be assigned to the magnitude of the elastically scattered component. Values of ρ at $E=E_0$ have been displayed in Fig. 6 for various targets as a function of the incident electron energy E_0. The decline in ρ with increasing energy E_0 and with decreasing target atomic number Z agrees qualitatively with a formula obtained by Dashen[14] and with a similar expression obtained earlier by Bothe.[13] However, the curves of Fig. 6 decrease more rapidly than the Z/E_0 dependence predicted by these theories. In view of the approximations employed in the theory, close agreement is not expected.

No theoretical treatment presently available offers an adequate quantitative description of the data contained in this and the previous paper.[1] Apparently, the energy range from about 500 eV to 10 MeV contains most of the interesting variation in the retrofugal-flux coefficient $\rho(Z,E_0,\theta,E)$. In this range the effect of the binding energy of the target atomic electrons is important and directly influences the generation of energetic secondary electrons. Except for the secondary electrons from *e-e* collisions, these have been ignored in theoretical treatments so far, but evidently the secondary electrons make a substantial contribution to the retrofugal flux. Berger,[15] using Monte Carlo methods, has calculated the spectrum of backscattered electrons from aluminum for 0.5-MeV primaries. He obtains an elastically scattered component consistent with the present data although the most probable energy E_w is somewhat higher than the present measurements indicate. Again, the presence of secondary electrons could account for the difference in magnitude between the measured and the calculated retrofugal-flux coefficient as well as the differences in the spectrum profile. Other theoretical treatments by Bothe,[13] by Thümmel,[12] and by Dashen[14] yield results which also are deficient at the lower energy portion of the spectrum. Since all of these neglect the generation of secondary electrons in the target, a discrepancy of this type is expected.

ACKNOWLEDGMENT

Appreciation is expressed for the able assistance of A. B. Grijalva in maintaining the Linac as a reliable instrument for these investigations.

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Stopping Power of M Electrons*

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Explicit formulas are obtained for the atomic M-shell form factor as a function of energy loss and momentum transfer of a charged particle in the Bethe-Born approximation. The M-shell binding corrections to Bethe's energy-loss formula are calculated. The validity of the calculation is limited by the use of hydrogenic wave functions.

I. INTRODUCTION

The removal of inner-shell electrons from atoms by impinging protons or other heavy ions has been studied experimentally and theoretically from time to time during the past fifty years.[1] The process itself, manifested by the emission of characteristic x rays, has received some attention, but most interest has centered around inner-shell excitation and ionization as a mechanism by which charged particles lose energy as they penetrate matter. As is well known, the contribution of the relatively slowly moving outer electrons to the stopping power of a particle incident with charge ze and velocity v is accurately taken into account by Bethe's simple formula[2] for the energy loss per unit path length,

$$-dE/dx=(4\pi e^4z^2/mv^2)NB\,,$$

with $B=Z\ln(2mv^2/I)$. N is the number of stopping atoms per unit volume, Z the atomic number, I an average ionization potential, and m the electron mass. The contributions of the inner-shell electrons are, on the other hand, not properly represented in this formula and must be calculated separately. The contributions of the inner shells, notably K and L, but more recently also M, to the stopping power of charged particles have remained a subject of investigation since Bethe's pioneering work.[3]

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[2] H. A. Bethe, Ann. Physik **5**, 325 (1930).

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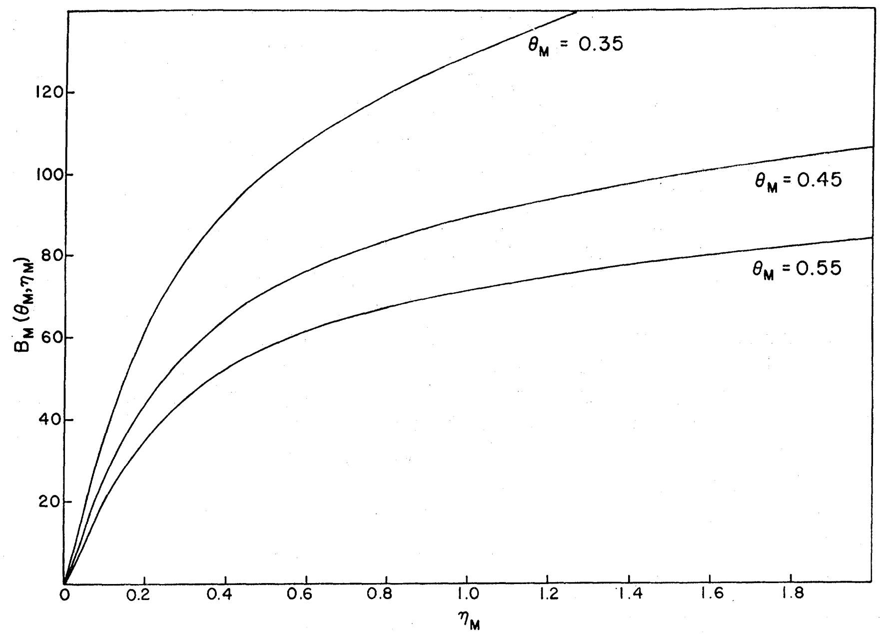

