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THEORY OF THE PASSAGE OF FAST CORPUSCULAR RAYS THROUGH MATTER

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TRANSLATION OF

Zur Theorie des Durchgangs schneller
Korpuskularstrahlen durch Materie

by

H. Bethe

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THEORY OF THE PASSAGE OF FAST CORPUSCULAR RAYS THROUGH MATTER

by

H. Bethe

The inelastic collision of a fast charged particle (electron, proton, α-particle) with an atom is treated according to Born's theory of wave mechanics. A very simple procedure is given for evaluating the matrix elements involved in the theory (section 3) and the close relationship to the intensity of the Compton effect is determined (section 5). The theory is developed in detail for collisions of hydrogen atoms and, in as far as possible, for complex atoms. The following are computed: the angular distribution of the inelastically (sections 6, 7, and 17) and elastically (section 16) scattered particles, the excitation cross sections for the excitation of the optical (sections 9 and 17) and x-ray (section 15) levels by electron collision, the sum of all inelastic and elastic collisions, and also the number of the primarily (sections 10 and 18) and secondarily (section 19) formed ions, the velocity distribution of the secondary electrons (section 18) and, finally, the braking of the colliding particles by gas atoms (sections 10, 12, and 13). The agreement of this theory with experiment is satisfactory to good. (For more detail see the summary in section 20).

I. GENERAL

1. Introduction

Essentially three types of processes take place during the passage of electrons through matter:

1. Elastic collisions: directional change of the electron without appreciable*) change of its velocity, no change of the excitation state of the atom. The elastically scattered electrons are capable of interference.

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*) Of course, during collision with an atom at rest there is always a small decrease in velocity according to the law of energy momentum.

2. Inelastic collisions: braking and generally minor changes (cf. section 6) in direction of the electron accompanied by excitation or ionization of the atom that has experienced collision. The inelastically scattered electrons are not capable of interference.

3. Bremsung of the electron with emission of wave radiation (x-ray bremsung spectrum).

There is analogy to all three processes in the interaction of light and matter, namely:

1. coherent scattering capable of interference without change in wavelength,

2. incoherent scattering, generally with an increase in wavelength (Raman or Compton effect),

3. photoeffect, i. e., absorption of wave radiation with acceleration of an electron from an atom.

Here, the analogy between fast electrons and shortwave light is quite close: The number of elastic electron collisions is closely related to the intensity of the coherently scattered x-rays of the same wavelength (cf. ref. [1], section 8 and refs. [2-4]), and the number of inelastic collisions is also closely related to the intensity of the scattering with a change in wavelength (cf. section 5).

α-rays also experience elastic and inelastic collisions in passing through matter, but because of their large mass, bremsung with emission of wave radiations is only of minor importance. Instead, the possibility exists that an electron will be captured from an atom. This "charge exchange" of the α-particles has been treated satisfactorily by Oppenheimer [5] on the basis of quantum mechanics; in this paper we shall disregard both this charge exchange and the emission of x-ray bremstrahlung and limit ourselves to the theory of elastic and, especially inelastic collisions, deceleration*) of the colliding particle caused by

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*) Although we neglect emission of the x-ray bremsung here, we should get nearly the total bremsung, because the energy used in the emission of the x-ray bremsung spectrum is very small (approximately 1/1000 of the kinetic energy of the particles).

these collisions, and excitation and ionization of the atoms by the colliding particle.

Theories are plentiful for this case as well. They are developed either on a purely classical basis, e.g., Bohr [6, 7], or they make some use of quantum-theoretical points of view [8-11]. However, in all these papers*) rather arbitrary assumptions had to be made about the interaction between the colliding particle and the atom. Therefore it seemed expedient, in view of the numerous experimental works in this field, to develop Born's strictly wave-mechanical collision theory [12] as extensively as possible. This lead to results that differ somewhat**) from those of the classical theory but which are more precise in any event. Further, computation is far simpler than by the classical method in its familiar form: Wave mechanics yields the desired information, i.e., the statistics of the collision process, immediately, without first introducing a collision parameter in addition to the physically significant magnitudes and only then averaging over all the values of this parameter.

The present theory is limited to the case of high velocity of the colliding particle (only in this case does Born's collision theory yield a dependable result, even in the first approximation which was employed here). For, as Distel of this institute will show in his paper (soon to be published), the Born process is a development by descending powers of v^2/v_0^2, where v is the velocity of the particle and v_0 the velocity of an electron in a "Bohr orbit" of the atom. The process, therefore, does not converge any better, e.g., for α-particles with a certain velocity than for electrons with the same velocity. In general, in analogy to optics, one would sooner expect a development according to descending powers of the wave number, or, perhaps even development according to descending powers of the kinetic energy. Thus, we always presuppose $v \gg v_0$.

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*) Except for Elsasser, who uses Born's collision theory as do we. However, his computations for the scattering of fast particles have not been carried out explicitly. His derivation may also be simplified essentially.

**) Contrary to Gaunt's opinion (cf. [10]).

2. Notation

We shall use the following notation consistently:

a = radius of the innermost Bohr orbit in the hydrogen atom

$$\alpha = \frac{1}{a}, \quad \alpha_0 = \frac{2\pi}{h}\sqrt{-2mE_0}, \quad \alpha_n = \frac{2\pi}{h}\sqrt{-2\pi E_n},$$

$$\alpha_{0n} = \sqrt{\alpha_0^2 - \alpha_n^2} \text{ [vgl. (12)]}, \quad \alpha_{nl} = \frac{2\pi}{h}\sqrt{-2\pi E_{nl}}.$$

E_n = energy (eigenvalue) of the n^{th} atomic state

E_0 = eigenvalue of the ground state

$E_{n\ell}$ = eigenvalue (negative ionization potential) of the $(n\ell)$-shell

ε_n = matrix element, corresponding to the transition from the ground state to the n^{th} excited state; for definition, cf. (11)

$\varepsilon_{n\ell, n'\ell'}$ = matrix element, corresponding to the transition of an electron from the $n\ell$-shell to the $n'\ell'$-shell

$dE(q)$ = the energy transferred to the atom from the particle during collision with a change in momentum between q and $q + dq$.

E = total energy transferred to the atom per unit time

$f_{m,n}$ = generalized oscillator strength, corresponding to the transition from atomic state m to state n (definition (45))

$f_{n\ell, n'\ell'}$ = oscillator strength, corresponding to the transition of an electron from the $n\ell$-shell to the $n'\ell'$-shell (definition (61a))

$f_{n\ell} = \sum_{n'\ell'} f_{n\ell,n'\ell'}$ = sum of the oscillator strengths for all transisitions of an electron of the $n\ell$-shell (cf. (62))

F = atomic form factor of the x-ray scattering theory

$d\Phi(q)$ = differential effective cross section = number of collisions with transfer of momentum between q and $q + dq$ (section 7)

Φ = integral effective cross section for all inelastic collisions (section 10)

Φ_n = integral effective cross section for excitation of the n^{th} atomic state (section 3 ff. , section 9)

$\Phi^{n\ell}_{n'\ell'}$ = effective cross section for the transition of an electron from the $n\ell$-shell into the $n'\ell'$-shell (cf. section 14)

$\Phi^{n\ell}$ = effective cross section for all possible excitations of an $n\ell$-electron (cf. section 15)

φ_n = generalized transition probability (definition (34))

$\mathfrak{K} = \frac{2\pi}{h} M\mathfrak{v}$ = propagation vector of the de Broglie wave of the motion of the particle with respect to the atom before collision

$\mathfrak{K} = \frac{2\pi}{h}M\mathfrak{v}'$ = propagation vector after collision

$K = |\mathfrak{K}|$, $K' = |\mathfrak{K}'|$ = wave numbers of the colliding particle

k = wave number of the secondary electron

ℓ = azimuthal quantum number

$\lambda = \frac{h}{mv} = \frac{2\pi}{K}$ = wavelength of the de Broglie wave of the colliding particle

m = mass of the electron

M_1 = mass of the colliding particle

M_2 = mass of the atom which has been struck

$M = \frac{M_1 M_2}{M_1 + M_2}$ = effective mass of the colliding particle

$\mathfrak{q} = \mathfrak{K} - \mathfrak{K}' = \frac{2\pi}{h}M(\mathfrak{v} - \mathfrak{v}')$ = collision vector = (geometric) change of the momentum of the colliding particle in units $h/2\pi$, $q = |\mathfrak{q}|$

$\mathfrak{R}$ = position vector of the colliding particle, reckoned from the nucleus of the struck atom

$\mathfrak{r}_j$ = position vector of the j^{th} electron

s_0 = number of the primarily formed ions per centimeter of path

s = number of all ions formed per centimeter of path

$T = \frac{M_1}{2}v^2$ = kinetic energy of the particle

$T_r = \frac{M}{2}v^2$ = kinetic energy of the motion of the particle relative to the atom

$d\tau_{\mathfrak{R}}$ = volume element in the space of the colliding particle

$d\tau_j$ = volume element in the space of the j^{th} electron, $d\tau = \prod_j d\tau_j$

u = time dependent wave function of the total system (atom + colliding particle)

$\mathfrak{v}$ = velocity of the particle before the collision, $v = |\mathfrak{v}|$

$\mathfrak{v}'$ = velocity after collision, $v' = |\mathfrak{v}'|$

ze = charge of the colliding particle

Ze = charge of the atomic nucleus

$Z_{n\ell}$ = number of electrons in the $n\ell$-shell

Ψ_n = eigenfunction of the atom in the n^{th} state

$\psi_{n\ell}$ = eigenfunction of an electron in the $n\ell$-shell (n = principal quantum number, ℓ = azimuthal quantum number)

ψ_k = continuous eigenfunction of an electron (wave number k)

3. General Scattering Formula

Neglecting the interaction between a colliding particle and an atom, the wave function of the system atom + particle is

$$u_0 = \sqrt{\frac{2\pi M}{hK}}\, e^{i(\mathfrak{K}\mathfrak{R})}\, \Psi_0(\mathfrak{r}_j)\, e^{-\frac{2\pi i}{h}Wt} \qquad (1)$$

$$W = \frac{h^2}{8\pi^2 M}K^2 + E_0 .$$

Expression (1) is normalized such that one particle passes through the unit surface per unit time. If the "interaction" is "switched on" at time t = 0, the wave function at time t can be expanded over the eigenfunctions χ, without interaction (method of variation of the constants):

$$u(t) = \sum_{n,\,\mathfrak{K}'} a_n(\mathfrak{K}', t)\,\chi_n(\mathfrak{K}';\ \mathfrak{R},\ \mathfrak{r}_j) \qquad (2)$$

$$\chi_n(\mathfrak{K}') = \sqrt{\frac{MK'}{2\pi h^2}}\, e^{i(\mathfrak{K}'\mathfrak{R})}\, \Psi_n(\mathfrak{r}_j)\, e^{-\frac{2\pi i}{h}W't}$$

$$W' = E_n + \frac{h^2}{8\pi^2 M}K'^2 . \qquad (3)$$

Expression (3) is normalized per energy interval $dW' = \frac{h^2}{4\pi^2 M}K'dK'$ and per solid angle element $d\omega'$ (relative to the velocity and direction of the particle after collision). Coefficients $a_n(\mathfrak{K}')$ in (2) are obtained from the time-dependent Schrödinger equation to a first approximation (V is the interaction energy):

$$\frac{h}{2\pi i}\cdot\frac{d a_n(\mathfrak{K}' t)}{dt} = \int V u_0\, \overline{\chi}_n(\mathfrak{K}')\, d\tau \cdot d\tau_{\mathfrak{R}} .$$

$$a_n(\mathfrak{K}', t) = \frac{e^{-\frac{2\pi i}{h}(W-W')t} - 1}{W' - W}\sqrt{\frac{M^2 K'}{h^3 K}}\, e^2 z \cdot V_{on}(\mathfrak{K}, \mathfrak{K}') . \qquad (4)$$

$$\left\{\begin{array}{l} V_{on}(\mathfrak{K}, \mathfrak{K}') = V_{on}(\mathfrak{q}) = \int \left(\frac{Z}{|\mathfrak{R}|} - \sum_{j=1}^{Z} \frac{1}{|\mathfrak{R} - \mathfrak{r}_j|} \right) \\ \qquad\qquad \cdot\, \Psi_0(\mathfrak{r}_j)\, \overline{\Psi}_n(\mathfrak{r}_j)\, e^{i(\mathfrak{K} - \mathfrak{K}',\, \mathfrak{R})}\, d\tau \cdot d\tau_{\mathfrak{R}} . \end{array}\right. \qquad (5)$$

If we proceed to large times t, the energy theorem

$$W = W' = E_0 + \frac{h^2}{8\pi^2 M}K^2 = E_n + \frac{h^2}{8\pi^2 M}K'^2 , \qquad (6)$$

will be satisfied to a significant degree, and by integration of $|a_n(\mathfrak{K}')|^2$ over a certain energy interval $\Delta W' \gg \frac{h}{2\pi t}$ and by differentiation of the integral with respect to time we obtain, in the familiar manner, the transition probability to the $(n, \mathfrak{K}')$-state, i. e., the number of particles that are scattered per unit time in direction $\mathfrak{K}'$ and thereby excite the atom to the n^{th} quantum state:

$$d\Phi_n(\mathfrak{q}) = d\omega' \frac{d}{dt} \int dW' \, |a_n(\mathfrak{K}', t)|^2$$

$$= \frac{4\pi^2}{h} \cdot \frac{M^2 K'}{h^3 K} \cdot 2\pi \sin\vartheta \, d\vartheta \cdot e^4 z^2 \cdot |V_{on}(\mathfrak{q})|^2$$

$$d\Phi_n(\mathfrak{q}) = \frac{1}{2\pi} \alpha^2 \left(\frac{M}{m} z\right)^2 \sin\vartheta \, d\vartheta \, |V_{on}|^2 \frac{K}{K'} \tag{7}$$

$d\Phi_n(\mathfrak{q})$ has the dimension of a surface (number of collisions per unit time in the flow of a particle through the unit surface per unit time). It means the effective cross section of the atom for scatterings at the angle ϑ with simultaneous excitation of the n^{th} atomic state, which we shall define as the differential effective cross section.

Usually, the matrix elements V_{0n} of the interaction energy are now evaluated by integrating first over the coordinates of the atomic electron and only then over those of the colliding particle [13] or else, by expanding $e^{i(\mathfrak{K} - \mathfrak{K}', \mathfrak{R})}$ according to spherical functions and then by finishing the integrations over the angular coordinates, and next the radial integrations [11].

The following method is much simpler and also demonstrates directly the relation to x-ray scattering:

First, we integrate over the space of the particle and note that, e. g.,

$$\varphi_{\mathfrak{q}}(\mathfrak{r}_j) = \int \frac{1}{|\mathfrak{R} - \mathfrak{r}_j|} e^{i(\mathfrak{q}\mathfrak{R})} \, d\tau_{\mathfrak{R}} \tag{8}$$

is the potential of a charge distributed with density

$$\rho_{\mathfrak{q}}(\mathfrak{R}) = e^{i(\mathfrak{q}\mathfrak{R})} \tag{8a}$$

at the point $\mathfrak{r}_j$. However, from

$$\Delta \varphi_{\mathfrak{q}}(\mathfrak{r}) = -4\pi\rho = -4\pi e^{i(\mathfrak{q}\mathfrak{r})} \tag{8b}$$

$$\varphi_{\mathfrak{q}}(\mathfrak{r}) = \frac{4\pi}{q^2} e^{i(\mathfrak{r}\mathfrak{q})}. \tag{9}$$

follows directly, i.e., the differential effective cross section becomes

$$d\,\Phi_n(\mathfrak{q}) = \frac{8\pi\alpha^2}{q^4}\left(\frac{M}{m}z\right)^2 \frac{K'}{K}\,|\,\varepsilon_n(\mathfrak{q})|^2 \sin\vartheta\, d\vartheta \tag{10}$$

with

$$\varepsilon_n(\mathfrak{q}) = \int \left(Z - \sum_j e^{i(\mathfrak{q}\,\mathfrak{r}_j)}\right)\Psi_0\,\bar{\Psi}_n(\mathfrak{r}_j)\prod_j d\tau_j, \tag{11}$$

where we need only to integrate over coordinates of the atomic electrons.

The step (8) to (9) may seem somewhat bold, since the integral in (8) does not converge. In fact, if we set $\mathfrak{r} = \mathfrak{R} - \mathfrak{r}_j$ and introduce a system of polar coordinates with the axis $\mathfrak{q}$, we will have

$$\begin{aligned} \varphi_{\mathfrak{q}}(\mathfrak{r}_j) &= e^{i(\mathfrak{q}\,\mathfrak{r}_j)}\int_0^\infty r^2\,dr\int_0^\pi 2\pi\sin\vartheta\,d\vartheta\cdot\frac{1}{r}\,e^{iqr\cos\vartheta} \\ &= \frac{4\pi e^{i(\mathfrak{q}\,\mathfrak{r}_j)}}{q}\int_0^\infty \sin qr\cdot dr. \end{aligned}$$

However, we can easily obtain convergence in the usual manner by letting the value q of the collision vector pass through a certain range $q - \Delta q$ to $q + \Delta q$ and averaging φ_q over this range, and also by reversing the integrations over q and r:

$$\begin{aligned} &\lim_{\Delta q = 0}\frac{1}{2\Delta q}\int_{q-\Delta q}^{q+\Delta q} dq'\,\varphi_{\mathfrak{q}'}(\mathfrak{r}_j) \\ &= \lim_{\Delta q = 0}\frac{4\pi e^{i(\mathfrak{q}\,\mathfrak{r}_j)}}{2q\,\Delta q}\int_0^\infty dr\int_{q-\Delta q}^{q+\Delta q}\sin q'r\,dq' \\ &= \lim_{\Delta q = 0}\frac{4\pi e^{i(\mathfrak{q}\,\mathfrak{r}_j)}}{2q\,\Delta q}\int_0^\infty \frac{dr}{r}\left(\cos(q-\Delta q)r - \cos(q+\Delta q)r\right) \\ &= \lim_{\Delta q = 0}\frac{4\pi e^{i(\mathfrak{q}\,\mathfrak{r}_j)}}{2q\,\Delta q}\ln\frac{q+\Delta q}{q-\Delta q} = \frac{4\pi e^{i(\mathfrak{q}\,\mathfrak{r}_j)}}{q^2}. \end{aligned}$$

Thus formula (10) is justified. This will be discussed in section 5.

4. Energy Relationships

First we must consider the relationships implied by energy theorem (6) among the collision vector q, the scattering angle ϑ, and the excitation energy transferred to the atom:

$$E_n - E_0 = \frac{h^2}{8\pi^2 m}(\alpha_0{}^2 - \alpha_n{}^2) = \frac{h^2}{8\pi^2 m}\alpha_{0n}^2. \tag{12}$$

The reciprocal lengths α_0, α_n, and α_{0n} defined by (12), are of the order of magnitude of the reciprocal atomic radius (10^8 cm^{-1}) for discrete atomic states n. With excitation to a state k of the continuous spectrum (ionization), $-\alpha_n^2$ must be replaced by k^2 (wave number of the secondary electron) and (12a)

$$E_k - E_0 = \frac{h^2}{8\pi^2 m}(\alpha_0{}^2 + k^2). \tag{12a}$$

The energy theorem (6) requires

$$K^2 - K'^2 = \frac{M}{m}\alpha_{0n}^2. \tag{13}$$

By definition

$$\mathfrak{q} = \mathfrak{K} - \mathfrak{K}' \tag{14}$$

$$q^2 = K^2 + K'^2 - 2KK'\cos\vartheta,$$

i. e.,

$$q^2 = 2K^2 - \frac{M}{m}\alpha_{0n}^2 - 2K\sqrt{K^2 - \frac{M}{m}\alpha_{0n}^2}\cos\vartheta. \tag{14a}$$

For elastic collisions ($E_n = E_0$, $\alpha_{0n} = 0$) this is identical to

$$q = 2K\sin\frac{\vartheta}{2} = \frac{4\pi\sin\frac{\vartheta}{2}}{\lambda} = \frac{4\pi M}{h}v\sin\frac{\vartheta}{2}. \tag{14b}$$

Indeed, this magnitude is known from the theory of x-ray scattering, in which the scattering intensity at the angle ϑ is a function of this magnitude.

