# Asymptotic Expression for the Stopping Power of K-Electrons

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An asymptotic form for the high energy stopping number of K-electrons (for any element) is determined by using the Born approximation expressions for the excitation and ionization probabilities of the K shell. The stopping number takes the form  $B_K(\theta, \eta) = A(\theta) \ln \eta + B(\theta) + C(\theta)(1/\eta) + \cdots$ , where  $\eta$  is a dimensionless quantity proportional to the energy of the incident particle and  $\theta$  is proportional to the observed ionization energy of the K shell. Other results include the stopping number for hydrogen, obtained by sum-rule methods, to order  $(1/\eta)$ , and results of M. C. Walske, obtained by numerical methods, for the low energy stopping number of K-electrons.

## I. INTRODUCTION

THE stopping power formula of Bethe<sup>1</sup> is valid without correction only if  $E \gg (M/m)E_{el}$  for each electron in the atom; here  $E_{el}$  is the ionization potential of an electron in the atom, *m* the electronic mass, *E* and *M* the energy and mass of the incident particle. For many important cases this condition is not well fulfilled, particularly for the *K*-electrons of the heavier elements, and it is useful therefore to obtain separately the contribution of the *K*-electrons, in order that the formula can be corrected.<sup>2</sup>

Curves for the stopping number,  $B_K$ , of the K-electrons have already been published in reference 1, and this new calculation of an asymptotic expression for large incident energies is undertaken to provide more accurate results in this energy region and to extend the former results to heavier elements.

### **II. GENERAL THEORY**

If we measure all energies in units of the "ideal ionization potential" of the K shell,  $Z_{eff}^2 Ry$ , the contribution to the stopping number due to excitation of K-electrons is<sup>1</sup>

$$B_K = \int_{\theta}^{\epsilon_{\max}} \epsilon d\epsilon \int_{Q_{\min}}^{Q_{\max}} \frac{dQ}{Q^2} |F_n(Q)|^2, \qquad (1)$$

where  $\epsilon = E_n - E_1$  is the energy given to the atomic electron,  $Q = (\mathbf{p} - \mathbf{p}')^2/2m$ , **p** and **p'** being the momenta of the incident particle before and after the collision,  $Q_{\min} = \epsilon^2/4\eta$  is the smallest possible value of Q for a given  $\epsilon$ ,  $Q_{\max} = 4\eta$ , with  $\eta = mv^2/2$ , v being the velocity of the incident particle. The minimum energy transferable to a K-electron,  $\theta$ , is the observed ionization energy of the K shell.

If we use hydrogenic wave functions for the evaluation of the form factor  $F_n(Q)$ , the contribution which arises from the continuum states  $\epsilon > 1$  will be the same (in our units) as the continuum contribution in the case of hydrogen. The integral over  $\epsilon$  from  $\theta$  to 1 will be evaluated using the excitation functions for hydrogen; however, the principal quantum number, n, of the excited state must be allowed to vary continuously.

The asymptotic expression for  $B_K$  will be obtained as an expansion in  $\eta$  which will take the form

$$B_{K}(\theta, \eta) = A(\theta) \ln \eta + B(\theta) + C(\theta)(1/\eta) + \cdots \qquad (2)$$

and we shall obtain A, B, and C.

The work will consist of several parts: (a) The excitation function

$$\Phi_n = \kappa \int_{Q_{\min}}^{Q_{\max}} \frac{dQ}{Q^2} |F_n(Q)|^2, \quad \kappa = \frac{2\pi e^4 z^2}{mv^2}, \quad (3)$$

will first be evaluated for discrete, non-integral, values of n. It will be shown that the  $\eta$ -dependence arising from the upper limit occurs first in  $O(1/\eta^5)$  and that the integral may therefore be extended to  $\infty$  and the  $\eta$ -dependence,  $A(\theta)$  and  $C(\theta)$  in Eq. (2), obtained from a small Q approximation. (b) An asymptotic expansion of  $\Phi_n$  for large *n* will be obtained, which will be useful for n > 5. (c) The integration over  $\epsilon$  will be performed to obtain the contribution of the states  $\theta \leq \epsilon \leq 1$  to  $B_K$ . (d) The total stopping power of hydrogen will be found, by sum-rule methods, to order  $1/\eta$ . (e) The contribution of the discrete states to  $B_K$  for hydrogen will be found. This will be subtracted from the total  $B_K$  for hydrogen, obtained by sum-rule methods, and the continuum contribution will thus be obtained. This will be added to the result of Section V for several values of  $\theta$ , and will constitute our final result.

