Contribution to the Theory of the Compton-Line

F. BLOCH, Department of Physics, Stanford University (Received July 24, 1934)

Starting from Wentzel's theory of the Compton scattering of bound electrons, and assuming that the motion of the electrons in the atom can be described by hydrogenic eigenfunctions, general formulae are developed for the calculation of the intensity distribution in the Compton line. It is shown that the interaction of the electrons with the atomic nucleus gives not only a broadening of the Compton line but makes it also asymmetrical, shifting at the same time the position of the maximum intensity from Compton's value $\Delta \lambda = (h/m_0 c)(1 - \cos \theta)$. The "defect of the Compton shift" is shown to be quadratic in the wave-length of the incident radiation. This law as well as the value of the constant entering into it are found to agree satisfactorily with experiment.

1. INTRODUCTION

I N the original form of the theory of the Compton effect, as given by Compton¹ and Debye,² it is assumed that the southering electronic assumed that the scattering electrons can be considered as free and at rest before the scattering process. This assumption is justified if the energy of the electrons after having scattered is very large compared with their binding energy in the atom, and leads to the well-known formula for the increase in wave-length of the radiation, observed at an angle θ with respect to the primary radiation:

$$\Delta \lambda = (h/m_0 c)(1 - \cos \theta) \tag{1}$$

(h =quantum of action, $m_0 =$ mass of the electron, c = velocity of light). In this approximation, where the binding forces are neglected, one should expect that monochromatic primary radiation under every angle would give rise to a *sharp* Compton line,³ the position of which is given by formula (1). The more detailed analysis of the Compton line, however, as performed in recent years⁴ has shown a distinct broadening and shape for the Compton line. Moreover, the position of the maximum intensity of the line is not given by (1) but, according to the measurements of Ross and Kirkpatrick,⁵ by the corrected formula

$$\Delta \lambda = (h/m_0 c) (1 - \cos \theta) - D\lambda^2, \qquad (2)$$

D being a constant which depends on the scattering substance, and λ the wave-length of the primary radiation. For the wave-lengths and observation angles used the order of magnitude of the "defect of the Compton shift"

$$\delta \lambda = D \lambda^2 \tag{3}$$

is of the order of magnitude of 1 percent of the total shift $\Delta\lambda$.

It is clear that both the broadening of the line and the defect of the shift are due to the binding forces, acting on the scattering electrons. As DuMond⁶ showed, the broadening of the line can easily be understood by ascribing it to the Doppler effect, due to motion of the electrons in the atom and therefore proportional to their velocities. Indeed, the observation of the broadening of the Compton line may be said to give direct information about the velocity distribution of the electrons in the atom. Since the average speed of an electron is essentially proportional to the square root of its binding

¹ A. H. Compton, Phys. Rev. 21, 483 (1923).

² P. Debye, Phys. Zeits. 24, 161 (1923)

² P. Debye, Fnys. Zetts. 24, 101 (1925).
³ The very small broadening of the line, due to the reaction of the scattered radiation on the electron can here be entirely neglected. Compare I. Waller, Zeits. f. Physik 88, 436 (1934).
⁴ G. E. M. Jauncey, Phys. Rev. 25, 314 (1925); 31, 723 (1928); H. M. Sharp, ibid. 26, 691 (1925); Jesse W. M. DuMond, ibid. 33, 643 (1929); 36, 146 (1930); F. L. Nutting, ibid. 36, 1267 (1930).
⁵ See the preceding paper of P. A. Ross and Paul Kirkpatrick.
⁶ Jesse W. M. DuMond, Rev. Mod. Phys. 5, 1 (1933).

energy, the broadening of the Compton line is also proportional to this square root. It is obvious that the consideration of the Doppler effect can only explain a symmetrical broadening of the line around the position of its center of gravity as given by (1), since the average of the electronic velocities in the atom vanishes.

In order to get an explanation of the defect of the shift $\delta \lambda$, one has to go one step further. By a simple consideration, Ross and Kirkpatrick' obtained for the constant D in (2) and (3)

$$D = \kappa E/hc, \tag{4}$$

where E is the binding energy of the electron under consideration and κ a numerical constant of the order of magnitude 1, the exact value of which could not be obtained by their semiclassical method. Nevertheless, formulae (3) and (4) account for the observed order of magnitude of the defect $\delta \lambda$, and for its dependence on λ . Since the broadening of the line is essentially proportional to \sqrt{E} while $\delta\lambda$ is proportional to E, the latter may be said to be a higher order effect, provided the binding energy is considered small compared with the recoil energy of the electron after the scattering process.

A consistent wave-mechanical scheme of the Compton effect of bound electrons has been given by Wentzel.⁸ However, he worked out his formulae only for the case of a K-electron, as in the hydrogen atom, and furthermore restricted himself to an approximation which accounted for the broadening but not for the defect of the shift of the Compton line. In order to make possible a quantitative comparison between the theory and the measured data for Be and C⁵ we have generalized his results for the case of higher electronic orbits, assuming that the forces acting on each electron can be approximately described by a Coulomb field with properly chosen screening constant. The method represents a series-expansion in powers of the binding energy, which goes far enough to allow a calculation of the defect $\delta\lambda$; in this approximation the law (3) is verified and the constant D is determined in satisfactory agreement with experiment.

2. GENERAL FORMULAE FOR THE INTENSITY OF RADIATION, SCATTERED BY AN ELECTRON IN A COULOMB FIELD

We consider an electron with principal quantum number n and angular momentum $lh/2\pi$ before the scattering process in a Coulomb field with effective nuclear charge Ze; its binding energy is then given by

$$E = 2\pi^2 Z^2 e^4 m_0 / n^2 h^2. \tag{5}$$

We call the frequencies of the incident and scattered radiations ν and ν' , respectively, and the energy of the electron after the scattering process

$$W = h^2 k^2 / 8\pi^2 m_0 = h\nu - h\nu' - E.$$
(6)

It will be assumed that

$$h\nu \ll m_0 c^2, \tag{7}$$

so that all relativistic effects can be neglected; furthermore we assume

$$E \ll W. \tag{8}$$

We shall see later that, in order to account for the defect of the Compton shift, it is sufficient to consider in the expression for the scattered intensity only terms of the relative order of magnitude 1 and $(E/W)^{\frac{1}{2}}$. In this approximation, as in Wentzel's paper (G), we still need only to consider Dirac's "true scattering" processes.