With constant excitation energy,

$$\sin\vartheta\, d\vartheta = \frac{q\,dq}{KK'}. \tag{15}$$

results from (14). It can be seen that when (15) is introduced into (10), the wave number K' of the particle is completely eliminated after the collision:

$$d\Phi_n(q) = \frac{8\pi\alpha^2}{K^2}\left(\frac{M}{m}z\right)^2\frac{dq}{q^3}\,|\varepsilon_n(q)|^2. \tag{16}$$

Thus, if the differential effective cross section is conceived of as the number of particles whose momentum during collision experiences a change between $\frac{h}{2\pi}q$ and $\frac{h}{2\pi}(q + dq)$ rather than the number of particles deflected into a certain solid angle element $d\vartheta \times \sin\vartheta$, the effective cross section will be a function of the excitation of the atom produced by the collision only by virtue of the matrix element $\varepsilon_n(q)$. This considerably facilitates the formation of the total cross section by integration over ϑ or q (sections 7 and 8). In view of this anticipated integration, we now determine the limits of integration:

1. The smallest possible collision vector q_{min} (scattering angle $\vartheta = 0$) depends (cf. (14a)) on the excitation energy $E_n - E_0$. As long as this excitation energy is of the order of magnitude of the ionization potential, i.e., as long as either a discrete atomic state is excited, or, in the case of ionization, only a small kinetic energy (i.e., of the order of magnitude of the ionization potential) is imparted to the detached secondary electron, $K \gg \alpha_{0n}\frac{M}{m}$ is surely valid and because $M \geq m$, $K^2 \gg \frac{M}{m}\alpha_{0n}^2$. We had to assume (see end of section 1) that the velocity $v = \frac{hK}{2\pi M}$ of the particle is large versus the velocity of an electron in a Bohr orbit of the atom, which must be defined analogously by the expression $v_0 = \frac{h\alpha_0}{2\pi m}$, to permit us to operate solely with the first approximation of the Born procedure. Thus, in (14a) we can expand over

$$\frac{M\alpha_{0n}^2}{mK^2} = \frac{E_n - E_0}{T_r}$$

and get

$$q^2 = \left(2K^2 - \frac{M}{m}\alpha_{0n}^2\right)(1 - \cos\vartheta) + \frac{1}{4}\left(\frac{M\alpha_{0n}^2}{mK}\right)^2\cos\vartheta + \cdots \tag{17a}$$

$$q_{\min} = q_{\vartheta=0} = \frac{M\alpha_{0n}^2}{2mK}. \tag{17}$$

Because $K \gg \frac{M}{m}\alpha_{0n}$,

$$q_{\min} \ll \alpha_{0n},$$

holds, and $q_{\min}$ decreases with the transferred excitation energy and decreases with increasing velocity of the particle (as in ref. [11, p. 537]).

2. For the overwhelming majority of collisions with a <u>small</u> collision vector q, the above assumption that the energy transfer is approximately equal to the ionization potential and, therefore, is small relative to the kinetic energy of the particle is certainly correct (cf. section 6). The most common inelastic collisions with a <u>large</u> q (i. e., with a large deflection of the colliding particle), however, are those in which the momentum theorem is almost satisfied for the colliding particle and the secondary electrons. Except for the factor $h/2\pi$, q is the change of momentum of the colliding particles, thus the momentum of the secondary electron must be almost $\frac{h}{2\pi}q$ with a wave number $k \approx q$. Then, since $\alpha_0 \ll q$, α_{0n} is also approximately equal to q and, by substitution in (18a), we obtain

$$\begin{cases} \cos\vartheta = \dfrac{K^2+K'^2-q^2}{2KK'} = \dfrac{K^2\left(1-\dfrac{m}{M}\right)+K'^2\left(1+\dfrac{m}{M}\right)}{2KK'} \\ \qquad\qquad = \dfrac{2K^2-q^2\left(1+\dfrac{M}{m}\right)}{2K\sqrt{K^2-q^2\dfrac{M}{m}}}\,. \end{cases} \tag{18}$$

for the angle ϑ between the azimuths of the colliding particle before and after the collision. The same applies to the angle φ between the direction q of the secondary electron and the original azimuth $\mathfrak{K}$ of the primary electron according to the cosine law

$$\cos\varphi = \frac{K^2+q^2-K'^2}{2Kq} = \frac{q\left(1+\dfrac{M}{m}\right)}{2K}\,. \tag{18a}$$

a) If the colliding particle is an electron, because M = m, we get

$$q = K\sin\vartheta = K\cos\varphi, \quad K' = K\cos\vartheta. \tag{19}$$

This is the law of classical theory [14] which states that after collision the azimuths of the primary and secondary electrons are perpendicular to each other. The greatest possible scattering angle $\vartheta_{\max}$ is 90° and the maximum collision vector $q_{\max} = K$.

b) If the colliding particle is a heavy (α or H) particle, $M \gg m$. Then, it follows from (18a) that with a small transfer of momentum the secondary electron leaves the atom perpendicularly to the direction of the α-particle, while with a larger collision vector q it receives an increasing momentum component in the primary direction. The greatest possible collision vector results when the electron is ejected along the continuation of the path of the oncoming particle ($\varphi = 0$), in which case

$$q_{\max} = 2K \frac{m}{M+m} \approx 2K \frac{m}{M}, \tag{20}$$

i. e., the secondary electron precedes the α-particle with the velocity $\frac{hq}{2\pi m} \approx 2 \times \frac{hK}{2\pi M} = 2v$. This, of course, is in full agreement with the result of classical theory, which was indeed based on the law of energy momentum. The angle of deflection ϑ of the colliding particle varies only within a very small range:*) when the transferred momentum grows from 0 to $\frac{q_{\max}}{\sqrt{2}}$ (and φ decreases from 90° to 45°), the scattering angle increases from 0 to $\vartheta_{\max} = \arcsin \frac{m}{M}$, only to decrease again to zero during a further increase of the momentum transfer to $q_{\max}$.

The energy loss $E_n - E_0$ of the colliding particle by excitation or ionization of the atom, discussed so far, refers only to the decrease of the relative velocity of the colliding particle to the atom from v to v' ("collision with the electrons of the atom" in classical theory). However, if the atom was initially at rest, this is no longer the case after the collision, and, consequently, the energy decrease of the colliding particle is somewhat greater still in a system at rest: A transfer of kinetic energy from the particle to the atom occurs according to the classical law of energy momentum. The velocity

$$\frac{M_1}{M_1 + M_2}\mathfrak{v}$$

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*) According to the sine law, $\sin\vartheta/\sin\varphi = q/K'$.

of the center of gravity of atom and colliding particle relative to a system at rest and the [velocity]

$$\frac{M_2}{M_1+M_2}\mathfrak{v}'$$

of the particle relative to the center of gravity, are added vectorially to constitute the particle velocity $\mathfrak{v}''$ after the collision in a system at rest:

$$\begin{aligned} v''^2 &= \frac{1}{(M_1+M_2)^2}(M_1^2 v^2 + M_2^2 v'^2 + 2M_1 M_2 v v' \cos\vartheta) \\ &= v^2 - \frac{M_1 M_2}{(M_1+M_2)^2}(v^2 + v'^2 - 2v v' \cos\vartheta) \\ &\qquad - \frac{M_2}{M_1+M_2}(v^2 - v'^2). \end{aligned}$$

The total loss of kinetic energy in a system at rest is, therefore,

$$\left\{\begin{aligned} \frac{M_1}{2}(v^2 - v''^2) &= \frac{M_1}{M_1+M_2}\cdot\frac{M}{2}\cdot|\mathfrak{v}-\mathfrak{v}'|^2 + \frac{M}{2}(v^2 - v'^2) \\ &= \frac{M_1}{M_1+M_2}\cdot\frac{h^2}{8\pi^2 M}q^2 + \frac{h^2}{8\pi^2 M}(K^2 - K'^2) \\ &= \frac{h^2}{8\pi^2 M_2}q^2 + E_n - E_0. \end{aligned}\right. \tag{21}$$

As we have seen, the second term, the transferred excitation energy is of the order of magnitude of $\frac{h^2}{8\pi^2 m}q^2$ (in the case of large q) or $\frac{h^2}{8\pi^2 m}a_0^2$ (when $q \ll a_0$), i.e., the first term is always smaller than the second by at least the factor $m/M_2 = \frac{\text{electron mass}}{\text{atomic mass}}$, just as in classical theory the energy loss due to the scattering on the nucleus is smaller than the loss due to the scattering on the electrons.

5. Collisions and X-Ray Scattering

Now we shall discuss the formula (10), or (16), for the differential effective cross section and relate the latter to the intensity of x-ray scattering:

1) For elastic collisions, we get (cf. (11))

$$\varepsilon_0(q) = Z - \int \sum_j e^{i(q\mathfrak{r}_j)}\,|\Psi_0|^2 d\tau = Z - F. \tag{22}$$

That is, the following theorem holds with respect to (14b):

The effective cross section for elastic collisions at a definite deflection angle ϑ is

$$d\Phi_0(q) = \frac{2\pi e^4 z^2}{16 T_r^2} \frac{(Z-F)^2}{\sin^4 \frac{\vartheta}{2}} \sin \vartheta \, d\vartheta, \tag{23}$$

where Z is the atomic number and F the atomic form factor (dependent on q) of the theory of x-ray scattering. The elastic scattering of corpuscular particles differs from that of x-rays by the addition of the "scattering by the nucleus" to the "scattering by the electron cloud of the atom" (Z - F instead of F) and by the characteristic factor

$$\frac{1}{\sin^4 \frac{\vartheta}{2}}$$

of Rutherford's formula.

2) For inelastic collisions, the "scattering by the nucleus"

$$\int Z \Psi_0 \overline{\Psi_n} \, d\tau$$

vanishes, owing to the orthogonality of the eigenfunctions; we get

$$-\varepsilon_n = \sum_j \int e^{i(\mathfrak{q}\mathfrak{r}_j)} \Psi_0 \overline{\Psi_n}(\mathfrak{r}_j) \, d\tau \tag{24}$$

equal to the matrix element [15 et alibi, 16] critical for the incoherent x-ray scattering (Compton effect).

The differential effective cross section for inelastic collisions, except for the "Rutherford factor" $1/\sin^4 \frac{\vartheta}{2}$, is proportional to the intensity of the Compton scattering of x-rays. Here, collisions with identical change of momentum $\frac{h}{2\pi} q$ (of the particle or the light quantum) must be compared. (In a region of medium angles, q is proportional to sin $\vartheta/2$.)*)

3) When the angles of deflection are small and the energy transfer to the atom $E_n - E_0$ is not too large, the collision vector q, as noted in (17a) and (17), is small compared with the "reciprocal

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*) That is, when (17a) still holds (i. e., $q \ll a_0$) but the first term of (17) predominates, viz., $q \gg q_{min} \approx a_0^2/2K \times M/m$.

atomic radius." In this case, which includes most collisions, we may expand the exponential functions in (11) or (24)

$$e^{i(\mathfrak{q}\,\mathfrak{r}_j)} = e^{iqx_j} = 1 + iq\,x_j \pm \cdots$$

because of the factor $1/q^4$ in (10) for the differential collision cross section, and break them off after the first term. Then

$$\varepsilon_n(q) = iq \int \sum_j x_j \Psi_0 \overline{\Psi_n}(\mathfrak{r}_j)\,d\tau \tag{25}$$

holds, where

$$\begin{cases} d\Phi_n(q) = \dfrac{8\pi\alpha^2}{q^4}\left(\dfrac{M}{m}z\right)^2 \dfrac{K'}{K}\sin\vartheta\,d\vartheta\cdot q^2\cdot|x_{0n}|^2 \\ \qquad = \dfrac{8\pi\alpha^2}{K^2}\cdot\left(\dfrac{M}{m}z\right)^2 |x_{0n}|^2\dfrac{dq}{q}, \end{cases}$$

$$x_{0n} = \int \sum_j x_j \Psi_0 \overline{\Psi_n}(\mathfrak{r}_j)\,d\tau \quad . \tag{26}$$

is the matrix element of the sum of the electron coordinates (or that of the electric moment of the atom). Thus, for small collision vectors q (i.e., small changes in momentum of the colliding particle), the collision probability is proportional to the square of the coordinate matrix, i.e., proportional to the optical transition probability for the respective excitation of the atom*) and, because of 1/q, the integral collision cross section also becomes almost proportional to this magnitude (cf. sections 9 and 14).

II. COLLISION WITH HYDROGEN ATOMS

6. Evaluation of the Matrix Elements

In a study of the Compton effect, Wentzel evaluated the matrix elements $\varepsilon_n(q)$ that enter into the differential effective cross section (20) and are defined by (11) for transitions from the ground state of the hydrogen atom to the states of the continuous spectrum in a parabolic coordinate. Here, it must be noted that a continuous group of eigenfunctions ψ_{km}, belonging to a definite continuous eigenvalue

$$E_k = \frac{h^2}{8\pi^2 m}k^2$$

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*) This theorem has already been derived for hydrogen by Elsasser [11, pp. 537, 538], who also presumed it to be universally valid.

differ in their parabolic quantum numbers m. Hence, the square of the matrix element (normalized per dk) becomes, for the transition from the ground state to the E_k state (cf. [15, p. 365]),

$$|\varepsilon_k(q)|^2 = \int_{-\infty}^{+\infty} dm\, |\varepsilon_{0,km}(q)|^2 \tag{27}$$

By elementary evaluation of Wentzel's formula (28), and taking his formulas (27), (25), and (19) into account, we obtain,*)

$$\left\{\begin{aligned} |\varepsilon_{0,km}(q)|^2 &= \frac{256\, k^2 q^2 a^5\, e^{-2\frac{a}{k}\operatorname{arc\,tg}\frac{2ak}{q^2-k^2+a^2}}}{[(q+k)^2+a^2]^3\,[(q-k)^2+a^2]^3}\cdot a(m) \\ a(m) &= \frac{q^2+4k^2m^2}{(1+e^{-2\pi(n+m)})(1+e^{-2\pi(n-m)})},\quad n=\frac{a}{2k}. \end{aligned}\right. \tag{28}$$

The integration over m anticipated in (27)

$$|\varepsilon_k(q)|^2 = c(k,q)\int_{-\infty}^{+\infty} a(m)\, dm \tag{28a}$$

requires evaluation of integrals of the type

$$J_\mu = \int_{-\infty}^{+\infty} \frac{m^\mu\, dm}{(1+e^{-2\pi n}\cdot e^{-2\pi m})\,(1+e^{-2\pi n}\cdot e^{+2\pi m})}\ (\mu = 0{,}2) \tag{28b}$$

(path of integration is a real axis). This can easily be done with complex terms, in analogy to ref. [15, footnote 2, p. 365]. Thus,

$$\left\{\begin{aligned} &\int \frac{(m+i)^\nu\, dm}{(1+e^{-2\pi n}e^{-2\pi(m+i)})\,(1+e^{-2\pi n}\cdot e^{+2\pi(m+i)})} \\ &\quad -\int \frac{m^\nu\, dm}{(1+e^{-2\pi n}e^{-2\pi m})(1+e^{-2\pi n}\cdot e^{+2\pi m})} \\ &\quad = \sum_{\mu=0}^{\nu-1}\binom{\nu}{\mu} i^{\nu-\mu} J_\mu \\ &\quad = \oint \frac{m^\nu\, dm}{(1+e^{-2\pi n}\cdot e^{-2\pi m})(1+e^{-2\pi n}\cdot e^{+2\pi m})} \end{aligned}\right. \tag{29a}$$

where we have to take the last, closed integral along the real axis from $+\infty$ to $-\infty$ and back along the parallel displaced by $+i$. Then the two poles

$m_1 = +n + \frac{i}{2}$ with the residue $\dfrac{-\left(n+\frac{i}{2}\right)^\nu}{2\pi(1-e^{-4\pi n})}$

$m_2 = -n + \frac{i}{2}$ " " " $\dfrac{\left(-n+\frac{i}{2}\right)^\nu}{2\pi(1-e^{-4\pi n})}$

---

*) Here q stands for Wentzel's $|\Delta k|$. For hydrogen, the reciprocal radius a of the innermost Bohr orbit is identical to the a_0 used in section 4 and defined by (12).

are both circumscribed in the negative direction so that

$$\oint = i\,\frac{\left(n+\frac{i}{2}\right)^{\nu}-\left(-n+\frac{i}{2}\right)^{\nu}}{1-e^{-4\pi n}}. \tag{29b}$$

By using formula (29b) for $\nu = 1$ and 3,

$$\begin{cases} J_0 = \dfrac{2n}{1-e^{-4\pi n}} \\ J_2 = \dfrac{n}{6}\cdot\dfrac{1+4n^2}{1-e^{-4\pi n}} \end{cases} \tag{29c}$$

follows directly from (29a) so that when n is replaced by its value $\alpha/2k$,

$$|\varepsilon_k(q)|^2 = \frac{2^8 k q^2 \alpha^6\left(q^2+\frac{1}{3}(\alpha^2+k^2)\right)}{[(q+k)^2+\alpha^2]^3[(q-k)^2+\alpha^2]^3}\cdot\frac{e^{-2\frac{\alpha}{k}\operatorname{arc\,tg}\frac{2\alpha k}{q^2-k^2+\alpha^2}}}{1-e^{-2\pi\frac{\alpha}{k}}}. \tag{30}$$ *)

For $q \gg \alpha$, $|\varepsilon_k(q)|^2$ has a sharp maximum at $k \approx q$ and then passes into the formula derived by Wentzel [15, bottom of p. 365]. For $q \approx 0$, (30) becomes q^2 times the usual optical transition probability (square of the element of the coordinate matrix) (cf. section 5, paragraph 3).

$$\begin{cases} \lim\limits_{q=0} |\varepsilon_k(q)|^2 = q^2 |x_{0k}|^2 \\ |x_{0k}|^2 = \dfrac{2^8}{3}\,\dfrac{\alpha^6\cdot k}{(\alpha^2+k^2)^5}\cdot\dfrac{e^{-4\frac{\alpha}{k}\operatorname{arc\,tg}\frac{k}{\alpha}}}{1-e^{-2\pi\frac{\alpha}{k}}}. \end{cases} \tag{31}$$

We shall postpone the discussion of (30) and (31) until the end of this section and first evaluate the matrix elements

$$\varepsilon_n = \int e^{iqx}\psi_0\bar{\psi}_n\,d\tau = \frac{\alpha^{\frac{3}{2}}}{\sqrt{2}}\int e^{iqx-\alpha r}\bar{\psi}_n(\xi+\eta)\,d\xi\,d\eta \tag{32}$$

for discrete transitions, also in parabolic coordinates

$$x = \frac{1}{2}(\xi-\eta),\ y = \sqrt{\xi\eta}\cos\varphi,\ z = \sqrt{\xi\eta}\sin\varphi,\ r = \frac{1}{2}(\xi+\eta),$$

Here we need consider only eigenfunctions ψ_n that are independent of φ. These are as follows (cf., e.g., [17, p. 181 ff.]):

$$\psi_n = \frac{1}{\sqrt{2n\cdot n_1!\,n_2!}}\left(\frac{\alpha}{n}\right)^{\frac{3}{2}} e^{-\frac{\alpha}{2n}(\xi+\eta)} L_{n_1}\left(\frac{\xi\alpha}{n}\right) L_{n_2}\left(\frac{\alpha\eta}{n}\right) \tag{32a}$$

n_1 and n_2 are the parabolic quantum numbers, $n = n_1 + n_2 + 1$. The equation

---

*) Read tg as tangent.

$$\varepsilon_{n_1, n_2}(q) = \frac{1}{2 n^2 n_1! \, n_2!} \int e^{-\frac{\alpha \xi}{2}\left(1+\frac{1}{n}-\frac{iq}{\alpha}\right)-\frac{\alpha \eta}{2}\left(1+\frac{1}{n}+\frac{iq}{\alpha}\right)} \cdot L_{n_1}\left(\frac{\alpha \xi}{n}\right) L_{n_2}\left(\frac{\alpha \eta}{n}\right) \cdot \alpha(\xi+\eta)\, \alpha \, d\xi \, \alpha \, d\eta$$

may then be used, for example, by employing the generating function of the Laguerre polynomials: with $\varrho = \frac{\alpha}{n}\xi$ or $\frac{\alpha}{n}\eta$, $p = n_1$ or n_2, $\beta = 0$ or 1, we have

$$\left\{\begin{aligned} & \sum_p \int \frac{L_p(\varrho)}{p!} t^p e^{-\frac{\varrho}{2}\left(n+1-i\frac{qn}{\alpha}\right)} \varrho^\beta d\varrho \\ & = \frac{1}{1-t} \int e^{-\varrho\left(\frac{t}{1-t}+\frac{1}{2}\left(1+n-i\frac{qn}{\alpha}\right)\right)} \varrho^\beta d\varrho \\ & = (1-t)^\beta \beta! \, 2^{\beta+1}\left[n+1-i\frac{qn}{\alpha}-t\left(n-1-i\frac{qn}{\alpha}\right)\right]^{-(\beta+1)}. \end{aligned}\right. \tag{32b}$$

By finding the coefficient t^p with respect to t in the expansion of the right side of (32b), we obtain, after short computation,

$$\left\{\begin{aligned} \varepsilon_{n_1, n_2} = {} & 4n \cdot \frac{\left(n-1-i\frac{qn}{\alpha}\right)^{n_1}\left(n-1+i\frac{qn}{\alpha}\right)^{n_2}}{\left(n+1-i\frac{qn}{\alpha}\right)^{n_1}\left(n+1+i\frac{qn}{\alpha}\right)^{n_2}} \\ & \cdot \left(\frac{n_1+1}{n+1-i\frac{qn}{\alpha}} - \frac{n_1}{n-1-i\frac{qn}{\alpha}} + \frac{n_2+1}{n+1+i\frac{qn}{\alpha}} \right. \\ & \left. - \frac{n_2}{n-1+i\frac{qn}{\alpha}}\right). \end{aligned}\right. \tag{32c}$$

which appears to be very similar to Wentzel's corresponding formula (28) for the transitions to the continuous spectrum, if we also carry out the differentiation with respect to α. By elementary transformation we obtain

$$\left\{\begin{aligned} |\varepsilon_{n_1, n_2}(q)|^2 = {} & \left(\frac{q}{\alpha}\right)^2 \cdot 2^8 n^6 \cdot \frac{\left[(n-1)^2+\left(\frac{qn}{\alpha}\right)^2\right]^{n-3}}{\left[(n+1)^2+\left(\frac{qn}{\alpha}\right)^2\right]^{n+3}} \\ & \cdot \left((n_1-n_2)^2+\left(\frac{qn}{\alpha}\right)^2\right). \end{aligned}\right. \tag{32d}$$

Finally, summation over all values possible at the given n: $n_1 - n_2 = -n+1, -n+3, \ldots, n = 3, n-1$, yields

$$\left\{\begin{aligned} |\varepsilon_n(q)|^2 = \sum_{n_1+n_2=n-1} |\varepsilon_{n_1, n_2}(q)|^2 = {} & \left(\frac{q}{\alpha}\right)^2 \cdot 2^8 \cdot n^7\left[\frac{1}{3}(n^2-1)\right. \\ & \left. +\left(\frac{qn}{\alpha}\right)^2\right] \frac{\left[(n-1)^3+\left(\frac{qn}{\alpha}\right)^2\right]^{n-3}}{\left[(n+1)^2+\left(\frac{qn}{\alpha}\right)^2\right]^{n+3}} \end{aligned}\right. \tag{33}$$

In order to discuss the dependence of the matrix elements $\varepsilon_n(q)$ or the differential effective cross section $d\Phi_n(q)$ on the collision vector q, we shall consider the dimensionless magnitude

$$\varphi_n(q) = \frac{a^2}{q^2} \, | \varepsilon_n(q) |^2 \tag{34}$$

and designate it as generalized transition probability; for $q = 0$, $\varphi_n(q)$ coincides (except for the factor a^2, introduced to obtain dimensionlessness) with what is usually called the square of the matrix element of the coordinate, since

$$\varphi_n(0) = \frac{2^8 n^7 (n-1)^{2n-5}}{3\,(n+1)^{2n+5}} \tag{34a}$$

is essentially the familiar intensity formula for the Lyman series. The differential effective cross section is related to the generalized transition probability (cf. (16), (34)) by

$$d\Phi_n(q) = \frac{8\pi}{K^2} \left(\frac{M}{m} z \right)^2 \frac{dq}{q} \, \varphi_n(q) \tag{34b}$$

Most of the collisions (55%) at smallest angles ($q = 0$) are those in which the two-quantum level is excited, 17% of all collisions lead to the excitation of higher discrete levels, 28% to ionization. Of the latter, only 4% impart a kinetic energy greater than the simple ionization potential to the secondary electron.