#### **III. EXCITATION FUNCTION**

The excitation function for a hydrogen-like atom is<sup>3</sup>

$$\Phi_{n} = \frac{2^{8}\kappa}{n^{3}} \int_{Q_{\min}}^{Q_{\max}} \frac{dQ}{Q} \begin{bmatrix} \frac{1}{3}(1-1/n^{2}) + Q \end{bmatrix} \times \frac{[(1-1/n)^{2} + Q]^{n-3}}{[(1+1/n)^{2} + Q]^{n+3}}$$
(4)

<sup>3</sup> H. A. Bethe, Handbuch der Physik (1933), Vol. 24, p. 507.

<sup>&</sup>lt;sup>1</sup> For a general discussion of the stopping power theory to which this paper is a supplement, see M. S. Livingston and H. A. Bethe, Rev. Mod. Phys. 9, 263-265 (1937).

<sup>&</sup>lt;sup>2</sup> J. O. Hirschfelder and J. L. Magee, Phys. Rev. **73**, 207 (1948) have used the previously published (reference 1) stopping power for K-electrons, modifying it for the L, M, etc. shells, to construct directly, shell by shell, the stopping power of a number of substances for low energy protons.

We shall write this as

$$\Phi_{n} = A_{n}\psi_{1} + B_{n}\psi_{2}$$
(5)  

$$\psi_{1} = \int_{Q_{\min}}^{Q_{\max}} \frac{dQ}{Q} \frac{(a+Q)^{n-3}}{(b+Q)^{n+3}},$$
(5a)  

$$\psi_{2} = \int_{Q_{\min}}^{Q_{\max}} dQ \frac{(a+Q)^{n-3}}{(b+Q)^{n+3}},$$
(5a)  

$$A_{n} = (2^{8}\kappa/3n^{3})(1-1/n^{2}), \quad B_{n} = 2^{8}\kappa/n^{3},$$
(5b)  

$$a = (1-1/n)^{2}, \quad b = (1+1/n)^{2}.$$

We now examine the limits of integration. For a fixed value of  $\epsilon = E_n - E_1$ ,

$$2M\epsilon = \mathbf{p}^2 - \mathbf{p}'^2 = (\mathbf{p} - \mathbf{p}') \cdot (\mathbf{p} + \mathbf{p}').$$

If we let  $q_{\min} = p - p'$ , with  $p = |\mathbf{p}|$ , then

$$q_{\min} = \frac{p^2 - p'^2}{p + p'} = \frac{2M\epsilon}{2p - q_{\min}} \approx \frac{\epsilon}{v} \left(1 + \frac{q_{\min}}{2p}\right) = \frac{\epsilon}{v} (1 + \epsilon/2pv).$$

Thus  $Q_{\min} = q_{\min}^2/2m = \epsilon^2/4\eta$ ; the next term, being of relative order  $\epsilon(m/M)(1/\eta)$ , has been neglected. For the upper limit,  $Q_{\max}$ , we may take the maximum energy which a heavy particle can transfer to a free electron, namely,  $2mv^2 = 4\eta$ . We may note, however, that if we take  $Q_{\max}$  to be infinite we make an error in  $\psi_2$  of

$$\int_{4\eta}^{\infty} \frac{dQ}{Q^6} \frac{(1+a/Q)^{n-3}}{(1+b/Q)^{n+3}} = \int_{4\eta}^{\infty} \frac{dQ}{Q^6} [1+O(1/Q)] = O(1/\eta^5).$$

Similarly, the error in  $\psi_1$  is  $O(1/\eta^6)$ . Since we wish to compute only to order  $1/\eta$ , we may take  $Q_{\max} = \infty$ .

For the above reason, assuming  $\eta$  to be large, we can obtain the  $\eta$ -dependence of  $\Phi_n$  by expanding the integrand for small Q.

$$\begin{split} \psi_2 &= \int_{Q_{\min}} dQ \frac{(a+Q)^{n-3}}{(b+Q)^{n+3}} \\ &= \frac{a^{n-3}}{b^{n+3}} \int_{Q_{\min}} dQ \frac{(1+Q/a)^{n-3}}{(1+Q/b)^{n+3}} \\ &= \frac{a^{n-3}}{b^{n+3}} \int_{Q_{\min}} dQ \Big\{ 1 + Q \Big[ n \Big( \frac{1}{a} - \frac{1}{b} \Big) \\ &- 3 \Big( \frac{1}{a} + \frac{1}{b} \Big) \Big] + \cdots \Big\}, \\ B_n \psi_2 / \kappa &= \frac{2^8}{n^3} \frac{a^{n-3}}{b^{n+3}} [\text{const.} - Q_{\min}] \end{split}$$

$$= |x_{0n}|^{2} \{ \text{const.} - 3(1 - 1/n^{2})/4\eta \} \quad (6)$$

where  $x_{0n}$  is the dipole moment,<sup>3</sup>

$$x_{0n}|^{2} = \left[ 2^{8}n^{7}(n-1)^{2n-5} \right] / \left[ 3(n+1)^{2n+5} \right].$$
(7)