Using formulae (10), (12), (12a) of G, and considering that the primary radiation is unpolarized,

⁷ P. A. Ross and Paul Kirkpatrick, Phys. Rev. **45**, 223 (1934). ⁸ G. Wentzel, Zeits. f. Physik **43**, 1, 779 (1927); Zeits. f. Physik **58**, 348 (1929). (We shall refer to this paper from now on as "G".)

F. BLOCH

we can write the intensity scattered by our electron at an angle θ with the direction of the incident radiation into a frequency range between ν' and $\nu' + d\nu'$ in the form

$$dI_{nla} = I_P \frac{2\pi^2 e^4}{m_0 c^4 r^2} \cdot \frac{1 + \cos^2 \theta}{hk} d\nu' \int_{-\infty}^{+\infty} |\epsilon_{nla, km}(\Delta k)|^2 dm,$$
(9)

where I_P is the intensity of the primary radiation, r the distance from the scattering atom, k the quantity defined by (6). $\epsilon_{nla, km}(\Delta k)$ is the matrix-element, associated with transitions of the electron from the initial state (n, l, a) to the final state (k, m). As in G, we use parabolic coordinates ξ, η, φ to describe the position of the electron; if \mathbf{v} and \mathbf{v}' are vectors with an absolute value equal to the frequencies and directed in the direction of propagation of the incident and scattered radiations, respectively, the azimuth φ of our parabolic system of coordinates is measured around an axis in the direction of the vector

$$\Delta \boldsymbol{k} = (2\pi/c)(\boldsymbol{v} - \boldsymbol{v}'). \tag{10}$$

The quantity a in (9) is the azimuthal quantum number of the initial state with respect to this axis, m is a parabolic quantum number, related to the direction of momentum of the recoil electron, Δk is the absolute value of the vector Δk , defined by (10). The matrix-element $\epsilon_{nla, km}(\Delta k)$ is then given by⁹

$$\epsilon_{nla, km}(\Delta k) = \frac{1}{4} \int_0^{2\pi} d\varphi \int_0^{\infty} d\xi \int_0^{\infty} d\eta (\xi + \eta) e^{i\Delta k(\xi - \eta)/2} \psi_{kma}(\xi \eta \varphi) \psi^*{}_{nla}(\xi \eta \varphi).$$
(11)

 $\psi^*{}_{nla}$ is the conjugate-complex of the normalized eigenfunction ψ_{nla} of the initial state, ψ_{kma} is the eigenfunction of the final state. We add here the azimuthal quantum number a to the two quantities (k, m), used before to describe the final state in order to remember that the component of the angular momentum in the direction of Δk remains unchanged during the scattering process, due to the fact that the perturbation function $e^{i\Delta k(\xi-\eta)/2}$ does not contain the azimuth φ . Writing

$$\psi_{kma}(\xi\eta\varphi) = u_{kma}(\xi\eta)e^{ia\varphi},\tag{12}$$

$$\psi^*{}_{nla}(\xi\eta\varphi) = u_{nla}(\xi\eta)e^{-ia\varphi},\tag{12a}$$

we can perform in (11) the integration over φ , finding

$$\epsilon_{nla, km}(\Delta k) = \frac{\pi}{2} \int_0^\infty d\xi \int_0^\infty d\eta (\xi + \eta) e^{i\Delta k(\xi - \eta)/2} u_{kma}(\xi\eta) u_{nla}(\xi\eta).$$
(11a)

According to (8) the final state (*kma*) has to be assumed to be in the continuous spectrum. Using the well-known methods developed by Schrödinger,¹⁰ the eigenfunction $u_{kma}(\xi\eta)$ can be represented as in G by complex integrals. We write

$$u_{kma}(\xi\eta) = C_{kma}(\xi\eta)^{a/2} (ik)^{-2a} f_{kma}(\xi) g_{kma}(\eta)$$
(13)

with

$$f_{kma}(\xi) = (1/2\pi i) \oint e^{t_1\xi} (t_1 + ik/2)^{(a-1)/2 + i(\beta+m)} (t_1 - ik/2)^{(a-1)/2 - i(\beta+m)} dt_1$$

$$g_{kma}(\eta) = (1/2\pi i) \oint e^{t_2\eta} (t_2 + ik/2)^{(a-1)/2 + i(\beta-m)} (t_2 - ik/2)^{(a-1)/2 - i(\beta-m)} dt_2$$
(14)

and

$$\beta = (1/2k)(4\pi^2 Z m_0 e^2/h^2). \tag{15}$$

⁹ Compare G, formulae (4) and (26).

¹⁰ E. Schrödinger, Ann. d. Physik 4, 361 (1926); 4, 437 (1926).

The same considerations which lead to formula (24) in G give the constant of normalization, entering into (13)

$$C_{kma} = \frac{1}{2}\pi^{-\frac{3}{2}}k^{a+1}e^{\pi\beta} |\Gamma\lfloor(1-a)/2 + i(\beta+m)\rfloor| |\Gamma\lfloor(1-a)/2 + i(\beta-m)\rfloor|.$$
(14a)

With this normalization and the condition, that

$$\frac{1}{4} \int_{0}^{2\pi} d\varphi \int^{\infty} d\xi \int_{0}^{\infty} d\eta (\xi + \eta) |\psi_{nla}(\xi \eta \varphi)|^{2} = 1$$
(16)

it can be shown, as in G, that under the assumption (8)

$$\int_{0}^{\infty} dk \int_{-\infty}^{+\infty} dm \left| \epsilon_{n l a, k m}(\Delta k) \right|^{2} = 1, \qquad (17)$$

which, using (6) and (9) gives for the total intensity scattered at the angle θ

$$I_{nla} = \int dI_{nla} = I_P (e^4 / 2m_0^2 c^4 r^2) (1 + \cos^2 \theta).$$
(18)

This is Thomson's formula for the scattering of free electrons. We shall see later, that in our approximation, although the spectral distribution is changed, the total intensity is still given by (18), since (17), in this approximation, remains valid.

