}
$3p, k$	1.94×10^{-5}	1.15×10^{-4}	4.16	1.03	1.64	1.95	1.89	1.57	1.20×10^{-3}	8.59×10^{-4}	5.95×10^{-4}
$3s, k$(II)	5.91×10^{-6}	3.12×10^{-5}	1.14×10^{-4}	3.00	4.72	4.91	3.90	2.63	1.71	1.07×10^{-4}	6.66×10^{-5}
$3s, k$(III)	4.50×10^{-6}	2.15×10^{-5}	7.59	2.18×10^{-4}	4.09	5.09	4.58	3.42	2.39	1.58	1.04×10^{-4}
$2p, k$	1.30×10^{-4}	6.70	2.20×10^{-3}	5.19	8.31×10^{-3}	1.04×10^{-2}	1.07×10^{-2}	9.51×10^{-3}	7.69	5.77	4.16×10^{-3}
$2s, k$(II)	7.82×10^{-5}	3.65×10^{-4}	1.15×10^{-3}	2.50	3.53	3.37	2.58	1.71	1.10×10^{-3}	6.84×10^{-4}	4.25×10^{-4}
$2s, k$(III)	5.74×10^{-5}	2.46×10^{-4}	7.72	1.94×10^{-3}	3.21	3.63	3.12	2.27	1.57	1.03×10^{-3}	6.71×10^{-4}
$1s, k$(II)	6.46×10^{-1}	9.13	9.97	8.92	6.94	4.83	3.18	1.96	1.22×10^{-1}	7.39×10^{-2}	4.51×10^{-2}
$1s, k$(III)	4.56×10^{-1}	7.43	9.53	9.93	8.67	6.59	4.65	3.03	1.96	1.23×10^{-1}	7.78×10^{-2}

0 \ E_p (Erskine)	250	500	750	1000	1250	1500
$1s, k$	6.21×10^{-1}	3.92	2.90	2.27	1.91	1.65×10^{-1}

with $Z_\alpha=2$; thus the cross section for protons, Q_p, is

$$Q_p(E_0,\mu_2)=\frac{1}{Z_\alpha^2}Q_\alpha(E',\mu). \tag{8b}$$

Equation (8b) relates the ionization cross section for protons of energy E_0 to the corresponding cross section for α particles of energy E'; E_0 and E' being energies in the center-of-mass system. (Actually, there is a difference in the value of $k_{\max}$ for the two cases, but this is unimportant, since the differential cross sections, dQ/dk, decrease to negligible values for $k\ll k_{\max}$ in both cases.)

Erskine's results translated to the proton case are shown in Fig. 1. These points practically coincide with the curve of Case III. It thus seems safe to conclude that Case III gives the most accurate ionization cross sections of the three cases treated in this paper. A qualitative reason for the close agreement between the two results is obtained by comparison of the final state wave functions. The s-wave part is the same, for $l\geq2$ this paper uses $Z_3=1$, and Erskine uses $Z_3=Z_1$; however, as Erskine showed, the p-wave contribution is the significant one for the high-energy range. Now the field $V(r)$ is essentially $V(r)=-e^2/r$ for $r>a_0$; so with the additional assumption that significant contributions to the p-wave cross section occur over a large range of the radial coordinate, it is seen why the results of Erskine's paper and Case III of this paper agree so closely.

The cross section for excitation to the $2s, k$ state is roughly 0.01 of the ionization cross section. This agrees with the calculated values of Lamb and Skinner,[11] and the experimental work of Hagstrum,[12] both for electron impact, and the experimental work of Dieterich[13] for proton impact. Lamb and Skinner used the results of Massey and Mohr[3] for the ionization cross section, and calculated $Q_0^{2s,k}$ by a sudden approximation method, whereas Hagstrum and Dieterich failed to observe any $2\,^2S_{\frac{1}{2}}$ states of He^+. From the remarks under Case II relevant to the similarity of the electron and proton Born amplitudes, it appears that the ratio, $Q_0^{2s,k}/Q_0^{1s,k}$, should be nearly the same for the two cases. The effective field, $V(r)$, for the $2\,^2S_{\frac{1}{2}}$ state of He^+ is:

$$V(r)=-e^2\left[\frac{1}{r}+\left(\frac{3}{2a_0}+\frac{1}{r}+\frac{r^2}{a_0^3}+\frac{r}{a_0^2}\right)\exp\left(-\frac{2r}{a_0}\right)\right].$$

