The Quantum Mechanical Cross Section for Ionization of Helium by Electron Impact

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By using Born's collision theory without exchange the effective ionization cross section is calculated for helium when the resulting ion is left in the normal state. A plane wave is used as a mathematically manageable substitute for the hyperbolic functions previously employed to represent the ejected electron. A comparison is made of the calculated cross section with the experimental values obtained by P. T. Smith. The maximum of the calculated curve falls at approximately three times the ionization potential. The calculation predicts that the maximum probability of ionization occurs when the energy transfer is about 3.5 volts greater than the ionization potential.

INTRODUCTION

ALTHOUGH a number of papers on the probability of elastic and inelastic scattering of electrons by atoms have appeared in the literature,[1] only one attempt has been made to evaluate a cross section for ionization. This is the work of Ochiai[2] who made certain calculations on the effective cross section for ionization of atomic hydrogen. Ochiai used the hyperbolic solutions for hydrogen to represent the ejected electron but was unable, because of their complexity, to bring his calculations to a satisfactory conclusion. Because of the difficulties involved, no experimental measurements have as yet been made on the probability for ionization of atomic hydrogen and therefore no check on the values obtained by Ochiai is possible.

It is the purpose of this paper to apply Born's theory (neglecting exchange) to calculate the cross section of helium for the case when the ion is left in an unexcited state. In order to avoid the difficulties encountered by Ochiai a plane wave is used to represent the electron ejected from the atom. That this method of attack leads to reasonable results will be shown by a comparison of the calculated cross section with the experimental measurements of P. T. Smith.[3]

PROCEDURE

If we represent the ejected atomic electron by a plane wave Born's formula for the ionization cross section becomes

$$\sigma(k)=(m^2/2\pi h^4k)\int k'|U|^2k''^2dk''d\Omega''d\Omega', \tag{1}$$

where

$$U=\int \psi_a e^{i\mathbf{k}\cdot\mathbf{r}_1}\tilde{V}\psi_i^* e^{-i\mathbf{k}'\cdot\mathbf{r}_1}e^{-i\mathbf{k}''\cdot\mathbf{r}_2}dv. \tag{2}$$

Here m is the mass of an electron. k, k' and k'' are equal respectively to $2\pi m/h$ times the velocity of the colliding, deflected and ejected electrons. ψ_a is the wave function of the normal atom and ψ_i that for the ionized atom. $d\Omega'=\sin\theta' d\theta' d\phi'$ and $d\Omega''=\sin\theta'' d\theta'' d\phi''$ where θ' and ϕ', and θ'' and ϕ'' are the direction angles of the vectors k' and k'', respectively, in a fixed set of cartesian axes to be specified later. The origin for all coordinate systems is chosen at the atomic nucleus.

In the particular problem we are considering where the ion is left in the state of lowest potential energy, ψ_i will be given by the solution for the ground state of the hydrogenic atom of double nuclear charge. Thus

[1] For references, see P. M. Morse, Rev. Mod. Phys. **4**, 577 (1932).

[2] K. Ochiai, Proc. Phys.-math. Soc. Japan **11**, 43 (1929).

[3] P. T. Smith, Phys. Rev. **36**, 1293 (1930).

$$\psi_i = (\beta^3/\pi)^{\frac{1}{2}} e^{-\beta r_3},$$

where $\beta = 2/a_0$, a_0 being the radius of the first Bohr orbit in hydrogen. Hylleraas'[4] first approximation representing the ground state of helium is chosen for ψ_a. This is

$$\psi_a = (\alpha^3/\pi) e^{-\alpha(r_2+r_3)},$$

where $\alpha = 27/16a_0$.

The perturbation energy is[5]

$$\tilde{V} = e^2(2/r_1 - 1/r_{21} - 1/r_{31}).$$

On substituting these values into Eq. (2) we may integrate over the coordinates of the colliding electron by using Bethe's[6] formula

$$\int (e^{i\mathbf{q}\cdot\mathbf{r}_1}/r_{n1}) dv_1 = (4\pi/q^2) e^{-i\mathbf{q}\cdot\mathbf{r}_n},$$

where, in this problem, $\mathbf{q} = \mathbf{k} - \mathbf{k}'$.