If we proceed to the finite changes of momentum q of the colliding particle, where q should still be much smaller than a, the largest transition probability φ_2 decreases somewhat, the transitions to the discrete states with $n \geq 4$ increase very slightly, ionization increases somewhat more, as may easily be found by logarithmic differentiation of (30) or (33) with respect to q. If q acquires the order of magnitude of the reciprocal hydrogen radius a, all discrete excitation probabilities ϕ_n decrease greatly, but probabilities of transition φ_k into the continuous spectrum, especially the transfer of greater kinetic energy to the secondary electron, increase. Here, as will be demonstrated in the next section, the sum of all (discrete and continuous) transition probabilities decreases continuously with increasing q.

At q = 2α the discrete transitions comprise only 2% of all transitions; with even greater momentum transfer, excitation of the discrete spectrum is practically precluded. Then, according to (30), the transitions with $q \approx k$ are by far the most probable, i.e., those transitions for which the secondary electron receives the momentum transferred by the colliding particle (cf. the analogy in the Compton effect [15] *et alibi*; cf. also section 4 of this paper). The transition matrix is then

$$|\varepsilon_k(q)|^2 = \frac{8}{3\pi}\,\frac{\alpha^5}{[\alpha^2 + (q-k)^2]^3} \tag{34c}$$

as in Wentzel's formula, and decreases essentially with the sixth power of the difference between the momentum of the secondary electron and the change in momentum of the primary electron.

The following table gives the transition probabilities $\varphi_n(q)$ for some values of q for the first four discrete transitions and for four selected continuous transitions. The latter are normalized per *energy interval*; therefore,

$$\frac{\varphi_k(q)\,d\,k}{k\,d\,k} = \frac{\varphi_k}{k} = \frac{\alpha^2}{q^2}\,\frac{|\,\varepsilon_k(q)\,|^2}{k}\,.$$

Besides, the sum of all transition probabilities

$$\left\{\begin{aligned} \varphi(q) = \sum_n \varphi_n(q) + \int d\,k\,\varphi_k(q) = \frac{\alpha^2}{q^2}\Big(\sum_n |\,\varepsilon_n(q)\,|^2 \\ + \int d\,k\,|\,\varepsilon_k(q)\,|^2\Big) \end{aligned}\right. \tag{35}$$

is given, and also the percentage of the discrete transitions in this total probability.

Table 1

Generalized transition probabilities φ_n from the ground state of hydrogen

	$\frac{q^2}{\alpha^2} = 0$	$^1/_4$	$^1/_2$	1	2	4
$n = 2$	0,555	0,328	0,202	0,088	0,0230	0,0034
3	,089	,075	,054	,0267	,0073	,0011
4	,031	,0285	,0218	,0113	,0033	,0005
5	,0145	,0136	,0109	,0058	,0017	,00025
$k = 0$	1,563	1,588	1,300	0,720	0,216	0,032
$^1/_2$	0,688	0,925	0,944	0,677	,245	,038
1	,116	,195	,276	,374	,278	,059
2	,0017	,0024	,0034	,0062	,0183	,064
φ	1,000	0,862	0,751	0,590	0,401	0,234

Table 1 (cont.)

Component of the discrete transitions in the total transition probability $\varphi_n(q)$ in percent

$n =$ 2	55,5	38,1	26,9	15,0	5,7	1,45
3	8,9	8,7	7,2	4,5	1,8	0,47
4	3,1	3,3	2,9	1,9	0,82	0,20
5	1,45	1,58	1,45	0,98	0,42	0,11

7. Collisions at a Definite Angle

The formula

$$d\Phi_n(q) = \frac{8\pi\alpha^2}{K^2}\left(\frac{M}{m}z\right)^2 \frac{dq}{q^3}\,|\varepsilon_n(q)|^2 \qquad (16)$$

gives the number of the collisions with a transfer of momentum between q and q + dq that lead to the excitation of the n-quantum state of the atom. The total number of all inelastic collisions with a transfer of momentum between q and q + dq may be obtained easily by application of the completeness relation for the eigenfunctions of the hydrogen atom, since

$$\begin{aligned} \varepsilon(q) &= \sum_{n=2}^{\infty} |\varepsilon_n(q)|^2 + \int dk\, |\varepsilon_k(q)|^2 \\ &= \sum_{n=2}^{\infty} \left| \int e^{iqx}\,\psi_0\,\bar{\psi}_n\,d\tau \right|^2 + \int dk \left| \int e^{iqx}\,\psi_0\,\bar{\psi}_k\,d\tau \right|^2 \\ \varepsilon(q) &= 1 - F^2, \end{aligned} \qquad (36)$$

where*)

$$F = \int \psi_0^2\, e^{iqx}\, d\tau = \frac{1}{\left(1 + \frac{q^2}{4\alpha^2}\right)^2} \qquad (37)$$

is the atomic form factor for a hydrogen atom in the ground state. (For the total (generalized) transition probability defined in (35) we get

$$\left\{ \begin{aligned} \varphi(q) &= \frac{\alpha^2}{q^2}\,\varepsilon(q) = \frac{\alpha^2}{q^2}\left(1 - \frac{1}{\left(1 + \frac{q^2}{4\alpha^2}\right)^4}\right) \\ &= \frac{1 + \frac{3}{2}\,\frac{q^2}{4\alpha^2} + \left(\frac{q^2}{4\alpha^2}\right)^2 + \frac{1}{4}\left(\frac{q^2}{4\alpha^2}\right)^3}{\left(1 + \frac{q^2}{4\alpha^2}\right)^4} \end{aligned} \right. \qquad (38)$$

---

*) Formula (37), which may be obtained easily, is derived in ref. [1, section 11] together with the atomic form factors of the excitated states of the hydrogen atom.

and by a limiting process (cf. (26), (34))

$$\begin{cases} \varphi(0) = \sum\limits_n \varphi_n(0) + \int dk\, \varphi_k(0) \\ \qquad = \alpha^2 \left(\sum\limits_n |x_{0n}|^2 + \int dk\, |x_{0k}|^2 \right) = \alpha^2 \int x^2 \psi_0{}^2\, d\tau = 1 . \end{cases} \tag{38a}$$

Of course, this last relation may also be derived directly (ref. [1, section 10]). Hence, the effective cross section for all inelastic collisions with a transfer of momentum between q and q + dq is

$$d\,\Phi(q) = \frac{8\pi\alpha^2}{K^2} \left(\frac{M}{m} z \right)^2 \frac{dq}{q^3} \left(1 - F^2(q)\right) . \tag{39}$$

Correspondingly, the effective cross section for elastic collisions with the same transfer of momentum is, according to (16) and (22),

$$d\,\Phi_0(q) = \frac{8\pi\alpha^2}{K^2} \left(\frac{M}{m} z \right)^2 \frac{dq}{q^3} \left(1 - F(q)\right)^2 . \tag{40}$$

Of course, formula (39) will not be valid unless the transitions to *all* quantum states of the discrete and continuous spectrum, or at leat all transitions with appreciable transition probability, are actually possible energetically at the given value of q; otherwise, the completeness relation must not be used. Therefore, (cf. (17)),

$$q > q_{\min}(k) = \frac{M}{2mK} (\alpha^2 + k^2)$$

must hold for all states k with appreciable transition probability $\varphi_k(0)$, let us say, for all $k \leq 2\alpha$, i.e.,

$$q > \frac{5M\alpha^2}{2mK} .$$

Hence, for comparatively fast particles, (39) is valid even for collisions in which q is much smaller than α.

1. In the case of scattering at a *small* angle ($q \ll \alpha$), K' is almost equal to K and

$$1 - F = \frac{q^2}{2\alpha^2} , \tag{37a}$$

$$1 - F^2 = \frac{q^2}{\alpha^2} , \tag{37b}$$

i.e., the effective cross section for inelastic collisions becomes (in view of (15))

$$\left\{\begin{aligned} d\,\Phi(q) &= \frac{8\pi}{K^2}\left(\frac{M}{m}z\right)^2\frac{dq}{q} \\ &= 8\pi\left(\frac{M}{m}z\right)^2\frac{\sin\vartheta\,d\vartheta}{q^2} \approx \frac{8\pi}{K^2}\left(\frac{M}{m}z\right)^2\frac{d\vartheta}{\sin\vartheta}; \end{aligned}\right. \tag{39a}$$

and for elastic collisions

$$d\,\Phi_0(q) = \frac{2\pi}{K^2a^2}\left(\frac{M}{m}z\right)^2 q\,dq = 2\pi a^2\left(\frac{M}{m}z\right)^2\sin\vartheta\,d\vartheta. \tag{40a}$$

That is, while the differential effective cross section for elastic collisions approaches a constant boundary value independent of ϑ and K, which is of the same order of magnitude as the gas kinetic cross section, for inelastic collisions the effective cross section increases proportionally to $1/q^2$ per solid angle element $\sin\vartheta\, d\vartheta$ with decreasing scattering angle ϑ. Only at very small scattering angles is a boundary value

$$\left\{\begin{aligned} \lim_{q=0} d\,\Phi(q) &= 8\pi\left(\frac{M}{m}z\right)^2\sin\vartheta\,d\vartheta\cdot\overline{\frac{1}{q_{\min}^2}} \\ &\approx 8\pi a^2\left(\frac{M}{m}z\right)^2\sin\vartheta\,d\vartheta\left(\frac{mK}{Ma}\right)^2 \end{aligned}\right. \tag{41}$$

reached, which in the ratio $\left(\frac{mK}{Ma}\right)^2 = \frac{v^2}{v_0^2}$ is greater than the elastic effective cross section.*)

2. With scattering at large angles ("single scattering"), $q \gg a$ and F is nearly zero (cf. (37)), i.e., the contribution of Schrödinger's density distribution of the atomic electron to the elastic scattering is almost completely canceled by the interference of the contributions of the individual volume elements. Then we get

$$d\,\Phi_0(q) = d\,\Phi(q) = \frac{8\pi a^2}{K^2}\left(\frac{M}{m}z\right)^2\frac{dq}{q^3}. \tag{42}$$

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*) Our formulas (39) ff. are no longer valid for $\vartheta = 0$, since at $\vartheta = 0$ q depends on the excitation energy. However, the first relation (41) is exact when we define

$$\overline{\frac{1}{q_{\min}^2}} = \sum_n \frac{\varphi_n(0)}{q_{\min}^2(n)} + \int dk\,\frac{\varphi_k(0)}{q_{\min}^2(k)}$$

When the transferred momentum is large, elastic and inelastic collisions with identical transfer of momentum occur with the same frequency.*)

From the standpoint of physics, the number of inelastic collisions with constant transfer of momentum between q and q + dq is less interesting than the number of scatterings in a definite angular region from ϑ to $\vartheta + d\vartheta$. At large scattering angles, for inelastic collisions (cf. section 4)

$$\cos\vartheta = \frac{2K^2 - q^2\left(1 + \frac{M}{m}\right)}{2K\sqrt{K^2 - q^2\frac{M}{m}}}, \tag{18}$$

is valid for colliding particles of any effective mass M, or

$$q = K\sin\vartheta, \tag{19}$$

for colliding electrons. For the latter we obtain, from (39) with respect to M = m, z = 1 (or directly from (10)),

$$d\Phi(\vartheta) = \frac{8\pi a^2}{K^4}\left[1 - F^2(K\sin\vartheta)\right]\frac{\cos\vartheta\, d\vartheta}{\sin^3\vartheta}. \tag{39b}$$

as the effective cross section for inelastic scatterings at angle ϑ, while the effective cross section for elastic scatterings is, according to (40) and (14b)

$$\left\{\begin{aligned} d\Phi_0(\vartheta) &= \frac{8\pi a^2}{K^4}\left[1 - F\left(2K\sin\frac{\vartheta}{2}\right)\right]^2\frac{\sin\vartheta\, d\vartheta}{16\sin^4\vartheta/2} \\ &= \frac{8\pi a^2}{K^4}\left[1 - F\left(2K\sin\frac{\vartheta}{2}\right)\right]^2\frac{\sin\vartheta\, d\vartheta}{4(1-\cos\vartheta)^2} \end{aligned}\right. \tag{40b}$$

For sufficiently large scattering angles, for which $F \approx 0$, (40b) becomes the Rutherford formula, and the ratio of inelastic to elastic collisions is

$$\frac{d\Phi(\vartheta)}{d\Phi_0(\vartheta)} = \frac{4\cos\vartheta(1-\cos\vartheta)^2}{\sin^4\vartheta} = \frac{4\cos\vartheta}{(1+\cos\vartheta)^2}. \tag{42a}$$

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*) Elsasser thought that the inelastic scattering (in contrast to the elastic scattering) might disappear at large angles; probably he did not give adequate consideration to transitions into the continuous spectrum.

For $\vartheta =$	0°	45°	60°	75°	80°	85°	90° and more
$\frac{d\Phi(\vartheta)}{d\Phi_0(\vartheta)} =$	1	0.97	0.89	0.65	0.50	0.30	0

i.e., the number of elastic and inelastic electron collisions is practically equal at the same scattering angle up to an angle of approximately 60°; above 90°, there are only elastic collisions (nuclear scattering), because of the approximate validity of the classical law of energy momentum; there are no inelastic ones (collisions with the atomic electrons).

However, in the case of a collision of a heavy particle (α-particle), only a very small angular region can be involved in inelastic scattering (section 4). Therefore, single scattering (scattering at large angles) is always nuclear scattering (elastic scattering) in this case.*)

8. Generalized f-Sum Rule

For our subsequent computation of the deceleration of a colliding particle, i.e., the energy per centimeter of path transferred during passage through a gas, let us find not only the number of collisions with a transfer of momentum between q and q + dq (cf. section 7), but also the total energy transferred by such collisions to the hydrogen atom through such collisions:

$$d\,E(q) = \sum_n (E_n - E_0)\,d\,\Phi_n(q). \tag{43}$$

Here, the evaluation based on the completeness relation for the eigenfunctions leads to a formula even simpler than that for the number of collisions. For the general case,**) we immediately compute

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*)However, this is due to the approximate validity of the classical law of momentum for colliding particle and secondary electron in theoretical collisions with large transfer of momentum and is, therefore, not a quantum-theoretical phenomenon.

**)Evidently (according to (16)), the equation

$$d\,E(q) = \frac{8\pi R h}{K^2}\left(\frac{M}{m}z\right)^2 \frac{d\,q}{q} f_0(q) \tag{43a}$$

is determined by evaluating (44) in the special case m = 0. (The sum over n should also include the continuous spectrum.)

$$\left\{\begin{aligned} f_m(q) &= \sum_n f_{mn}(q) = \sum_n \frac{E_n - E_m}{Rh} \varphi_{mn}(q) \\ &= \frac{\alpha^2}{q^2 Rh} \sum_n (E_n - E_m) \,|\, \varepsilon_n(q) \,|^2 . \end{aligned}\right. \tag{44}$$

Since the $\varphi_{mn}(q)$'s are generalized transition probabilities, the expression

$$f_{mn}(q) = \frac{E_n - E_m}{Rh} \varphi_{mn}(q) = \frac{1}{R} \nu_{mn} \varphi_{mn}(q) \tag{45}$$

can be defined as the generalized oscillator strength for the transition mn. For q = 0, this definition agrees with the definition common in dispersion theory:

$$f_{mn}(0) = \frac{\nu_{mn} \varphi_{mn}(0)}{R} = \frac{\alpha^2}{R} \nu_{mn} \,|\, x_{mn} \,|^2 = \frac{8\pi^2 m}{h} \nu_{mn} \,|\, x_{mn} \,|^2 . \tag{45a}$$

In order to evaluate (44), we proceed as when setting up the usual f-sum rule, from the Schrödinger equations

$$\Delta \psi_m + \frac{8\pi^2 m}{h^2}(E_m - V)\psi_m = 0$$
$$\Delta \psi_n + \frac{8\pi^2 m}{h^2}(E_n - V)\psi_n = 0$$

with an arbitrary potential V and only presuppose that E_m is a discrete eigenvalue, so that from now on we can neglect all surface integrals. Then

$$\left\{\begin{aligned} &(E_n - E_m)\int \psi_m \bar{\psi}_n e^{iqx}\, d\tau \\ &= \frac{h^2}{8\pi^2 m}\int (\bar{\psi}_n \Delta \psi_m - \psi_m \Delta \bar{\psi}_n) e^{iqx}\, d\tau \\ &= -\frac{h^2}{8\pi^2 m} iq \int \left(\bar{\psi}_n \frac{\partial \psi_m}{\partial x} - \psi_m \frac{\partial \bar{\psi}_n}{\partial x}\right) e^{iqx}\, d\tau \\ &= Rha^2 \Big(-2iq \int \frac{\partial \psi_m}{\partial x} \bar{\psi}_n e^{iqx}\, d\tau \\ &+ q^2 \int \psi_m \bar{\psi}_n e^{iqx}\, d\tau\Big) . \end{aligned}\right. \tag{45b}$$

$$\begin{aligned} f_m(q) &= \sum_n f_{mn}(q) = \frac{\alpha^2}{q^2 Rh} \sum_n (E_n - E_m) \left| \int e^{iqx} \psi_m \bar{\psi}_n \, d\tau \right|^2 \\ &= \frac{1}{q^2} \sum_n \Big(-2iq \int \frac{\partial \psi_m}{\partial x} \bar{\psi}_n e^{iqx}\, d\tau \\ &+ q^2 \int \psi_m \bar{\psi}_n e^{iqx}\, d\tau\Big) \cdot \int e^{-iqx} \bar{\psi}_m \psi_n \, d\tau \\ &= -2\frac{i}{q} \cdot \int \frac{\partial \psi_m}{\partial x} \bar{\psi}_m \, d\tau + \int |\, \psi_m \,|^2 \, d\tau . \end{aligned}$$

$$f_m(q) = \sum_n f_{mn}(q) = 1. \tag{46}$$

The sum of the generalized oscillator strengths $f_{mn}(q)$ for all transitions from one level of a hydrogen atom is equal to 1, as is the sum of the oscillator strengths $f_{mn}(0)$, defined in the usual manner.

Therefore, (43) becomes

$$dE(q) = \frac{8\pi R h}{K^2}\left(\frac{M}{m} z\right)^2 \frac{dq}{q} = \frac{4\pi e^4 z^2}{m v^2}\,\frac{dq}{q}. \tag{47}$$

which is the energy transferred by a stream of one particle per unit time and surface per unit time to a hydrogen atom as a result of <u>those collisions</u> in which the momentum of the particle changes by an amount between $\frac{h}{2\pi}q$ and $\frac{h}{2\pi}(q + dq)$. It has the dimension energy times surface.

On the average, during every collision with a change in momentum of the colliding particle between q and q + dq, the energy

$$\frac{dE(q)}{d\Phi(q)} = \frac{q^2 R h a^2}{1 - F^2(q)} \tag{48}$$

is transferred, i. e., with large deflections ($F \approx 0$)

$$\frac{dE(q)}{d\Phi(q)} = \frac{q^2}{a^2} R h = \frac{h^2}{8\pi^2 m} q^2. \tag{48a}$$

This result is self-evident, since we know that in nearly all cases when q is large the secondary electron receives the momentum $\frac{h}{2\pi}q$, i. e., the energy $\frac{h^2}{8\pi^2 m}q^2$. In the case of small deflections we get, according to (37b), simply

$$\frac{dE(q)}{d\Phi(q)} = Rh, \tag{48b}$$

i. e., on the average the simple ionization potential is transferred.

