The Scattering of Fast Electrons by Heavy Elements. II

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If fast electrons impinge on a mercury atom, the external electrons will modify the nuclear scattering, at least for small angles. We have determined the amount of scattering to be expected, as a function of angle, for 100-kv electrons and for 230-kv electrons. For the former, shielding is effective below 60°, and for the latter, below 15°. For the determination of phase shifts, the electron may be pictured as moving in an effective (Dirac) field, which involves zero, first, and second derivatives of the ordinary (Hartree) field. Three methods were used: (1) integration with the differential analyzer, (2) the WKB procedure, and (3) the first-order Born approximation. Methods (1) and (2) lead to results in good agreement with each other for all angular momenta, and method (3) gives good results for large angular momenta, despite the fact that the first-order correction to the wave function is large. The summation of the series for the scattering amplitudes was accomplished by noting that the phase shifts decreased in an exponential manner for large values of the angular momentum.

IF fast electrons undergo single elastic scattering from an atom, then we expect the angular distribution at sufficiently large angles to be determined by the effect of the nucleus alone, since large deflections accompany close distances of approach. For small angle scattering, however, the outside electrons will exert the controlling influence. In a previous research,[1] the single scattering of fast electrons by mercury nuclei was calculated. In this paper, we present results which include the contributions made by the extranuclear electrons. Since an easy technique for calculation of scattering for electrons of arbitrary energy has not yet been evolved, we have limited ourselves to energies of 100 kv and 230 kv.

For the mercury atom, a Hartree model is used. The spin-orbit interaction and other relativistic characteristics of the incident electron may be included (as will be shown) in an effective central field which acts on this electron. The phase shift caused by this field can then be found, as a function of angular momentum and of incident energy, and the series for the scattering amplitudes summed.

To determine the phase shifts, it is necessary to integrate numerically. The differential equation has a singular point at the origin, but the actual field is approximately Coulomb in the neighborhood, so that the Gordon[2] solutions of Dirac's equation may be used. From $r=0.002$ (atomic unit) to $r=0.26$ (in some cases $r=0.65$) the solution was carried outward on the Massachusetts Institute of Technology differential analyzer. For greater values of the radius, the WKB method has sufficient validity, and was therefore employed.

HARTREE FIELD

The potential energy of an electron at radius r, denoted by Z_p/r, has been tabulated by Hartree.[3] We have fitted these values by means of exponential functions (in order to facilitate differentiation) and find that the effective atomic number Z_p can be represented adequately by the equation $2Z_p=33.7e^{-17.376r}+95.9e^{-3.892r}+30.3e^{-1.253r}$. Near the origin (in the range $r\leq 0.02$) a single exponential suffices, i.e., $Z_p=80e^{-6.325r}$.

DIRAC FIELD

Darwin[4] writes the Dirac equations for an electron in a central field $V(r)$ as

$$\begin{aligned}(1/\hbar c)(W+eV+m_0c^2)F&\\ +(dG/dr)-(l/r)G=0,&\quad(1)\\ -(1/\hbar c)(W+eV-m_0c^2)G&\\ +(dF/dr)+[(l+2)/r]F=0.&\end{aligned}$$

If l is a positive integer, then Eqs. (1) have

[1] J. H. Bartlett and R. E. Watson, Phys. Rev. **56**, 612 (1939); Proc. Am. Acad. **74**, 53 (1940).
[2] W. Gordon, Zeits f. Physik **48**, 11 (1928).
[3] D. R. Hartree, Phys. Rev. **46**, 743 (1934), Table III.
[4] C. G. Darwin, Proc. Roy. Soc. London **A118**, 654 (1928). We have used l instead of k for the Legendre polynomial subscript.

solutions regular at the origin. The Dirac angular momentum quantum number j' is equal to $-l-1$ for $j=l+\frac{1}{2}$, and to l for $j=l-\frac{1}{2}$. The solutions of (1) which refer to the state $j=l+\frac{1}{2}$ (or $j'=-l-1$) are denoted by Darwin as F_l, G_l, while those for $j=l-\frac{1}{2}$ (or $j'=l$) are F_{-l-1}, G_{-l-1}. Let us now substitute as follows: $\psi_1=rF$, $\psi_2=-rG$, $\Pi=(1/\hbar c)\times(W+eV+m_0c^2)$, and $\Phi=(1/\hbar c)(W+eV-m_0c^2)$. Then

$$\Pi\psi_1-(d\psi_2/dr)-(j'/r)\psi_2=0, \qquad (2)$$
$$\Phi\psi_2+(d\psi_1/dr)-(j'/r)\psi_1=0.$$