In polar coordinates, $r\vartheta$, the function u_{nla} in (12a) is given by¹¹

$$u_{nla} = C_{nla} e^{-\alpha r/2} (\alpha r)^l P_l^a (\cos \vartheta) L_{l+n}^{2l+1} (\alpha r)$$
⁽¹⁹⁾

where the constant $C_{n la}$ has to be determined such that (16) is fulfilled and α is given by

$$\alpha = 8\pi^2 Z m_0 e^2 / nh^2. \tag{20}$$

In order to get a general expression for the quantity (11a) consider the expression

$$q_{la}(k, m, \Delta k, t) = \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{\epsilon_{nla, km}(\Delta k)}{C_{nla}(n+l)!} t^{n-l-1}.$$
(21)

Performing the summation under the integral in (11a) and using the formula¹²

$$\sum_{n=1}^{\infty} L_{n+l}^{2l+1}(\alpha r) \frac{t^{n-l-1}}{(n+l)!} = \frac{(-1)^{2l+1}}{(1-t)^{2l+2}} e^{-\alpha r t/(1-t)}$$

and (19), we find

$$q_{la}(k, m, \Delta k, t) = \frac{(-1)^{2l+1}}{(1-t)^{2l+2}} \int_0^\infty d\xi \int_0^\infty d\eta (\xi+\eta) e^{i\Delta k(\xi-\eta)/2} u_{kma}(\xi\eta) (\alpha r)^l P_l^a(\cos\vartheta) e^{-(\alpha r/2)(1-t)/(1+t)}.$$
 (22)

In order to express the variables r and ϑ , entering in (22), by means of the parabolic coordinates ξ and η , we use the expressions

$$r = \xi + \eta/2, \qquad \cos \vartheta = (\xi - \eta)/(\xi + \eta).$$
 (23)

Writing

$$P_{l^{a}}(\cos\vartheta) = (1 - \cos^{2}\vartheta)^{a/2} \sum_{p=0}^{l-a} c_{p} \cos^{p}\vartheta, \qquad (24)$$

¹¹ Cf. A. Sommerfeld, *Wave Mechanics*, page 60 ff. ¹² E. Schrödinger, Ann. d. Physik **4**, 437 (1926).

where the quantities c_p are certain numbers defining the spherical harmonics P_i^a , we find, using (13), (14), (22), (23) and (24)

After having performed the integrations over ξ and η , the remaining integrand in the integrals over t_1 and t_2 have simple poles for

$$t_1' = \frac{\alpha}{4} \frac{1+t}{1-t} - \mu_1 - \frac{i\Delta k}{2}$$
 and $t_2' = \frac{\alpha}{4} \frac{1+t}{1-t} - \mu_2 + \frac{i\Delta k}{2}$, respectively.

The application of the theorem of residues gives¹³

$$q_{la}(k, m, \Delta k, t) = (ik)^{-2a} \frac{\alpha^{l}}{2^{l-a}} C_{kma} \frac{(-1)^{2l+1}}{(1-t)^{2l+2}} \sum_{p=0}^{l-a} c_{p} \left(\frac{\partial}{\partial\mu_{1}} + \frac{\partial}{\partial\mu_{2}}\right)^{1+l-a-p} \left(\frac{\partial}{\partial\mu_{1}} - \frac{\partial}{\partial\mu_{2}}\right)^{p} \frac{\partial^{2a}}{\partial\mu_{1}^{a}\partial\mu_{2}^{a}} \\ \times \left(\frac{\alpha}{4} \frac{1+t}{1-t} - \mu_{1} - i\frac{\Delta k - k}{2}\right)^{(a-1)/2 + i(\beta+m)} \left(\frac{\alpha}{4} \frac{1+t}{1-t} - \mu_{1} - \frac{i(\Delta k + k)}{2}\right)^{(a-1)/2 - i(\beta+m)} \\ \times \left(\frac{\alpha}{4} \frac{1+t}{1-t} - \mu_{2} + i\frac{\Delta k + k}{2}\right)^{(a-1)/2 + i(\beta-m)} \left(\frac{\alpha}{4} \frac{1+t}{1-t} - \mu_{2} + i\frac{\Delta k - k}{2}\right)^{(a-1)/2 - i(\beta-m)}.$$
(26)

This expression can be simplified, if we restrict ourselves to the zero and first power terms in an expansion with respect to β , which according to (15), (5) and (6) is of the order of magnitude of $(E/W)^{\frac{1}{2}}$ and, accepting (8), can be considered as small compared with unity. Since we have to expect a considerable contribution to the scattered intensity only, if $\Delta k - k$ is of the order of magnitude of α , i.e. if the momentum transferred to the nucleus is of the order of magnitude of the momentum which the electron has in its initial orbit, we can write $\gamma = \alpha/2(\Delta k + k) \cong \alpha/2k$ or, according to (15) and (20)

$$\gamma = 2\beta/n. \tag{27}$$

In the expansion of (26) we can then neglect all terms which are quadratic or of higher order in β

¹³ Cf. the analogous considerations, which lead to formula (28) of G.

and γ . With

$$v = (2/\alpha)(\Delta k - k); \quad \tau_1 = -4\mu_1/\alpha; \quad \tau_2 = -4\mu_2/\alpha,$$
 (28)

and using (14a), we find in our approximation:

$$q_{la}(k, m, \Delta k, t) = 8\pi^{-\frac{3}{2}} (-2)^{l} \left(\frac{\alpha}{2}\right)^{-2+2mi} \frac{1}{(1-t)^{2l+2}} \frac{k^{1-a}}{(\Delta k+k)^{1-a+2mi}} \left| \Gamma\left[\frac{1-a}{2} + i(\beta+m)\right] \right| \\ \times \left| \Gamma\left[\frac{1-a}{2} + i(\beta-m)\right] \right| \lim_{\tau_{1}, \tau_{2} \to 0} \sum_{p=0}^{l-a} c_{p} \left(\frac{\partial}{\partial\tau_{1}} + \frac{\partial}{\partial\tau_{2}}\right)^{1+l-a-p} \left(\frac{\partial}{\partial\tau_{1}} - \frac{\partial}{\partial\tau_{2}}\right)^{p} \frac{\partial^{2a}}{\partial\tau_{1}^{a}\partial\tau_{2}^{a}} \\ \times \left(\frac{1+t}{1-t} + \tau_{1} - iv\right)^{(a-1)/2+im} \left(\frac{1+t}{1-t} + \tau_{2} + iv\right)^{(a-1)/2+im} \\ \times \left\{ 1 + i\beta \lg \frac{1+t+(1-t)(\tau_{1} - iv)}{1+t+(1-t)(\tau_{2} + iv)} + i\gamma \left(\frac{a-1}{2} - im\right)(\tau_{1} - \tau_{2}) \right\}.$$
(29)

