with a copper crystal placed between the Al_2O_3 sample and our movable counter, oriented as in the copper annihilation experiments. No Laue peaks were observed in this "correlation-absorption" curve, taken with the same statistical accuracy as the original copper $N_{\hat{n}}(\theta)$.

We conclude therefore that the observed high-momentum anisotropies in copper can be attributed to a large extent to HMC annihilations with the conduction band and that the observed order of magnitude of these HMC is in agreement with simple independent particle computations. It is clear that a far better theoretical calculation is needed to include the following effects neglected in our model: (a) k-dependent Fourier components obtained from a "first-principle" band computation, which includes s-d hybridization both for the "s" and the "$3d$" bands and the effect of the large energy gaps on the (111) faces, combined with anisotropic positron wave functions[17]; (b) k-dependent enhancement factors due to positron-electron correlation.[18]

The authors thank A. Thompson and J. M. Weingart for technical assistance during the experiments.

[17] Similarly to the computation of Ref. 9 for Si.
[18] J. P. Carbotte and S. Kahana, Phys. Rev. 139, A213 (1965).

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Straggling of Heavy Charged Particles: Comparison of Born Hydrogenic-Wave-Function Approximation with Free-Electron Approximation*

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Statistical fluctuations in the energy loss of heavy charged particles in thin absorbers resulting from collisions with atomic electrons are determined for collision cross sections obtained from the first Born approximation calculated with hydrogenic wave functions. A comparison is given with the results calculated with a $1/\epsilon^2$ collision spectrum.

1. INTRODUCTION

STRAGGLING functions describe the statistical fluctuations of the energy losses of fast charged particles. Landau[1] has introduced a transport equation describing the behavior of the straggling function $f(x,\Delta)$ for energy losses Δ small compared to the initial energy T of the incident particle:

$$\frac{\partial f(x,\Delta)}{\partial x}=\int_0^\infty w(\epsilon)f(x,\Delta-\epsilon)d\epsilon-f(x,\Delta)\sigma_t, \quad (1)$$

where $f(x,\Delta)$ is the probability density function of particles that have penetrated a thickness x of the absorber and have experienced an energy loss Δ; $w(\epsilon)d\epsilon$ is the differential collision cross section for single collisions, with an energy loss ϵ; and $\sigma_t=\int_0^\infty w(\epsilon)d\epsilon$ is the total collision cross section. This equation has recently been discussed by Tschalär,[2] and Kellerer.[3]

In experiments, for example, N_0 particles penetrate an absorber of a given thickness x. The number dN of particles emerging with energy losses between Δ and $\Delta+d\Delta$ is given by $dN=N_0f(\Delta)d\Delta$. Often, only the mean energy loss $\langle\Delta\rangle=\int f(\Delta)\Delta d\Delta$ is of interest. It is closely related to the stopping power S: $\langle\Delta\rangle\simeq xS$.

The collision cross section $w(\epsilon)$ is of great importance in the solution of Eq. (1). The simple approximation $w(\epsilon)=k/\epsilon^2$ used so far[1,2,4] and a more realistic function obtained from calculation in first Born approximation using hydrogenic wave functions are therefore discussed in Sec. 2. It may be noted, though, that the true collision cross section $w(\epsilon)d\epsilon$ for single atoms is zero below an energy ϵ_l equal to the difference in energy between the lowest possible excited state and the ground state of the atoms, and also vanishes rapidly for $\epsilon>\epsilon_m\simeq 2mv^2$. Similarly, $f(x,\Delta-\epsilon)$ must be equal to zero for $\epsilon>\Delta$. The limits of integration introduced by Vavilov have to be understood from these conditions.

The solution of the transport equation using the Laplace transform[1,4] is

$$f(x,\Delta)=\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty}\exp\left[p\Delta-x\int_0^\infty w(\epsilon)(1-e^{-p\epsilon})d\epsilon\right]dp. \quad (2)$$

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[1] L. Landau, USSR J. Phys. 8, 201 (1944).
[2] C. Tschalär, Nucl. Instr. Methods 61, 141 (1968).
[3] A. Kellerer, G. S. F. Bericht *B*-1 Strahlenbiologisches Institut der Universität München.
[4] P. V. Vavilov, Zh. Eksperim. i Teor. Fiz. 32, 920 (1957) [English transl.: Soviet Phys.—JETP 5, 749 (1957)]. Extensive tabulations of the Vavilov functions are given by Seltzer and Berger, Natl. Acad. Sci.—Natl. Res. Council, Publ. 1133, 187 (1967), 2nd printing.

The derivation is discussed by Landau and Vavilov. It should be noted that $c \to 0$ can be used in the limits of the integral. For a general collision cross section, numerical integration is required. Landau[1] and Vavilov[4] achieved an analytic form for the integral over ϵ, using $w(\epsilon)=k/\epsilon^2$, but performed a numerical integration for the integral over p. Blunck and Leisegang[5] and Shulek *et al.*[6] introduced corrections due to resonance effects in $w(\epsilon)$. In this paper we progress further by exploring the effects of cross sections calculated in first Born approximation, using hydrogenic wave functions. It is possible to express the solution for a general $w(\epsilon)$ in terms of a correction applied to the Vavilov solution. Therefore Vavilov's method is discussed in Sec. 3. The numerical integration of the integral over ϵ in Eq. (2) is discussed in Sec. 4. A generalization of the method of Blunck and Leisegang and Shulek *et al.* is discussed in Sec. 5, and the modified straggling function is given in Sec. 6. Quantities calculated with $w(\epsilon)=k/\epsilon^2$ are denoted with primes, e.g., $f'(x,\Delta)$, I_2'.

2. ATOMIC COLLISION CROSS SECTIONS

The practical results for straggling calculations so far have been obtained with the use of the classical electron cross section,[1,4] modified by estimates[5,6] of the influence of the "resonance effects" on the second moment M_2 of $w(\epsilon)$. The collision cross section $d\sigma'$ describing the collision of a heavy charged particle of charge ze, kinetic energy T, and velocity $v=\beta c$ with a free electron of mass m and charge $-e$ is given by

$$\begin{aligned} d\sigma' &= w(\epsilon)d\epsilon = k_1\epsilon^{-2}d\epsilon, \quad \text{for } \epsilon_l<\epsilon<\epsilon_m \\ d\sigma' &= 0, \quad \text{for all other } \epsilon, \end{aligned} \tag{3}$$

where $k_1=2\pi z^2e^4/mv^2$. Since we are concerned with low energies, a sufficient approximation for ϵ_m is given by $\epsilon_m=2mv^2$. For the further applications in Eq. (13), the moments M_n' of $w(\epsilon)=k_1/\epsilon^2$ for $n>1$ will be required. They are calculated for an absorber containing N atoms per cm^3 of atomic number Z,

$$M_n'=k\int_0^{\epsilon_m}\epsilon^{-2}\epsilon^n d\epsilon=\frac{k\epsilon_m{}^{n-1}}{(n-1)}, \tag{4}$$

where $k=k_1NZ$, and $\epsilon_l=0$, as assumed in the previous papers.