For $r>3.50$, $V(r)\doteq-e^2/r$; consequently, on the basis of the discussion of ionization cross sections, it seems reasonable to suppose that a $Z_3>1$ for $l\geq1$ (Case III) in the final state functions might provide a more accurate cross section. Similar remarks can be made relevant to the cross section $Q_0^{3s,k}$.

Cross sections for double excitation by electron impact have been calculated in Born approximation by Massey and Mohr.[14] For final states other than S-states, they obtained fair agreement with experiment by using as a final state wave function:

$$\psi=\frac{1}{\sqrt{2}}[\phi_{n_1l_1m_1}(Z_3|\mathbf{r}_1)\phi_{n_2l_2m_2}(Z_2|\mathbf{r}_2)+\phi_{n_1l_1m_1}(Z_3|\mathbf{r}_2)\phi_{n_2l_2m_2}(Z_2|\mathbf{r}_1)],$$

with the one-electron principal quantum numbers $n_1>n_2$, and $Z_3=1$, $Z_2=2$. About the only justification for using the final state wave functions of this paper in the calculation of $Q_0^{2p,k}$, $Q_0^{3p,k}$, and $Q_0^{3d,k}$, is the fact that they are orthogonal to ψ_0. The S-state part of the final state functions could have been modified; however, such a project was considered inadvisable in the light of the reasonableness of the relative magnitudes of the cross sections, as well as the fact that no measured results exist. For example, the one-electron transition $1s\rightarrow2p$ is optically allowed and $1s\rightarrow2s$ is disallowed, and a glance at Fig. 2 shows that $Q_0^{2p,k}$ is indeed larger than $Q_0^{2s,k}$. It is questionable just how much the approximation to the final state wave function should be improved without likewise improving the approximation to the ground state function. One fact is clear, an improvement of the ground state will greatly increase the numerical labor.

In conclusion, the author wishes to mention that all integrals over the variable A under Cases I through III were calculated on the IBM-704 by the Service Bureau Corporation of IBM in New York City.

The numerical results are listed in Table I.

[11] W. E. Lamb, Jr. and M. Skinner, Phys. Rev. **28**, 539 (1950).
[12] Homer D. Hagstrum, Phys. Rev. **104**, 309 (1956).
[13] Ernest J. Dieterich, Phys. Rev. **103**, 632 (1956).
[14] H. S. W. Massey and C. B. O. Mohr, Proc. Cambridge Phil. Soc. **31**, 604 (1935).

Note added in proof.—Cross sections for ionization and excitation of Helium by protons to the levels $2p, k$, $3p, k$, $4p, k$, $3d, k$, and $4d, k$ have been calculated by A. Dalgarno and M. R. C. McDonald.[15] Their results differ considerably from the corresponding calculations of this paper. This is not surprising since the calculated cross-sections of this paper can vary from zero ($Z_3=1.6875$) to a maximum value for some choice of Z_3. In conclusion the author expresses his gratitude to Professor A. Dalgarno for informing him of these calculations.

[15] E. B. Armstrong and A. Dalgarno, *The Airglow and The Aurorae* (Pergamon Press, New York, 1955).