Similarly,

$$\psi_{1} = \int_{Q_{\min}} \frac{dQ}{Q} \frac{(a+Q)^{n-3}}{(b+Q)^{n+3}}$$
  
=  $\frac{a^{n-3}}{b^{n+3}} \{ \text{const.} - \ln Q_{\min} + 2Q_{\min}n^{2}(n^{2}+3)/(n^{2}-1)^{2} \},$ 

$$A_{n}\psi_{1}/\kappa = |x_{0n}|^{2} \{\text{const.} + \ln\eta + 2(1+3/n^{2})/4\eta\}.$$
 (8)

Combining (6) and (8), according to (5), and denoting the constant by G(n), we obtain the result

$$\Phi_n/\kappa = |x_{0n}|^2 \{G(n) + \ln\eta - (1 - 9/n^2)/4\eta\}.$$
(9)

Expression (9) is valid for any value of n, and there remains the evaluation of the part independent of  $\eta$ ,  $|x_{0n}|^2 G(n)$ . This is somewhat lengthy as no approximations can be made concerning Q in the integrand. We can, however, set  $Q_{\max} = \infty$ .

Introduce the variable

$$z=Q/\gamma(b+Q),$$

with

$$\gamma = (n-1)^2/4n.$$
  
 $dQ = \gamma b dz/(1-\gamma z)^2, \quad dQ/Q = dz/z(1-\gamma z),$   
 $1+Q/b = 1/(1-\gamma z), \quad 1+Q/a = (1+z)/(1-\gamma z).$ 

Equation (4) becomes

$$\Phi_{n}/\kappa = |x_{0n}|^{2} \int_{Q_{\min}}^{\infty} \frac{dQ}{Q} [1+3Q/(ab)^{\frac{1}{2}}] \frac{(1+Q/a)^{n-3}}{(1+Q/b)^{n+3}}$$
$$= |x_{0n}|^{2} \left\{ \int_{z_{0}}^{1/\gamma} \frac{dz}{z} (1-\gamma z)^{5} (1+z)^{n-3} + 3[\gamma(\gamma+1)]^{\frac{1}{2}} \int_{z_{0}}^{1/\gamma} dz (1-\gamma z)^{4} (1+z)^{n-3} \right\}, \quad (10)$$

with  $z_0 = Q_{\min}/\gamma(b+Q_{\min}) \ll 1$ . Let

$$L_{k}(n) = \int_{z_{0}}^{1/\gamma} dz (1-\gamma z)^{k} (1+z)^{n-3},$$

$$M_{n} = \int_{z_{0}}^{1/\gamma} (1+z)^{n-3} dz/z.$$
(11)

Then, as

$$(1-\gamma z)^{5}-1=-\gamma z\sum_{k=0}^{4}(1-\gamma z)^{k},$$
$$\int_{z_{0}}^{1/\gamma}(1-\gamma z)^{5}(1+z)^{n-3}dz/z=M_{n}-\gamma\sum_{k=0}^{4}L_{k}(n),$$

and

$$\Phi_{n}/\kappa = |x_{0n}|^{2} \{ M_{n} + 3 [\gamma(\gamma+1)]^{\frac{1}{2}} L_{4}(n) - \gamma \sum_{k=0}^{4} L_{k}(n) \}.$$
(12)

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with

In  $L_k(n)$ , the lower limit can now be replaced by  $1.75 \le n \le 5$  by the expression zero. Integrating repeatedly by parts we obtain,

$$L_{k}(n) = \frac{(1+z)^{n-2}}{(n-2)} \left\{ (1-\gamma z)^{k} + \frac{\gamma k}{(n-1)} (1-\gamma z)^{k-1} (1+z) + \cdots + \frac{\gamma^{k} k! (1+z)^{k}}{(n-1)n \cdots (n-2+k)} \right\} \Big|_{0}^{1/\gamma} + \frac{\gamma^{k} k! (1+z)^{k}}{(n-1)n \cdots (n-2+k)} + \frac{k! \gamma^{k} [1-(1+1/\gamma)^{n-2+k}]}{(n-2)(n-1)} + \frac{k! \gamma^{k} [1-(1+1/\gamma)^{n-2+k}]}{(n-2)(n-1) \cdots (n-2+k)}$$