It is the intent of this paper to investigate the modifications necessary in the Vavilov theory caused by the use of more realistic collision cross sections. As a first, improved approximation, the values calculated with the first Born approximation,[7,8] using hydrogenic wave functions,[9,10] are used. Using Walske's notation,[9]

$$d\sigma=kJ(\eta,W)dW, \tag{5}$$

where $W=\epsilon/(Z-d)^2R$ is the energy ϵ lost by the particle expressed in suitable units, $\eta=mv^2/[2(Z-d)^2R]$ is the energy of an electron having the same velocity as the incident particle; $R=13.6$ eV is the Rydberg constant; d is a shielding factor for the nuclear charge of the absorber, depending on the electron shell; k is proportional to the number of electrons under consideration.

The excitation function J is defined by

$$J(\eta,W)=\int|F(\eta,\mathbf{q})|^2Q^{-2}dQ, \tag{6}$$

where $\mathbf{q}$ is the change in momentum of the incident particle, $Q=q^2/2m$; $|F(\eta,\mathbf{q})|^2$ is the matrix element for the transition from the ground state to the excited state of energy W of the atom. Notice that the energy E of the secondary electron (δ ray) is $E=\epsilon-I$, where I is the ionization energy of the atomic shell. The excitation functions have been recalculated for the K and L shells.[11] The difference between k_1/ϵ^2 and J can be appreciated from a plot of $d\sigma/d\sigma'=JW^2$ as a function of W. This is given in Figs. 1 and 2. The increase for small W corresponds to the resonance effects discussed by Bohr.[12] No simple analytic expression can be given for J or for its moments M_n:

$$M_n=k\int_{W_l}^{\infty}J(\eta,W)W^ndW. \tag{7}$$

The lower limit is now exactly the lowest possible excitation energy W_l of the atomic shell; the upper limit can be set at ∞, because J drops off rapidly near $W_m=4\eta=2mv^2/(Z-d)^2R$. It is to be expected, though, that, for large η, the tail beyond 4η (see Figs. 1 and 2) will contribute increasingly to the higher moments.

The total collision cross section σ_t, equal to the moment M_0, has been discussed, e.g., by Merzbacher and Lewis[13] and by Brandt and Laubert.[14] The stopping power S, equal to the first moment M_1, is discussed in many papers.[9,15] The stopping number $B=M_1/k$ is compared with the expression $\ln 2mv^2/I$, used frequently in simplified stopping-power theory, in Fig. 3.

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[5] O. Blunck and S. Leisegang, Z. Physik **128**, 500 (1950).
[6] P. Shulek, B. M. Golovin, L. A. Kulyukina, S. V. Medved, and P. Pavlovich, Yadern. Fiz. **4**, 564 (1966) [English transl.: Soviet J. Nucl. Phys. **4**, 400 (1967)].
[7] U. Fano, Ann. Rev. Nucl. Sci. **13**, 1 (1963).
[8] H. Bethe, Ann. Physik **5**, 325 (1930).
[9] M. C. Walske, Phys. Rev. **88**, 1283 (1952); **101**, 940 (1956).
[10] G. S. Khandelwal and E. Merzbacher, Phys. Rev. **144**, 349 (1966); **151**, 12 (1966).
[11] Unpublished calculations by the author, available on computer tape. Approximate values can be obtained from Figs. 1 and 2.
[12] N. Bohr, Kgl. Danske Videnskab. Selskab, Mat.-Fys. Medd. **18**, No. 8 (1953).
[13] E. Merzbacher and H. W. Lewis, in *Encyclopedia of Physics*, edited by S. Flügge (Springer-Verlag, Berlin, 1958), Vol. 34.
[14] W. Brandt and R. Laubert, Phys. Rev. **178**, 225 (1969).
[15] H. Bichsel, American Institute of Physics Handbook, 3rd ed. (to be published).

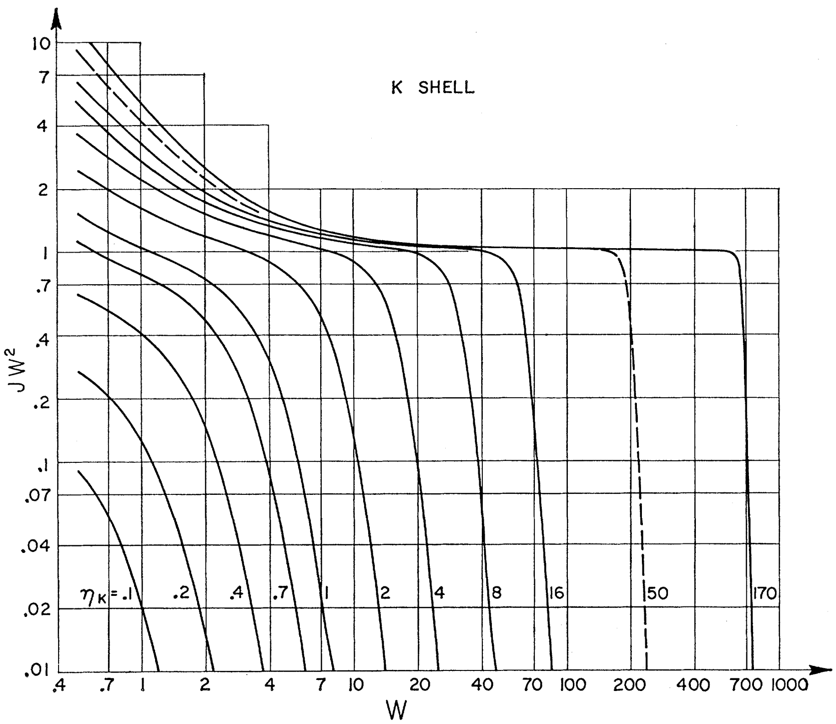

FIG. 1. The excitation function J_K for the K shell. Plotted is the product $J_K W^2$, where W is the electron energy in a suitable unit: $W = \epsilon / [(13.6 \text{ eV}) \times (Z-0.3)^2]$. The parameter $\eta_K = 18\,800\beta^2/(Z-0.3)^2$ is the value of W for an electron of the same velocity $v=\beta c$ as the incident particle. The energy $\epsilon_m = 2mv^2$ for a free electron corresponds to $W_m = 4\eta_K$. The lower limit for the integrals is $W_l = W_{\min} = I_K/(13.6 \text{ eV}) \times (Z-0.3)^2$, where I_K is the energy to lift a K-shell electron to the lowest unoccupied level of the atom with atomic number Z. The asymptotic value for large $W < 4\eta_K$ is $JW^2 \to 1$.