PHYSICAL REVIEW VOLUME 109, NUMBER 4 FEBRUARY 15, 1958

Hfs Anomaly of Sb^{121} and Sb^{123} Determined by the Electron Nuclear Double Resonance Technique

J. EISINGER AND G. FEHER
Bell Telephone Laboratories, Inc., Murray Hill, New Jersey

(Received July 16, 1957)

The ratios of the hyperfine interaction constants "a" and the nuclear g factors of the stable isotopes of antimony have been measured. From these measurements the hyperfine structure anomaly, defined as $\Delta=(a_{121}/a_{123})(g_{123}/g_{121})-1$, was found to be $(-0.352\pm0.005)\%$. Δ has its origin in the difference in the spatial distribution of the nuclear magnetic dipole for the two isotopes, which is related to the structure of the two nuclei. The experimental result is compared with theoretical values of Δ based on a variety of nuclear models.

The determination of a_{121}/a_{123} makes use of the electron nuclear double resonance technique (ENDOR) which is discussed in some detail. The sample used in the experiment was silicon doped with antimony and the microwave resonances were observed at ~9000 Mc/sec at a temperature of 1.2°K.

The ratio of the nuclear g factors was determined by conventional nuclear magnetic resonance techniques.

A. INTRODUCTION

THE hyperfine interaction constant a is a measure of the strength of the interaction between the nuclear magnetic dipole moment μ_I and the moment due to the orbital electron. For two isotopes (subscripts 1 and 2) of the same element in the same electronic state one might expect $(a_1/a_2)=(g_1/g_2)$, where we have written $g=\mu_I/I$.

By measuring the ratio of the interaction constants (e.g., by methods described in this paper or by atomic beams) and the ratio of the nuclear g factors (e.g., by nuclear magnetic resonance experiments) to high precision, deviations from this equality have been found.

It was pointed out by Kopfermann[1] and Bitter[2] that one should expect $(a_1/a_2)=(g_1/g_2)(1+\Delta)$ for certain pairs of isotopes, where Δ is of the order of a fraction of one percent and is usually called the hyperfine structure (hfs) anomaly. Physically the origin of Δ can be traced to nuclear size effects, the most important of which is due to the difference in the distribution of the magnetic moment inside the nuclei under consideration.[1–3] A quantitative discussion of Δ from a theoretical point of view is left to a later section. Suffice it to say that such a calculation usually depends on the particular nuclear model chosen so that an experimental determination of the hfs anomaly should be capable of adding to our knowledge of nuclear structure.

Hfs anomalies have been measured for several pairs of isotopes. Such experiments have been restricted until now to elements which lend themselves to detection in atomic beam experiments, i.e., mostly alkalies.[2,4–7] Recent advances in the techniques of paramagentic resonance experiments[8] have made it possible to measure "a" with greater precision than had previously been possible. The method employed is called electron nuclear double resonance (ENDOR)[8] and will be described in detail in a later section.

In the present experiment[9] the precise ratio of the hyperfine interaction constants was determined by the ENDOR technique and the ratio of the nuclear g factor was redetermined by the NMR method for the two stable isotopes of antimony, Sb^{121} and Sb^{123}. The experimental value of Δ obtained in this manner was compared with values based on a variety of nuclear models.

B. ENERGY LEVELS AND TRANSITIONS

The magnetic interaction of an atom whose angular momentum $J=\frac{1}{2}$ and whose nucleus has a magnetic

[1] H. Kopfermann, *Kernmomente* (Akademische Verlagsgesellschaft, Leipzig, 1940).
[2] F. Bitter, Phys. Rev. **76**, 150 (1949).
[3] A. Bohr and V. F. Weisskopf, Phys. Rev. **77**, 94 (1950).
[4] Ochs, Logan, and Kusch, Phys. Rev. **78**, 184 (1950).
[5] Eisinger, Bederson, and Feld, Phys. Rev. **86**, 73 (1952).
[6] Jaccarino, Stroke, Edmonds, and Weiss, Phys. Rev. **105**, 590 (1957).
[7] Y. Ting and H. Lew, Phys. Rev. **105**, 581 (1957).
[8] G. Feher, Phys. Rev. **103**, 83 (1956).
[9] A preliminary account of this work has been given [J. Eisinger and G. Feher, Bull. Am. Phys. Soc. Ser. II, **2**, 31 (1957)].