Thus the result for  $\Phi_n/\kappa$ , apart from the  $\eta$ -dependence, is

$$\Phi_n/\kappa = |x_{0n}|^2 \{ M_n - 3 [\gamma(\gamma+1)]^{\frac{1}{2}} f_1(n) + 5\gamma f_2(n) - \gamma(1+1/\gamma)^{n-2} f_3(n) ] \quad (13)$$

where

$$f_{1}(n) = -L_{4}(n) = \frac{1}{n-2} \left\{ 1 + \frac{4\gamma}{(n-1)} + \frac{12\gamma^{2}}{(n-1)n} + \frac{24\gamma^{3}}{(n-1)n(n+1)} + \frac{24\gamma^{4}[1-(1+1/\gamma)^{n+2}]}{(n-1)n(n+1)(n+2)} \right\}, \quad (13a)$$

$$f_{2}(n) = \frac{1}{n-1} \left\{ 1 + \frac{2\gamma}{(n-1)} + \frac{4\gamma^{2}}{(n-1)n} + \frac{6\gamma^{3}}{(n-1)n(n+1)} + \frac{24}{5} \frac{\gamma^{4}}{(n-1)n(n+1)(n+2)} \right\}, \quad (13b)$$

$$f_{3}(n) = \frac{1}{n-2} \left\{ 1 + \frac{(1+\gamma)}{(n-1)} + \frac{2(1+\gamma)^{2}}{(n-1)n} + \frac{6(1+\gamma)^{3}}{(n-1)n(n+1)} + \frac{24(1+\gamma)^{4}}{(n-1)n(n+1)(n+2)} \right\}.$$
 (13c)

Unfortunately, the integral  $M_n$  can be calculated exactly only for certain discrete values of n. A tabulation of the numerical value of the part of  $M_n$  which is independent of  $\eta$  is given in Table I for those values of *n* for which  $M_n$  was integrated in closed form.

Bethe<sup>3</sup> gives expressions for  $\Phi_n$  for n=2, 3, 4, 5. These have been evaluated and the numerical results for  $|x_{0n}|^2$ , and for the part of  $\Phi_n$  which is independent of  $\eta$ , are given also in Table I.

The constant part of  $\Phi_n/\kappa$  (the term independent of  $\eta$ ) may be represented within 0.1 percent in the range

$$|x_{0n}|^2 G(n) = 2.31197(1/n^3) + 3.17662(1/n^5) + 0.75111(1/n^7) + 7.3743(1/n^9) - 54.117(1/n^{11})$$
(14)

## IV. ASYMPTOTIC EXPANSION OF $\Phi_n$

Expression (9) for  $\Phi_n$  is valid for any bound excited state, and G(n) has been determined for  $n \leq 5$ . In this part of the work we will get an asymptotic expression for G(n) which will be useful for n > 5.

We write Eq. (4) in the form

$$\Phi_{n}/\kappa = \frac{2^{8}}{n^{3}} \int_{Q_{\min}}^{Q_{\max}} \frac{dQ}{Q} \frac{(1-1/n^{2})/3 + Q}{[(1-1/n)^{2} + Q]^{3}[(1+1/n)^{2} + Q]^{3}} \times \left[\frac{(1-1/n)^{2} + Q}{(1+1/n)^{2} + Q}\right]^{n} \cdot (15)$$

The last factor in the integral of (15) can be expanded for large values of *n* as

$$\left[1+4(Q-\frac{1}{3})/n^2(1+Q)^3\right]e^{-4/(1+Q)}$$

Expanding also the remaining factors of the integrand we obtain

$$\Phi_n/\kappa = \frac{2^8}{n^3} \int_{q_{\min}}^{q_{\max}} \frac{dQ}{Q} \frac{Q + \frac{1}{3}}{(1+Q)^6} e^{-4/(1+Q)} + \frac{2^8}{3n^5} \int_{q_{\min}}^{q_{\max}} \frac{dQ}{Q} \times \frac{-19Q^3 + 3Q^2 + 15Q + 11/3}{(1+Q)^9} e^{-4/(1+Q)}.$$
 (16)

If we now make the substitutions y=1/(1+Q),  $y_0 = 1/(1+Q_{\min}), y_1 = 1/(1+Q_{\max})$ , we get, after some simplification:

$$\Phi_n/\kappa = \frac{2^8}{3n^3} \int_{y_1}^{y_0} y^4 e^{-4y} dy [2 + 1/(1-y)] + \frac{2^8}{9n^5} \int_{y_1}^{y_0} y^5 e^{-4y} dy \times [-32y^2 + 112y - 68 + 11/(1-y)]. \quad (17)$$

TABLE I. Calculated values of several quantities.