An approximation for the second moment has been given in Livingston and Bethe[16]; for the higher moments, $M_n = M_n'$ is usually chosen. This is not a good assumption, as mentioned above. The second and third moments for the L shell are given in Figs. 4 and 5; some higher moments are listed in Table I.

For solids, the excitation function for valence electrons will be modified for energy losses below 50 or 100

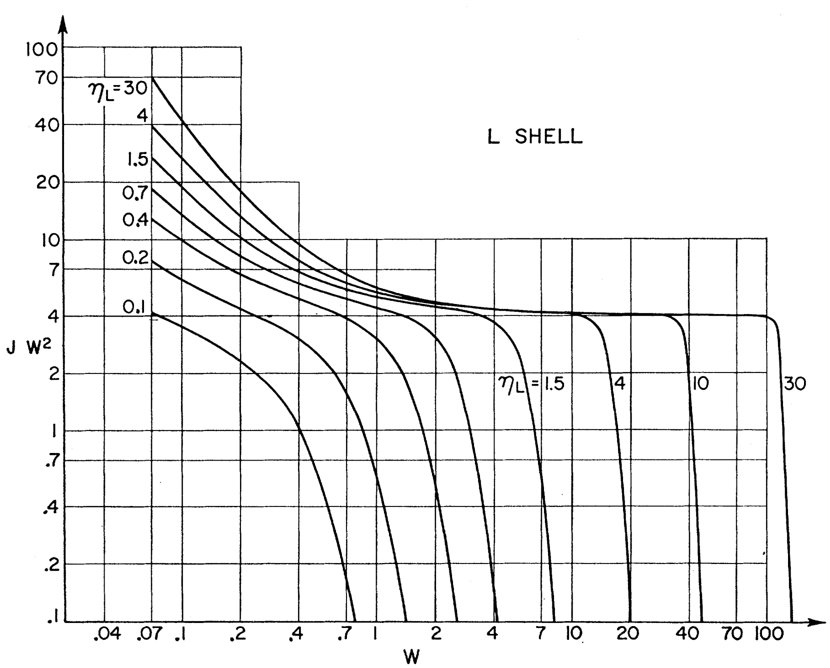

FIG. 2. The product $J_L W^2$ for the L shell. The units are the same as defined for the K shell, except that $(Z-0.3)^2$ is to be replaced by $(Z-4.15)^2$. Notice that J_L as well as J_K extends beyond $4\eta_L$. There is a small probability of collisions with energy transfer $\epsilon > 2mv^2$. W_l depends on Z: for Al, $W_{\min} \simeq 0.0926$, for Pb, $W_{\min} \simeq 0.167$. The asymptotic value of $J_L W^2$ is 4.

[16] M. S. Livingston and H. Bethe, Rev. Mod. Phys. 9, 263 (1937).

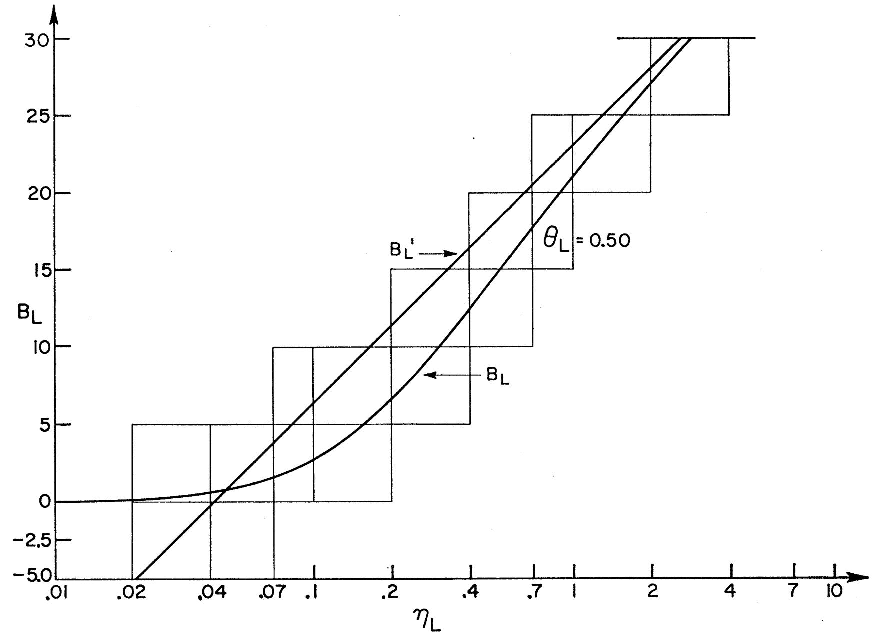

FIG. 3. The stopping number B_L as a function of η_L for $Z\simeq50$, compared with $B_L'=3.37\times\ln(2mv^2/I_L)$. The shell correction C_L is the difference between B_L and B_L': $C_L=B_L'-B_L$.

eV to resemble a resonance-type cross-section curve,[17,18] with a finite slope toward low energies. For single atoms, sharp peaks are expected in the cross section at energy losses equal to the excitation energies.[19] Although these effects are quite important for σ_T and S, they produce relatively small changes in the higher moments $M_2, M_3, \ldots$.