9. Excitation of Certain Energy Levels

We integrate the differential effective cross section over ϑ (or over q) and thus obtain the total effective cross section for the excitation of a definite level n, i. e., the excitation functions for excitation by collision of fast electrons

$$\Phi_n = \int_{q_{\min}}^{q_{\max}} d\Phi_n(q) = \frac{2^{10}\pi}{3K^2}\left(\frac{M}{m}z\right)^2 n^7 \cdot A \tag{49}$$

$$A = \int_{q_{\min}}^{q_{\max}} [n^2 - 1 + 3x]\,\frac{[(n-1)^2 + x]^{n-3}}{[(n+1)^2 + x]^{n+3}}\,\frac{dx}{x} \tag{49a}$$

by using (33) and (16); $x = (\frac{qn}{a})^2$. Equation (49a) can be stated in an elementary manner:

$$\begin{aligned} A &= \int (n^2 - 1 + 3x) \sum_{k=0}^{n-3} \binom{n-3}{k} \frac{(-4n)^k}{[(n+1)^2 + x]^{6+k}}\,\frac{dx}{x} \\ &= \int \frac{dx}{x}(n^2-1)c_0' - (n^2-1)\sum_{\tau=0}^{n+2} \frac{c_\tau'\,dx}{[(n+1)^2+x]^{\tau+1}} \\ &\quad + 3\sum_{\tau=5}^{n+2}\binom{n-3}{\tau-5}(-4n)^{\tau-5}\,\frac{dx}{[(n+1)^2+x]^{\tau+1}}, \end{aligned}$$

$$\begin{aligned} c_\tau' &= \sum_{k=\tau-5}^{n-3}\binom{n-3}{k}\frac{(-4n)^k}{(n+1)^{2(k+6-\tau)}} \\ &= \frac{(n-1)^{2(n-3)}}{(n+1)^{2(n+3-\tau)}}\left[1 - \left(\frac{n+1}{n-1}\right)^{2n-6}\sum_{k=0}^{\tau-6}\binom{n-3}{k}\left(\frac{-4n}{(n+1)^2}\right)^k\right]. \end{aligned}$$

$$\left\{\begin{aligned} A = \frac{(n-1)^{2n-5}}{(n+1)^{2n+5}}\Bigg| & \ln x - \ln[(n+1)^2 + x] \\ & + \sum_{\tau=1}^{n+2}\frac{c_{n\tau}}{\tau\left(1 + \frac{x}{(n+1)^2}\right)^\tau}\Bigg|_{q_{\min}}^{q_{\max}}, \end{aligned}\right. \tag{49b}$$

$$\left\{\begin{aligned} c_{n\tau} = 1 - \left(\frac{n+1}{n-1}\right)^{2n-6} & \left[\sum_{k=0}^{\tau-6}\binom{n-3}{k}\left(\frac{-4n}{(n+1)^2}\right)^k\right. \\ & \left. + 3\binom{n-3}{\tau-5}\left(\frac{-4n}{(n+1)^2}\right)^{\tau-5}\frac{n+1}{n-1}\right]. \end{aligned}\right. \tag{50a}$$

Finally, the excitation probability becomes (cf. (34a))

$$\left\{\begin{aligned} \Phi_n = \frac{4\pi}{K^2}\left(\frac{M}{m}z\right)^2 \alpha^2 |x_{0n}|^2 & \left[F_n\left(1 + \left(\frac{n}{n+1}\,\frac{q_{\max}}{\alpha}\right)^2\right)\right. \\ & \left. - F_n\left(1 + \left(\frac{n}{n+1}\,\frac{q_{\min}}{\alpha}\right)^2\right)\right], \end{aligned}\right. \tag{50}$$

where

$$F_n(y) = \ln\frac{y-1}{y} + \sum_{\tau=1}^{n+2}\frac{c_{n\tau}}{\tau y^\tau}\,. \tag{50b}$$

In particular:

$$\begin{cases} F_2(y) = \ln \frac{y-1}{y} + \frac{1}{y} + \frac{1}{2y^2} + \frac{1}{3y^3} + \frac{1}{4y^4} \\ F_3(y) = F_2(y) - \frac{1}{y^5}, \\ F_4(y) = F_2(y) - \frac{116}{45\,y^5} + \frac{32}{27\,y^6} \\ F_5(y) = F_2(y) - \frac{697}{160\,y^5} + \frac{85}{24\,y^6} - \frac{25}{32\,y^7}\,. \end{cases} \tag{50c}$$

Formulas (50c) completely agree in construction with the formulas given by Elsasser [11, p. 532] for the excitation cross sections of the first transitions. In that respect Elsasser's formulas are somewhat more complete than ours, since he computes the transitions according to partial levels with different azimuthal quantum numbers ℓ separately, while we obtain only the total excitation probability of the levels of the hydrogen atom defined by the principal quantum number n, because we used parabolic instead of polar coordinates. On the other hand, we have gained so much in simplicity that we can derive the general formula for the effective cross section (50, 50a, 50b) and can easily write the explicit representation of the excitation functions even for higher series terms.*)

Thus far in this section we have performed Born's approximation without omissions. Now we shall concentrate again on fast particles, introduce for q_{min} the value from (17) ($a_{0n}^2 = a^2(1 - 1/n^2)$ for hydrogen), set $q_{max} \approx 2K$ and disregard all powers of $\frac{aM}{Km} = \frac{v}{v_0}$ beginning with the fourth. We get

$$\Phi_n = \frac{4\pi\alpha^2}{K^2}\left(\frac{M}{m}z\right)^2 |x_{0n}|^2 \ln a_n \left(\frac{2Km}{\alpha M}\right)^2 \tag{51}$$

$$\ln a_n = 2\ln\frac{n}{n-1} - \sum_{\tau=1}^{n+2}\frac{c_{n\tau}}{\tau}, \tag{51a}$$

$$\Phi_n = \frac{8\pi R h z^2}{m v^2}|x_{0n}|^2 \ln\frac{2a_n m v^2}{Rh} \tag{51b}$$

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*) Our formula for Φ_2 obviously coincides with Elsasser's sum $\Phi(2,0) + (2,1)$; however, the formula for Φ_3 does not agree with Elsasser's $\Phi(3,0) + \Phi(3,1) + \Phi(3,2)$. (Our y is Elsasser's x, our q_{max}/a his S_1, and our q_{min}/a his S_0. In his formula for F_1 the sign should be reversed.) Since Elsasser's derivation is much more complicated than ours, we are inclined to suspect an error in his formulas.

$|x_{0n}|^2$ is the square of the coordinate matrix (cf. table 1). For the a_n's we get numerically

$n =$	2	3	4	5
$\ln a_n =$	− 0,697	− 0,272	− 0,115	− 0,042
$a_n =$	0,498	0,762	0,891	0,959

It now seems that $\lim_{n=\infty} a_n = 1$.

The excitation cross section is nearly proportional to the optical transition probability and inversely proportional to the square of the velocity of the particle; in addition, there appears - as in Bohr's deceleration theory - a logarithmic term whose argument is proportional to v^2 and in addition is weakly dependent on the level n which is to be excited. This latter dependence somewhat decreases the excitation cross section for the strongest transitions (small n's), although the lower integration limit q_{min} in (49a) is lower for these transitions than for those to higher levels.

10. Total Number of Collisions and Deceleration

We now compute the total of all inelastic collisions in general:

$$\Phi = \sum_n \int_{q_{\min}}^{q_{\max}} d\Phi_n(q). \tag{52}$$

We divide the integration into two partial integrations from q_{min} to q_0 and from q_0 to q_{max}. On the one hand, we choose q_0 so large, that for all $q > q_0$, the differential effective cross sections $d\Phi_n(q)$ for the excitations of the different levels n can be summed to $d\Phi(q)$ by application of the completeness relation, i. e., $q_0 \gg \alpha^2/K \times M/m$. On the other hand, let $q_0 \ll \alpha$, so that for all $q > q_0$ the generalized transition probabilities $\varphi_n(q)$ (cf. (33), (34)) may be replaced by the usual transition probabilities $\varphi_n(0) = \alpha^2 |x_{0n}|^2$. Then according to (34), (17), and (38a)

$$\left\{\begin{aligned} \Phi' &= \sum_n \int_{q_{\min}}^{q_0} d\Phi_n(q) = \frac{8\pi}{K^2}\cdot\left(\frac{M}{m}z\right)^2\cdot\sum_n \varphi_n(0)\int_{q_{\min}}^{q_0}\frac{dq}{q} \\ &= \frac{8\pi}{K^2}\cdot\left(\frac{M}{m}z\right)^2\sum_n \varphi_n \ln\frac{2q_0 K m}{\alpha^2 M\left(1-\frac{1}{n^2}\right)} \\ &= \frac{4\pi}{K^2}\left(\frac{M}{m}z\right)^2\left[\ln\frac{4q_0^2K^2m^2}{\alpha^4M^2} - 2\sum_{n=2}^{\infty}\varphi_n \ln\frac{n^2-1}{n^2}\right. \\ &\qquad\left. -2\int_0^{\infty} dk\cdot\varphi_k \ln\left(1+\frac{k^2}{\alpha^2}\right)\right]. \end{aligned}\right. \tag{52a}$$

Also, by (40), (19), and (37):

$$\Phi'' = \int_{q_0}^{q_{\max}}\sum_n d\Phi_n(q) = \frac{8\pi\alpha^2}{K^2}\left(\frac{M}{m}z\right)^2\int_{q_0}^{q_{\max}}\frac{dq}{q^3}\left(1-\frac{1}{\left(1+\frac{q^2}{4\alpha^2}\right)^4}\right)$$

$$= \frac{4\pi}{K^2}\left(\frac{M}{m}z\right)^2\left|\ln\frac{q^2}{4\alpha^2+q^2} + \frac{\frac{3}{4}}{1+\frac{q^2}{4\alpha^2}} + \frac{\frac{1}{4}}{\left(1+\frac{q^2}{4\alpha^2}\right)^2} + \frac{\frac{1}{12}}{\left(1+\frac{q^2}{4\alpha^2}\right)^3}\right|_{q_0}^{q_{\max}\gg\alpha},$$

$$\Phi'' = \frac{4\pi}{K^2}\left(\frac{M}{m}z\right)^2\left(\ln\frac{4\alpha^2}{q_0^2} - \frac{13}{12}\right) \tag{52b}$$

Except for magnitudes of the order of α^2/K^2:

$$\Phi = \Phi' + \Phi'' = \frac{4\pi}{K^2}\left(\frac{M}{m}z\right)^2 \ln\frac{4m^2K^2}{b\,M^2\alpha^2} \tag{52c}$$

$$\ln b = -\ln 4 + \frac{13}{12} + 2\sum_{n=2}^{\infty}\varphi_n \ln\frac{n^2-1}{n^2} + 2\int_0^{\infty} dk\,\varphi_k \ln\left(1+\frac{k^2}{\alpha^2}\right).$$

$$\left\{\begin{aligned} \ln b &= -\ln 4 + \frac{13}{12} - \frac{2^9}{3}\left[\sum_{n=2}^{\infty}\frac{n^7(n-1)^{2n-5}}{(n+1)^{2n+5}}\ln\frac{n^2}{n^2-1}\right. \\ &\qquad\left. -\int_0^{\infty}\cdot\frac{k\,dk\,\alpha^8}{(\alpha^2+k^2)^5}\cdot\frac{e^{-4\frac{\alpha}{k}\operatorname{arctg}\frac{k}{\alpha}}}{1-e^{-2\pi\frac{\alpha}{k}}}\cdot\ln\left(1+\frac{k^2}{\alpha^2}\right)\right]. \end{aligned}\right. \tag{52d}$$

We find by numerical evaluation

$$\underline{b = 0{,}638\,,}$$

$$\Phi = \frac{8\pi R h a^2 z^2}{m v^2}\ln\frac{2mv^2}{0{,}638\,Rh} = \frac{2\pi e^4 z^2}{Rh\cdot m v^2}\ln\frac{2mv^2}{0{,}638\,Rh}\,. \tag{53}$$

Multiplying by the number of atoms N per unit volume, we obtain the number NΦ of inelastic collisions per centimeter path of the particle, i.e., the reciprocal mean free path. Essentially, this is inversely proportional to the square of the velocity of the particle and it also contains a logarithmic term. A corresponding logarithmic term also occurs in the number of the ions formed primarily from the particle per centimeter path, in contrast to Bohr's and Thomson's classical theory (cf. [18], [7, p. 606]). We obtain the number of primary ions

$$s_0 = N\Phi_i = N \int_0^{\infty} dk \int_{q_{\min}}^{q_{\max}} d\,\Phi_k(q)$$

most simply by subtracting the number of the discrete excitations

$$N\Phi_a = N \sum_{n=2}^{\infty} \int_{q_{\min}}^{q_{\max}} d\,\Phi_n(q)$$

from NΦ. The result is

$$N\Phi_a = 0{,}715 \cdot \frac{2\pi e^4 z^2 N}{Rh \cdot m v^2} \ln \frac{2 m v^2}{1{,}79\, Rh} \tag{54a}$$

for the total number of excitations, and

$$N\Phi_i = s_0 = 0{,}285 \cdot \frac{2\pi e^4 z^2 N}{Rh \cdot m v^2} \cdot \ln \frac{2 m v^2}{0{,}048\, Rh} \tag{54b}$$

for the total number of ions formed per centimeter path. Likewise (integrating (40) over q),

$$N\Phi_0 = \frac{4\pi N}{K^2} \left(\frac{M}{m} z\right)^2 \cdot \frac{7}{12} = 0{,}583 \cdot \frac{2\pi e^4 z^2 N}{Rh \cdot m v^2} \tag{54c}$$

is the total number of elastic collisions per centimeter path; therefore, the latter does not contain any logarithmic term.

Now we compute quite analogously the total energy loss

$$E = \sum_n (E_n - E_0) \int_{q_{\min}}^{q_{\max}} d\Phi_n(q) \tag{55a}$$

of the particle flux per unit time. With respect to (45) and (46) we find, by analogy to (52a),

$$E' = \sum_n \int_{q_{\min}}^{q_0} d\Phi_n(q)(E_n - E_0) \tag{55b}$$

$$= \frac{8\pi R h}{K^2}\left(\frac{M}{m} z\right)^2 \cdot \left[\ln \frac{2 q_0 K m}{\alpha^2 M} - \sum_n \varphi_n \left(1 - \frac{1}{n^2}\right) \ln \frac{n^2 - 1}{n^2} - \int dk\, \varphi_k \cdot \left(1 + \frac{k^2}{\alpha^2}\right) \ln \left(1 + \frac{k^2}{\alpha^2}\right)\right].$$

Also, according to (47) and (20),

$$E'' = \int_{q_0}^{q_{\max}} d\,E(q) = \frac{8\pi R h}{K^2}\left(\frac{M}{m} z\right)^2 \ln \frac{2K}{q_0} \frac{m}{M + m}. \tag{55c}$$

Therefore,

$$E = \frac{8\pi R h}{K^2}\left(\frac{M}{m} z\right)^2 \ln \frac{4K^2}{c\,\alpha^2} \frac{m^2}{M(M + m)},$$

$$\ln c = \frac{2^9}{3} \sum_{n=2}^{\infty} \frac{n^5 (n-1)^{2n-4}}{(n+1)^{2n+4}} \ln \frac{n^2 - 1}{n^2}$$

$$+ \frac{2^9}{3} \int_0^{\infty} \frac{dk \cdot k \cdot \alpha^6}{(\alpha^2 + k^2)^4} \cdot \frac{e^{-4 \frac{\alpha}{k} \operatorname{arctg} \frac{k}{\alpha}}}{1 - e^{-2\pi \frac{\alpha}{k}}} \ln \left(1 + \frac{k^2}{\alpha^2}\right),$$

$$c = 1{,}105,$$

$$E = \frac{4\pi e^4 z^2}{m v^2} \ln \frac{(2)\, m v^2}{c R h}, \tag{55}$$ *)

where the 2 in parentheses appears only for the collision of heavy particles, while it is disregarded in the case of electron collision.

The loss in kinetic energy per centimeter path is

$$-\frac{dT}{dx} = N E = \frac{4\pi e^4 z^2 N}{m v^2} \ln \frac{(2)\, m v^2}{c R h}. \tag{56}$$

This is almost exactly double the value derived by Henderson for the stopping cross section. Since Henderson's values are approximately half of the observed stopping cross section [9], our result agrees quite well with observation. Formula (56) differs from Bohr's formula for deceleration in that the argument of the logarithm contains v^2 instead of v^3.

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*) Read arctg as arc tangent.

The mean energy loss of the particle per collision becomes

$$\bar{E} = \frac{E}{\Phi} \approx 2Rh. \tag{57}$$

Since 28.5% of all collisions lead to ionization [(53) and (54b)], the energy consumption for each primarily formed ion is approximately 2Rh/0.285; which is seven times the ionization potential. This is the case with very high particle velocities; otherwise, the energy [illegible] smaller [illegible] is appreciably larger [illegible]

III. MORE COMPLEX ATOMS

11. f-Sum Rules

In this section we extend our results to more complex atoms, but, strictly speaking, we can do this for only a few points. In general we shall have to assume that the eigenfunctions of the atom may be represented as the sum of the products of the eigenfunctions of individual electrons, owing to which the simultaneous excitation of two electrons of the atom by the collision process is precluded from the very beginning. In numerical computation frequently we must go one step further - a precarious step - and replace the eigenfunctions of each electron by the hydrogen eigenfunctions of the corresponding quantum numbers. In all other cases we shall consider the eigenfunctions of an electron to be approximately the eigenfunctions computed by the Hartree method for a suitable potential field of the atom.

First we apply the generalized f-sum rule to atoms with several electrons; i.e., as in section 8, we are looking for the total energy transfer by collisions with a change in momentum between q and q + dq:

$$E(q) = \frac{8\pi}{K^2} \left(\frac{M}{m} z\right)^2 \frac{dq}{q} Rh \sum_k f_{0k}(q), \tag{58}$$

$$f_{mk} = \frac{E_k - E_m}{Rh} \cdot \frac{a^2}{q^2} \cdot \left| \int \sum_j e^{iqx_j} \psi_m \overline{\psi_k} \, d\tau \right|^2. \tag{58a}$$

Since no assumption had to be made about the potential V of Schrödinger's equation in deriving (45b), V in particular (as well as Ψ) depend on more than three coordinates and (45b) applies directly to our case

$$\begin{cases} (E_k - E_m)\int \Psi_m \overline{\Psi_k} e^{iqx_j} d\tau \\ = Rh\, a^2 \left(-2iq \int \frac{\partial \Psi_m}{\partial x_j} \overline{\Psi_k} e^{iqx_j} d\tau + q^2 \int \Psi_m \overline{\Psi_k} e^{iqx_j} d\tau\right). \end{cases} \tag{58b}$$

Furthermore, from this we obtain

$$\begin{aligned} f = \sum_k f_{mk} = \sum_k \Big(&-\frac{2i}{q}\int \sum_j e^{iqx_j} \cdot \frac{\partial \Psi_m}{\partial x_j} \overline{\Psi_k}\, d\tau \\ &+ \int \sum_j e^{iqx_j} \cdot \Psi_m \overline{\Psi_k}\, d\tau\Big) \cdot \int \sum_l e^{-iqx_l} \cdot \overline{\Psi}_m \Psi_k\, d\tau, \\ f = \sum_j \sum_l \Big(&-\frac{2i}{q}\int \frac{\partial \Psi_m}{\partial x_j} \overline{\Psi_m} e^{iq(x_j - x_l)} + \int \Psi_m \overline{\Psi_m} e^{iq(x_j - x_l)}\Big). \end{aligned}$$

Since f is real by definition, it may easily be shown that in the first integral $2\overline{\Psi}_m \dfrac{\partial \Psi_m}{\partial x_j}$ may be replaced by $\dfrac{\partial |\Psi_m|^2}{\partial x_j}$. Then, through partial integration we find that

$$-\frac{i}{q}\int \frac{\partial |\Psi_m|^2}{\partial x_j} e^{iq(x_j - x_l)} d\tau = \begin{cases} -\int |\Psi_m|^2 e^{iq(x_j - x_l)} & \text{for } j \neq \ell \\ 0 & \text{for } j = \ell \end{cases}$$

i.e.,

$$f = \int \sum_j e^{iq(x_j - x_j)} \, |\Psi_m|^2 \, d\tau$$

$$f = \sum_k f_{mk}(q) = Z. \tag{59}$$

The sum of the generalized oscillator strengths (58a) for all transitions from one level of any atom is equal to the number Z of the electrons.

The transitions of a heavy atom from the ground state break down according to their transition frequency into different groups separated from each other to some extent, depending on whether an electron from the K, L, M, etc. shell is excited. It is questionable whether the oscillator strengths (58a) may also be summed by a simple process for each of these individual groups of transitions. Such a "partial f-sum rule" would be important for computing the total stopping cross section of an atom by integration over all possible collision vectors q. Since the lower integration boundary q_{min} depends on the transferred excitation energy (17), it is advantageous to combine transitions with neighboring transition frequencies (excitation energies) before integration over q.