n	$M_n$	$ x_{0n} ^2$	G(n)	$ x_{0n} ^2 G(n)$
1.75	0.177425	1.217489	0.470380	0.572682
2.00		0.554929	0.689255	0.382488
2.25	0.979248	0.305527	0.845516	0.258328
2.50	1.38629	0.188806	0.960383	0.181326
3.00		0.088989	1.113891	0.099124
3.50	2.98629	0.049766	1.208570	0.060145
4.00		0.030924	1.270918	0.039302
4.50	4.44946	0.020644	1.314077	0.027128
5.00		0.014519	1.345081	0.019529

Letting

$$I_{k} = \int_{y_{1}}^{y_{0}} y^{k} e^{-4y} dy \text{ and } R = \int_{y_{1}}^{y_{0}} e^{-4y} dy/(1-y),$$

we note that

$$\int_{y_1}^{y_0} y^k e^{-4y} dy/(1-y) = \int_{y_1}^{y_0} (y^k - 1) e^{-4y} dy/(1-y) + R,$$

and

$$(y^{k}-1)/(1-y) = -\sum_{l=0}^{k-1} y^{l}$$

Thus

$$\int_{y_1}^{y_0} y^k e^{-4y} dy/(1-y) = R - \sum_{l=0}^{k-1} I_l,$$

and

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$$\Phi_n/\kappa = \frac{2^8}{3n^3} \{ 2I_4 - \sum_{l=0}^3 I_l + R \} + \frac{2^8}{9n^5} \{ -32I_7 + 112I_6 - 68I_5 - 11 \sum_{l=0}^4 I_l + 11R \}.$$
(18)

The integrals  $I_k$  are elementary, and the integral R can be evaluated, giving

$$R = -e^{-4} [Ei(4(1-y_0)) - Ei(4(1-y_1))].$$

Keeping terms to relative order  $1/n^2$ , the final expression for *n* large becomes:

$$|x_{0n}|^2 n^3 G(n) = 2.31197 + 3.17662(1/n^2).$$
 (19)

This agrees with the results obtained in Section III, Eq. (14) to order  $1/n^2$  and agrees with the exact result, given in Table I, for n=5 within 0.1 percent.

# V. CONTINUOUS SPECTRUM CONTRIBUTION TO $B_K$

We will now obtain the contribution to  $B_K$  of the part of the continuous spectrum between  $\theta$  and 1. This is given by

$$D_{K}(\theta) = \frac{1}{\kappa} \int_{\theta}^{1} \epsilon d\epsilon \Phi_{n}(\epsilon) = \frac{1}{\kappa} \int_{(1-\theta)^{-\frac{1}{2}}}^{\infty} (1-1/n^{2}) \Phi_{n} dn. \quad (20)$$

 $\Phi_n$  is given by (9) with  $|x_{0n}|^2$  defined by (7); G(n) is given by (14) for  $1.75 \le n \le 5$ , and by the first two terms

of (14) for n > 5. To perform the integration for the  $\ln \eta$  and the  $1/\eta$ -terms it is convenient to expand  $|x_{0n}|^2$  to order  $1/n^{10}$  as follows:

$$n^{3} | x_{0n} |^{2} = 1.56294 + 5.73076(1/n^{2}) + 13.1634(1/n^{4}) + 24.2952(1/n^{6}) + 39.4260(1/n^{8}) + 58.8077(1/n^{10}). (21)$$

We obtain, finally,

$$D_{K}(\theta) = \begin{bmatrix} 1.15599(1-\theta) + 1.37215(1-\theta)^{2} \\ + 0.654622(1-\theta)^{3} + 1.01568(1-\theta)^{4} \\ - 4.67429(1-\theta)^{5} + 4.50977(1-\theta)^{6} \end{bmatrix} \\ + \ln\eta \begin{bmatrix} 0.781468(1-\theta) + 1.04196(1-\theta)^{2} \\ + 1.23877(1-\theta)^{3} + 1.39148(1-\theta)^{4} \\ + 1.51307(1-\theta)^{5} + 1.61515(1-\theta)^{6} \end{bmatrix} \\ - (1/\eta) \begin{bmatrix} 0.195367(1-\theta) - 0.618662(1-\theta)^{2} \\ - 1.25324(1-\theta)^{3} - 1.74256(1-\theta)^{4} \\ - 2.12640(1-\theta)^{5} - 2.43323(1-\theta)^{6} \end{bmatrix}, \quad (22)$$