3. VAVILOV SOLUTION

In order to solve Eq. (2) it will be useful to consider separately the integral over ϵ:

$$I_1\equiv\int_0^\infty w(\epsilon)(1-e^{-p\epsilon})d\epsilon. \quad (8)$$

Since p is imaginary, I_1 is complex. In general, the uncertainty in the knowledge of $w(\epsilon)$ is greater at small values of ϵ. Landau and Vavilov therefore extract the first moment M_1 of $w(\epsilon)$ from I_1,

$$M_1\equiv\int w(\epsilon)\epsilon d\epsilon, \quad (9)$$

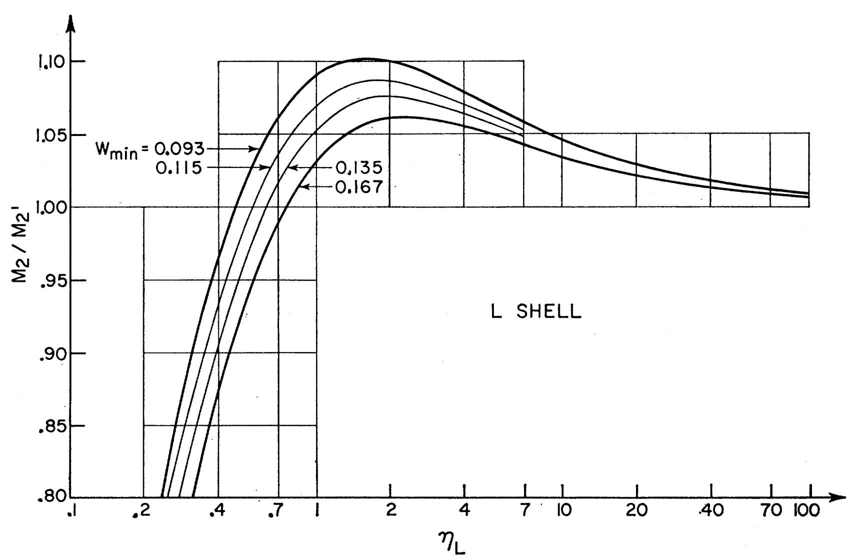

FIG. 4. The ratio $r_2=M_2/M_2'$ of the cross section as calculated in this paper and of the free-electron cross section for the L shell. The four curves are drawn for $W_l\equiv W_{\min}=0.093$ (silicon), 0.115 (copper), 0.135 (silver) and 0.167 (lead). For $\eta_L>4$, the expression of Ref. 16 agrees approximately with the curves given here, but deviates strongly at smaller η_L.

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[17] P. Nozières and D. Pines, Phys. Rev. **113**, 1254 (1959).
[18] R. E. Burge and D. L. Misell, Phil. Mag. **18**, 251 (1968).
[19] J. T. Park and F. D. Schowengerdt, Phys. Rev. **185**, 152 (1969).

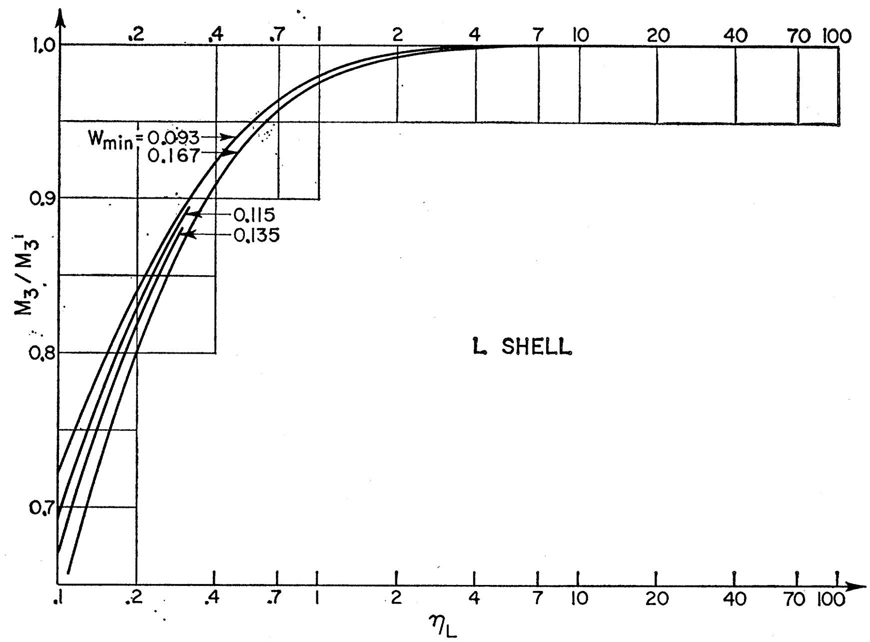

FIG. 5. The ratio $r_3=M_3/M_3'$ for the L shell. The same values for $W_{\min}$ are used as for Fig. 4.

by adding and subtracting $p\epsilon$ in the parentheses:

$$I_1=p\int w(\epsilon)\epsilon d\epsilon+\int w(\epsilon)(1-e^{-p\epsilon}-p\epsilon)d\epsilon, \qquad (10)$$

with

$$I_2\equiv\int w(\epsilon)(1-e^{-p\epsilon}-p\epsilon)d\epsilon, \qquad (11)$$

and, since M_1 is the stopping power S of the material, we obtain

$$I_1=pS+I_2. \qquad (12)$$

The behavior of $w(\epsilon)$ at small values of ϵ is less important in I_2, and for S an experimental value can be chosen, thus eliminating uncertainties in $w(\epsilon)$ for the first moment. For the method described in Sec. 5, the

TABLE I. Higher moments M_n of the quantum-mechanical collision cross section. M_n depend very little on $W_{\min}$. Tabulated is M_n/M_n'.

η_L	n = 4	5	6	7	8	9	10
0.1	1.08	1.97	4.57				
0.2	1.04	1.51	2.65				
0.25	1.026	1.42	2.30	4.62	26.2	1926	...
0.4	1.012	1.27	1.80				
0.9	1.003	1.12	1.35				
1.5	1.001	1.074	1.210	1.434	1.821	2.85	25.5
4	1.0005	1.03	1.08				
10	1.0005	1.01	1.032	1.061	1.102	1.16	1.24
20	1.0005	1.01	1.016				
40	1.0005	1.003	1.008				
100	1.000	1.000	1.002	1.004	1.008	1.0115	1.016

power-series expansion of I_2 will be needed:

$$I_2=-\sum_{n=2}^{\infty}(-1)^n\frac{p^n}{n!}\int w(\epsilon)\epsilon^n d\epsilon=-\sum_{n=2}^{\infty}(-1)^n\frac{p^nM_n}{n!}, \qquad (13)$$

where the $M_n=\int w(\epsilon)\epsilon^n d\epsilon$ [see also Eqs. (4) and (7)] are the moments[3,5] of the collision cross-section spectrum $w(\epsilon)$.