This gives

$$U = (4e^2\alpha^3\beta^{\frac{3}{2}}/\pi^{\frac{1}{2}} q^2)(2I_a - I_b - I_c),$$

where

$$I_a = \int e^{-\gamma r_3} dv_3 \int e^{-\alpha r_2} e^{-i\mathbf{k}''\cdot\mathbf{r}_2} dv_2,$$

$$I_b = \int e^{-\gamma r_3} dv_3 \int e^{-\alpha r_2} e^{i(\mathbf{q}-\mathbf{k}'')\cdot\mathbf{r}_2} dv_2,$$

$$I_c = \int e^{-\gamma r_3} e^{i\mathbf{q}\cdot\mathbf{r}_3} dv_3 \int e^{-\alpha r_2} e^{-i\mathbf{k}''\cdot\mathbf{r}_2} dv_2,$$

and $\gamma = \alpha + \beta$.

Let us choose the polar axis to which r_2 is referred to be in the direction of $\mathbf{k}''$ in the cases of integrals I_a and I_c. For the evaluation of I_b choose the polar axis to be in the direction of the vector $\mathbf{l} = \mathbf{q} - \mathbf{k}''$. The exponents containing the scalar product $\mathbf{k}''\cdot\mathbf{r}_2$ and $\mathbf{l}\cdot\mathbf{r}_2$ may then be written as $ik''r_2 \cos\theta_2$ and $ilr_2 \cos\Theta_2$ and dv_2 is replaced by $r_2^2 \sin\theta_2 dr_2 d\theta_2 d\phi_2$ and $r_2^2 \sin\Theta_2 dr_2 d\Theta_2 d\Phi_2$, respectively. The integrals are then easily evaluated to give

$$U = (A/q^2)\{[2/(\alpha^2+k''^2)^2] - [\gamma^4/(\alpha^2+k''^2)^2(\gamma^2+q^2)^2] - [1/(\alpha^2+l^2)^2]\},$$

where $A = 256e^2\alpha^4\beta^{\frac{3}{2}}\pi^{\frac{3}{2}}/\gamma^3$.

A choice of $\mathbf{k}$ as the polar axis from which θ' is measured allows us to write $q^2 = k^2 + k'^2 - 2kk' \cos\theta'$.

This choice of axis defines θ' as the usual scattering angle for the deflected electron. Similarly, taking $\mathbf{q}$ as the polar axis for θ'' permits us to write $l^2 = q^2 + k''^2 - 2qk'' \cos\theta''$, which on differentiation gives

$$\sin\theta''\, d\theta'' = ldl/qk''. \tag{3}$$

Since, with this definition of polar axes, the integrand of Eq. (1) is independent of ϕ' and ϕ'' we may integrate over these two coordinates and on substituting Eq. (3) obtain

$$\sigma(k) = (2\pi m^2/h^4 k) \int (k'k''/q) |U|^2 dk'' \sin\theta'\, d\theta'\, ldl. \tag{4}$$

[4] E. Hylleraas, Zeits. f. Physik **54**, 347 (1929).

[5] It should be noted that if our wave functions really satisfied the proper orthogonality relations the first term in $\tilde{V}$, representing the contribution of the nucleus to the inelastic scattering would vanish on integrating Eq. (2). That we must retain it in the following can be made plausible by interpreting Eq. (2) as the result of the interaction of the colliding electron with a system of generalized electrical moments representing the atom as a whole. Actually this term is partially cancelled in the integration by other terms which also arise from the lack of orthogonality of the wave function.

[6] H. Bethe, Ann. d. Physik **5**, 325 (1930).