We can set up a partial f-sum rule if we assume, as indicated above, that the atomic eigenfunction may be represented as a sum of products of the eigenfunctions of individual electrons. Let us classify the latter by the principal quantum number n and the azimuthal quantum number ℓ, and also a magnetic quantum number m (which is insignificant because of the azimuthal degeneracy); let $Z_{n\ell}$ be the number of electrons in an atom in the ground state in the $(n\ell)$-shell, let $\overrightarrow{Z}_{n\ell}$ and $\overleftarrow{Z}_{n\ell}$ be the numbers of $(n\ell)$-electrons of the individual spin directions*) $(Z_{n\ell} = \overrightarrow{Z}_{n\ell} + \overleftarrow{Z}_{n\ell})$, and let $g_{n\ell} = 2\ell + 1$ be the "weight" of the electron state $(n\ell)$. Then it may easily be shown that the square of the matrix element for the transition of an electron from the $n\ell$-shell to n', ℓ' is given by

$$\left\{ \begin{aligned} & |\varepsilon_{nl,n'l'}(q)|^3 \\ & \quad = \left[\overrightarrow{Z}_{nl}\left(1-\frac{\overrightarrow{Z}_{n'l'}}{g_{n'l'}}\right)+\overleftarrow{Z}_{nl}\left(1-\frac{\overleftarrow{Z}_{n'l'}}{g_{n'l'}}\right)\right] |\varepsilon^1_{nl,n'l'}(q)|^2; \end{aligned} \right. \tag{60}$$

$$|\varepsilon^1_{nl,n'l'}(q)|^2 = \frac{1}{g_{nl}} \cdot \sum_{m=-l}^{+l} |\int \psi_{nlm} \bar{\psi}_{n'l'm} e^{iqx} d\tau|^2 \tag{60a}$$

is the square of the matrix element for the case where <u>one</u> electron is in the $(n\ell)$-state and the $(n'\ell')$-state is unoccupied, i.e., for the case which always applies for the hydrogen atom.**) The factor which occurs

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*) In the case of the ground state, these numbers may be given individually. Since the ground term is a term of the highest multiplicity, when → gives the direction of the total spin, $\overrightarrow{Z}_{n\ell}$ must be as large as possible, i.e., $\overrightarrow{Z}_{n\ell} = Z_{n\ell}$ when $Z_{n\ell} < g_{n\ell}$; and $\overrightarrow{Z}_{n\ell} = g_{n\ell}$ when $Z_{n\ell} > g_{n\ell}$.

**) As in (60a), averaging over m should also be done for the hydrogen atom. If we do not combine all transitions from the $n\ell$-shell, but consider transitions from each individual quantum cell (characterized by n, ℓ, m, and the spin direction) individually, the matrix element becomes even simpler, viz.,

$$\varepsilon_{nlm,n'l'm} = \int e^{iqx} \psi_{nlm} \bar{\psi}_{n'l'm}. \tag{60b}$$

when ℓm is occupied and n'ℓ'm empty, but it is zero when nℓm is unoccupied or n'ℓ'm is occupied (or both), i.e., it is as though only the one "jumping" electron were present in the atom. However, the distribution of electrons to individual places with a different m within an $(n\ell)$-level cannot be given and, therefore, averaging must be done over all electron position distributions possible with the given total number of electrons in the $(n\ell)$-shell. This averaging yields (60, 60a).

both in (60a) and (60) and depends both on the number of electrons in the initial level and the number of vacant positions in the final level is quite evident from the viewpoint of the Pauli principle.

From (60) we may compute the sum of the oscillator strengths for all transitions in which an electron from the $(n\ell)$-shell is excited:

$$\left\{\begin{aligned} f_{nl} &= \sum_{n'l'} f_{nl,n'l'} = \frac{\alpha^2}{q^2 R h} \sum_{n'l'} (E_{n'l'} - E_{nl}) \, |\varepsilon_{nl,n'l'}(q)|^2 \\ &= \frac{\alpha^2}{q^2 R h} \left(Z_{nl} \sum_{n'l'} (E_{n'l'} - E_{nl}) \, |\varepsilon^1_{nl,n'l'}(q)|^2 \right. \\ &\quad \left. - \sum_{n'l'} \frac{\overrightarrow{Z}_{nl}\overrightarrow{Z}_{n'l'} + \overleftarrow{Z}_{nl}\overleftarrow{Z}_{n'l'}}{g_{n'l'}} (E_{n'l'} - E_{nl}) \, |\varepsilon^1_{nl,n'l'}(q)|^2 \right). \end{aligned}\right. \tag{61a}$$

The first summand may be computed in exact analogy to the derivation of the f-sum rule for hydrogen (section 8) and is found to be $Z_{n\ell}$; furthermore, if

$$\left\{\begin{aligned} f^1_{nl,n'l'} &= (E_{n'l'} - E_{nl}) \frac{\alpha^2}{q^2 R h} |\varepsilon^1_{nl,n'l'}(q)|^2 \\ &= \frac{\alpha^2}{q^2 R h} (E_{n'l'} - E_{nl}) \\ &\quad \cdot \frac{1}{g_{nl}} \sum_{m} \left| \int \psi_{nlm} \bar{\psi}_{n'l'm} \, e^{iqx} \, d\tau \right|^2, \end{aligned}\right. \tag{61}$$

we will have

$$\left\{\begin{aligned} f_{nl} &= Z_{nl} - \sum_{n'l'} \frac{\overrightarrow{Z}_{nl}\overrightarrow{Z}_{n'l'} + \overleftarrow{Z}_{nl}\overleftarrow{Z}_{n'l'}}{g_{n'l'}} \cdot f^1_{nl,n'l'} \\ &= \sum_{n'l'} f^1_{nl,n'l'} \, \zeta. \end{aligned}\right. \tag{62}$$

The sum of the oscillator strengths of all transitions in which an electron from the $(n\ell)$-shell is excited is equal to the number $Z_{n\ell}$ of the electrons in this shell, less the oscillator strengths of the transitions from the $n\ell$-state forbidden by the Pauli principle. If all $n''\ell''$-shells are occupied and all others are vacant, $\vec{Z}_{n''\ell''} = \overleftarrow{Z}_{n''\ell''} = g_{n''\ell''}$ and

$$f_{nl} = Z_{nl} \left(1 - \sum_{n''l''} f^1_{nl,n''l''} \right). \tag{62a}$$

The partial sum $f_{n\ell}$ of the oscillator strengths is smaller or greater than the number of electrons $Z_{n\ell}$ in the $(n\ell)$-shell, depending on whether

$(n\ell)$ is an inner or an outer shell of the atom. If $(n\ell)$ is an inner shell, the oscillator strengths $f^{1}_{n\ell,\, n'\ell'}$ are positive for all transitions forbidden by the Pauli principle because $E_{n'\ell'} > E_{n\ell}$, and the reverse is true for outer shells.[*)] If we sum the oscillator strengths for all possible transitions of the atom, we obtain

$$f = \sum_{nl} f_{nl} = \sum_{nl} Z_{nl} - \frac{u^2}{q^2 Rh} \sum_{nl} \sum_{n'l'} \frac{\vec{Z}_{nl}\vec{Z}_{n'l'} + \overleftarrow{Z}_{nl}\overleftarrow{Z}_{n'l'}}{g_{nl}\, g_{n'l'}}$$

$$\cdot (E_{n'l'} - E_{nl}) \sum_{m} \left| \int e^{iqx} \psi_{nlm} \bar{\psi}_{n'l'm}\, d\tau \right|^2 = Z\,.$$

The deviations of the partial sums $f_{n\ell}$ from the numbers of electrons $Z_{n\ell}$ in the individual shells necessarily become more prominent when all oscillator strengths of the atom are summed.

We give the oscillator sums $f_{n\ell}/Z_{n\ell}$ for the individual $(n\ell)$-shell of various atoms[**)] in table 2 to establish a criterion for the order of magnitude of the expected effects. They are greatest (up to 1.7) for outer shells of high azimuthal quantum numbers, since the transition probabilities in the hydrogen atom are greatest for transitions from $(n-1,\ \ell = n-2)$ to $(n,\ \ell = n-1)$ and because the oscillator sum $f_{n,\, n-1}$ increases by the oscillator strength of this transition when it is forbidden. On the other hand, outer (ns)-shells have oscillator sums that are not appreciably greater than 1, because the transition probabilities $n-1,\ 1 \rightarrow n,\ 0$ are very small, as is generally true of the probabilities of all transitions in which the principal and secondary quantum numbers vary inversely with respect to one another. Oscillator sums for inner shells in heavy atoms decrease to approximately 0.3 to 0.4 per

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[*)] I was reading the proofs of the present paper when I learned that this law had already been discovered by R. de L. Kronig and H. A. Kramers [19]. This law has also been confirmed experimentally: Dispersion and absorption measurements in the x-ray region show the sum of the oscillator strengths of the K-series to be considerably smaller than 2 (see the literature cited in [19]).

[**)] The number of forbidden transitions increases with the atomic number, and the oscillator sums change accordingly. In computing the oscillator strengths (61), we introduced hydrogen eigenfunctions for the $\psi_{n\ell m}$; the transition probabilities were taken from the numerical tables of Kupper [20].

electron,*) then a K-electron, for example, may be raised practically only to a state of the continuous spectrum and not to one of the discrete spectrum; thus, practically the only remaining oscillator strengths are those of the transitions to the continuous spectrum.

Table 2

Oscillator sums for several levels in various atoms

	Be	B	C	N	O	F	Ne	Na	Mg
$1s$ . . .	1,000	,931	,861	,792	,723	,653	,584	,584	,584
$2s$ . . .	1,000	1,000	1	1	1	1	1,	1,	1
$2p$ . . .	—	1,136	1,136	1,136	1,136	1,136	1,136	1,120	1,122
$3s$ . . .	—	—	—	—	—	—	—	1,040	1,040

	Ne	Ar	Cu	Kr	Ag	Xe	Au	Em
$1s$	.584	,505	,505	,476	,476	,463	,463	,455
$2s$	1,000	,565	,565	,462	,462	,420	,420	,398
$2p$	1,136	1,122	,426	,423	,301	,300	,256	,256
$3s$	—	1,040	1,040	,566	,566	,446	,446	,394
$3p$	—	1,171	1,171	1,138	,533	,526	,387	,387
$3d$	—	—	1,418	1,407	1,407	1,405	,408	,408
$4s$	—	—	—	1,103	1,103	,560	,422	,422
$4p$	—	—	—	1,220	1,220	1,070	,450	,450
$4d$	—	—	—	—	1,437	1,464	1,464	1,456
$4f$	—	—	—	—	—	—	1,712	1,712

12. Deceleration

We compute the total energy transferred from the particle flux to the atom per unit time

$$E = \frac{8\pi\alpha^2}{K^2}\left(\frac{M}{m}z\right)^2 \sum_k (E_k - E_0) \int_{q_{\min}}^{q_{\max}} \frac{dq}{q^3} \, |\varepsilon_{0k}(q)|^2 \qquad (63)$$

in a manner quite similar to that used in section 10 for the hydrogen atom: We divide the integration region $q_{\min}$ to $q_{\max}$ by a point of intersection into two parts; in the first part ($q_{\min}$ to the point of intersection) we first integrate over q for each transition separately and only then sum over all possible transitions k. Starting from the point of intersection, we use the partial f-sum rule of the preceding section to combine all those transitions in which an electron of the ($n\ell$)-shell is excited, and only then integrate over q. We do not choose the point

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*) If we do not introduce hydrogen eigenfunctions but consider the screening, the forbidden transitions become weaker and all oscillator sums approach unity (cf. [19]).

of intersection itself for all transitions of the atom equal to (q_0) as in section 10, but only for those transitions in which an ($n\ell$)-electron is excited ($q_{n\ell}$); the $q_{n\ell}$'s may be different for various $n\ell$-shells. We determine each point of intersection $q_{n\ell}$ such that practically all excitations of the ($n\ell$)-electron are possible, from the standpoint of energy, for all $q > q_{n\ell}$; thus,

$$q_{nl} \gg \frac{\alpha^2_{nl} M}{2Km},$$

where

$$\alpha^2_{nl} = -\frac{8\pi^2 m}{h^2} E_{nl}$$

and $-E_{n\ell}$ is the ionization potential of the $n\ell$-shell.*) On the other hand, the transition probabilities for all $q < q_{n\ell}$ should be indicated by their value at $q = 0$, viz., by the elements of the coordinate matrix, i. e., $q_{n\ell} \ll \alpha_{n\ell}$ (cf. the corresponding choice of the point of intersection q_0 for the hydrogen atom). Then (cf. (55b), (55c)) in view of (61a) and (62), we will have

$$\left\{\begin{aligned}
E = {} & \frac{8\pi R h}{K^2}\left(\frac{M}{m} z\right)^2 \sum_{nl} \left(\sum_{n'l'} f_{nl,\,n'l'}(0) \cdot \ln \frac{2 q_{nl} K m}{(\alpha^2_{nl} - \alpha^2_{n'l'}) M} \right. \\
& \left. \qquad + \int_{q_{nl}}^{q_{\max}} f_{nl}(q) \frac{dq}{q} \right) \\
= {} & \frac{8\pi R h}{K^2}\left(\frac{M}{m} z\right)^2 \sum_{nl} \left(f_{nl}(0) \ln \frac{2 q_{nl} K m}{\alpha^2_{nl} \cdot M} \right. \\
& \qquad + \sum_{n'l'} f_{nl,\,n'l'}(0) \ln \frac{-E_{nl}}{E_{n'l'} - E_{nl}} \\
& + Z_{nl} \ln \frac{2Km}{q_{nl}(M+m)} - \sum_{n''l''} \int_{q_{nl}}^{q_{\max}} f_{nl,\,n''l''}(q) \frac{dq}{q} \\
& \left. \qquad \cdot \frac{\overrightarrow{Z}_{nl} \overrightarrow{Z}_{n''l''} + \overleftarrow{Z}_{nl} \overleftarrow{Z}_{n''l''}}{g_{n''l''}} \right).
\end{aligned}\right. \tag{63a}$$

Here, due to definition (61a) of $f_{n\ell,\, n'\ell'}$, the sum over $n'\ell'$ applies to all vacant electron states, while the sum over $n''\ell''$ applies to the occupied states. Since, according to (61),

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*) $\alpha_{n\ell}$ is of the type of reciprocal lengths α_n in section 4 that relate to the state of the atom (electron), not of the type of the $\alpha_{0n'}$s in section 4 that relate to transitions.

of intersection itself for all transitions of the atom equal to (q_0) as in section 10, but only for those transitions in which an ($n\ell$)-electron is excited ($q_{n\ell}$); the $q_{n\ell}$'s may be different for various $n\ell$-shells. We determine each point of intersection $q_{n\ell}$ such that practically all excitations of the ($n\ell$)-electron are possible, from the standpoint of energy, for all $q > q_{n\ell}$; thus,

$$q_{nl} \gg \frac{a^2_{nl} M}{2Km},$$

where

$$a^2_{nl} = -\frac{8\pi^2 m}{h^2} E_{nl}$$

and $-E_{n\ell}$ is the ionization potential of the $n\ell$-shell.*) On the other hand, the transition probabilities for all $q < q_{n\ell}$ should be indicated by their value at $q = 0$, viz., by the elements of the coordinate matrix, i.e., $q_{n\ell} \ll a_{n\ell}$ (cf. the corresponding choice of the point of intersection q_0 for the hydrogen atom). Then (cf. (55b), (55c)) in view of (61a) and (62), we will have

$$\left\{\begin{aligned} E &= \frac{8\pi Rh}{K^2}\left(\frac{M}{m}z\right)^2 \sum_{nl} \left(\sum_{n'l'} f_{nl,n'l'}(0) \cdot \ln \frac{2 q_{nl} K m}{(a^2_{nl} - a^2_{n'l'}) M} \right. \\ &\qquad\qquad \left. + \int\limits_{q_{nl}}^{q_{\max}} f_{nl}(q) \frac{dq}{q} \right) \\ &= \frac{8\pi Rh}{K^2}\left(\frac{M}{m}z\right)^2 \sum_{nl} \left(f_{nl}(0) \ln \frac{2 q_{nl} K m}{a^2_{nl} \cdot M} \right. \\ &\qquad\qquad + \sum_{n'l'} f_{nl,n'l'}(0) \ln \frac{-E_{nl}}{E_{n'l'} - E_{nl}} \\ &\quad + Z_{nl} \ln \frac{2Km}{q_{nl}(M+m)} - \sum_{n''l''} \int\limits_{q_{nl}}^{q_{\max}} f_{nl,n''l''}(q) \frac{dq}{q} \\ &\qquad\qquad \left. \cdot \frac{\vec{Z}_{nl}\vec{Z}_{n''l''} + \overleftarrow{Z}_{nl}\overleftarrow{Z}_{n''l''}}{g_{n''l''}} \right). \end{aligned}\right. \tag{63a}$$

Here, due to definition (61a) of $f_{n\ell,\, n'\ell'}$, the sum over $n'\ell'$ applies to all vacant electron states, while the sum over $n''\ell''$ applies to the occupied states. Since, according to (61),

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*) $a_{n\ell}$ is of the type of reciprocal lengths a_n in section 4 that relate to the state of the atom (electron), not of the type of the a_{0n}'s in section 4 that relate to transitions.

$$g_{nl} f^1_{nl,\,n''l''} = - g_{n''l''} f^1_{n''l'',\,nl}, \tag{63b}$$

by combining two terms each in the sum over $n''\ell''$ which correspond to the transition $n\ell \rightarrow n''\ell''$ and to the inverse transition, we get

$$\left\{\begin{aligned} & - \int\limits_{q_{nl}}^{q_{\max}} \frac{f^1_{nl,\,n''l''}(q)}{g_{n''l''}} \frac{dq}{q} - \int\limits_{q_{n''l''}}^{q_{\max}} \frac{f^1_{n''l'',\,nl}(q)}{g_{nl}} \frac{dq}{q} \\ & \qquad\qquad\qquad\qquad = \int\limits_{q_{n''l''}}^{q_{nl}} \frac{f^1_{nl,\,n''l''}(q)}{g_{n''l''}} \frac{dq}{q} \\ & \approx \int\limits_{q_{n''l''}}^{q_{nl}} \frac{f^1_{nl,\,n''l''}(0)}{g_{n''l''}} \frac{dq}{q} = - \frac{f^1_{nl,\,n''l''}(0)}{g_{n''l''}} \ln \frac{2Km}{q_{nl}(M+m)} \\ & \qquad\qquad - \frac{f^1_{n''l'',\,nl}(0)}{g_{nl}} \ln \frac{2Km}{q_{n''l''}(M+m)}. \end{aligned}\right. \tag{63c}$$

(The substitution of $f^1_{n\ell,\,n''\ell''}(0)$ for $f^1_{n\ell,\,n''\ell''}(q)$ is permissible for $q < q_{n\ell}$ or $q_{n''\ell''}$ because the points of intersection $q_{n\ell}$ are chosen such that the generalized oscillator strengths there do not yet deviate essentially from their value at $q = 0$ (i.e., from the oscillator strengths defined in the usual manner)). Therefore, in view of (62)

$$\left\{\begin{aligned} & E = \frac{8\pi Rh}{K^2} \left(\frac{M}{m} z\right)^2 \sum_{nl} f_{nl} \\ & \cdot \left(\ln \frac{4K}{\alpha^2_{nl}} \frac{m^2}{M(M+m)} + \frac{1}{f_{nl}} \sum_{n'l'} \zeta f^1_{nl,\,n'l'} \ln \frac{-E_{nl}}{E_{n'l'} - E_{nl}}\right), \end{aligned}\right. \tag{63d}$$

where the oscillator strengths $f^1_{n\ell,\,n'\ell'}$ and the partial oscillator sums $f_{n\ell}$ mean the values of these quantities at $q = 0$. In order to write (63d) more conveniently, we define the mean excitation energy of the $(n\ell)$-shell:

$$\left\{\begin{aligned} & f_{nl} \ln A_{nl} = f_{nl} \ln(-E_{nl}) \\ & + \sum_{n'l'} f^1_{nl,\,n'l'} \left(Z_{nl} - \frac{\overleftarrow{Z}_{nl}\overleftarrow{Z}_{n'l'} + \overrightarrow{Z}_{nl}\overrightarrow{Z}_{n'l'}}{g_{n'l'}}\right) \cdot \ln \frac{E_{n'l'} - E_{nl}}{-E_{nl}}. \end{aligned}\right. \tag{64}$$

For an outer shell, the mean excitation energy is generally somewhat lower than the ionization potential $-E_{n\ell}$ of the shell. The transitions to the next higher discrete levels (especially to $n' = n + 1$, $\ell' = \ell + 1$) have the highest oscillator strengths $f^1_{n\ell,\,n'\ell'}$; however, for these transitions $E_{n'\ell'} < 0$, i.e., $\ln \frac{E_{n'\ell'} - E_{n\ell}}{-E_{n\ell}} < 0$, therefore, if the level $n'\ell'$ is vacant, these transitions yield a large negative contribution to the sum in (64), in comparison to which the positive contribution of the transitions to the continuous spectrum is negligible.*) In any case, the mean excitation energy is greater (even for outer shells) than the energy for the initial excitation (excitation of the "resonance line"), as may easily be seen from (64). We may safely assume that the mean excitation energy is greater than that of the excitation potential of the resonance line by a factor of 1.2 to 1.5; at any rate, rough computations using hydrogen eigenfunctions give this result.**)

For inner shells, ionization is practically the only effect possible; the mean excitation energy is approximately 30 to 60% higher than the ionization potential.