For a Coulomb field, $(eV/\hbar c)=\alpha/r$, where $\alpha=(Ze^2/\hbar c)$. In this case, the equations are

$$(d\psi_1/dr)-(j'/r)\psi_1 = [-(1/\hbar c)(W-mc^2)-(\alpha/r)]\psi_2,$$
$$(d\psi_2/dr)+(j'/r)\psi_2=[(1/\hbar c)(W+mc^2)+(\alpha/r)]\psi_1.$$

These are the same as those of Gordon (reference 2, Eq. (1)). Let us now drop the primes from the j's. The function ψ_1 may be eliminated from (2). We have

$$\left(\frac{d}{dr}-\frac{j}{r}\right)\Pi^{-1}\left(\frac{d\psi_2}{dr}+\frac{j}{r}\psi_2\right)=-\Phi\psi_2.$$

This results in a second-order equation for ψ_2, namely,

$$\frac{d^2\psi_2}{dr^2}+\Pi\left[\frac{d}{dr}\left(\frac{1}{\Pi}\right)\right]\frac{d\psi_2}{dr}+\Pi\left[\frac{d}{dr}\left(\frac{j}{\Pi r}\right)\right]\psi_2 - \frac{j^2}{r^2}\psi_2+\Pi\Phi\psi_2=0. \qquad (3)$$

Equation (3) is of the form

$$\psi_2''+p(r)\psi_2'+q(r)\psi_2=0,$$

where $p(r)=-(d/dr)\log\Pi$, and

$$q(r)=\Pi\Phi-[j(j+1)/r^2]-(j\Pi'/r\Pi).$$

By means of the substitution

$$\psi_2=y\Pi^{\frac{1}{2}}, \qquad (4)$$

one can obtain[5] an equation with no first-order term. It is

$$y''+Q^2(r)y=0, \qquad (5)$$

where

$$Q^2(r)=q-\tfrac{1}{2}p'-\tfrac{1}{4}p^2 = \Pi\Phi-\frac{j(j+1)}{r^2}-\frac{j}{r}\frac{d}{dr}\log\Pi + \frac{1}{2}\frac{d^2}{dr^2}\log\Pi-\frac{1}{4}\left[\frac{d}{dr}\log\Pi\right]^2. \qquad (6)$$

In atomic units, $\hbar=1$, $m_0=1$, $e=1$, and $c=137$. Also, by definition, $p=k\hbar=k$. Accordingly,[6]

$$\Pi\Phi=(1/c^2)[(E-V)^2-c^4] = k^2-(2EV/c^2)+(V^2/c^2),$$

since $E=c[p^2+c^2]^{\frac{1}{2}}$, and hence

$$1-E^2/c^4=-k^2/c^2. \qquad (7)$$

Equation (6) might be written as

$$Q^2(r)=k^2-V_{\text{eff}},$$

where V_{eff} is an effective field in which the electron moves. This field, which we may call the Dirac field, includes all the relativistic effects, and is dependent on the energy. Our expression for $Q^2(r)$ does not agree with that deduced by Rose and Bethe,[7] but it does give the right behavior of the solution near the origin, and must hence be correct.

Near $r=0$, $V=-(Z/r)$, $\Pi=(Z/cr)$, $(dV/dr)=(Z/r^2)$, $(d^2V/dr^2)=-(2Z/r^3)$ and therefore

$$Q^2(r)=k^2+(2EZ/c^2r)+[(\tfrac{1}{4}-\rho^2)/r^2],$$

where $\rho=(j^2-\alpha^2)^{\frac{1}{2}}$. Equation (5) is then solved by the confluent hypergeometric function, which behaves near the origin as $r^{\rho+\frac{1}{2}}$. The function $\psi_2=y\Pi^{\frac{1}{2}}$ then behaves as r^ρ, which result was obtained in another manner by Gordon.[2]

Coulomb Solutions

At $r=0.00195$, the effective atomic number Z_p is[3] 78.95, so that the field is nearly Coulomb out to this point. We have assumed $Z_p=80$ out to $r=0.002$, and have calculated $(y'/y)_{r=0.002}$ from the Gordon solutions.