from which

$$D_{K}(0.7) = 0.377789 \ln \eta + 0.488121 + 0.051963(1/\eta)$$
  

$$D_{K}(0.75) = 0.287153 \ln \eta + 0.385488 + 0.018884(1/\eta)$$
  

$$D_{K}(0.8) = 0.210696 \ln \eta + 0.291738 - 0.000677(1/\eta)$$
  

$$D_{K}(0.9) = 0.089961 \ln \eta + 0.130034 - 0.011899(1/\eta).$$

#### VI. TOTAL STOPPING POWER OF HYDROGEN

We now obtain the total stopping number of hydrogen to order  $1/\eta$ . Following the method of Bethe,<sup>4</sup> we break the stopping number

$$B_H = \sum_{\substack{\text{all} \\ \text{states}}} (E_n - E_1) \int_{Q_{\min}}^{Q_{\max}} \frac{dQ}{Q^2} |F_n(Q)|^2 \qquad (24)$$

into two parts (introducing  $q^2 = Q$ ) as follows:

$$B_{H} = 2 \int_{q_{0}}^{q_{\max}} \frac{dq}{q^{3}} \sum_{n} |F_{n}(q)|^{2} (E_{n} - E_{1})$$
$$-2\sum_{n} \int_{q_{0}}^{q_{\min}(n)} \frac{dq}{q^{3}} |F_{n}(q)|^{2} (E_{n} - E_{1}) \quad (25)$$

where  $q_0$  may be chosen arbitrarily, and will be taken to be small. In the first term, integration and summation have been interchanged, as  $q_0$  and  $q_{\max}$  are independent of *n*. Bethe<sup>5</sup> has shown that

$$\sum_{n} |F_{n}(q)|^{2} (E_{n} - E_{1}) = q^{2}$$

so that the first term can be integrated directly giving  $2 \ln(q_{\text{max}}/q_0)$ .

To evaluate the second term in (25), expand  $\varphi_n(q^2) = (E_n - E_1) |F_n(q)|^2 / q^2$  about zero in Taylor's series, getting  $\varphi_n(q^2) \approx \varphi_n(0) + q^2 (d/dq^2) \varphi_n(q^2) |_{q^2=0}.$  (26)

The second term in (25) then becomes

$$-2\sum_{n} \varphi_{n}(0) \ln(q_{\min}/q_{0}) - \sum_{n} q_{\min}^{2} (d \varphi_{n}/dq^{2}) |_{q^{2}=0}$$

<sup>4</sup> Reference 3, p. 520.

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<sup>&</sup>lt;sup>5</sup> H. A. Bethe, Ann. d. Physik 5, 325 (1930).

As  $q_{\min}^2 = (E_n - E_1)^2 / 4\eta$ , we must evaluate the sum

$$\sum_{n} (E_{n} - E_{1})^{3} \frac{d}{dq^{2}} \frac{|F_{n}(q)|^{2}}{q^{2}} = \sum_{n} (E_{n} - E_{1})^{3} \frac{d}{dq^{2}} \frac{|(e^{iqx})_{1n}|^{2}}{q^{2}}.$$
(27)

With Hamiltonian H and wave functions  $\psi_n$ ,

$$(E_n - E_1) \int e^{iqx} \psi_n^* \psi_1 d\tau = (He^{iqx} - e^{iqx}H)_{1n} = \{e^{iqx} [q^2 - 2iq(\partial/\partial x)]\}_{1n} = K_{1n}$$

(using atomic units throughout), and

$$(E_n - E_1)^2 \int e^{iqx} \psi_n^* \psi_1 d\tau = (HK - KH)_{1n},$$
  
$$HK - KH = [H, e^{iqx}] [q^2 - 2iq(\partial/\partial x)] + e^{iqx} [H, q^2 - 2iq(\partial/\partial x)] = e^{iqx} [q^2 - 2iq(\partial/\partial x)]^2 + 2iqe^{iqx}(\partial V/\partial x).$$

Thus,

$$(E_n - E_1)^3 \left| \int e^{iqx} \psi_n^* \psi_1 d\tau \right|^2 = \left\{ \int \psi_1^* [q^2 - 2iq(\partial/\partial x)] e^{-iqx} \psi_n d\tau \right\} \left\{ \int \psi_n^* e^{iqx} \{ [q^2 - 2iq(\partial/\partial x)]^2 + 2iq(\partial V/\partial x) \} \psi_1 d\tau \right\} \cdot Making use of closure,$$

$$\sum_{n} (E_n - E_1)^3 |(e^{iqx})_{1n}|^2 = \int \psi_1^* [q^2 - 2iq(\partial/\partial x)] \{ [q^2 - 2iq(\partial/\partial x)]^2 + 2iq(\partial V/\partial x) \} \psi_1 d\tau$$