The evaluation of Eq. (11) using the free-electron collision spectrum has been given by Vavilov and is repeated here. The real and imaginary parts, $\Re(I_2')$ and $\Im(I_2')$, are written separately, with $p=iy$, $t=y\epsilon_m$:

$$\Re(I_2')=k\int_0^{\epsilon_m}\frac{1-\cos y\epsilon}{\epsilon^2}d\epsilon=ky\left(\frac{\cos t-1}{t}+\mathrm{Si}(t)\right)$$
$$=\frac{k}{\epsilon_m}[\cos t-1+t\,\mathrm{Si}(t)], \qquad (14)$$

where

$$\mathrm{Si}(t)\equiv\int_0^t\frac{\sin t'}{t'}dt',\quad \mathrm{Si}(0)=0,$$

$$\Im(I_2')=k\int_0^{\epsilon_m}\frac{\sin y\epsilon-y\epsilon}{\epsilon^2}d\epsilon=\frac{k}{\epsilon_m}$$
$$\times\{t-\sin t+t[\mathrm{Ci}(t)-\ln t-\gamma]\}, \qquad (15)$$

where

$$\mathrm{Ci}(t)\equiv\int_0^t\frac{\cos t'-1}{t'}dt'+\ln t+\gamma,\quad \text{for } \gamma=0.577216. \qquad (16)$$

The functions $\mathcal{R}$ and $\mathcal{J}$ are plotted in Figs. 6 and 7 for several values of ϵ_m.

For any given collision spectrum $w(\epsilon)$, two procedures can be used to determine I_2: (a) Direct numerical evaluation of Eq. (11), discussed in Sec. 4, and (b) calculations based on the use of Eq. (13), similar to the methods used in Refs. 5 and 6, and discussed in Sec. 5.

4. TRANSFORM OF BORN-APPROXIMATION COLLISION CROSS SECTIONS

The integral I_2 defined in Eq. (11) has been calculated numerically for the collision cross section $J(W)$ defined in Sec. 2 for a number of purely imaginary values of p, $0<|p|<1000$. Since only a limited number of values of $J(W)$ are available at $W=W_n$, $n=1, 2, 3, \ldots,$ and since $(1-e^{-p\epsilon}-p\epsilon)$ oscillates rather strongly, the mean-value theorem has to be used for the integral:

$$I_2(p,\eta)\approx k\sum_n J(W_n,\eta)\int_{a_n}^{b_n}(1-e^{-pW}-pW)dW$$
$$=k\sum_n J(W_n,\eta)[b_n-a_n+p^{-1}(e^{-pa_n}-e^{-pb_n})-\tfrac{1}{2}p(a_n^2-b_n^2)],\quad(17)$$

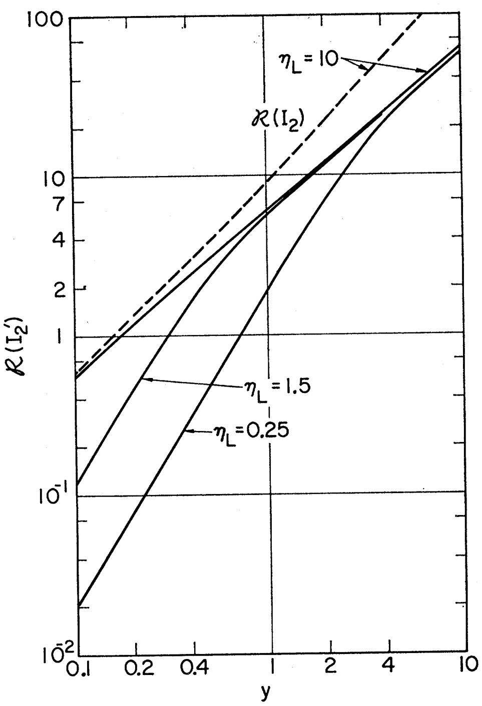

FIG. 6. The real part $\mathcal{R}(I_2')$ of the integral I_2' for three values of $W_m=4\eta_L$, as a function of the Laplace-transform parameter y. The electron energies corresponding to W_m are $\epsilon_m=W_m\times13.6$ eV $\times(Z-4.15)^2$. The dotted line is $\mathcal{R}(I_2)$ for the cross section calculated here, for $\eta_L=10$. This function is the exponent in the integrand of Eq. (24).

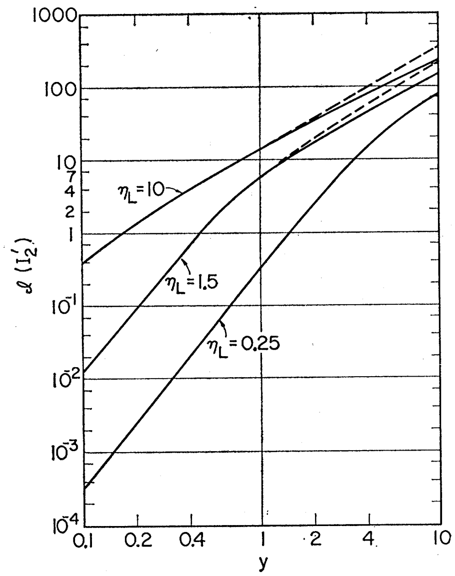

FIG. 7. The imaginary part of the integral I_2' for three values of W_m. The dotted lines show the function for I_2. This function, added to $y(\Delta-\bar{\Delta})$, forms the argument of the cosine in Eq. (24).

where $a_n=(W_nW_{n-1})^{1/2}$, $b_n=(W_nW_{n+1})^{1/2}$, since the W_n follow a geometrical progression. The ratios $r=\mathcal{R}(I_2)/\mathcal{R}(I_2')$ and $r_i=\mathcal{J}(I_2)/\mathcal{J}(I_2')$ are given in Figs. 8 and 9 for L-shell electrons. The numerical accuracy of the results can be estimated from a comparison of the evaluation of Eq. (17), using $J'=1/W^2$, with results calculated with Eqs. (14) and (15). The agreement is within 0.1%; a slightly larger error for I_2 is expected because of the faster change of $J(W)$ at small W.

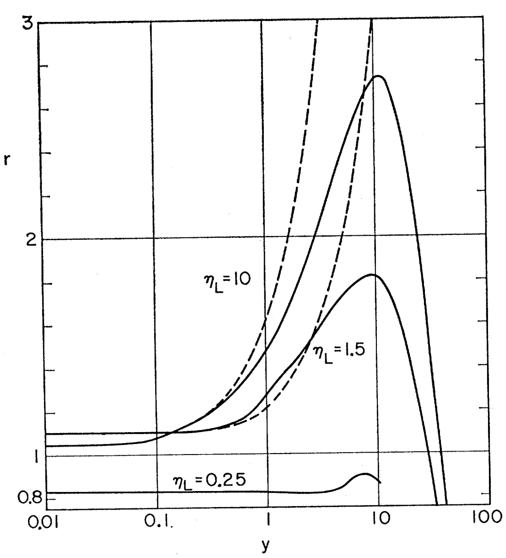

FIG. 8. The ratio r of the real part of I_2 and the real part of I_2'. The dotted lines indicate the correction by Shulek *et al.* (Ref. 6). $W_l=0.095$.