[5] E. T. Whittaker and G. N. Watson, *Modern Analysis* (Cambridge University Press, 1935), p. 194.

[6] Note the slight change of notation, $W\rightarrow E$, $eV\rightarrow -V$.

[7] M. E. Rose and H. A. Bethe, Phys. Rev. **55**, 277 (1939). The substitution (4) must be used if the first-order term is to be eliminated, so that the disagreement must be caused by some error in the work of Rose and Bethe.

TABLE I. *Initial conditions:* $(z'/z)_{r=0.002}$ *and* $(y'/y)_{r=0.26\ (\text{or } 0.65)}$.

j	(z'/z)	(y'/y)	j	(z'/z)	(y'/y)	j	(z'/z)	(y'/y)
	$E=100$ kv			$E=100$ kv			$E=100$ kv	
1	−335.4	666.4	9	−206.5	−319.8	−1	−96.2	−91.22
2	−243.5	67.16	11	−214.0	150.7	−2	27.15	−265
3	−212.6	−68.71	15	−232.7	−129.2	−3	60.57	82.6
4	−205.6	149.2	19	−254.5	2.0*	−4	76.63	−57.7
5	−198.8	−53.01	24	−282.9	−20.2*	−5	86.14	162.3
7	−201.2	−89.23	29	−312.1	−105.5*	−6	92.5	−51.06
8	−203.2	54.20				−8	100.29	
	$E=230$ kv			$E=230$ kv			$E=230$ kv	
1	−349.3	−28.00	8	−196.0		−2	4.12	
2	−250.0	−278.9	11	−204.4	23.06	−3	42.77	
3	−216.9	145.1	15	−221.2		−4	61.44	
4	−203.7	−113.3	19	−240.1		−5	72.51	
5	−194.6	198.2	−1	−139.7	221.7	−6	79.9	
						−12	98.2	30.51

* (y'/y) for $r=0.65$ rather than 0.26.

In Eq. (3), the solution ψ_2 is determined except for an arbitrary multiplying factor, which might be complex. Since the phase of this factor has no physical significance, we shall take ψ_2 to be real. Inspection of Eqs. (2) then shows that ψ_1 will be real, and the equations are consistent in this respect. The ratio $\psi_1:\psi_2$ is therefore also real.

From (4), we have $y=\psi_2\Pi^{-\frac{1}{2}}$, and

$$y'=(d\psi_2/dr)\Pi^{-\frac{1}{2}}-\tfrac{1}{2}\psi_2\Pi'\Pi^{-\frac{3}{2}}$$
$$=[-(j\psi_2/r)+\Pi\psi_1-\tfrac{1}{2}\psi_2\Pi'\Pi^{-1}]\Pi^{-\frac{1}{2}}.$$

It follows that

$$(y'/y)=-(j/r)+\Pi(\psi_1/\psi_2)-\tfrac{1}{2}(\Pi'/\Pi). \quad (8)$$

This ratio is likewise real.

As in our previous paper,[1] $q=(\alpha/\beta)$ and $q'=q(1-\beta^2)^{\frac{1}{2}}$, where $\beta=(v/c)$. Now $E=mc^2=c^2(1-\beta^2)^{-\frac{1}{2}}$, from which we may conclude that $\beta^2=(m^2-1)/m^2$, so that $q=\alpha m(m^2-1)^{-\frac{1}{2}}$, or $-iq=\alpha m(1-m^2)^{-\frac{1}{2}}$. Then $-iq'=\alpha(1-m^2)^{-\frac{1}{2}}$. Gordon's Eq. (7), which defines n', now becomes $-n'=\rho+iq$.