We obtain, finally,

$$-\sum_{n} (E_n - E_1)^3 |\langle e^{iqx} \rangle_{1n}|^2 = -q^6 + 4q^4 \langle \nabla^2 \rangle_{11} - 2iq^3 \langle \partial V / \partial x \rangle_{11} - (4/3)q^2 \langle \nabla^2 V \rangle_{11} - 4q^2 \langle (\partial V / \partial x) (\partial / \partial x) \rangle_{11}.$$
(28)

These expectation values can be obtained easily, giving,

$$\langle \nabla^2 \rangle_{11} = -1, \quad \langle \nabla^2 V \rangle_{11} = 8, \quad \left\langle \frac{\partial V}{\partial x} \frac{\partial}{\partial x} \right\rangle_{11} = -\frac{4}{3}, \quad \left\langle \frac{\partial V}{\partial x} \right\rangle_{11} = 0,$$

$$(1/q^2) \sum_n (E_n - E_1)^3 |(e^{iqx})_{1n}|^2 = +q^4 + 4q^2 + 16/3, \tag{29}$$

and thus

$$\sum_{n} q_{\min}^{2} (d\varphi_{n}/dq^{2}) |_{q^{2}=0} = 1/\eta, \qquad (30)$$



FIG. 1. Parametric curves of  $B_{\mathcal{K}}(\theta, \eta)$ .

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and

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$$B_H = 2 \ln(4\eta)^{\frac{1}{2}} q_{\max} - 1/\eta - 2\sum_n \varphi_n(0) \ln(1 - 1/n^2).$$
(31)

The last sum in (31) has been evaluated numerically (observe that  $\varphi_n(0) = |x_{0n}|^2 (1-1/n^2)$ ) and is equal to 0.096990. We set  $q_{\max} = (4\eta)^{\frac{1}{2}}$  in (31), and obtain, finally,

$$B_H = 2\ln\eta + 2.57861 - 1/\eta. \tag{32}$$

# VII. CONTRIBUTION OF DISCRETE STATES TO $B_K$ FOR HYDROGEN

We next obtain the contribution of the discrete states to the asymptotic stopping number of hydrogen; this is given by  $\sum_{\substack{\text{discrete}\\\text{states}}} (1-1/n^2)\Phi_n/\kappa$ . Bethe<sup>3</sup> gives formulas for  $\Phi_n$  for n=2, 3, 4, 5 which we have evaluated, and which

agree with (9). These give

$$\Phi_{2}/\kappa = 0.554929 \ln \eta + 0.382488 + 0.173415(1/\eta),$$

$$\Phi_{3}/\kappa = 0.0889893 \ln \eta + 0.0991244,$$

$$\Phi_{4}/\kappa = 0.0309238 \ln \eta + 0.0393016 - 0.0033823(1/\eta),$$

$$\Phi_{5}/\kappa = 0.0145191 \ln \eta + 0.0195294 - 0.0023231(1/\eta),$$

$$1/\kappa^{2}\Phi_{5}/\kappa = 0.528228 \ln \eta + 0.420570 + 0.124661(1/\kappa).$$
(33)

 $\sum_{n=6}^{\infty} f(n) = \int_{6}^{\infty} f(n) dn + f(6)/2$ 

$$\sum_{n=2}^{5} (1 - 1/n^2) \Phi_n / \kappa = 0.538228 \ln \eta + 0.430570 + 0.124661(1/\eta).$$
(34)

For n > 5 we approximate the sum over discrete states by an integral. For  $\Phi_n$  we use the asymptotic form of (9),  $|x_{0n}|^2 G(n)$  being given by (19) and  $|x_{0n}|^2$  by (21). The expression used

 $\begin{array}{c} n^{3}\Phi_{n}/\kappa = 2.31197 + 3.17662(1/n^{2}) \\ + \left[1.56294 + 5.73076(1/n^{2}) + 13.1634(1/n^{4})\right] \\ \times \left[\ln\eta - (1 - 9/n^{2})/4\eta\right] \end{array} (35)$ 

$$+ \Delta^{1}/12 - \Delta^{3}/720 + \cdots \quad (36)$$
with  $f(n) = (1 - 1/n^{2}) \Phi_{n}/\kappa$ ,  $\Delta^{r} = -f^{(r)}(6)$ , gives
$$\sum_{n=1}^{\infty} (1 - 1/n^{2}) \Phi_{n}/\kappa = 0.026778 \ln \eta$$

gives agreement with the exact value at n=5 to within 0.1 percent. The Euler-Maclaurin summation formula,

$$+0.038120 - 0.0057038(1/\eta).$$
 (37)



FIG. 2. Parametric curves of  $C_K(\theta, \eta)$ .

The error in approximating the sum by (36) is better than 0.01 percent.