Integrating over l from $l_{\min}=q-k''$ to $l_{\max}=q+k''$ the above expression becomes

$$\sigma(k)=\frac{B}{h}\int_0^{k''_{\max}}\int_0^{\pi}\frac{k'k''}{q^5}\left\{2qk''\left(\frac{4}{(\alpha^2+k''^2)^4}+\frac{\gamma^8}{(\gamma^2+q^2)^4(\alpha^2+k''^2)^4}-\frac{4\gamma^4}{(\gamma^2+q^2)^2(\alpha^2+k''^2)^4}\right)\right.$$
$$+\left(\frac{\gamma^4}{(\alpha^2+k''^2)^2(\gamma^2+q^2)^2}-\frac{2}{(\alpha^2+k''^2)^2}\right)\cdot\left(\frac{1}{\alpha^2+(q-k'')^2}-\frac{1}{\alpha^2+(q+k'')^2}\right)$$
$$\left.+\frac{1}{6}\left(\frac{1}{[\alpha^2+(q-k'')^2]^3}-\frac{1}{[\alpha^2+(q+k'')^2]^3}\right)\right\}dk''\sin\theta'\,d\theta'. \quad (5)$$

Here $B=(27/2\gamma)^6(\alpha^2/4a_0^{11})$.

Numerical Computations and Comparison with Experiment

Although it is possible to carry the analytical integration further, the expression becomes unwieldy and since a numerical evaluation at this point yields interesting information, that method of procedure was adopted. In order that the calculations may be compared directly with experiment, it is convenient to make a change of variables given by

$$k^2=CV_c;\quad k'^2=CV\quad\text{and}\quad k''^2=CV_e,$$

where $C=8\pi^2me/300h^2$. Also let $\theta'=2\pi\theta/360$. Now θ is measured in degrees, and V_c, V and V_e in volts (i.e., not electron volts, as they are no longer expressed in energy units). From the energy relation we have $dV=dV_e$.

Eq. (5) may be written as

$$\sigma(V_c)=\int_0^{V_{\max}}\int_{0°}^{180°}f(\theta,\ V,\ V_c)dVd\theta, \quad (6)$$

where $f(\theta,\ V,\ V_c)$ is equal to the integrand of Eq. (5) multiplied by $2\pi eB/300\times 360$.

Let us define $F(V,\ V_c)$ by the relation

$$F(V,\ V_c)=\int_{0°}^{180°}f(\theta,\ V,\ V_c)d\theta. \quad (7)$$

$f(\theta,\ V,\ V_c)$ was evaluated for $V_c=50$, 75, 100, 200, 350 and 500 volts. In each case several values of θ were used. Figs. 1 and 2 give the result for $V_c=75$ and $V_c=200$ volts, respectively. $f(\theta,\ V,\ V_c)$ is proportional to the probability of an electron which has fallen through a potential of V_c volts, striking an atom of helium, ionizing it and coming away from the ion with an energy in electron volts numerically equal to V at an angle θ measured from the original direction of travel. The ejected electron comes away from the ion at an unspecified angle but with an energy in electron volts equal numerically to V, which, in accordance with the law of conservation of energy, satisfies the equation

$$V_e=V_c-V_i-V,$$

where V_i is the ionization potential of helium.

Having plotted the function $f(\theta,\ V,\ V_c)$ the integration indicated in Eq. (7) was carried out by use of a planimeter to evaluate $F(V,\ V_c)$. Fig. 3 shows the complete set of points obtained in this manner. $F(V,\ V_c)$ is proportional to the probability of an electron, which has fallen through a potential of V_c volts, colliding with an atom of helium, ionizing it and coming away from the ion at an unspecified angle with an energy in electron-volts numerically equal to V. The area under a curve of Fig. 3 when multiplied by (V_c-V_i) gives a final value for $\sigma(V_c)$. These values are plotted on Fig. 4.

For purposes of comparison, Smith's values[3] for the experimental total cross section, together with values calculated from Thomson's formula[7] are also plotted on Fig. 4. The experimental values include all possible types of ionization while Thomson's curve and the curve obtained with the present theory include only ionization without excitation. One should expect therefore, that the calculated will fall below the experimental values although just how much below it is impossible to state. Bleakney[8] has found that, up to several hundred volts, the contribution to the total cross section due to double ionization is less

[7] J. J. Thomson, Phil. Mag. **23**, 449 (1912).

[8] Walker Bleakney, Phys. Rev. **36**, 1303 (1930).