The substitutions of Gordon are: $\psi_1=(1-m)^{\frac{1}{2}}\times(\sigma_1-\sigma_2)$ and $\psi_2=(1+m)^{\frac{1}{2}}(\sigma_1+\sigma_2)$. If ψ_2 is real, the following results are true: $\sigma_1+\sigma_2=a$ is real, ψ_1 is real, $\sigma_1-\sigma_2=ib$ is imaginary,

$$2\sigma_1=a+ib, \quad 2\sigma_2=a-ib, \quad \sigma_2=\sigma_1^*, \quad (9)$$

and, using (7),

$$\frac{\psi_1}{\psi_2}=\left(\frac{1-m}{1+m}\right)^{\frac{1}{2}}\frac{ib}{a}=-\frac{k}{c(1+m)}\frac{b}{a}. \quad (10)$$

Let

$$F(\alpha,\beta,z)=1+\frac{\alpha z}{1!\beta}+\frac{\alpha(\alpha+1)z^2}{2!\beta(\beta+1)}+\cdots.$$

Gordon's solutions are

$$\sigma_1=c_0^{(1)}r^\rho e^{-ikr}F(\rho+iq+1,\ 2\rho+1,\ 2ikr),$$
$$\sigma_2=c_0^{(2)}r^\rho e^{-ikr}F(\rho+iq,\ 2\rho+1,\ 2ikr), \quad (11)$$

$$\frac{c_0^{(1)}}{c_0^{(2)}}=-\frac{j-iq'}{\rho-iq}=e^{2i\theta+i\pi}, \quad (12)$$

$$2\theta=\tan^{-1}(q/\rho)-\tan^{-1}(q'/j)$$
$$=\tan^{-1}(j'q-\rho q')/(j\rho+qq'). \quad (13)$$

(We have used the equation $j^2+q'^2=\rho^2+q^2$, which is true because $q'^2=q^2-\alpha^2$.)

Determination of (y'/y)

Let us use the symbol Ph for the phase. Also, let

$$v_{\kappa,\rho}(z)=e^{-\frac{1}{2}z}F(\tfrac{1}{2}+\rho-\kappa,\ 2\rho+1;\ z)$$
$$=z^{-\frac{1}{2}-\rho}M_{\kappa,\rho}(z), \quad (14)$$

where M is the confluent hypergeometric function.

From (9),

$$(b/a)=\tan Ph\sigma_1=\tan(Phc_0^{(1)}+Phv). \quad (15)$$

An application of Kummer's formula[8] leads to the result that $(\sigma_1/c_0^{(1)})=(\sigma_2^*/c_0^{(2)*})$. Therefore, from Eq. (9), $c_0^{(1)}=c_0^{(2)*}$, and

$$Phc_0^{(1)}=\theta+\tfrac{1}{2}\pi. \quad (16)$$

The function $v_{\kappa,\rho}(z)$ satisfies the equation

$$v''+[(2\rho+1)/z]v'+[-\tfrac{1}{4}+(\kappa/z)]v=0.$$

A series solution in ascending powers of $z(=2ikr)$ may be found, and is

$$v=1-\frac{\kappa}{\eta}(2ikr)+\frac{\frac{1}{4}\eta+\kappa^2}{2\eta(\eta+1)}(2ikr)^2$$
$$-\frac{\kappa(\frac{3}{4}\eta+\frac{1}{2})+\kappa^3}{6\eta(\eta+1)(\eta+2)}(2ikr)^3+\cdots,$$

where $\eta=2\rho+1$.

This series was summed numerically for $q=0.8$ and $q=1.0564$, and for all values of ρ which were used. From this and Eqs. (8), (10), (15), and (16), the values of $(y'/y)_{r=0.002}$ were computed. These were used as initial conditions for the differential analyzer solutions. They are given in Table I.

[8] Reference 5, p. 338.

WKB Solutions

The WKB method for solving equations such as (5) has been discussed very thoroughly by Langer.[9,10] The usual procedure is to set $y=e^{\int f dr}$, and to expand f in an ascending power series in $\hbar$. As an alternative, we can expand in a descending power series in k, or in Q, which is still better. The equation in f is

$$f'+f^2+Q^2=0. \text{ If } Q^2>0, \text{ put } f=iQ+g,$$

where g satisfies the equation

$$iQ'+g'=-2iQg-g^2. \tag{17}$$

Expand $g=g_1/Q+g_2/Q^2+\cdots$ and compare like powers of Q, obtaining $g_1=-\frac{1}{2}Q'$, and

$$g_l'-(l-1)g_{l-1}=-2ig_{l+1}-\sum_k g_k g_{l-k}$$

in general. From this recursion formula we may determine the successive coefficients in the power series. This series will converge rapidly when Q is large. When we are not in the neighborhood of the turning point $r_1(Q^2=0)$, it usually suffices to take

$$f=iQ-\tfrac{1}{2}(Q'/Q), \tag{18}$$

and the second term here contributes little.