Once the expression (29) has been determined for given numbers l and a, we obtain readily the quantity $\epsilon_{nla, km}(\Delta k)$ by differentiation with respect to t. Indeed, according to (21) we find

$$\epsilon_{nla, km}(\Delta k) = \pi^{\frac{3}{2}}(-1)^{l} 2^{-3-l} (A_{nla})^{\frac{1}{2}} \frac{\partial^{n-l-1} q_{la}(k, m, \Delta k, t)}{\partial t^{n-l-1}} \bigg|_{t=0}.$$
(30)

The constant $(A_{n \, la})^{\frac{1}{2}}$ of (30) stands in a simple relation to the constant of normalization $C_{n \, la}$ appearing in (21). Instead of determining $C_{n \, la}$ from the Eq. (16), we can determine $A_{n \, la}$ by the equivalent Eq. (17) after having calculated $\epsilon_{n \, la, \ km}(\Delta k)$ from (30). The fact, that relation (17) remains valid when all quadratic and higher terms in β and γ are neglected can be seen from (29). Indeed, by the substitutions $\tau_1 \rightarrow \tau_2, \ \tau_2 \rightarrow \tau_1, \ v \rightarrow -v$ all the terms in (29) not containing β or γ do not change, while the terms with β or γ change their sign and vice versa. Those terms in $|\epsilon|^2$ which are linear in β or γ are therefore uneven functions of v and therefore their integral over v, or over k as in (17), vanishes, thus giving no contribution to the total scattered intensity.

3. Scattering of Electrons in the K- and L-Shell

We proceed now to calculate the contribution to the Compton scattering of electrons in the different orbits of the K- and L-shells. Assuming hydrogenic orbits, we can express the constants β and γ entering in (29) and (30) in terms of the observed binding energy E, using (5) and (15) and (27). These constants are, of course, different for different orbits and elements.

(a) s-electrons

.

Here, we have l=a=0; in the sum $\sum_{p=0}^{l-a}$ of (29), there appears only the term with p=0 and it is, according to (24), $c_0=1$ since P_0^0 (cos θ)=1.

A straightforward differentiation with respect to τ_1 and τ_2 and taking the limit τ_1 , $\tau_2 \rightarrow 0$ gives:

$$q_{00}(k, m, \Delta k, t) = 8\pi^{-\frac{3}{2}} \left(\frac{\alpha}{2}\right)^{-2+2mi} \frac{k}{(\Delta k+k)^{1+2mi}} |\Gamma[\frac{1}{2}+i(\beta+m)]||\Gamma[\frac{1}{2}+i(\beta-m)]| \\ \times \frac{1}{(1-t)^{2}} \left[\left(\frac{1+t}{1-t}\right)^{2}+v^{2}\right]^{-\frac{3}{2}+im} \left\{\left(\frac{1+t}{1-t}\right)(-1+2im)\left(1+i\beta \lg \frac{1+t-(1-t)iv}{1+t+(1-t)iv}\right)-2\beta v\right\}.$$
(31)

In order to obtain explicit expressions for the scattered intensity of the *s*-electrons in the K- and L-shells, we have to treat the two cases separately.

(a) K-shell. Since n=1, l=0, we obtain from (30), taking simply the expression (31) for t=0 and noticing

$$i\beta \lg [(1-iv)/(1+iv)] = 2\beta \arctan v$$

$$\epsilon_{100, km}(\Delta k) = (A_{100})^{\frac{1}{2}}(\alpha/2)^{-2+2mi}(k/(\Delta k+k)^{1+2mi}) |\Gamma[\frac{1}{2}+i(\beta+m)]|\Gamma[\frac{1}{2}+i(\beta-m)]|(1+v^2)^{-\frac{3}{2}+im} \times \{-1-2\beta \arctan v - 2\beta v + 2mi(1+2\beta \arctan v)\}.$$
(32)

Taking the absolute square of (32), we neglect again all quadratic and higher terms in β . It can be easily seen, that in this approximation the terms containing β in the Γ -functions of (32) can be neglected.

We use the relation¹⁴

$$|\Gamma(\frac{1}{2}+im)|^{2} = |\Gamma(\frac{1}{2}-im)|^{2} = \pi/ch\pi m, \quad \text{and further}$$

$$k = \Delta k - \frac{1}{2}\alpha v = \Delta k(1 - \alpha/2\Delta kv) \cong \Delta k(1 - \gamma v)$$

$$\Delta k + k = 2\Delta k - \frac{1}{2}\alpha v = 2\Delta k(1 - \alpha v/4\Delta k) \cong 2\Delta k(1 - \frac{1}{2}\gamma v). \quad (33)$$

Eqs. (33) follow from (28) and (27) which, for n=1 gives $\gamma = 2\beta$. Hence we obtain

$$|\epsilon_{100, km}(\Delta k)|^{2} \cong A_{100}(\alpha/2)^{-4}(\pi^{2}/4) [(1+v^{2})^{-3}/ch^{2}\pi m] \{(1+4m^{2})(1+4\beta \operatorname{arctg} v)+2\beta v\}.$$
(34)

For the following integrations over m, we make use of the formula¹⁵

$$\int_{-\infty}^{+\infty} \frac{m^{g}dm}{ch^{2}\pi m} - \int_{-\infty}^{+\infty} \frac{(m+i)^{g}dm}{ch^{2}\pi m} = -\frac{4}{\pi}g\left(\frac{i}{2}\right)^{g},$$

which, applied for g=1, 3, 5 gives

$$\int_{-\infty}^{+\infty} \frac{dm}{ch^2 \pi m} = \frac{2}{\pi}, \qquad \int_{-\infty}^{+\infty} \frac{m^2 dm}{ch^2 \pi m} = \frac{1}{6\pi}, \qquad \int_{-\infty}^{+\infty} \frac{m^4 dm}{ch^2 \pi m} = \frac{7}{120\pi}.$$
 (35)

With the help of (35) we find

$$|\epsilon_{100}(k,\Delta k)|^{2} = \int_{-\infty}^{+\infty} |\epsilon_{100,km}(\Delta k)|^{2} dm = A_{100}(\alpha/2)^{-4} (\pi/(1+v^{2})^{3}) \{ (5/6)(1+4\beta \arctan v) + \beta v \}.$$
(36)

In order to satisfy (17) we have to choose the constant A_{100} such, that according to (28)

$$\int_{0}^{\infty} |\epsilon_{100}(k, \Delta k)|^{2} dk \cong (\alpha/2) \int_{-\infty}^{+\infty} |\epsilon_{100}(k, \Delta k)|^{2} dv = 1.$$

$$(37)$$

Since $1+v^2$ is an even function of v, while arctg v and v are uneven, the terms of (36) containing β give no contribution to the integral (37).