If we use the mean excitation energy, (63d) becomes

$$E = \frac{4\pi e^4 z^2}{m v^2} \sum_{nl} f_{nl} \ln \frac{(2)\, m v^2}{A_{nl}}. \qquad (65)$$

The 2 in parentheses in the logarithm stands for the case of collision of heavy particles only (see (55)) and does not apply to electron collision.

Hence, the total energy loss of the particle per centimeter path

$$-\frac{dT}{dx} = N E = \frac{4\pi e^4 z^2 N}{m v^2} \sum_{nl} f_{nl} \ln \frac{(2)\, m v^2}{A_{nl}} \qquad (66)$$

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*) The case where 1s is the outermost shell (H, He) is an exception. Here, the excitation energy for discrete transitions differs very little from the ionization potential (by 25% at most), while it lies considerably above the ionization potential, on the average, for the high energy transitions into the continuous spectrum; therefore, the continuous transitions here yield the greater contribution to the sum in (64) and the mean excitation energy becomes somewhat greater (10%) than the ionization potential (cf. section 10, formula (55)).

**) The stopping cross section is not sensitive to errors in the mean excitation energy.

is composed of the energy losses to individual shells. The energy loss to each shell is not proportional to the number of electrons in the shell, but rather to the oscillator sum $f_{n\ell}$ which differs somewhat from it (cf. table 2); in addition, the stopping cross section (energy loss) for every shell contains a logarithmic term, as in classical theories. Both the logarithmic term and the replacement of the number of electrons $Z_{n\ell}$ by the oscillator sum $f_{n\ell}$ cause the outer shells to have a greater stopping cross section than the inner ones; however, the stopping cross sections of the outer and inner shells relative to the fast particles do not differ by orders of magnitude, but at most by a factor of about 5.

13. Comparison of the Stopping Cross Section with Earlier Theories and with Observation

Our formula for the stopping cross section

$$-\frac{dT}{dx} = -M_1 v \frac{dv}{dx} = \frac{4\pi e^4 z^2 N}{m v^2} \sum_{nl} f_{nl} \ln \frac{2 m v^2}{A_{nl}} \tag{66a}$$

is most like that of Henderson [8]. This is quite natural, since Henderson's theory goes beyond all previous ones in the use of quantum-theoretical propositions. Equation (66) differs from Henderson's formula chiefly by a factor of 2; this factor makes our formula agree well with observation, since Fowler [9] has shown that the stopping cross section computed according to Henderson turns out to be about 50% too low (cf. below). Henderson's idea is to compute the transfer of energy from the particle to an electron of the atom by classical means but to regard only collisions with a transfer of energy greater than the ionization potential as admissible by quantum theory; this idea has a basis in fact. According to wave mechanics, the f-sum rule for the transfer of energy to an $(n\ell)$-electron in collisions in which the particle momentum changes by $M(\mathfrak{v} - \mathfrak{v}')$ between $\frac{h}{2\pi}q$ and $\frac{h}{2\pi}(q + dq)$ gives us*)

$$E(q) = \frac{4\pi e^4 z^2}{m v^2} \frac{dq}{q} \cdot \frac{f_{nl}(q)}{Z_{nl}}. \tag{67}$$

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*) Provided that q is large enough to permit all transitions of the $(n\ell)$-electron.

Moreover, classically each of these collisions involves an energy loss*)

$$\begin{cases} Q = \frac{M_1}{2}(v^2 - v'^2) = \frac{m\,M_1^2}{2\,(m+M_1)^2}\,|v - v'|^2 \\ \quad = \frac{m\,M_1^2}{M^2\,(m+M_1)^2}\,\frac{h^2}{8\pi^2}\,q^2 = \mathrm{const}\cdot q^2 \end{cases} \tag{67a}$$

and, except for the replacement of the oscillator sums $f_{n\ell}$ by the electron numbers $Z_{n\ell}$, we get the <u>same</u> formula classically as we do wave mechanically (cf. [9, p. 526]) for the energy loss during these collisions. W(Q) is the probability of the collisions.

$$E(Q) = Q \cdot W(Q) = \frac{2\pi e^4 z^2}{m\,v^2}\,\frac{dQ}{Q}. \tag{67b}$$

Computing the smallest "classically transferable energy" from the minimum change of momentum permitted by quantum mechanics,

$$q_{\min} \approx \frac{Ma^2_{n\ell}}{2mK}$$

(cf. (17)), we obtain

$$Q_{\min} \approx \frac{m}{M^2}\,\frac{h^2}{8\pi^2}\,q^2_{\min} = \frac{m}{4M}\cdot\frac{E^2_{nl}}{T_r}, \tag{67c}$$

Thus, contrary to Henderson's hypothesis, the minimum transferable energy is very much lower than the ionization potential, consequently our stopping cross section is twice as large as Henderson's.**)

Curiously, Gaunt [10] obtains a result completely different from ours. Treating the colliding particle as a corpuscle and the atom wave mechanically, for hydrogen he again obtains Bohr's formula for deceleration

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*) Classically, the inelastic collisions are treated as elastic collisions between the particle and an atomic electron. Thus, from our formula (21) for the total energy lost by a particle during collision, only the first (classical) term appears on the right side; however, in this term we have to substitute m for M_2 (mass of the struck particle) and $M_1 m/m+M_1$ for M (effective mass of the colliding particle).

**) Besides, integration of the classical formula from our $Q_{\min}$ to $Q_{\max} = m/2\,v^2$ gives a correct result only for electrons. For α-particles, the the classical hypothesis of "collision with the atomic electron according to the momentum principle" is too crude for small deflections - in the logarithm one obtains one factor M/m too many.

$$-\frac{dT}{dx} = \frac{4\pi e^4 z^2 N}{m v^2} \ln \frac{m v^3}{0{,}08 \cdot 2\pi \cdot R \cdot e^2 z} \tag{68}$$

which, with respect to the argument in the logarithm, differs from our formula by the factor*)

$$\frac{1{,}12 \cdot h v}{2\pi e^2 z} \tag{68a}$$

Perhaps the reason is that Gaunt disregards the fate of the particle during the collision and thus includes collisions in which the energy balance is not fulfilled at all, i. e., in which the classically-treated particle loses less energy than is gained (quantum mechanically) by the atom. Furthermore, he complicates his calculation needlessly by mixing classical and quantum mechanical methods.

To compare our theory with experiment, like Fowler ([9]) we do not compute the total range, which would naturally be given by integral logarithm of the initial velocity of the particle, but rather the path length X needed to decelerate an α-particle of radium C' from the initial velocity v = 1. 922 x 10^9 cm $\sec^{-1}$ to 90% of this value. Then, in the logarithm on the right side of (66) we can replace v^2 by a mean value. We express $m/2\ v^2$ in electron volts - it is the energy of an electron having the same velocity as the α-particle. According to Fowler,

$$\frac{m}{2}\overline{v^2} = \overline{W} = 940 \text{ volts}$$

and we obtain

$$\frac{v_0^4 - v^4}{X} = \frac{16\pi e^4 z^2 N}{m M_1} \sum_{nl} f_{nl} \ln \frac{4\overline{W}}{A_{nl}} \tag{69}$$

and, by substituting constants (for 15°C),

$$\left\{\begin{aligned} B &= \sum_{nl} f_{nl} \cdot {}^{10}\log \frac{4W}{A_{nl}} = \\ &= \frac{0{,}4343 \cdot (1{,}922)^4 \cdot 10^{36} \cdot (1-0{,}9^4) \cdot 4 \cdot 1830 \cdot 0{,}81 \cdot 10^{-54} \cdot 2{,}24 \cdot 10^4 \cdot 288}{16 \cdot 3{,}14\,(4{,}77)^4 \cdot 10^{-40} \cdot 2^2 \cdot 6{,}1 \cdot 10^{23} \cdot 273 \cdot X} = \frac{45}{X}. \end{aligned}\right. \tag{69a}$$

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*) Although for normal α-particles (v = 1 to 2 x 10^9 cm $\sec^{-1}$) the factor is of the order of magnitude of 2 to 4 (i. e., since it is contained in the logarithm, it is of but little consequence), the form of the law is nevertheless considerably changed.

Table 3 gives the experimental and the theoretical values of the stopping cross section B for several elements.[*)] The oscillator sums $f_{n\ell}$ are taken from table 2, i.e., computed on the basis of hydrogen eigenfunctions; for the mean excitation potentials we substituted the resonance potential, increased by a factor of 1.5, in outer shells and the ionization potential, increased by a factor of 1.5, in inner shells; we used the values given by Fowler in [9] for both the excitation and the ionization potentials.

Table 3

Stopping Cross Sections

Z	Substance	$B_{\text{obs.}}$	$B_{\text{cal.}}$	Error %
1	½ H_2	2,67	2,42	− 9
2	He	5,03	4,24	− 15
7	½ N_2	—	13,4	—
7,2	½ Luft	12,0	13,8	+ 15
8	½ O_2	13,3	15,4	+ 15
10	Ne	—	18,4	—
13	Al	18,7	20,7	+ 11
18	A	24	27,1	+ 13
29	Cu	31,7	49,9	+ 57
79	Au	48,4	95,6	+ 97

For H_2, He, air, O_2, Al, and Ar, our formula is in very good agreement with experiment; in the case of heavier elements, it systematically yields excessive values for the stopping cross section. The partial oscillator sums for all transitions proceeding from one level would probably be considerably closer to 1 if, instead of the hydrogen eigenfunctions, we used eigenfunctions that are more suitable for computing oscillator strengths, e.g., Hartree's eigenfunctions. This would reduce the stopping cross section of the outer shells as well as the total stopping cross section. The error that may be caused by incorrect values for the mean excitation potential can be smaller. Errors

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[*)] Although the expression $\frac{v_0^4 - v^4}{X}$ is generally designated as the stopping cross section, it is cumbersome owing to its magnitude. Our stopping cross section differs from Fowler's S-value by a factor of $0.217 = \frac{1}{2} \times {}^{10}\log e$.

are more likely to arise from our use of formulas taken from Born's collision theory for the middle shells as well, although there our hypothesis (ionization potential small relative to $\frac{m}{2}v^2$) no longer holds. At any rate, it is gratifying that the agreement with observation is best in the case of light atoms, for which our hypotheses are most likely to be correct.

On the other hand, our formula does not offer a basis for deriving a general law of the dependence of the stopping cross section on the atomic number. We can only observe from the increasing number of sum terms in formula (66) that the stopping cross section grows with increasing atomic number, but not as rapidly as Z (since the individual terms (the logarithms) are very much smaller for inner than for outer shells, and since in more complex atoms it is mainly new <u>inner</u> shells that are added). A particularly large stopping cross section should be found in all atoms having many electrons in the outer shells, i.e., in noble gases (in agreement with observation) as well as in elements with closed 18-electron shells, e.g., Cu, Ag, and Au (contrary to observation).

The particle's energy loss per centimeter of path is less dependent on <u>velocity</u> for heavy decelerating atoms than for light atoms, for if we rewrite (66) as

$$-\frac{dT}{dx} = \frac{4\pi e^4 z^2}{m v^2} Z \ln \frac{2 m v^2}{E}, \tag{70}$$

the mean excitation energy of the atom E is defined by[*)]

$$Z \ln E = \sum_{nl} f_{nl} \ln A_{nl} \tag{70a}$$

and it increases with the number of inner shells having a high excitation potential. Hence, in heavy atoms the mean excitation energy E is more nearly equal to the energy $W = \frac{m}{2}v^2$, so that if the velocities

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[*)] On the right side, only the terms $A_{n\ell} < \frac{m}{2}v^2$ are to be computed; correspondingly, Z should be replaced by $\Sigma f_{n\ell}$ for all those $n\ell$-shells for which this inequality holds.

v are not excessively large, the logarithm in (70) becomes relatively small; the change of the logarithm with velocity, however, is always

$$\frac{d}{dv}\ln\frac{m v^2}{E} = \frac{2}{v}$$

i. e., independent of the decelerating atom, and thus the relative change is greater with heavy atoms than with light atoms. Therefore, owing to the factor $1/v^2$, the decrease of the stopping cross section at a reasonable particle velocity v is partially balanced by an increase in the logarithm. The increase is relatively larger in the case of deceleration by heavy atoms than by light atoms; therefore, in heavy atoms the resulting decrease in the stopping cross section with increasing velocity is smoother and the range of the particle varies with a lower power of the velocity than in the case of light atoms, as indicated by observation.*) For very large particle velocities (fast electrons), the change of the logarithm in (70) with velocity becomes insignificant, the energy loss becomes proportional to $1/v^2$, and the range proportional to v^4; this is the Thomson-Whiddington law [22, 23]. If we compute the constant of this law**)

$$\frac{\varrho Z}{A}\cdot b = \frac{v_0^4 - v^4}{x} = \frac{16\pi e^4 L}{m^2}\cdot\frac{\varrho Z}{A}\cdot\ln\frac{m v^2}{E} \tag{70b}$$

e. g., for the velocity 10^{10} cm $\sec^{-1}$ = 30, 000 volts, we obtain for air (mean excitation energy E = 35 volts) b = 14 x 10^{42} and for Cu (E ≈ 80 volts) b = 12.5 x 10^{42}, which in both cases is somewhat higher than the experimental results (10 to 11 x 10^{42}) [24, 25]. The constant b should increase slightly with increasing velocity (e. g., by 1 x 10^{42} if the kinetic energy of the electron is doubled), but the experiments do not allow a decision on this.

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*) Cf. [21]. The principle that the range is proportional to v^3 (i. e., that the stopping cross section is proportional to 1/v) is satisfied well in the case of air, but this must be considered a coincidence.

**) L is the Loschmidt number, ρ is the density, and A is the atomic weight of the decelerating substance.

14. Excitation of Optical Levels

According to (60), the differential effective cross section for the excitation of an electron to the $n'\ell'$-state is

$$d\Phi^{n\,l}_{n'l'}(q) = \frac{8\pi a^2}{q^3 K^2}\,dq\left(\frac{M}{m}z\right)^2\cdot\zeta\cdot|\varepsilon^1_{nl,\,n'l'}(q)|^2 \tag{71}$$

where $|\varepsilon^1_{n\ell,\,n'\ell'}(q)|^2$ is given by (60a) and ζ is defined in (62). The total probability (the integral excitation cross section) for this transition is obtained by integration over q. When $n'\ell'$ is a discrete atomic state, the region $q \gg a_{n\ell}$ is not involved because its matrix elements for discrete transitions almost disappear, owing to interference by the contributions of the individual volume elements to $\int \psi_{n\ell}\overline{\psi}_{n'\ell'}e^{iqx}d\tau$ (see sections 6 and 9); the factor $1/q^3$ is also in (71). Moreover, since

$$\left\{\begin{aligned} |\varepsilon^1_{nl,\,n'l'}(q)|^2 &= \frac{1}{g_{nl}}\sum_m \left|\int e^{iqx}\psi_{nlm}\bar{\psi}_{n'l'm}\,d\tau\right|^2 \\ &= \frac{q^2}{g_{nl}}\sum_m \left|\int \psi_{nlm}\bar{\psi}_{n'l'm}\,x\,d\tau\right|^2 = q^2\,|x_{nl,n'l'}|^2 \end{aligned}\right. \tag{71a}$$

is q^2-times the optical transition probability for $q \ll a_{n\ell}$, it follows by approximation that[*)]

$$\Phi^{n\,l}_{n'l'} \approx \frac{8\pi a^2}{K^2}\left(\frac{M}{m}z\right)^2\cdot\zeta\cdot|x_{nl,n'l'}|^2\int_{q_{\min}}^{a_{nl}}\frac{dq}{q}$$

$$\left\{\begin{aligned} \Phi^{n\,l}_{n'l'} &\approx \frac{8\pi Rh}{mv^2}z^2\,|x_{nl,n'l'}|^2 \\ &\qquad\left(Z_{nl} - \frac{\overrightarrow{Z_{nl}}\,\overrightarrow{Z_{n'l'}} + \overleftarrow{Z_{nl}}\,\overleftarrow{Z_{n'l'}}}{g_{n'l'}}\right)\ln\frac{2mv^2}{E_{n'l'} - E_{ln}} \end{aligned}\right. \tag{72}$$

i.e., the excitation cross section for a collision of fast electrons or α-particles is approximately proportional to the optical transition probability, and, furthermore, is inversely proportional to the square of the velocity of the electron and proportional to the logarithm of the quotient of the kinetic energy of the electron over the excitation potential. Hence, strong optical transitions are excited with particular intensity, especially the transition corresponding to the emission of the "resonance line" (cf., e.g., [26]).

[*)] That is, except for one factor of the order of 1.

Of course, excitation of transitions without an optical transition probability, i.e., without a dipole moment, is not entirely forbidden; for the excitation cross section of a transition with a quadrupole moment, we get, e.g.,

$$\sum_m \left| \int e^{iqx} \psi_{nlm} \bar{\psi}_{n'l'm} d\tau \right|^2 = \frac{q^4}{4} \sum_m \left| \int x^2 \psi_{nlm} \bar{\psi}_{n'l'm} d\tau \right|^2$$
$$= \frac{q^4}{4} \left| x^2_{nlm, n'l'm} \right|^2$$

for $q \ll a_{n\ell}$, while interference of the contributions of the individual volume components causes the integral on the left to approach zero again at large values of q. Thus, for such transitions

$$\left\{ \begin{aligned} \Phi^{nl}_{n'l'} &\approx \frac{2\pi a^2}{K^2} \left(\frac{M}{m} z \right)^2 \left| x^2_{nl, n'l'} \right|^3 \zeta \int_{q_{\min}}^{a_{nl}} q\, dq \\ &= \frac{2\pi R h z^2}{m v^2} \left| x^2_{nl, n'l'} \right|^2 a^2_{nl} \zeta \end{aligned} \right. \tag{72a}$$

i.e., the excitation cross section for transitions with a quadrupole moment differs from that of transitions with dipole moment because it lacks the logarithmic factor of the order of 10 and in general has a smaller numerical factor, in accordance with Elsasser's computations of the excitation of forbidden transitions (1, 0) → (n, 2) and (1, 0) → (n, 0) in hydrogen.

On the contrary, in our approximation it is not possible for two electrons to be excited simultaneously by the collision process, for we have assumed that the eigenfunctions of the atom are given as the sum of the products of the electron eigenfunctions orthogonal to one another, i.e., if j enumerates the electrons, the eigenfunction of the ground state must be

$$\Psi_0 = \sum_{(a)} c_{(a)} \prod_j \psi_{a_j}(r_j)$$

where ψ_a must be summed over all possible permutations (a), and where the eigenfunction of the excited state must be

$$\Psi_n = \sum_{(\beta)} c_{(\beta)} \prod_j \psi_{\beta_j}(r_j)$$

Then

$$\varepsilon_{0n}(q) = \int \Psi_0 \overline{\Psi}_n \sum_i e^{iqx_i} d\tau$$
$$- \sum_{(\alpha)} \sum_{(\beta)} \sum_l c_{(\alpha)} c_{(\beta)} \int \prod_j d\tau_j \psi_{\alpha_j}(r_j) \overline{\psi}_{\beta_j}(r_j) e^{iqx_l}$$

and all integrals on the right side in which we do not have

$$\alpha_j = \beta_j \text{ for all } j \neq \ell,$$

are zero, i.e., only one electron eigenfunction in the excited state may be changed relative to the ground state, unless all integrals are to vanish.

Furthermore, a transition to another term system of the atom cannot be excited by electron collision,*) because perturbation by the oncoming electron is definitely symmetrical in all atomic electrons. According to Wigner [28], a transition to another term system cannot be effected by such perturbations as long as spin is not explicitly included in the computation.