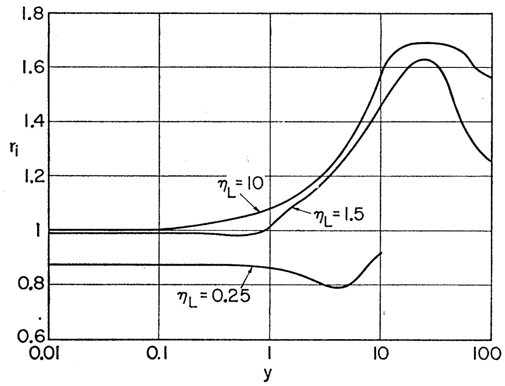

FIG. 9. The ratio $r_i = \mathcal{J}(I_2)/\mathcal{J}(I_2')$ of the imaginary part of I_2 and I_2'.

For very small values of p, I_2 can be written as:

$$\mathcal{R}(I_2) \approx -\tfrac{1}{2}p^2 M_2, \quad (18)$$

$$\mathcal{J}(I_2) \approx p^3 M_3/6i, \quad (19)$$

derived from Eq. (13), and therefore $\mathcal{R}(I_2)/\mathcal{R}(I_2') \approx M_2/M_2'$ and $\mathcal{J}(I_2)/\mathcal{J}(I_2') \approx M_3/M_3'$.

5. METHOD OF MOMENTS

The direct evaluation of Eq. (13) is not practical, because quite a large number of terms would have to be calculated. Blunck and Leisegang[5] and Shulek *et al.*[6] suggested the comparison of M_2 with the moment M_2' of the free-electron cross section. This method can readily be extended to all moments. Using $\delta_n \equiv M_n - M_n'$, with M_n from Eq. (7) and M_n' from Eq. (4), we obtain

$$I_2 = -\sum_{n=2}^{\infty} \frac{(-1)^n M_n' p^n}{n!} - \sum_{n=2}^{\infty} \frac{(-1)^n p^n \delta_n}{n!}. \quad (20)$$

The first sum is exactly I_2', and the last sum, therefore, is the contribution due to the difference in the higher moments of the true collision cross section from the free-electron value $1/\epsilon^2$. It is convenient to introduce

$$D_n = \delta_n / M_n' = (M_n/M_n') - 1$$

to modify the second sum

$$-S_2 \equiv \sum \frac{(-1)^n p^n \delta_n}{n!} = k \sum \frac{(-1)^n p^n \epsilon_m{}^n D_n}{[n!(n-1)\epsilon_m]}. \quad (21)$$

D_n can be obtained from Figs. 4 and 5 and Table I.

Using the substitution $p = it/\epsilon_m$, we obtain

$$-S_2 = \epsilon_m{}^{-1} k \sum_{n=2}^{\infty} \frac{(-1)^n (it)^n D_n}{[n!(n-1)]}. \quad (22)$$

Shulek *et al.*[6] have used this approach, introducing only a second moment

$$M_2 = k[\epsilon_m Z_{\text{eff}}/Z + \sum_i 2.667 I_i f_i \ln(\epsilon_m/I_i)],$$

first discussed in Ref. 16, to get a second approximation to I_2. Corresponding curves, using the more appropriate second moments from Fig. 4, are shown in Fig. 8, for $\eta_L = 1.5$ and 10. Since the region $1 < p < 10$ is still quite important for the convergence of Eq. (2) (see Fig. 14), this procedure is usually not satisfactory. The imaginary part is unchanged, since it does not contain M_2. The use of higher moments in Eq. (20) leads to problems; D_4 is quite small (Table I), whereas the higher moments give larger contributions and lead to wild fluctuations of S_2 for p above 0.5 or 1.0. As elegant as the method may appear, it is not practical.

6. MODIFICATIONS OF VAVILOV FUNCTION

With the function I_2 defined in Eq. (11), it is now possible to write Eq. (2) in the form

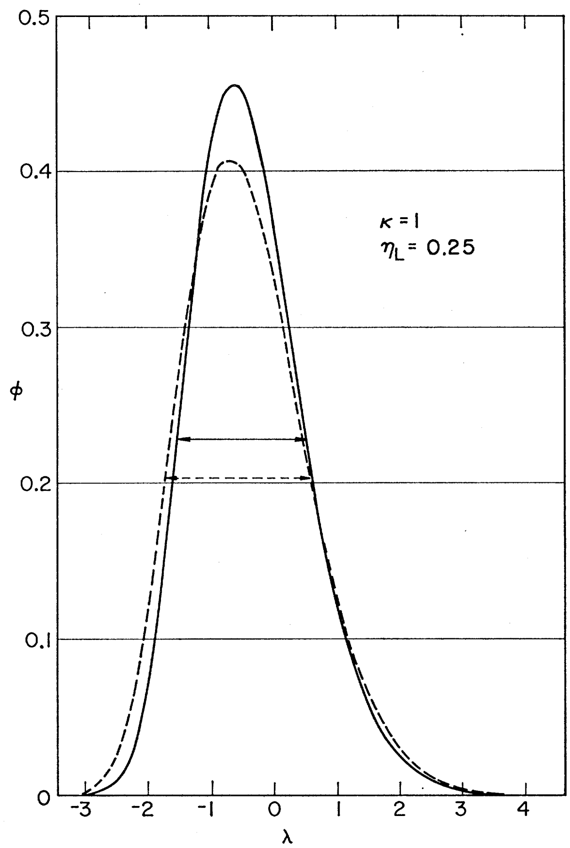

FIG. 10. Straggling function $f(x,\Delta)$ for low-energy particles in a thin detector. The abscissa is $\lambda = (\Delta - \bar{\Delta})/xk + \langle\lambda\rangle$, where $\langle\lambda\rangle = 0.577216 - \beta^2 - 1 - \ln \kappa$. The solid line represents results of my theory; the dotted line is the Vavilov curve for $\beta^2 = 0$. The difference for a slightly larger β^2 is very small. The full width at half-maximum (FWHM) of f' is 11% larger than that of f. Example: protons in an argon-filled counter. With $\eta_L = mv^2/[2R(Z-4.15)^2] \simeq 40T$ (MeV)$/(Z-4.15)^2$, the energy of the proton is about 1.2 MeV. Since $\kappa = 1$, $x \simeq 0.02$ mg/cm² or 1 cm at about 40 Torr. The mean energy loss amounts to about 3 keV, and would be affected seriously by δ-ray escape. The narrowing of the straggling curve predicted here for the L shell would be partially compensated by a widening contributed by the M-shell electrons. $D_2 = -0.018$.