The contribution of the discrete states to the hydrogen stopping number is thus, adding (34) and (37),

$$\sum_{n=2}^{\infty} (1 - 1/n^2) \Phi_n / \kappa = 0.565006 \ln \eta + 0.468690 + 0.118957(1/\eta). \quad (38)$$

Subtracting this from the total stopping number (32), we obtain the continuum contribution

$$E_{\kappa} = \sum_{\text{continuum}} (1 - 1/n^2) \Phi_n / \kappa = 1.43499 \ln \eta + 2.10992 - 1.11896(1/\eta). \quad (39)$$

When (39) is added to Eq. (23), we obtain the asymptotic expression for the stopping power of K-electrons of any element,  $B_K(\theta, \eta)$ :

 $B_K(0.7, \eta) = 1.81278 \ln \eta + 2.59804 - 1.06699(1/\eta),$  $B_K(0.75, \eta) = 1.72215 \ln \eta + 2.49540 - 1.10007(1/\eta),$ (40) $B_K(0.8, \eta) = 1.64569 \ln \eta + 2.40165 - 1.11963(1/\eta),$  $B_K(0.9, \eta) = 1.52495 \ln \eta + 2.23995 - 1.13085(1/\eta).$ 

## VIII. RESULTS

In Fig. 1 we give the results of M. C. Walske<sup>6</sup> for  $B_K(\theta, \eta)$  for  $\theta = 0.7$ , 0.8, 0.9, and for  $0 \leq \eta \leq 1.5$ , for

<sup>6</sup> We wish to thank Mr. Walske for making available to us his results, which have not previously been published.

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TABLE II. Percentage difference between Eq. (40) and the results of Walske.

	$\theta = 0.7$	0.8	0.9
$\eta = 2.5$	13.9	12.5	12.0
5	7.5	6.4	5.8
10	4.0	3.0	2.6

which, of course, the expressions (40) are not valid. These curves, having an absolute accuracy of 0.01 in  $B_K$ , were obtained from a numerical evaluation of (1), using for  $|F_n(Q)|^2/Q$  expression (755) of reference 1. Walske has carried his calculations up to  $\eta = 10$ , and for  $\eta > 1$  his values lie below those given by (40). As a guide to the energy region where (40) may be applied, we give in Table II the error in (40) for several values of  $\eta$ .

For large values of  $\eta$  it is convenient to write  $B_K(\theta, \eta)$ in the form

$$B_{K}(\theta, \eta) = A(\theta) \ln \eta + B(\theta) - C_{K}(\theta, \eta), \qquad (41)$$

where  $-C_K(\theta, \eta)$  approaches the  $1/\eta$ -term in (40) as  $\eta$ increases. In Fig. 2 we plot  $C_K(\theta, \eta)$  as a function of  $(1/\eta).$ 

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# Photo-Disintegration of Deuterium by 4.5 to 20.3 Mev X-Rays\*†‡

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A study is made of the angular distributions and the distribution in energy of the photo-protons arising from the photo-disintegration of deuterium by the continuous x-ray spectrum produced when electrons accelerated in the betatron to a kinetic energy of 20.3 Mev impinged on a 0.005 in. Pt target. The collimated x-ray beam passed through a deuterium gas-filled reaction chamber in which nuclear emulsions were placed to detect the resulting photo-protons. The angular distributions for six photon energy intervals are consistent with a differential cross section in the center of mass system of the form:  $\sigma(\theta) \approx a + \sin^2\theta (1 + \alpha \cos\theta)$ . Assuming an intensity spectrum for the betatron radiation of the shape determined by Koch and Carter a curve for the relative cross section for the photo-disintegration of deuterium as a function photon energy was determined. This curve falls off more slowly than does the Bethe-Peierls expression. The discrepancy, however, is within the experimental errors and the uncertainties in the spectrum of the betatron radiation.

# I. INTRODUCTION

'HE photo-disintegration process in deuterium, i.e., the process  $D(\hbar\omega, n)P$ , has been the subject of considerable experimental study during the last few years. Most of this work has been done with photons having energies below 3 Mev. Both the photo-neutrons<sup>1</sup>

and the photo-protons<sup>2</sup> have been observed and their angular distributions studied. At these low energies both the observed angular distributions and the total cross sections<sup>3</sup> seem to be in general agreement with the theoretically predicted values.

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<sup>‡</sup> Deuterium gas obtained on allocation from the U.S. Atomic Energy Commission. <sup>1</sup> B. Hammermesh and A. Wattenberg, Phys. Rev. **75**, 1290

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FIG. 2. Parametric curves of  $C_K(\theta, \eta)$ .