Applying the first of the following formulae

$$\int_{-\infty}^{+\infty} \frac{dv}{(1+v^2)^3} = \frac{3\pi}{8}, \qquad \int_{-\infty}^{+\infty} \frac{dv}{(1+v^2)^4} = \frac{5\pi}{16}, \qquad \int_{-\infty}^{+\infty} \frac{dv}{(1+v^2)^5} = \frac{35\pi}{128}$$
(38)

we find

$$(\alpha/2) \int_{-\infty}^{+\infty} |\epsilon_{100}(k, \Delta k)|^2 dv = A_{100}(\alpha/2)^{-3}(5\pi^2/16) = 1,$$
(39)

¹⁴ G, page 359.

¹⁵ This equation, is a slightly different form of the equation, given in G in the footnote page 366.

therefore

$$A_{100} = (\alpha/2)^3 (16/5\pi^2) \tag{39a}$$

and from (36)

1

$$\epsilon_{100}(k, \Delta k) |^{2} = (16/3\pi\alpha) [1/(1+v^{2})^{3}] \{1+4\beta \arctan v + (6/5)\beta v\}$$
(40)

with $v = (2/\alpha)(\Delta k - k)$. Formula (40) becomes identical with formula (32) of G, if the terms with β are neglected.

(β) *L-shell*. Here we have n=2, l=0; in order to obtain $\epsilon_{200, km}(\Delta k)$ from (30), we have to derive the expression (31) once with respect to t and take the limit t=0. Instead of (32) we find thus

$$\epsilon_{200, km}(\Delta k) = (A_{200})^{\frac{1}{2}}(\alpha/2)^{-2+2mi}(k/(\Delta k+k)^{1+2mi}) |\Gamma[\frac{1}{2}+i(\beta+m)]|\Gamma[\frac{1}{2}+i(\beta-m)]|2(1+v^2)^{-\frac{1}{2}+im} \\ \times \left\{ -(1+2\beta \arctan v) \left(2-\frac{3}{1+v^2}+\frac{4m^2}{(1+v^2)^2}\right) - 2\beta v \left(1-\frac{5}{1+v^2}\right) + 2mi \left[(1+2\beta \arctan v) \left(2-\frac{4}{1+v^2}\right)-\frac{4\beta v}{1+v^2}\right] \right\}, \quad (41)$$

Keeping only the linear terms in β it follows that, instead of (34):

$$|\epsilon_{200, km}(\Delta k)|^{2} = 4A_{200}(\alpha/2)^{-4}\pi^{2} [(1+v^{2})^{-3}/ch^{2}\pi m] [k^{2}/(\Delta k+k)^{2}] \\ \times \left\{ [1+4\beta \arctan v] \left[4 - \frac{12}{1+v^{2}} + \frac{9}{(1+v^{2})^{2}} + 4m^{2} \left(4 - \frac{12}{1+v^{2}} + \frac{10}{(1+v^{2})^{2}} \right) + \frac{16m^{4}}{(1+v^{2})^{2}} \right] \\ + 4\beta v \left[2 - \frac{13}{1+v^{2}} + \frac{15}{(1+v^{2})^{2}} - \frac{12m^{2}}{1+v^{2}} + \frac{12m^{2}}{(1+v^{2})^{2}} \right] \right\}.$$

Integrating over *m* with the help of formulae (35) and using (33) with $\gamma = \beta$ according to (27) for n=2, we get

$$|\epsilon_{200}(k, \Delta k)|^{2} = \int_{-\infty}^{+\infty} |\epsilon_{200, km}(\Delta k)|^{2} dm = A_{200} \left(\frac{\alpha}{2}\right)^{-4} \frac{\pi}{(1+v^{2})^{3}} \times \left\{\frac{32}{3} \left[1+4\beta \operatorname{arctg} v\right] \left[1-\frac{3}{1+v^{2}}+\frac{12}{5}\frac{1}{(1+v^{2})^{2}}\right] + 16\beta v \left[\frac{4}{3}-\frac{5}{1+v^{2}}+\frac{32}{5}\frac{1}{(1+v^{2})^{2}}\right]\right\}.$$
 (42)

Applying (17) we obtain with the help of formulae (38) in a way, similar to (39) and (39a) the result:

$$(\alpha/2)\int_{-\infty}^{+\infty} |\epsilon_{200}(k, \Delta k)|^2 dv = A_{200}(\alpha/2)^{-3}\pi^2 = 1; \qquad A_{200} = (1/\pi^2)(\alpha/2)^3$$

and therefore

$$|\epsilon_{200}(k,\Delta k)|^{2} = \frac{64}{3\pi\alpha} \frac{1}{(1+v^{2})^{3}} \left\{ \left[1+4\beta \arctan v \right] \left[1-\frac{3}{1+v^{2}} + \frac{12}{5} \frac{1}{(1+v^{2})^{2}} \right] + \beta v \left[2-\frac{15}{2} \frac{1}{1+v^{2}} + \frac{48}{5} \frac{1}{(1+v^{2})^{2}} \right] \right\}.$$
 (43)

(b) *p*-electrons in the *L*-shell

Since in this case n-l-1=0, it is not necessary to carry out any differentiation with respect to t. It is sufficient therefore to consider the quantity q_{1a} , given by (29) only for t=0. Yet we have to

F. BLOCH

consider separately the two cases a=0 and a=1, which correspond to the orientations of the angular momentum in the initial state perpendicular and parallel, respectively, to the axis, given by the direction of the vector $\Delta \mathbf{k}$, defined by (10).