FIG. 1. $B_M(\theta_M,\eta_M)$, stopping-number contribution of M electrons as a function of the energy η_M of the incident particle for three values of the screening parameter θ_M.

The first quantum-mechanical calculation of the cross section of excitation and ionization was made by Bethe[2,4] for the K-shell electrons. The same method was applied to the L-shell electrons by Walske.[5] In Bethe's treatment, one uses plane waves to describe the impinging protons or heavy ions thereby neglecting any distortion of the projectile wave function by the Coulomb field of the nucleus. A further simplifying assumption is the use of hydrogenic wave functions for the atomic electrons in the vicinity of the nucleus.[6]

The extension of Bethe's method to the calculation of the ionization and excitation cross sections for M-shell electrons has for some time seemed desirable, but the complexity of the problem has so far been a deterrent against its solution. Since the main obstacle was the prodigious amount of algebra which could be expected on the basis of experience with the K- and L-shell calculations, one is led to think of using a computer for some of the algebraic operations.

The present paper contains the results of a calculation of the M-shell cross sections following the procedure and the assumptions used earlier by Bethe. Explicit formulas were obtained for the M-shell form factor as a function of energy loss and momentum transfer. The values of the stopping number B_M are exhibited in graphic and tabular form. Finally, approximate asymptotic formulas for the M-shell corrections to Bethe's stopping-power formula valid in the limit of high projectile energies are obtained.

[4] M. S. Livingston and H. A. Bethe, Rev. Mod. Phys. **9**, 263 (1937).
[5] M. C. Walske, Phys. Rev. **101**, 940 (1956).
[6] These assumptions and the prescription for including the effect of screening are discussed in the review article by Merzbacher and Lewis, Ref. 1.

II. THE EXCITATION FUNCTION AND STOPPING NUMBER

For an inelastic collision between an incident particle of mass M and energy E and an atom at rest, in which an electron from the M shell is promoted to a higher energy level, it is convenient to define an excitation function as

$$I(\eta_M,W)=\int_{Q_{\min}}^{Q_{\max}}\frac{dQ}{Q^2}|F_{WM}(Q)|^2. \quad (1)$$

The energy of the incident particle is measured in terms of

$$\eta_M=mE/MZ_M^2R_y, \quad (2)$$

where Z_M is the effective nuclear charge for the M shell which takes screening of the inner electrons summarily into account, and R_y is the Rydberg constant. W is the energy transferred to the atomic electron, in units $Z_M^2R_y$. The variable of integration Q in Eq. (1) is defined in terms of $\hbar q$, the change of the incident particle's momentum, by the relation

$$Q=(a_0^2/Z_M^2)q^2, \quad (3)$$

where a_0 is the first Bohr radius of the hydrogen atom.

The limits of integration in Eq. (1) can be obtained from conservation of energy and momentum. If, as may be assumed, the heavy charged particle loses in a single collision only a very small fraction of its initial energy, the lower limit of the Q integration becomes approximately $Q_{\min}=W^2/4\eta_M$. For the upper limit $Q_{\max}=\infty$ is a good approximation.

The so-called form factor $|F_{WM}(Q)|^2$, which appears in the integrand of (1), is the sum of the squares of the matrix elements of e^{iqz} between the nine distinct M-

shell states and the atomic states greater in energy by the amount W.

The calculation of the form factor, $|F_{WM}(Q)|^2$, follows the analogous work of Bethe[2] and Walske,[5,7] for the K and L shells, respectively, and is made with nonrelativistic hydrogenic wave functions. A GAT program was written performing the necessary algebra in obtaining $|F_{WM}(Q)|^2$ on a Univac 1105 computer. As a check, the program was required to reproduce the calculations of Walske[7] on the L shell. We quote only the final results here.