$$f(x,\Delta)=\frac{1}{2\pi i}\int_{-i\infty}^{i\infty}e^{p(\Delta-\bar{\Delta})-xI_2}dp\,, \qquad (23)$$

where $\bar{\Delta}=xS$ is the mean energy loss of a beam of particles. Further, using $\kappa=xk/\epsilon_m$ and $p=it/\epsilon_m$, we have

$$f(x,\Delta)=\frac{1}{2\pi\epsilon_m}\int_{-\infty}^{\infty}\exp\left[it\left(\frac{\Delta-\bar{\Delta}}{\epsilon_m}\right)-\kappa r[\cos t-1+t\,\mathrm{Si}(t)]-i\kappa r_i\{t-\sin t+t[\mathrm{Ci}(t)-\ln t-\gamma]\}\right]dt$$

$$=\frac{\kappa}{\pi\xi}\int_0^{\infty}\exp\{-\kappa r[\cos t-1+t\,\mathrm{Si}(t)]\}\times\cos\left[t\left(\frac{\Delta-\bar{\Delta}}{\epsilon_m}\right)+\kappa r_i[t\gamma-t+\sin t+t\ln t-t\,\mathrm{Ci}(t)]\right]dt. \qquad (24)$$

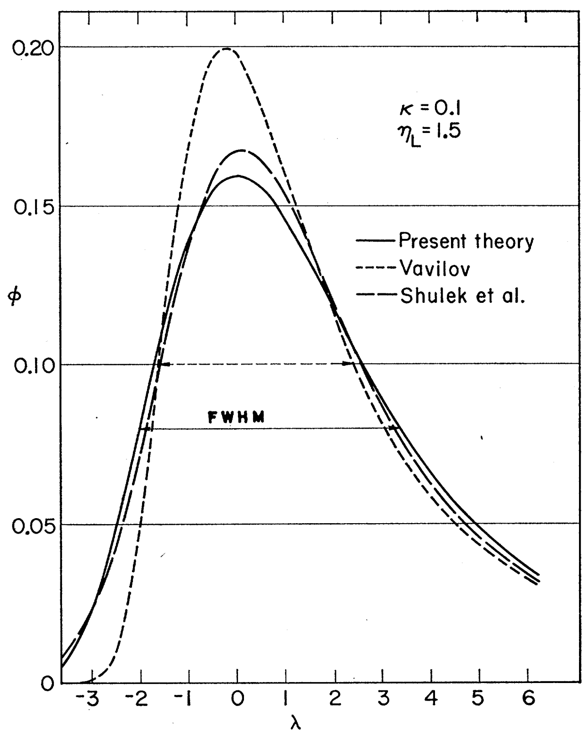

FIG. 11. Straggling function $f(x,\Delta)$ for L-shell electrons at $\eta_L=1.5$ (solid line). This is approximately the energy giving the maximum quantum mechanical effect (see Fig. 4). The FWHM of $f(x,\Delta)$ is about 34% wider than that of $f'(x,\Delta)$. Since the area under the curve [equal to the moment $M_0=\int f(x,\Delta)d\Delta$] is not very sensitive to the contributions from the tails of the function, the peak height of the normalized function from an experiment gives important information. To find it, determine the number of particles occurring in the peak channel (the spectrum is assumed to be measured in a multichannel analyzer) as a fraction of the total number of particles in the spectrum, multiply it with xk/c, where c is the width of a channel in the same units as xk, and compare with the maximum value of $f(x,\Delta)$. The measurement of FWHM or the determination of the standard deviation is more sensitive, though. $D_2=0.10$.

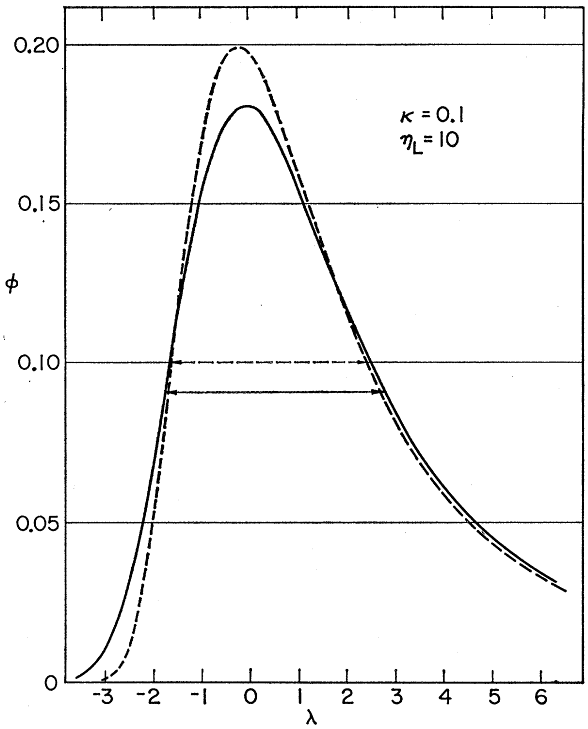

FIG. 12. Medium-energy particles in a thin detector (e.g., $\approx$25-MeV protons in a silicon detector of thickness $x\approx3.7$ mg/cm² with $\bar{\Delta}\approx63$ keV). My theory: solid line; Vavilov theory for $\beta^2=0$: dotted line. The theory by Shulek *et al.* differs by only a few percent from the solid line. The ratio of the FWHM is 1.12. $D_2=0.047$.

Note that the imaginary part of the integral is antisymmetric in t and therefore does not contribute to the integral. For $r=r_i=1$, Eq. (24) is exactly Vavilov's expression [Eq. (V-16)] for $\beta^2=0$. The terms containing β^2 in Eq. (V-16) appear because of the choice of $w(\epsilon)=k\epsilon^{-2}(1-\beta^2\epsilon/\epsilon_m)$ by Vavilov. This relativistic correction factor has been neglected here because the excitation function $J(W)$ is nonrelativistic. Notice that the factor e^κ outside of the integral in Eq. (V-16) is not constant in Eq. (24).