(a) a=0. Since $P_1^0(\cos \vartheta) = \cos \vartheta$, we have, according to (24) $c_0=0$; $c_1=1$. This means in (29) a differentiation with respect to τ_1 and τ_2 of the form $\frac{\partial^2}{\partial \tau_1^2} - \frac{\partial^2}{\partial \tau_2^2}$ and leads to the result

 $\epsilon_{210, km}(\Delta k) = -\pi^{\frac{3}{2}} 2^{-2} (A_{210})^{\frac{1}{2}} q_{10}(k, m, \Delta k, 0) = (A_{210})^{\frac{1}{2}} (\alpha/2)^{-2+2mi} (k/(\Delta k+k)^{1+2mi})$

$$\times \left| \Gamma \left[\frac{1}{2} + i(\beta + m) \right] \right| \Gamma \left[\frac{1}{2} + i(\beta - m) \right] \left| 2(-1 + 2mi)(1 + v^2)^{-\frac{5}{2} + im} \left\{ -mv(1 + 2\beta \operatorname{arctg} v) + m\gamma(1 + v^2) - \frac{2m\beta}{1 + 4m^2}(1 - v^2) + i \left[-\frac{3}{2}v(1 + 2\beta \operatorname{arctg} v) - \frac{1}{2}\gamma(1 + v^2) + \beta \frac{2 + 4m^2}{1 + 4m^2}(1 - v^2) \right] \right\}.$$
(44)

Taking the absolute square of (44) and keeping only terms linear in β we find

$$\begin{aligned} |\epsilon_{210, km}(\Delta k)|^{2} &\cong A_{210} \left(\frac{\alpha}{2}\right)^{-4} \pi^{2} \frac{(1+v^{2})^{-5}}{ch^{2}\pi m} \frac{k^{2}}{(\Delta k+k)^{2}} \{v^{2}(9+40m^{2}+16m^{4})(1+4\beta \operatorname{arctg} v) \\ &+ \gamma v(1+v^{2})(6+12m^{2}-32m^{4})-8\beta v(1-v^{2})(3+4m^{2})\}. \end{aligned}$$

The integration over m and the use of (33) and (35) leads, in a manner similar to that employed for obtaining (42) to the expression

$$|\epsilon_{210}(k, \Delta k)|^{2} = \int_{-\infty}^{+\infty} |\epsilon_{210, km}(\Delta k)|^{2} dm = A_{210} \left(\frac{\alpha}{2}\right)^{-4} \frac{\pi}{60(1+v^{2})^{4}} \left\{ 384 \left[1+4\beta \arctan v\right] \left[1-\frac{1}{1+v^{2}}\right] + \beta v \left[598-\frac{1216}{1+v^{2}}\right] \right\}.$$

The determination of A_{210} with the help of (17) gives

$$\frac{\alpha}{2} \int_{-\infty}^{+\infty} |\epsilon_{210}(k, \Delta k)|^2 dv = A_{210}(\alpha/2)^{-3} \pi^2/4 = 1,$$

 $A_{210} = (4/\pi^2)(\alpha/2)^3$ and therefore

$$|\epsilon_{210}(k, \Delta k)|^{2} = \frac{256}{5\pi\alpha} \frac{1}{(1+v^{2})^{4}} \Big\{ [1+4\beta \arctan v] \Big[1-\frac{1}{1+v^{2}} \Big] + \beta v \Big[\frac{299}{192} - \frac{19}{6} \frac{1}{1+v^{2}} \Big] \Big\}.$$
(45)

(β) a=1. Here again the summation over p in (29) contains only the term with p=0 and from (24) it follows that $c_0=1$. The differentiation with respect to τ_1 , τ_2 in (29) here takes the form

$$(\partial/\partial au_1 + \partial/\partial au_2)(\partial^2/\partial au_1 \partial au_2).$$

One finds

$$\begin{aligned} \varepsilon_{211, \ km}(\Delta k) &= -\pi^{\frac{3}{2}} 2^{-2} (A_{211})^{\frac{1}{2}} q_{11}(k, \ m, \ \Delta k, \ 0) = (A_{211})^{\frac{1}{2}} (\alpha/2)^{-2+2mi} (1/(\Delta k+k)^{2mi}) \left| \Gamma[i(\beta+m)] \right| \\ &\times \left| \Gamma[i(\beta-m)] \right| 2im(1+v^2)^{-2+im} \{ -m^2(1+2\beta \arctan v) + m^2\gamma v - im[1+2\beta \arctan v + \beta v - \gamma v] \}. \end{aligned}$$
(46)

By taking the absolute square of this expression and keeping only the terms linear in β and $\gamma = \beta$, it is again permissible to neglect the term with β in the Γ -functions of (46). From the formulae

$$\Gamma(1+z) = z\Gamma(z)$$
 and $\Gamma(z)\Gamma(1-z) = \pi/\sin \pi z$

it follows $|\Gamma(im)|^2 = |\Gamma(-im)|^2 = \pi/msh\pi m$ and we obtain from (46)

$$|\epsilon_{211, km}(\Delta k)|^{2} \cong A_{211}(\alpha/2)^{-4} 4\pi^{2} [(1+v^{2})^{-4}/sh^{2}\pi m] \{(m^{2}+m^{4})[1+4\beta \operatorname{arctg} v] - 2m^{4}\beta v\}.$$

For the integration over m, we make use of the formula

$$\int_{-\infty}^{+\infty} (m^{g} dm/sh^{2}\pi m) = 2^{g-1}/2^{g-1} - 1 \int (m^{g} dm/ch^{2}\pi m),$$

which for g=2 and g=4, with the help of (35) gives

$$\int_{-\infty}^{+\infty} m^2 dm/sh^2 \pi m = 1/3\pi, \qquad \int_{-\infty}^{+\infty} m^4 dm/sh^2 \pi m = 1/15\pi.$$
(47)

We find thus

$$|\epsilon_{211}(k, \Delta k)|^{2} = \int_{-\infty}^{+\infty} |\epsilon_{211, km}(\Delta k)|^{2} dm = A_{211}(\alpha/2)^{-4}(8\pi/15) [1/(1+v^{2})^{4}] \{3(1+4\beta \operatorname{arctg} v) - \beta v\}$$

and with the help of (38)

$$(\alpha/2)\int_{-\infty}^{+\infty} |\epsilon_{211}(k,\,\Delta k)|^2 dv = A_{211}(\alpha/2)^{-3}\pi^2/2 = 1,$$