15. Excitation of X-Ray Levels

Now we sum (71) over all possible excitations of the $(n\ell)$-electron. Taking the completeness relation of the eigenfunctions $\psi_{n'\ell'm}$ into consideration, we have

$$\left\{\begin{aligned} g_{nl} \sum_{n'l'} |\varepsilon^1_{nl,n'l'}(q)|^2 &= \sum_m \sum_{n'l'} \left|\int \psi_{nlm} \overline{\psi}_{n'l'm} e^{iqx} d\tau\right|^2 \\ &= \sum_m \left(1 - \left|\int |\psi_{nlm}|^2 e^{iqx} d\tau\right|^2\right) \end{aligned}\right. \tag{73a}$$

$$\sum_{n'l'} |\varepsilon^1_{nl,n'l'}(q)|^2 = 1 - F_{nl}^2(q) \tag{73}$$

$$F_{nl}^2(q) = |\varepsilon^1_{nl,nl}(q)|^2 = \frac{1}{g_{nl}} \sum_m \left|\int |\psi_{nlm}|^2 e^{iqx} d\tau\right|^2 \tag{74}$$

Hence, $F_{n\ell}(q)$ is the "atomic form factor for an $n\ell$-electron." Except for constant factors, (73) gives the intensity of the incoherent x-ray scattering or of inelastic corpuscular-ray scattering for an atom containing only one $(n\ell)$-electron. However, owing to the Pauli exclusion

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*) This is in agreement with the observation of Dymond and Watson [27].

principle, several transitions whose matrix elements we included in (73) are forbidden: i. e., the incoherent scattering becomes relatively smaller than for an atom with one electron. From (71) we obtain directly[*)]

$$\left\{\begin{aligned} d\Phi^{nl}(q) &= \sum_{n'l'} d\Phi^{nl}_{n'l'}(q) = \frac{8\pi a^2}{K^2}\frac{dq}{q^3}\left(\frac{M}{m}z\right)^2 Z_{nl} \\ &\cdot\left(1 - F_{nl}{}^2(q) - \sum_{n'l'}\frac{\vec{Z}_{nl}\vec{Z}_{n'l'} + \overleftarrow{Z}_{nl}\overleftarrow{Z}_{n'l'}}{g_{n'l'}Z_{nl}}\left|\varepsilon^1{}_{nl,n'l'}(q)\right|^2\right) \end{aligned}\right. \tag{75}$$

or, when levels n''ℓ'' are all occupied,

$$\left\{\begin{aligned} d\Phi^{nl}(q) &= \frac{8\pi a^2}{K^2}\frac{dq}{q^3}\left(\frac{M}{m}z\right)^2 Z_{nl} \\ &\cdot\left(1 - F^2_{nl}(q) - \sum_{n''l''}\left|\varepsilon^1_{nl,n''l''}(q)\right|^2\right). \end{aligned}\right. \tag{75a}$$

The total effective cross section for the excitation of an electron (especially from an inner shell) is greatly reduced in the case of small scattering angles ϑ and collision vectors q by prohibition of transitions to occupied states, since precisely the strongest transitions are forbidden in those shells. However, in the case of large scattering angles ($q \gg a_{n\ell}$), the matrix elements for all discrete transitions approach zero (cf. section 6); i. e., both the atomic form factor $F_{n\ell}$ and the sum over the occupied states n''ℓ'' vanish, and the differential effective cross section becomes proportional to the number $Z_{n\ell}$ of electrons in the nℓ-shell. However, collisions at a large angle contribute only slightly to the value for the integral effective cross section; on the contrary, because of the factor $1/q^3$ in (75a), it is mainly determined by collisions with $q \ll a_{n\ell}$. Here, however, we again have (cf. (25), (38a), etc.)

$$\left|\int \psi_{nlm}\bar{\psi}_{n'l'm}e^{iqx}\,d\tau\right|^2 \approx q^2\left|\int x\,\psi_{nlm}\bar{\psi}_{n'l'm}\,d\tau\right|^2$$

$$\int|\psi_{nlm}|^2 e^{iqx}\,d\tau \approx 1 - \frac{q^2}{2}\int x^2|\psi_{nlm}|^2\,d\tau$$

hence,

$$\lim_{q=0}\frac{1}{q^2}\left(1 - F^2_{nl}(q) - \sum_{n''l''}\left|\varepsilon^1_{nl,n''l''}(q)\right|^2\right) = \overline{x^2_{nl}} - \sum_{n''l''}\left|x_{nl,n''l''}\right|^2 \tag{76}$$

with

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*) Naturally, assuming as always that practically all transitions from the nℓ-level are permitted, as far as energy is concerned.

$$\left\{\begin{aligned} \overline{x_{nl}^2} &= \frac{1}{2l+1}\int x^2 \sum_m |\psi_{nlm}|^2 d\tau \\ &= \frac{1}{2l+1}\int x^2 \psi_{nl}^2(r) \sum_m |P_l^m(\cos\vartheta)|^2 d\tau = \frac{1}{3}\int r^2 \psi_{nl}^2(r) r^2 dr \\ |x_{nl,n''l''}|^2 &= \frac{1}{2l+1} \sum_{m=-l}^{+l} \left|\int \psi_{nlm} \bar{\psi}_{n''l''m} x \, d\tau\right|^2. \end{aligned}\right. \tag{76a}$$

(The last transformation of the magnitude $\overline{x^2_{n\ell}}$ presupposes that the potential field of the atom, including the eigenfunctions $\psi_{n\ell m}$, is spherically symmetric.) Integration over q, carried out in the ordinary manner (cf. sections 9, 10, and 12), yields

$$\Phi^{nl} = \frac{4\pi a^2}{K^2}\left(\frac{M}{m}z\right)^2 Z_{nl}\left(\overline{x_{nl}^2} - \sum_{n''l''} |x_{nl,n''l''}|^2\right) \ln \frac{2mv^2}{B_{nl}} \tag{77}$$

where $B_{n\ell}$ is an energy of the order of magnitude of the ionization potential. Hence, the probability of the excitation of an ($n\ell$)-electron for outer shells is essentially proportional to the cross section of the electron shell (to the averaged square of the "distance" from the nucleus, $\overline{r^2_{n\ell}}$), but is considerably smaller for inner shells. However, the total energy transferred from the particle to the electrons of one shell is still not the same as given in sections 11 and 12. In the latter case, the outer shells benefited from the energy deficiency of the inner shells (the partial f-sums are less than 1 for inner shells and greater than 1 for outer shells). On the other hand, our excitation probability for outer shells (77) is also somewhat less (albeit only slightly) than if the inner shells were not occupied; the forbidden transitions are completely lost to the excitation probability.

If we compute the matrices $x_{n\ell,\, n''\ell''}$ introducing hydrogen eigenfunctions with a suitable effective nuclear charge Z_{eff}, we get (cf. ref. [1, section 10]):

$$\overline{x^2} = \frac{1}{2}\,\frac{n^2 a^2}{Z^2_{\text{eff}}}\left(\frac{5n^2+1}{3} - l(l+1)\right). \tag{77a}$$

That is, the approximate total excitation probability for an electron in an outer shell is roughly proportional to n^4. For inner shells in which the electrons are forbidden strong discrete transitions and essentially only the continuous transitions are still possible, we obtain

$$\overline{x^2_{nl}} - \sum_{n''l''} |x_{nl,n''l''}|^2 = \text{about } 0{,}2\text{—}0{,}6 \cdot \frac{n^2 a^2}{Z^2_{\text{eff}}}, \tag{77b}$$

where the proportionality factor depends on the number and kind of the forbidden transitions, on the azimuthal quantum number ℓ, and (only slightly) on the principal quantum number n. Since

$$\frac{RhZ^2_{\text{eff}}}{n^2}$$

is the ionization potential of the shell $-E_{n\ell}$, we can write, analogously to (53),

$$\Phi^{nl} = \frac{2\pi e^4 z^2}{m v^2 \cdot (-E_{nl})} \cdot Z_{nl} \cdot b_{nl} \cdot \ln \frac{2 m v^2}{B_{nl}}, \tag{78}$$

where, in very rough approximation, $b_{n\ell} = 0.2$ to 0.6 for inner shells and is of the order of n^2 for the outermost shells. Table 4 gives the excitation factors of several atoms; we used hydrogen eigenfunctions for the computation.

Table 4

Excitation factors $b_{n\ell}$

Shell	H	Be	N	Ne	A	Cu	Kr	Ag	Xe	Em
1*s*	1	1	0,72	0,44	0,35	0,35	0,32	0,32	0,30	0,29
2*s*	—	3,5	2,37	1,25	0,47	0,47	0,33	0,33	0,28	0,26
2*p*	—	—	1,70	1,70	1,68	0,43	0,43	0,27	0,27	0,21
3*s*	—	—	—	—	1,63	1,63	0,53	0,53	0,34	0,27
3*p*	—	—	—	—	4,55	2,05	1,98	0,56	0,55	0,33
3*d*	—	—	—	—	—	2,83	2,81	2,81	2,81	0,48
4*s*	—	—	—	—	—	—	2,12	2,12	0,61	0,36
4*p*	—	—	—	—	—	—	8,50	2,50	2,35	0,36
4*d*	—	—	—	—	—	—	—	6,40	6,32	3,16
4*f*	—	—	—	—	—	—	—	—	—	3,66

Equation (78) is quite critical for the intensity of the characteristic x-ray radiation emitted by the atom during bombardment with fast particles (in general, electrons), or - more exactly - for the total intensity of the lines of an x-ray series with an identical final level. The latter depend on how many electrons are removed from the inner shells of the atom; the number of these is given by (78). Hence, with high velocity bombarding electrons, the intensity of the characteristic x-ray radiation is inversely proportional to the square of this velocity and is inversely proportional to the ionization potential. It seems that the logarithmic term, which also appears, is in even poorer agreement with Wisshak's experiments (cf. [29, 30]) than is the classical Thomson formula which does not contain this term. The increase in x-ray intensity with excess of bombarding energy over the ionization potential should be even more abrupt than in Thomson's theory, while in experiment it is somewhat smoother. It must be borne in mind that our formula is not valid in Wisshak's region, which lies slightly above the ionization potential. Because of the excitation factors $b_{n\ell}$, the <u>absolute values</u> of the excitation function appear to be lower at a small ratio of the bombarding potential to the ionization potential than in Thomson's theorem; this agrees with Wisshak's experiments.

16. Angular Distribution of Elastic Collisions

The number of particles deflected at an angle by elastic collisions is

$$\left\{\begin{aligned} d\,\Phi_0(\vartheta) &= \frac{2\pi e^4 z^2}{16\,T_r^2}\sin\vartheta\, d\vartheta \cdot \frac{(Z-F(q))^2}{\sin^4\frac{\vartheta}{2}} \\ q &= \frac{4\pi}{\lambda}\sin\frac{\vartheta}{2} = \frac{4\pi M v}{h}\sin\frac{\vartheta}{2}\,. \end{aligned}\right. \tag{23}$$

For computing the atomic form factor F, Mott [3] and Mark and Wierl [31] used the Thomas-Fermi statistical distribution of electrons in an atom and found it to be in good agreement with their experiments [32]. In this paper, we want only to compare the angular distribution of the scattered particles for scattering on heavy and light atoms, assuming the Thomas-Fermi distribution to be valid.

The number of electrons at a distance between r and r + dr from the atomic nucleus which have the nuclear charge Z is, in Fermi's notation ([33]; cf. also [34]):

$$4\pi r^2\, dr \cdot \psi\bar{\psi}(r) = \frac{r\,dr}{e}\cdot\frac{d^2}{dr^2}(v\,r) = \frac{\gamma\mu}{e}\,x\,dx\cdot\frac{d^2\varphi(x)}{dx^2},$$

where v is the potential at point r, $x = r/\mu$, $\varphi = x\frac{v}{\gamma}$, $\gamma\mu = Ze$, $\mu = \mu_0 Z^{-\frac{1}{3}}$, $\mu_0 = \frac{3^{\frac{2}{3}}\pi^{\frac{2}{3}}}{2^{\frac{7}{3}}} \times a = 0.87a = 0.466 \times 10^{-8}$ cm, and $\varphi(x)$ is a function computed numerically by Fermi. The atomic form factor becomes

$$F(q) = 2\pi \int_0^\infty r^2\,dr \int_0^\pi \sin\vartheta\, d\vartheta\, e^{-iqr\cos\vartheta}\, \psi\bar{\psi}(r)$$

$$= 4\pi \int_0^\infty r^2\,dr\, \psi\bar{\psi} \cdot \frac{\sin qr}{qr} = Z \int_0^\infty \frac{\sin \mu q x}{\mu q}\, \frac{d^2\varphi}{dx^2} \cdot dx$$

$$= Z \int_0^\infty \left(-\frac{d\varphi}{dx}\right) \cdot \cos \mu_0 q Z^{-\frac{1}{3}} x\, dx .$$

$$F(q) = Z\,\mathfrak{F}'\left(4\pi \frac{\mu_0}{\lambda} \sin\frac{\vartheta}{2} Z^{-\frac{1}{3}}\right) = Z \cdot \mathfrak{F}\left(\frac{\sin\frac{\vartheta}{2}}{\lambda} Z^{-\frac{1}{3}}\right), \qquad (79)$$

where

$$\mathfrak{F}(\xi) = \mathfrak{F}'(5{,}85\,\xi) = \int_0^\infty \left(-\frac{d\varphi}{dx}\right) \cdot \cos 5{,}85\,\xi\, x \cdot dx \qquad (80)$$

and λ is in Ångstroms.

Hence, according to Thomas and Fermi, the atomic form factor per electron, F/Z, becomes a universal function ℨ of the argument

$$\frac{\sin\frac{\vartheta}{2}}{\lambda} \cdot Z^{-\frac{1}{3}}$$

and no longer depends separately on $\frac{\sin\frac{\vartheta}{2}}{\lambda}$ and the atomic number Z. The function ℨ is tabulated in table 5 (after Bragg [35]); it is monotonic decreasing with increasing argument. If argument ξ is small, ℨ behaves as 1-const $\times\ \xi^2$, as can easily be seen from partial integration of (80):

$$\left\{\begin{aligned} &\mathfrak{F}(\xi) = -\,|\,\varphi \cdot \cos 5{,}85\,\xi\, x \cdot |_0^\infty - 5{,}85\,\xi \int_0^\infty \varphi \sin 5{,}85\,\xi\, x \cdot dx \\ &\lim_{\xi=0} \mathfrak{F}(\xi) = 1 - (5{,}85\,\xi)^2 \int \varphi\, x\, dx = \text{etwa } 1 - 160\,\xi^2 . \end{aligned}\right. \qquad (80a)$$

The same $\frac{\sin\frac{\vartheta}{2}}{\lambda}$ has corresponding smaller values of argument ξ for heavy atoms than for light atoms, i.e., larger values of the atomic form factor per electron $\mathfrak{F}$. The decrease of the atomic form factor inversely with the scattering angle is steeper in light atoms than in heavy atoms.

Table 5

$\xi = \frac{\sin\frac{\vartheta}{2}}{\lambda} Z^{-\frac{1}{3}}$	atomic form factor $\mathfrak{F}(\xi)$	scattering intensity according to Fermi $\frac{1-\mathfrak{F}}{\xi^2}$	Wentzel $\frac{(2\pi r_0)^2}{1+(2\pi r_0 \xi)^2}$
0	1	160	80
0,02	0,947	133	77
0,04	0,853	92	71
0,06	0,758	67	62
0,08	0,677	50,5	53
0,10	0,610	39,—	44
0,12	0,550	31,5	37
0,15	0,485	22,9	28,5
0,20	0,395	15,1	18,5
0,25	0,322	10,9	13,3
0,30	0,277	8,0	9,8
0,40	0,207	5,0	5,8
0,50	0,156	3,4	3,8

The number of particles elastically scattered in the range of angles from ϑ to $\vartheta + d\vartheta$ now becomes

$$d\,\Phi_0(\vartheta) = \frac{2\pi e^4 z^2 Z^2}{16 T_r^2 \sin^4\frac{\vartheta}{2}} \left(1 - \mathfrak{F}\left(\frac{\sin\frac{\vartheta}{2}}{\lambda} Z^{-\frac{1}{3}}\right)\right)^2 \sin\vartheta\, d\vartheta. \qquad (81)$$

As shown in refs. [13], [17, p. 231], and [36], (81) becomes the simple Rutherford formula for large angles of deflection; a "screening factor" $(1 - \mathfrak{F})^2$ is also involved when the angles are small. Since ξ is smaller and $\mathfrak{F}(\xi)$ is larger for heavy atoms than for light atoms in the case of identical $\frac{\sin\frac{\vartheta}{2}}{\lambda}$ (in contrast to Rutherford), the scattering power of heavy atoms diminishes more sharply than that of light atoms:

The decrease of the scattering intensity with the scattering angle is less steep for all atoms than according to Rutherford's formula, and even more gradual for heavy atoms than for light ones.

This theorem has been verified quite satisfactorily by the experiments of Mark and Wierl ([31]).

In making a more detailed study of the dependence of the scattering intensity on the angle, we can also combine Rutherford's factor

$\sin^4 \frac{\vartheta}{2}$ with $(1 - F^2)$ to advantage:

$$\left\{ \begin{aligned} d\,\Phi_0(\vartheta) &= \frac{a^2 Z^{\frac{2}{3}}}{32\,\pi^3} \left(\frac{M}{m} z\right)^2 \left(\frac{1 - F(\xi)}{\xi^4}\right)^2 \sin\vartheta\, d\,\vartheta \\ &= 0{,}00356 \left(\frac{M}{m} z\right)^2 \cdot Z^{\frac{2}{3}} \cdot \left(\frac{1-F(\xi)}{\xi^2}\right)^2 \sin\vartheta\, d\,\vartheta, \end{aligned} \right. \tag{81a}$$

if the effective cross section $d\Phi_0(\vartheta)$ is measured in $(\mathrm{\AA})^2$. In the third column of table 1, $1 - F/\xi^2$ is given as a function of

$$\xi = \frac{\sin\frac{\vartheta}{2}}{\lambda} Z^{-\frac{1}{3}}$$

Thus, this function gives the universal pattern of the decrease of scattering intensity with the scattering angle for the scattering of corpuscular radiation. For very small scattering angles, i.e., when ξ is small, (80a) holds and we have, approximately,

$$d\,\Phi_0(\vartheta) = 0{,}6 \cdot \left(\frac{M}{m} z\right)^2 Z^{\frac{2}{3}} \sin\vartheta\, d\,\vartheta (\mathrm{\AA})^2, \tag{81b}$$

In other words, the scattering power for inelastic collisions then becomes independent of ϑ and proportional to $Z^{2/3}$ (rather than to Z^2 when the scattering angle is large).*)

Naturally, use of the Thomas-Fermi distribution for electrons in the atom gives better results for the scattering power than does the summing combination of all electrons in the K-shell (using Wentzel's method). Wentzel obtains

$$d\Phi_0(\vartheta) = \frac{2\,\pi\, e^4 z^2 Z^2 \sin\vartheta\, d\,\vartheta}{16\, T_r^2 \left(\sin^2\frac{\vartheta}{2} + \left(\frac{\lambda}{2\,\pi\, r}\right)^2\right)^2}, \tag{82}$$

where the "atomic radius" r must be determined arbitrarily by experimentation. Then if we set $r = r_0 Z^{-1/3}$, $(r_0 = \sim 1\ \mathrm{\AA})$, we obtain

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*) However, this requires that $\frac{\sin\frac{\vartheta}{2}}{\lambda}$ be smaller than $0.01\ Z^{\frac{1}{3}}$, i.e., the observation must be made closer to the primary beam than the first point of interference in most metals (e.g., in Au, $\frac{\sin\frac{\vartheta}{2}}{\lambda} = 0.037\ Z^{\frac{1}{3}}$). Hence, no observation is possible.

$$d\,\Phi_0(\vartheta) = 0{,}00356\left(\frac{M}{m}z\right)^2 \cdot Z^{\frac{2}{3}} \cdot \frac{(2\pi r_0)^2}{1+(2\pi r_0\,\xi)^2}\sin\vartheta\,d\,\vartheta. \qquad (82a)$$

The function $\dfrac{(2\pi r_0)^2}{1+(2\pi r_0 \xi)^2}$, which replaces Thomas and Fermi's $1-F/\xi^2$, is given in table 3, column 4 for the arbitrary value $(2\pi r_0)^2 = 80$ Å^2; with the exception of small scattering angles, it agrees to some extent with the Thomas-Fermi function. Next, the more precise expression "the effective atomic radius is proportional to $1/\sqrt[3]{Z}$" from Fermi's theory is introduced into Wenzel's formula, since Wentzel's formula alone tells us nothing about r or about the variation of the decrease of the scattering intensity with the angle in light and heavy atoms.*)

17. Angular Distribution of Inelastic Scattering

We compute the total number of inelastically scattered particles that experience a change of momentum, of an amount between q and q + dq, due to scattering by summing the number of scatterings in the individual ($n\ell$)-shells (eq. (75)):

$$\left\{\begin{aligned} d\,\Phi(q) &= \sum_{nl}\sum_{n'l'} d\,\Phi^{nl}_{n'l'}(q) \\ &= \frac{8\pi a^2}{K^2}\,\frac{d\,q}{q^3}\left(\frac{M}{m}z\right)^2 \sum_{nl}\sum_{n'l'} |\varepsilon_{nl,n'l'}(q)|^2 \\ &= \frac{8\pi a^2}{K^2}\,\frac{d\,q}{q}\left(\frac{M}{m}z\right)^2 \Big(Z - \sum_{n} Z_{nl} F^2_{nl} \\ &\quad - \sum_{nl}\sum_{n'l'} \frac{\overrightarrow{Z}_{nl}\,\overrightarrow{Z}_{n'l'} + \overleftarrow{Z}_{nl}\,\overleftarrow{Z}_{n'l'}}{g_{nl}\,g_{n'l'}} \\ &\quad \cdot \sum_{m} \Big| \int \psi_{nlm}\,\bar{\psi}_{n'l'm}\,e^{iqx}\,d\tau \Big|^2 \Big). \end{aligned}\right. \qquad (83)$$

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*) We can say, however, that the effective atomic radius r cannot be either the radius of the K-shell or the effective radius critical for molecular distances (the former being proportional to Z^{-1}, the latter increasing with Z), but is approximately the radius of a sphere containing, e.g., half the total charge of the atomic electrons. This radius, however, can only be obtained from a statistical theory such as that of Thomas and Fermi. Wentzel's formula, on the other hand, is justified when the validity boundaries of Rutherford's formula are to be estimated; then, for r we have to set the radius of the K-shell $r = \frac{a}{Z}$, because with an increasing angle ϑ, the K-shell retains its scattering power longer than any other shell.