The function $f(x,\Delta)$ has been calculated for several values of κ for the values of η_L given in Fig. 8. The results are given in Figs. 10–13. For comparison, the Vavilov curves and curves including the correction for the second moment (Shulek *et al.*) are also given.

An impression of the problems encountered in the numerical integration of Eq. (24) can be obtained from a plot of the integral as a function of the upper limit. An example is shown in Fig. 14.

7. COMMENTS AND CONCLUSIONS

Straggling functions derived from the transport equation with the use of collision cross sections calculated in the first Born approximation, with hydrogenic wave functions, for the electrons in the atomic L shell, have been discussed in this paper. It is expected that similar

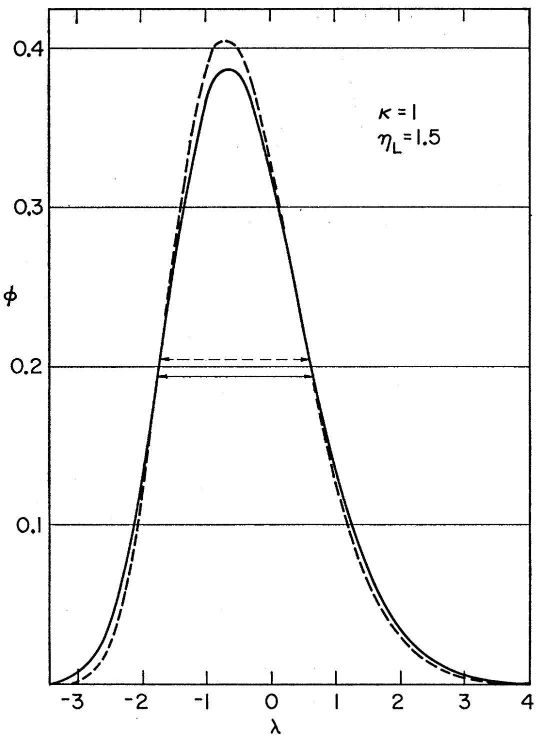

FIG. 13. Similar to Fig. 11, for $\kappa=1$. This would apply to 4-MeV protons in a silicon detector of 1 mg/cm^2, $\bar{\Delta}\approx 70$ keV. The ratio of the FWHM is about 1.05, the ratio of the peaks is about the same. $D_2=0.10$.

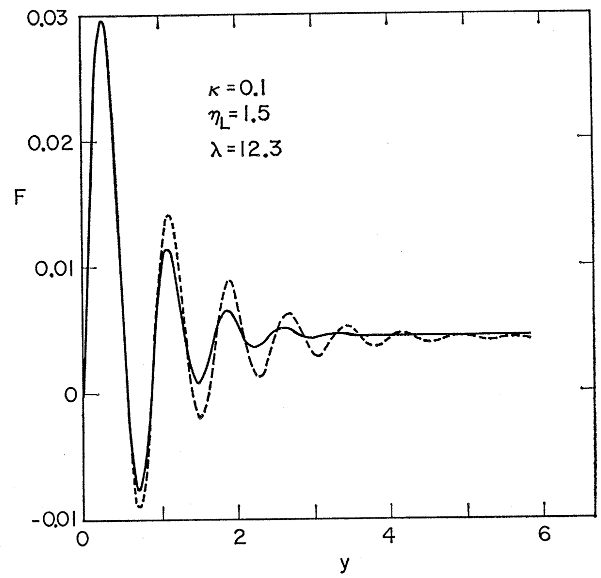

FIG. 14. The integral of the inverse Laplace transform for the straggling function $f(x,\Delta)$, Eq. (24), as a function of the upper limit, for $\kappa=0.1$, and $\lambda=12.3$. The solid line is used for the function with the quantum-mechanical cross section, the dotted line for the free-electron cross section. The large oscillation for $y<1$ requires great care in the numerical integration to avoid errors in the relatively small value of the integral. For smaller values of λ, the oscillations are less important.

results would be obtained for other shells. Substantial deviations from the Vavilov functions and the functions modified by Shulek *et al.* are found, especially for low-energy particles in thin absorbers. Further improvements in the theoretical treatment require better collision cross sections. For the application to any given atom it would be necessary to calculate the contribution for all the atomic shells. No reliable collision cross sections for the higher shells are presently available. A scaling procedure with adjustable parameters similar to the method used for the "shell corrections" in stopping power[15] or, alternatively, collision cross sections calculated from a statistical model of the atom,[20] might be used.

Existing experimental straggling data[21–25] are not at suitable energies, or, in general, accurate enough to confirm the trends discussed here. Relatively small corrections to the Vavilov curves occur in the examples presented here (Figs. 10–13). Very large modifications[26] have to be expected for $\kappa<D_2$ [this is equivalent to Eq. (10) of Ref. 5]. In Fig. 11 $\kappa=D_2$. The existing computer program is not suitable for $\kappa<0.01$.

For future straggling measurements, it will probably be necessary to determine the first moment (the stopping power) and the second moment (the standard deviation) from the experiment, because the calculation of collision cross sections with sufficient accuracy would be extremely time consuming. The third and fourth moments deviate only little from the free-electron moments and probably cannot be determined experimentally with sufficient accuracy (Fig. 5, Table I). For the higher moments, even very small amounts of slit-edge scattering, nuclear reactions, etc., contribute heavily to the experimental straggling. The derivation of further details of the collision cross sections from straggling measurements, thus, does not appear promising, except maybe in extremely thin absorbers,[18] with only a few collisions per particle. For this type of experiment, the Landau-Vavilov theory does not apply; Kellerer's convolution method[3] might be used instead.

[20] E. Bonderup, Kgl. Danske Videnskab. Selskab, Mat.-Fys. Medd. **35**, No. 17 (1967).
[21] T. J. Gooding and R. M. Eisberg, Phys. Rev. **105**, 357 (1957).
[22] L. P. Nielsen, Kgl. Danske Videnskab. Selskab, Mat.-Fys. Medd. **33**, No. 6 (1961).
[23] H. D. Maccabee, M. R. Raju, and C. A. Tobias, Phys. Rev. **165**, 469 (1968).
[24] J. J. Kolata, T. M. Amos, and H. Bichsel, Phys. Rev. **176**, 484 (1968).
[25] D. W. Aitken, W. L. Lakin, and H. R. Zulliger, Phys. Rev. **179**, 393 (1969).
[26] J. W. Hilbert, N. A. Baily, and R. G. Lane, Phys. Rev. **168**, 290 (1968).