 $A_{211} = (2/\pi^2)(\alpha/2)^3$ and therefore

$$|\epsilon_{211}(k, \Delta k)|^{2} = (32/5\pi\alpha)(1/(1+v^{2})^{4})\{1+4\beta \operatorname{arctg} v - \frac{1}{3}\beta v\}.$$
(48)

4. TOTAL INTENSITY AND DEFECT OF THE COMPTON-SHIFT FOR ELEMENTS WITH K- AND L-ELECTRONS

With the expressions (40), (43), (45) and (48) we are now able, according to (9) to give the intensitydistribution on the Compton line of any element with given numbers N_{nla} of electrons in an orbit (nla) of the K- or L-shell. Indeed, assuming the electrons as independent, as has been done in the previous paragraphs, we can write for the total intensity of the frequency range $d\nu'$:

$$dI = \sum_{nla} N_{nla} dI_{nla}.$$
 (49)

It has to be noticed, that for p-electrons in the *L*-shell all the three orientations of the angular momentum with respect to our chosen axis appear with the same weight. Calling N_3 the number of electrons in any one of the p-orbits, we have therefore in (49) to take:

$$N_{210} = N_3/3; \quad N_{211} = 2N_3/3.$$
 (50)

Furthermore, we have to remember that the constants α and β as well as the variables v, according to their definition (28) have different significance for different orbits, changing with the binding energy of the corresponding electron. In order to distinguish them, we write instead of α , β and v

Remembering that according to (28)

$$k = \Delta k - \frac{1}{2}v \cong \Delta k(1 - \alpha v / \Delta 2k) \cong \Delta k(1 - 2\beta v / n)$$

and using (9), (40), (43), (45), (48) and (50), we find for the total intensity of the range $d\nu'$ the following expression, which is correct, if all terms with second and higher powers in β are neglected:

F. BLOCH

$$dI = I_{P} \frac{2\pi^{2}e^{4}}{m_{0}c^{4}r^{2}} \frac{1 + \cos^{2}\theta}{h\Delta k} d\nu' \frac{16}{3\pi} \left\{ \frac{N_{1}}{\alpha_{1}} \frac{1}{(1 + v_{1}^{2})^{3}} \left[1 + 4\beta_{1} \arctan v_{1} + \frac{16}{5}\beta_{1}v_{1} \right] \right. \\ \left. + \frac{4N_{2}}{\alpha_{2}} \frac{1}{(1 + v_{2}^{2})^{3}} \left[(1 + 4\beta_{2} \arctan v_{2} + \beta_{2}v_{2}) \left(1 - \frac{3}{1 + v_{2}^{2}} + \frac{12}{5} \frac{1}{(1 + v_{2}^{2})^{2}} \right) \right. \\ \left. + \beta_{2}v_{2} \left(2 - \frac{15}{2} \frac{1}{1 + v_{2}^{2}} + \frac{48}{5} \frac{1}{(1 + v_{2}^{2})^{2}} \right) \right] + \frac{4N_{3}}{5\alpha_{3}} \frac{1}{(1 + v_{3}^{2})^{4}} \\ \left. \times \left[(1 + 4\beta_{3} \arctan v_{3} + \beta_{3}v_{3}) \left(5 - \frac{4}{1 + v_{3}^{2}} \right) + \beta_{3}v_{3} \left(\frac{283}{48} - \frac{38}{3} \frac{1}{1 + v_{3}^{2}} \right) \right] \right\}.$$
(51)

In order to obtain the relation between v and the wave-length of the scattered radiation λ' , we notice that according to (28) and (6) it is

$$v = \frac{2}{\alpha} (\Delta k - k) = \frac{2}{\alpha} \left\{ \left[\frac{8\pi^2 \nu^2}{c^2} (1 - \cos \theta) \right]^{\frac{1}{2}} - \left[\frac{8\pi^2 m_0}{h} \left(\nu - \nu' - \frac{E}{h} \right) \right]^{\frac{1}{2}} \right\}$$
(52)

since for $h\nu \ll mc^2$, i.e., $\nu \cong \nu'$ it follows from (10)

$$(\Delta k)^2 = (8\pi^2 \nu^2 / c^2) (1 - \cos \theta).$$
(53)

From (5) and (19) we get

$$(8\pi^2 m_0/\hbar^2) E = \alpha^2/4.$$
(54)

With the notation $\gamma = \alpha/2k \cong \alpha/2\Delta k$ used before, and

$$\lambda' - \lambda \leq c(\nu - \nu')/\nu^2 = x(h/m_0 c)(1 - \cos \theta)$$
(55)

we can therefore write (52) in the form

$$v = (1/\gamma) \{ 1 - (x - \gamma^2)^{\frac{1}{2}} \}.$$
(56)

Since we expect a considerable intensity only in the neighborhood of Compton's value (1), i.e., for $\Delta \lambda = \lambda' - \lambda = (h/m_0 c)(1 - \cos \theta)$, we write

$$x = 1 - \delta \tag{57}$$

and, expanding the square-root in (56), keeping only the terms with δ and γ^2 , we get

$$v = (1/2\gamma)(\delta + \gamma^2). \tag{58}$$

As long as one neglects all terms with β_1 , β_2 and β_3 in (51) and consequently with γ^2 in (56), one sees that the intensity is symmetrically distributed around Compton's value (1), namely, symmetrical around v=0 or $\delta=0$. Fig. 1 shows this symmetrical distribution for Be $(N_1=N_2=2, N_3=0)$ assuming for the binding energies the values: $E_1=122$ volts. $E_2=9.5$ volts. Fig. 2 is drawn for $C(N_1=N_2=N_3=2)$ with $E_1=285$ volts; $E_2=24.9$ volts; $E_3=11$ volts.