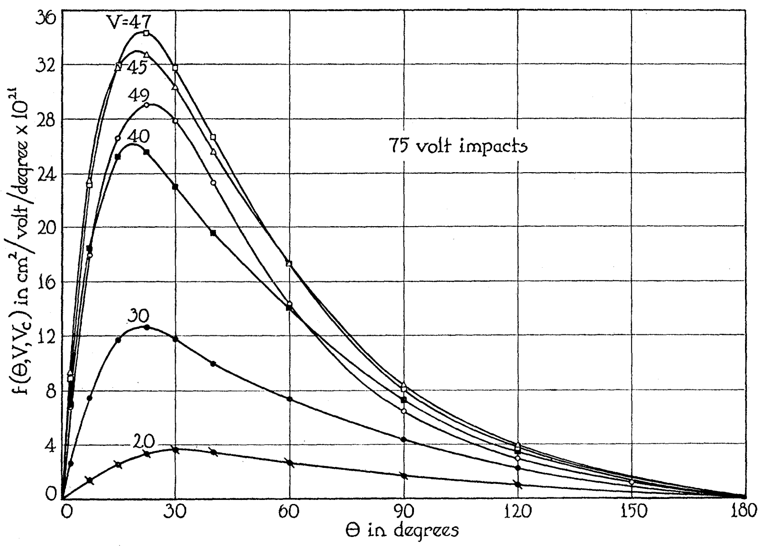

FIG. 1. Angular scattering of the deflected electron for 75-volt collisions in helium which result in simple ionization. V is the potential fall in volts necessary to stop the deflected electron.

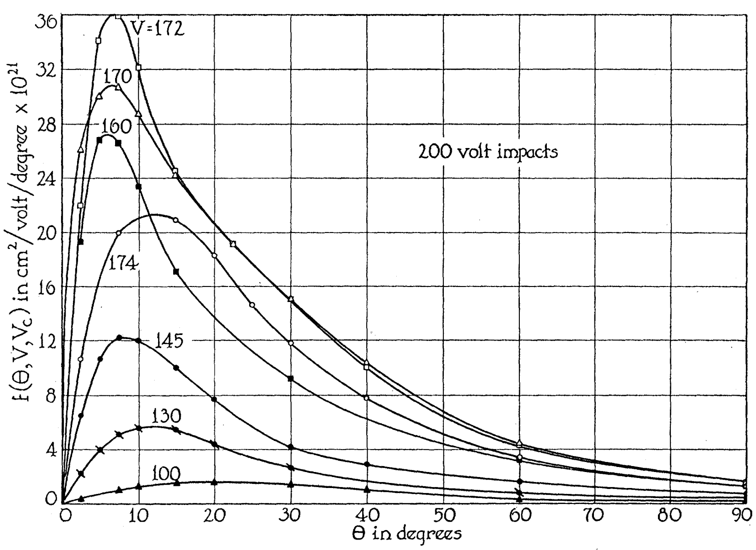

FIG. 2. Angular scattering of the deflected electron for 200-volt collisions in helium which result in simple ionization. V is the potential fall in volts necessary to stop the deflected electron.

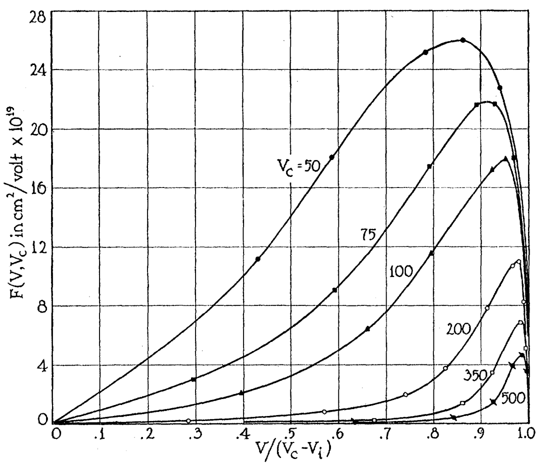

FIG. 3. Total probability of ionization for collisions of V_c volts. V is the potential fall in volts necessary to stop the deflected electron and V_i is the ionization potential.

than one percent of the total experimental cross section. No data are available on the contribution due to ionization plus excitation. As an estimation we may say that the calculated $\sigma(V_c)$ is too great by a factor somewhat less than two.