The expression in the parentheses, which is also critical for the intensity of the incoherent x-ray scattering, has already been derived in essence by Waller and Hartree [16], who employed the completeness relation for the eigenfunction of an atom, and the expression of the eigenfunction of the ground term of the atom, as the product of two determinants containing the eigenfunctions of the individual electrons. However, Waller and Hartree did not average the matrix elements over m (which must be done because of azimuthal degeneracy; they write

$$\left|\int \psi_{nlm}\bar{\psi}_{n'l'm}\,e^{iqx}\,d\tau\right|^2 \text{ instead of } \frac{1}{g_{nl}}\sum_{m=-l}^{+l}\left|\int \psi_{nlm}\bar{\psi}_{n'l'm}\,e^{iqx}\,d\tau\right|^2\Big),$$

but this is unnecessary for atoms with closed shells, which were investigated by Waller and Hartree in greater detail. For such atoms, from (83) we obtain

$$\left\{\begin{aligned} d\,\Phi(q) &= \frac{8\pi a^2}{K^2}\,\frac{dq}{q^3}\left(\frac{M}{m}z\right)^2\Big(Z-2\sum_{nl}(2l+1)F_{nl}^2(q) \\ &\quad -2\sum_{nl}\sum_{n'l'}\sum_{m}\left|\int \psi_{nlm}\bar{\psi}_{n'l'm}\,e^{iqx}\,d\tau\right|^2\Big), \end{aligned}\right. \tag{83a}$$

where the double sum must be taken over all the occupied shells $n\ell$ and $n'\ell'$ and where the possibility of two spin directions accounts for the factor 2. Formulas (83) and (83a) also indicate (see section 15) that the component of forbidden transitions must be subtracted from the inelastic scattering intensity $Z - \sum_{n\ell} Z_{n\ell} F^2_{n\ell}$ computed without considering Pauli's principle.

If the scattering angle is large, the matrix elements of the forbidden transitions and the atomic form factors $F_{n\ell}$ again approach zero and the scattering intensity becomes proportional to the number of electrons Z. Hence, we can state that at large angles every electron scatters classically, i.e., the energy momentum principle is satisfied for the colliding particle and the scattering electron (section 6) and the scattering cross section has the classical value for a scattering particle with the charge 1; the intensities of the scatterings of the various electrons are simply additive terms. At a large scattering angle (vanishing atomic form factor), the ratio of inelastic (83a) to elastic scattering (81) is $Z:Z^2$, as in classical theory. To be sure, we have not actually compared scattering at the same *angle*, but rather scattering with identical *momentum change* of the colliding particles; converting (as in section 7) to scattering at the same angle, in analogy to (42), we obtain for large ϑ

$$\frac{d\,\Phi\,(\vartheta)}{d\,\Phi_0\,(\vartheta)} = \frac{Z}{Z^2}\cdot\frac{4\cos\vartheta}{(1+\cos\vartheta)^2} \tag{84}$$

which differs little from $Z:Z^2$ (cf. the table for (42)). At a small scattering angle, we obtain the same result as for hydrogen: The inelastic scattering reaches a boundary value which exceeds the boundary value of the elastic scattering, e.g., in the ratio of kinetic energy of the colliding electrons to ionization potential of the atom. This agrees qualitatively with the experiments of Dymond [27] on inelastic electron scattering in He and with Arnot's experiments [37] on scattering in Hg: *Inelastic scattering predominates if the angle is small, especially if the energy of the colliding electrons is large and the ionization potential is small (Hg); elastic scattering predominates at a large scattering angle.* However, the inelastic scattering should be quantitatively more intensive relative to the elastic scattering than it is in the experiments, e.g., the ratio 2:4 is scarcely approached for He at large scattering angles. Of course, the electron velocities used may be too close to the ionization potential; it would be highly desirable to investigate the angular distribution of the inelastically scattered electrons at a high primary velocity.*)

18. Primary Ionization

We obtain the effective cross section for ionization in the ($n\ell$)-shell (i.e., the number of the atoms from which an ($n\ell$)-electron is removed by collision), by summing the transition probabilities (71)

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*) Dr. Kulenkampff of the Munich Institute of Technology has informed me that such experiments are currently in progress there.

over all states $n'\ell' = k$ of the continuous spectrum and integrating over q:

$$\Phi_i^{nl} = \frac{8\pi a^2}{K^2}\left(\frac{M}{m} z\right)^2 Z_{nl}\int_0^\infty dk \int_{q_{\min}}^{q_{\max}} \frac{dq}{q^3}\,|\varepsilon^1_{nl,k}(q)|^2, \tag{85}$$

$$|\varepsilon^1_{nl,k}(q)|^2 = \frac{1}{g_{nl}}\sum_m \left|\int \psi_{nlm}\bar{\psi}_{km}\, e^{iqx}\, d\tau\right|^2. \tag{85a}$$

For large q

$$\int dk\, |\varepsilon^1_{nl,k}(q)|^2 = \int |\psi_{nlm}|^2\, |e^{iqx}|^2\, d\tau = 1,$$

for the discrete transitions are then no longer substantial; hence, the integrand in (85) decreases with $1/q^3$. Integrating in the usual manner, we obtain approximately

$$\Phi_i^{nl} N = \frac{4\pi a^2}{K^2} N \left(\frac{M}{m} z\right)^2 Z_{nl}\int dk\, |x_{nl,k}|^2 \cdot \ln \frac{2mv^2}{C_{nl}}, \tag{85b}$$

for the number of primarily-formed (nℓ)-ions per centimeter path (cf. section 15); $x_{n\ell,k}$ is again the element of the coordinate matrix and $C_{n\ell}$ an energy of the order of magnitude of the ionization potential of the (nℓ)-subshell, or, to conclude from the corresponding formula (54b) for hydrogen, about one power of ten smaller. Conversion analogous to that from (77) to (78) yields

$$s_{nl} = N\Phi_i^{nl} = \frac{2\pi e^4 z^2 N}{mv^2} \cdot \frac{c_{nl} Z_{nl}}{-E_{nl}} \ln \frac{2mv^2}{C_{nl}}, \tag{86}$$

where

$$c_{nl} = \frac{Z^2_{\text{eff}}}{n^2 a^2}\int dk\, |x_{nl,k}|^2 \tag{86a}$$

is a constant (ionization factor), which is computed as approximately 0.05 to 0.3 by employing hydrogen eigenfunctions:

Subshell	1s	2s	2p	3s	3p	3d	4s	4p	4d	4f
	0,28	0,21	0,13	0,17	0,14	0,07	0,15	0,13	0,09	0,04

Subshells with a large azimuthal quantum number are more difficult to ionize than those with a small number (the extensively projecting electron of an s-shell offers, so to speak, a larger exposed surface);

in addition, the ionization probability is approximately inversely proportional to both the ionization potential and the square of the particle velocity further multiplied by a logarithmic factor. In the case of a high primary velocity, the classical formula of Thomson [18] gives instead

$$s_{nl} = \frac{2\pi N e^4 z^2}{m v^2} \frac{Z_{nl}}{-E_{nl}} \tag{87}$$

without the logarithmic factor (cf. end of section 15).

By summation over all nℓ-shells of the atom, we obtain

$$s_0 = \sum_{nl} s_{nl} = \frac{2\pi e^4 z^2 N}{m v^4} \sum_{nl} \frac{c_{nl} Z_{nl}}{-E_{nl}} \ln \frac{2 m v^2}{C_{nl}} . \tag{88}$$

from (86) for the total number of ions formed per centimeter of path. Because of the factor $\frac{1}{-E_{n\ell}}$, the probability of ionization in inner shells is one or more orders of magnitude smaller than that in outer shells, in contrast to the stopping cross section which is smaller for inner shells by a factor ≤ 5 (cf. section 12). Therefore, only the ionization of the outer shells need be considered on the whole.

When (66) is divided by (88), we obtain

$$E_0 = \frac{-\frac{dT}{dx}}{s_0} = \frac{2 \sum_{nl} f_{nl} \ln \frac{m v^2}{A_{nl}}}{\sum_{nl} \frac{c_{nl}}{-E_{nl}} Z_{nl} \ln \frac{2 m v^2}{C_{nl}}} . \tag{89}$$

for the energy consumed per primary ion. To a certain extent, the logarithms for kinetic energies of the primary electron, which are very large in comparison with the ionization potential of the innermost shell, become equal. Rough approximation independently of v yields

$$E_0 = 2 \frac{Z J_a}{Z_a c_a} , \tag{89a}$$

where Z_a, J_a, and c_a are the electron number, the ionization potential, and the ionization factor of the outermost shell, respectively.

This gives*)

$$2 \times \frac{7}{5 \times 0.13} \times 15 \approx 300 \text{ volts}$$

for N, while a more exact evaluation of (89) yields considerably less, viz., 81 volts at a primary energy of 30,000 volts. We cannot rely too heavily on this value either, since computation of the ionization factors by means of hydrogen eigenfunctions is very uncertain. It is certain, however, that the energy consumption per primary ion is a high multiple of the smallest ionization potential, as was also the case in hydrogen (a factor of 7; section 10).

The primary fault is that only a small part of the inelastic collisions leads to ionization; the larger part leads to excitation. What is more, a considerable portion of the energy supplied by the particle is consumed in excitation and ionization of inner shells, while the number of the primary ions must be furnished mainly by the ionization of the *outer* shells. Finally, about half of the energy is transformed into the kinetic energy of fast secondary electrons, i.e., electrons whose energy is large compared with the ionization potential.

The majority of all collision processes involving large momentum change of the colliding particle $q \gg a_{n\ell}$ leads to emission of secondary electrons with momentum q, i.e., with kinetic energies that are large relative to the ionization potential. Since we can set $Z_{n\ell} = f_{n\ell}$, the energy lost during such collisions is approximately

$$\begin{aligned} E' &= \frac{8\pi a^2}{K^2}\left(\frac{M}{m}z\right)^2 \sum_{nl} Z_{nl} \int_{a_{nl}}^{K\frac{m}{M+m}} \frac{dq}{q} \\ &= \frac{4\pi a^2}{K^2}\left(\frac{M}{m}z\right)^2 \sum_{nl} Z_{nl} \ln \frac{K^2 m^2}{a_{nl}^2 M^2}, \end{aligned}$$

i.e., about half the total transferred energy E.

However, although the *energy* converted into kinetic energy of fast secondary electrons constitutes a large part of the total energy

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*) The ionization potential and ionization factor of the L_2-subshell is assumed for all 5 L-electrons.

lost by the colliding particle, the fast electrons, judging by their number, make up but a small fraction of all secondary electrons. By far the greatest number of secondary electrons occurs in collisions in which the particle's momentum changes only slightly ($q \ll \alpha_{n\ell}$) (because of the factor $1/q^3$; see beginning of this section). In this case, however, the probability of formation of a secondary electron with the energy $\frac{h^2}{8\pi^2 m} k^2$ is given by the element of the coordinate matrix corresponding to the transition from one shell of the atom to the state k of the continuous spectrum; this is of considerable magnitude only for $k < \alpha_{n\ell}$ (cf. section 6), i.e., for secondary electrons whose energy is even smaller than the ionization potential.

The velocity distribution of the secondary electrons released from hydrogen molecules is calculated roughly for a primary velocity of approximately 10,000 volts ($\beta = 0.2$) and compared with Ishino's [38] data. In the computation it is assumed that the transition probabilities have the same form as in the case of the hydrogen atom and the only change required is that α^2 be replaced by $1.16\,\alpha^2$ in all formulas, because the energy 2.32 Rh = 2 x 1.16 Rh is required for removal of both the electrons of H_2. We obtain

Table 6

Velocity distribution of the secondary electrons of hydrogen

Retarding potential in volts	Number of secondary electrons which overcome the retarding potential		
	theor.	exper.	Thomson's theorem
0	100	100	100
10	25	20,6	61
20	17	12,7	44
40	11	7,74.	24
110	4,8	3,12	12,5
190	2,7	1,87	7,6
390	1.31	1,01	3,9
790	0,61	0,29	1,9
990	0,48	0,12	1,5
1190	0,42	0	1,2

Hence, the theoretically computed velocity distribution agrees quite well with experiment, in contrast to the distribution computed using Thomson's method; the remaining difference is caused by inclusion of the tertiary electrons (whose velocities are even somewhat smaller) in the experiments.

19. Secondary Ionization

It is well known that fast secondary electrons are themselves capable of repeated ionization. Likewise, an atom with an inner shell that has been excited primarily can be ionized by an Auger jump; in addition, it emits fast secondary electrons which in turn cause ionization. Collision of one internally excited atom with another might also cause ionization. For at least an estimate of the secondary ionization, let us make two assumptions:

1. Whenever the colliding primary particle, in an elementary process, transfers an energy of more than twice the smallest ionization potential to the atom, whether in the form of inner excitation or by transfer of relatively large kinetic energy to the secondary electron, this energy can be used for the secondary excitation or ionization of another atom.

2. The secondary processes should divide into excitations and ionizations in the same manner as the primary processes; on the average, the same energy should be consumed for each ionization as must be expended by the primary particle.

The latter assumption is supported by the fact that the energy loss per formed ion (89) does not depend essentially on the velocity of the colliding particle [39]. In any case, it is more satisfactory than the earlier classical assumption by Bohr, which had to assume a complete utilization of the energy of the secondary electrons for the ionization, in contrast to conditions in the primary ionization. However, it is doubtful whether our assumption No. 2 is even roughly valid for electrons with a kinetic energy about twice the ionization potential, especially since Born's method does not apply to that case. Although our assumptions are arbitrary, it seems that a better treatment of the very complex phenomenon of secondary ionization is not possible at present.

Hence, let κ be that fraction of the energy transferred from the primary particle, which according to our assumption No. 1 is available for secondary processes. It is composed of the energy converted into the kinetic energy of fast electrons (velocity greater than the smallest ionization potential) and used for the excitation of inner shells, minus twice the smallest ionization potential. However, we can omit this subtraction,[*)] since it is not important for either the ionization potential of inner shells or the kinetic energy of the fast electrons, and we get approximately

$$\varkappa = \frac{1}{2} + \frac{\sum' f_{nl} \ln \frac{m v^2}{A_{nl}}}{\sum f_{nl} \ln \frac{m v^2}{A_{nl}}}, \tag{90a}$$

where the primed sum is taken over the inner shells only and the unprimed sum over all shells. However, the energy consumed in the formation of one ion in the secondary processes must be of the same magnitude as in the primary processes; hence, the numerical ratio between the secondary and the primary ions must be κ:1. On the other hand, in the secondary processes, the fraction κ of the energy must be used again for excitations that can give rise to tertiary ionization, etc. Thus, the quotient of the total (primary, secondary, tertiary, etc. ionization) over the primary ionization becomes

$$\frac{s}{s_0} = 1 + \varkappa + \varkappa^2 + \ldots = \frac{1}{1-\varkappa} = \frac{2}{1 - \frac{\sum' f_{nl} \ln \frac{m v^2}{A_{nl}}}{\sum f_{nl} \ln \frac{m v^2}{A_{nl}}}}. \tag{90}$$

Hence, for atoms with no inner shells (H, He), the total ionization becomes approximately equal to twice the primary ionization; with N_2 we obtain [four inner electrons, $f_K \approx 2 \times 3/4 = 1.5$, four middle electrons (L_1, $f = 2$), for which one cannot avoid subtracting twice the smallest ionization potential mentioned in our assumption No. 2], at

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[*)] For compensation, we omit the electrons released from the outer shells through collisions with a momentum transfer $q < \alpha_{n\ell}$, with a kinetic energy greater than the simple ionization potential.

primary velocities of approximately 30, 000 volts ($\beta = 0.33$), $\kappa = 0.63$, $s/s_0 = 2.7$, while Wilson's counts yield 3 to 4. In the case of heavy elements with many inner electrons, the number of the secondary processes should be slightly larger. On the other hand, it should hardly depend on the primary velocity. For all the energy used per ion formed, we obtain from (89) and (90)

$$\bar{E} = \frac{-\frac{dT}{dx}}{s} = \frac{\sum'' f_{nl} \ln \frac{mv^2}{A_{nl}}}{\sum \frac{C_{nl}}{-E_{nl}} Z_{nl} \ln \frac{mv^2}{C_{nl}}}, \tag{91}$$

where the sum in the numerator (in practice also the sum in the denominator) is taken over the outer shells only. At a primary velocity of 30, 000 volts, for N_2

$$\bar{E} = \frac{85}{2.7} = 31.5 \text{ volts}$$

i. e., almost exactly the same as Eisl's experimental value (32 volts). Furthermore, $\bar{E}$, as in experiment, is almost completely independent of the primary velocity: at 10, 000 volts, $\bar{E} = 30$ volts. To be sure, the numerical agreement with experiment may be partly coincidental, since the more thoroughly substantiated stopping cross section (section 13) agrees less well, yet we can be well satisfied with the correlation.

20. Summary of the Results

1. The number of the inelastic collisions of a fast, charged particle with an atom is proportional to the intensity of the Compton effect for x-rays, which have the same wavelength and undergo the same deflection ϑ as the particle divided by the Rutherford factor $\sin^4 \frac{\vartheta}{2}$ (section 5).

2. In most inelastic collisions, the colliding particle is only slightly deflected: the sine of the mean deflection angle for inelastically scattered electrons is approximately equal to the root of the ionization potential divided by the kinetic energy of the electron (section 6)

$$\bar{q} \approx K \sin \bar{\vartheta} \approx \alpha_{nl}, \quad \sin \bar{\vartheta} \approx \frac{\alpha_{nl}}{K} = \sqrt{\frac{-E_{nl}}{\frac{1}{2} m v^2}}$$

3. In inelastic collisions with large deflection, the momentum principle for colliding particles and secondary electrons is nearly satisfied, in which case the nucleus of the atom is not involved (section 6).

4. In the case of large deflection angles, the number of the inelastic collisions is related to the number of the elastic collisions as $Z:Z^2$; if the deflection angles are small, the number of the inelastic collisions is larger than that of the elastic collisions by approximately the factor "kinetic energy of the particle divided by ionization potential of the atom" (sections 17 and 7).

5. The dependence of the number of the elastic collisions on the scattering angle can be represented by a universal function of $\frac{\sin\frac{\vartheta}{2}}{\lambda\sqrt[3]{Z}}$, using the Thomas-Fermi distribution for the electrons in the atom. The decrease of the collision count with increasing angle is more gradual for heavy atoms than for light atoms, in agreement with the experiments of Mark and Wierl; with a large scattering angle, the collision count is proportional to Z^2, and with a small angle, proportional to $Z^{2/3}$ (section 16).

6. The probability for the excitation of a certain transition of the atom due to collision of fast electrons is almost exactly proportional to the optical transition probability for this transition and inversely proportional to the kinetic energy of the electrons. Therefore, nearly all collisions cause excitation of the resonance line (sections 14, 5, and 9).

7. The probability of the excitation of an x-ray level (ionization of an atom in an inner shell) through collision of fast electrons is, in first approximation, inversely proportional to the ionization potential of the excited level and the kinetic energy of the electrons. Besides, a logarithmic term appears, which is not found in the classical theory (section 15).

8. The stopping cross section of an atom for α-particles and electrons is inversely proportional to the square of the velocity of the particle and proportional to a logarithmic term whose argument does not exactly agree with the one known from Bohr's theory (sections 12, 13, and 10).

9. The stopping cross section of an atom is composed additively of the stopping cross sections of the individual electron shells. The latter are proportional to the sum of the oscillator strengths of all transitions that can be made by the electrons of the shell rather than to the number of the electrons in each shell. The stopping cross section of an electron in an outer shell is greater than in an inner shell by a factor of 3 to 5 (section 12).

10. The stopping cross section for very fast electrons should be approximately proportional to Z; for slower electrons and for α-particles, it increases more slowly with Z. An explicit law cannot be given for this increase. The theoretical values for the stopping cross section seem to increase somewhat more rapidly with Z than do the experimental values. Theory and experiment are in agreement for the elements up to argon (section 13).

11. The stopping cross section of heavy atoms decreases more gradually with increasing velocity than that of light atoms; therefore, in a substance of high atomic weight, the range of a particle is proportional to a low power of the velocity, in agreement with observation. For very large velocities, the range is always proportional to v^4. The proportionality factor (the constant of the Thomson-Whiddington law) is slightly too high (section 13).

12. The number of primarily formed ions per centimeter of path formed by a fast particle is inversely proportional to the square of the velocity of the particle, inversely proportional to the ionization potential of the atoms, and proportional to a logarithmic term which is not found in the classical theory. In the argument of the

logarithm, the square of the particle velocity is divided by the smallest ionization potential of the atom (sections 18 and 19).

13. The ratio of the number of all the ions formed to the primary ions is, starting from a certain lower limit, almost independent of the velocity of the ionizing particle and increases from slightly more than 2:1 in hydrogen to approximately 3:1 in air and even more in heavy elements. In agreement with this, the experiments of Wilson give a ratio 3 to 4:1 for air (section 19).

14. The energy consumption for every primary ion in hydrogen, for very high velocities of the colliding particle, is greater by a factor of approximately 7 than the smallest ionization potential, and for heavier atoms the factor is even larger. For every ion formed (either primary or secondary), the energy consumption must be nearly independent of the velocity; for air, it is approximately 32 volts, in agreement with observation (sections 18, 19, and 10).

15. By far most of the secondary electrons have a kinetic energy of the order of magnitude of the simple ionization potential or even less. However, about half of the energy imparted by the colliding particle is converted into kinetic energy of fast secondary electrons (section 19).

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