For transitions to the continuum ($W=k^2+\frac{1}{9}$),

$$|F_{WM}(Q)|^2dW=\frac{2^7}{3^3(1-e^{-2\pi/k})}\times\frac{\exp\{-(2/k)\arctan[\frac{2}{3}k/(Q-k^2+\frac{1}{9})]\}}{[(Q-k^2+\frac{1}{9})^2+(4/9)k^2]^5}\times Q[Q^5+f_1(k)Q^4+f_2(k)Q^3+f_3(k)Q^2+f_4(k)Q+f_5(k)]dW, \quad (4)$$

where

$$f_1(k)=-\left(\frac{43}{27}+\frac{11}{3}k^2\right),$$

$$f_2(k)=\frac{518}{243}+\frac{412}{81}k^2+\frac{14}{3}k^4,$$

$$f_3(k)=-\left(\frac{442}{729}+\frac{310}{81}k^2+\frac{122}{27}k^4+2k^6\right),$$

$$f_4(k)=\frac{11443}{98415}+\frac{1652}{2187}k^2+\frac{4606}{3645}k^4+\frac{4}{27}k^6-\frac{1}{3}k^8,$$

$$f_5(k)=\frac{14923}{6200145}+\frac{1279}{59049}k^2+\frac{902}{3645}k^4+\frac{34848}{45927}k^6+\frac{71}{81}k^8+\frac{1}{3}k^{10}.$$

From the excitation function the total cross section for an inelastic collision leading to a removal of one of the electrons from the M shell is easily obtained:

$$\sigma_M=\frac{8\pi z^2}{Z_M{}^2\eta_M}a_0{}^2\int_{W_{\min}}^{\infty}I(\eta_M,W)dW. \quad (5)$$

The lower limit $W_{\min}$ of the integration over all possible energy losses is a critical quantity which in the absence of any interaction between the atomic electrons would have the value $\frac{1}{9}$. Screening by the atomic electrons, which effectively reduces this quantity, is accounted for by the definition of a screening number θ_M by the relation

$$I_M=\theta_M\tfrac{1}{9}Z_M{}^2R_y, \quad (6)$$

where I_M is the average ionization potential of the M shell. In the computations of this paper θ_M was chosen to have the values 0.35, 0.45, and 0.55, corresponding to three representative regions of the periodic table of elements. The proper choice for $W_{\min}$ then becomes

$$W_{\min}=\tfrac{1}{9}\theta_M. \quad (7)$$

Since $\theta_M<1$, this implies the use of expression (4) for negative values of k^2. As Bethe and Walske have shown such an extrapolation is permissible if the normalization factor $1/(1-e^{-2\pi/k})$ is simply omitted.

The stopping number for the M shell, which is the quantity of central interest in this paper, is defined as

$$B_M(\theta_M,\eta_M)=\int_{\frac{1}{9}\theta_M}^{\infty}WI(\eta_M,W)dW. \quad (8)$$

The results of computations of B_M are given in graphic and tabular forms in Fig. 1 and Table I, respectively. These calculations were made for values of η_M between 0.1 and 10.

By comparing Fig. 1 with similar curves for the K and L shells, given in the work of Walske,[5,8] it is seen that the initial rise in B as a function of η becomes sharper as one goes from the lower toward the higher atomic shells.

TABLE I. Stopping-number contribution of M electrons, $B_M(\theta_M,\eta_M)$.

η_M	$\theta_M=0.55$	$\theta_M=0.45$	$\theta_M=0.35$
0.1	20.85	26.44	36.70
0.2	36.13	44.97	62.43
0.3	45.53	56.52	79.08
0.4	52.02	64.61	91.12
0.5	56.87	70.74	100.48
0.6	60.94	75.87	108.13
0.7	63.93	79.78	114.60
0.8	66.67	83.32	120.22
0.9	69.01	86.37	125.12
1.0	71.10	89.10	129.53
1.1	72.97	91.55	133.52
1.25	75.44	94.80	138.84
1.5	78.91	99.39	146.42
1.75	81.81	103.25	152.84
2.0	84.30	106.57	158.39
2.5	88.36	112.03	167.60
3.5	94.45	120.24	181.54
5.0	100.91	128.95	196.37
10.0	113.38	145.83	225.07

[7] M. C. Walske, thesis, Cornell, 1951 (unpublished).

[8] M. C. Walske, Phys. Rev. 88, 1283 (1952).