The experimental curve in Fig. 4 has a maximum at 110 volts while the calculated maximum falls at approximately 75 volts. The addition of contributions due to ionization plus excitation would probably increase the voltage at which the calculated maximum falls and bring it to a better agreement with experiment.

When $F(V, V_c)$ is plotted against V instead of $V/V_c - V_i$ it is seen that, within the accuracy of the calculation, the maximum probability of ionization occurs when the energy transfer is 3.5 volts more than the ionization potential. At impacts of 200 volts or more it should be possible to separate experimentally two groups of electrons coming from the ion. One group should consist of slow electrons whose maximum distribution in energy comes at about 3.5 volts and the other of fast electrons whose volt energy V is given by $V \cong V_c - V_i - 3.5$. This value for the maximum is independent of V_c within the range of 50 to 500 volts.

Figs. 1 and 2 show a series of curves similar to those obtained in angular scattering measurements. For 75 volt collisions the average maximum of the high energy group occurs at about twenty degrees. For 200 volt collisions it has decreased to about ten degrees. This decrease in scattering angle with increased energy of the

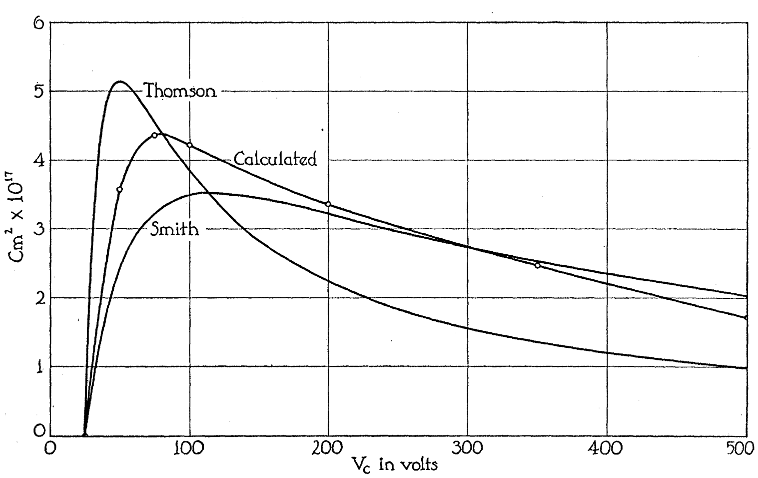

FIG. 4. The calculated cross section for simple ionization as a function of the accelerating potential applied to the colliding electron. Thomson's theoretical and Smith's experimental curves are plotted here for comparison.

colliding electron is in qualitative agreement with Tate and Palmer's work on mercury vapor.[9] The curves illustrated in the first two figures lead to the prediction that for any particular value of V_c, the maximum of the probability for scattering changes as V decreases, first occurring at de-

[9] J. T. Tate and R. R. Palmer, Phys. Rev. 40, 731 (1932).

creasing values of θ then at increasing values of θ. The smallest angle at which the maximum falls for any particular value of V_c corresponds to an energy transfer of about five volts more than the ionization energy of helium.

One may ask what influence the inclusion of "electron interchange" between the colliding and atomic electrons would have on our results. As we have not yet actually calculated this factor, we cannot be absolutely sure of the effect but it seems reasonable to expect that it would be small, except perhaps for energies of the colliding electron in the neighborhood of the ionization energy of the atom. Qualitatively we may expect this since, in our calculations, the probability that the deflected and ejected electrons leave the atom in nearly the same direction with nearly the same velocity is very small as soon as the energy of the impacting electron is more than 10–20 volts above the ionization potential. However, even though there should be no large change in the numerical results, the inclusion of exchange would completely eliminate any possible identification of the deflected and the impacting electrons such as we have employed in our integrations.

The results obtained seem to justify further calculations and it is intended to correct the present values for exchange effect as well as to extend the work to include some of the lower excited levels of the ion.

In conclusion the author wishes to express his gratitude to Professor John T. Tate who suggested the problem and to Professor E. L. Hill for his continued interest and assistance in its solution.