The appearance of uneven functions of $v_{1, 2, 3}$ in (51), however, makes the Compton line slightly asymmetrical. Furthermore, it changes the position of the maximum intensity and we are particularly interested in this maximum position, in order to compare it with the empirical results.⁵

Since this maximum will occur for very small values of the variables $v_{1, 2, 3}$ in (51) it is sufficient to consider in the bracket {} in (51) only the terms, linear and quadratic in $v_{1, 2, 3}$. Near the maximum the bracket becomes

$$Y = \frac{N_1}{\alpha_1} \left[1 - 3v_1^2 + \frac{36}{5}\beta_1 v_1 \right] + \frac{4N_2}{\alpha_2} \left[\frac{2}{5} - 3v_2^2 + \frac{61}{10}\beta_2 v_2 \right] + \frac{4N_3}{5\alpha_3} \left[1 - \frac{85}{48}\beta_3 v_3 \right].$$
(59)



FIG. 1. Intensity-distribution in the Compton-line of beryllium, neglecting all higher order effects, causing asymmetry and defect of the shift. The ordinates are plotted in arbitrary units, the abscissae measure the difference of the wave-length λ' and λ of the scattered and incident radiation, respectively, in units 0.0177 $\lambda(1 - \cos \theta)^{\frac{1}{2}}$, θ being the angle between the direction of the incident and scattered radiation. The scale of the abscissae is chosen such that at the origin $\lambda' = \lambda + (h/mc_0) \times (1 - \cos \theta)$. The binding energies are assumed to be for the K-electrons, 122 v; for the $L_{\rm I}$ electron, 9.5 v.

It is interesting to notice that the third term in (59) does *not* contain v_3^2 , the intensity curve for *p*-electrons near the maximum following a fourth power law.

In order to determine the maximum of Y and therefore of the intensity in the λ -scale, we calculate

$$\frac{\partial Y}{\partial \delta} = \frac{\partial Y}{\partial v_1} \frac{\partial v_1}{\partial \delta} + \frac{\partial Y}{\partial v_2} \frac{\partial v_2}{\partial \delta} + \frac{\partial Y}{\partial v_3} \frac{\partial v_3}{\partial \delta}$$

or, according to (54), (58) and (59)

$$4\Delta k \frac{\partial Y}{\partial \delta} = \frac{N_1}{\gamma_1^2} \left[-\frac{3}{\gamma_1} (\delta + \gamma_1^2) + \frac{18}{5} \gamma_1 \right] + \frac{4N_2}{\gamma_2^2} \left[-\frac{3}{\gamma_2} (\delta + \gamma_2^2) + \frac{61}{10} \gamma_2 \right] - \frac{17}{12} \frac{N_3}{\gamma_3}.$$



FIG. 2. Intensity distribution in the Compton-line of carbon under the same approximations and in the same scale as in Fig. 1. The binding-energies are assumed to be for the K-electrons, 285 v; for the $L_{\rm I}$ -electrons, 24.9 v; for the $L_{\rm II}$ -electrons, 11 v.

This expression vanishes for

$$\delta = \frac{1}{15} \frac{3N_1/\gamma_1 + 62N_2/\gamma_2 - (85/12)N_3/\gamma_3}{N_1/\gamma_1^3 + 4N_2/\gamma_2^3}.$$
(60)

Using finally (53), (54), (55), (27) and (57), we find for the position of the maximum intensity in the λ scale:

$$\lambda' = \lambda + \frac{h}{m_0 c} (1 - \cos \theta) - \frac{\lambda^2}{hc} \frac{1}{15} \frac{3N_1 / \sqrt{E_1 + 62N_2 / \sqrt{E_2} - (85/12)N_3 / \sqrt{E_3}}}{N_1 / \sqrt{E_1^3 + 4N_2 / \sqrt{E_2^3}}}.$$
(61)

We see that the defect of the Compton shift

$$\delta \lambda = \lambda - \lambda' + (h/m_0 c)(1 - \cos \theta),$$

as expected from formula (2) has indeed the form

$$\delta \lambda = D \lambda^2 \tag{62}$$

with

=

$$D = \frac{1}{15hc} \frac{3N_1/\sqrt{E_1 + 62N_2}/\sqrt{E_2 - (85/12)N_3}/\sqrt{E_3}}{N_1/\sqrt{E_1^3 + 4N_2}/\sqrt{E_2^3}}.$$
(63)

For the case of H and He, where $N_2 = N_3 = 0$, D can be written in the form (4) $D = \kappa E_1/hc$ with $\kappa = 3/5$. For higher atomic numbers, however, one has to treat the complete expression (63), D depending essentially on both the binding energies E_2 and E_3 of the L-electrons in a rather complicated way.

5. Comparison with the Experiment

Table I shows the numerical values of $\delta\lambda$, calculated for Be and C and the corresponding observed values for a primary radiation with $\lambda = 0.631$ A, the binding energies E_1 , E_2 , E_3 being given in elec-

TABLE I. Theoretical and observed values of $\delta\lambda$.								
	N_1	N_2	N_3	E_1	E_2	E_3	$\delta\lambda_{\text{theor.}}(A)$	$\delta\lambda_{\rm obs.}(A)$
Be C	2 2	$2 \\ 2$	0 2	122 285	9.5 24.9	11	2.8×10^{-4} 6.5×10^{-4}	2.3×10^{-4} 5.9×10^{-4}

tron-volts. The values $\delta \lambda_{obs}$ are taken from the preceding paper of Ross and Kirkpatrick. The dotted lines in their Fig. 4 show the Compton shift as expected from the theory here presented.

One will notice that in both cases of Be and C, the theoretical value lies about 10 to 20 percent higher than the measured value. It does not seem surprising that the theory here proposed will tend to give too high values of $\delta\lambda$. Indeed, with formulae (60) and (61), $\delta\lambda$ has been computed by using the binding energies, as given from spectroscopic data. These binding energies are meant as being the energies needed for removing a specified electron from its atomic orbit to infinity. However, in the solid state, the electrons ejected by the Compton-recoil will not be removed to infinity but into the neighborhood of other atoms in the crystal lattice, a fact which will tend to decrease the "effective binding energy" and therefore $\delta\lambda$. An approximate way of correcting our result might be to subtract from the binding-energies the electronic work function, i.e., the energy needed to bring a conduction electron from the interior of the crystal to infinity, which would account for the sign and the order of magnitude of the correction. We need not say, however, that a more accurate consideration of the forces, due to the interaction of different atoms in the lattice, would require much more elaborate calculations than we intended to give here.