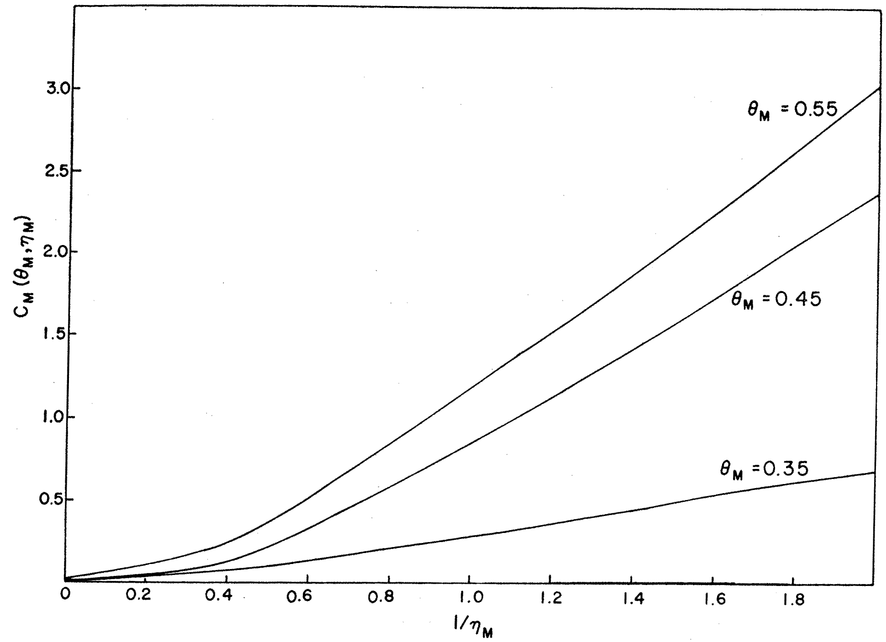

FIG. 2. Correction C_M to the high-energy stopping number for M electrons against $1/\eta_M$ for screening parameters $\theta_M=0.35$, 0.45, and 0.55.

III. ASYMPTOTIC FORMULA FOR $B_M(\theta_M,\eta_M)$

For large values of the projectile energy η_M, an asymptotic expression for B_M can be written in the form

$$B_M(\theta_M,\eta_M)=S_M(\theta_M)\ln\eta_M+T_M(\theta_M)-U_M(\theta_M)/\eta_M. \quad (9)$$

Approximate values for $S_M(\theta_M)$, $T_M(\theta_M)$, and $U_M(\theta_M)$ have been obtained by fitting an expression of this form to the highest computed values given in Table I for $\theta_M=0.35$, 0.45, and 0.55, respectively. No attempt was made to derive the asymptotic expansions from the theory. The resulting equations are

$$\begin{aligned} B_M(0.35,\eta_M)&=41.37\ln\eta_M+129.8-0.24/\eta_M,\\ B_M(0.45,\eta_M)&=24.29\ln\eta_M+89.92-0.39/\eta_M, \quad (10)\\ B_M(0.55,\eta_M)&=17.88\ln\eta_M+72.28-0.75/\eta_M. \end{aligned}$$

It should, however, be noted that the accuracy of Eqs. (10) depends on the accuracy of numerical values of B_M. Since the numerical values of B_M listed in Table I may contain errors of as much as 1%, the coefficient $U_M(\theta_M)$ in the last term of Eqs. (10) is not accurately determined. It is nevertheless useful to follow convention[8] and to extend the asymptotic expressions (10) by defining a quantity $C_M(\theta_M,\eta_M)$ for all η_M through the equations,

$$\begin{aligned} B_M(0.35,\eta_M)&=41.37\ln\eta_M+129.8-C_M(0.35,\eta_M),\\ B_M(0.45,\eta_M)&=24.29\ln\eta_M+89.92-C_M(0.45,\eta_M), \quad (11)\\ B_M(0.55,\eta_M)&=17.88\ln\eta_M+72.28-C_M(0.55,\eta_M). \end{aligned}$$

For low values of η_M, $C_M(\theta_M,\eta_M)$ was determined from the numerically evaluated B_M, and for $\eta_M>2$, $C_M(\theta_M,\eta_M)$ was taken to be proportional to η_M^{-1}, according to Eqs. (10). The results are shown in Fig. 2.

IV. CONCLUSIONS

The main result of this paper is Eq. (4) giving explicitly the plane-wave Born-approximation form factor for inelastic collisions of a charged particle with M-shell atomic electrons. The validity of the calculated cross section and stopping power is limited primarily by use of hydrogenic wave functions to represent the initial and final states of the ejected electron. More accurate calculations, using Hartree-Fock wave functions for the atomic electron are now probably feasible. In the meantime, the M-shell binding corrections presented in this paper may serve as reasonable estimates for protons and heavier ions stopping in high-Z elements.