Let

$$\xi=\int_{r_1}^{r} Q dr, \quad S(r)=Q^{-\frac{1}{2}}(r)\xi^{\frac{1}{2}},$$

and $\theta=S''/S$. Then

$$U(r;\alpha,\beta)=S\{\alpha\xi^{\frac{1}{2}}J_{-\frac{1}{3}}(\xi)+\beta\xi^{\frac{1}{2}}J_{\frac{1}{3}}(\xi)\} \tag{19}$$

satisfies the differential equation

$$U''+(Q^2-\theta)U=0.$$

This equation resembles (5) when $\theta\ll Q^2$. Langer[10] finds the asymptotic form of U and is thus able to establish the connection formula

$$|Q(r)|^{-\frac{1}{2}}\exp\left[-\int_r^{r_1}|Q|dr\right] \rightarrow 2Q^{-\frac{1}{2}}(r)\cos\left\{\int_{r_1}^{r}Qdr-\frac{\pi}{4}\right\}, \tag{20}$$

which gives the phase shift for a given Q. He shows that, in evaluating this phase shift, one must replace $l(l+1)$ by $(l+\frac{1}{2})^2$. However, if we use the WKB method for a region completely outside the turning point, the proper quantity to use is still $l(l+1)$, for the connection formula plays no part. Langer notes that when l is small or when E is large, the turning point is near to $r=0$, and the use of the connection formula is then questionable. We shall see that the WKB method is, with these exceptions, quite reliable.

Mott and Massey[11] state that "the condition for classical scattering at a given angle θ is that l_0 should be large, where l_0 is the value of l for which $(\partial\eta_l/\partial l)=\frac{1}{2}\theta$, *and that* η_l *should also be large for this value.*" From this, one infers that the WKB method should yield good results only when the phase shifts are large. Our work does not indicate this.

Phase Shifts

We have used the WKB method (1) to continue the differential analyzer solutions outward and (2) to determine the phase shifts in an independent way.

(1) Continuation of analyzer solutions

Let us denote initial values with the subscript i. As above, set

$$\xi=\int_{r_i}^{r} Q dr,$$

and

$$y=(Q_i/Q)^{\frac{1}{2}}(a\cos\xi+b\sin\xi). \tag{21}$$

Then $y_i=a$, and $y_i'=-\frac{1}{2}a(Q'/Q)_i+bQ_i$. If $a=1$,

$$bQ_i=(y'/y)_i+\tfrac{1}{2}(Q'/Q)_i\cong(y'/y)_i. \tag{22}$$

(The term Q'/Q is approximately $j(j+1)/2r^3Q^2$, and is usually negligible.)

If we put $\xi=kr-\delta(r)$, then $\delta(\infty)$ will be simply related to the phase shift η_κ, which is defined[12] so that it vanishes for a free particle, i.e.,

$$y_\kappa\cong rG_\kappa\sim\cos[kr-\tfrac{1}{2}(l+1)\pi+\eta_\kappa]. \tag{23}$$

From (21),

$$y\sim A\sin(kr-\delta)+B\cos(kr-\delta)$$
$$=(A\cos\delta+B\sin\delta)\sin kr$$
$$+(B\cos\delta-A\sin\delta)\cos kr.$$

[9] R. E. Langer, Bull. Am. Math. Soc. **40**, 574 (1934).
[10] R. E. Langer, Phys. Rev. **51**, 669 (1937).
[11] N. F. Mott and H. S. W. Massey, *Atomic Collisions* (Oxford University Press, 1933), pp. 92–94.
[12] M. E. Rose and H. A. Bethe, Phys. Rev. **55**, 280 (1939), Eq. (21).

TABLE II. *Phase shifts.*

a. $E=100$ kv

l	Differential Analyzer η_l	η_{-l-1}	Δ_l	WKB η_l	η_{-l-1}	Δ_l	Curve l	η_l	Born η_l
0		237.9							
1	199.2°	174.2°	25.0°	195.0°	176.0°	18.9°	Same as		
2	149.6	143.9	5.7	150.9	143.4	7.2	D.A.		
3	125.5	121.0	4.5	126.5	122.5	3.7	Up to		
4	110.3	108.1	2.2	109.3	106.9	2.4	$l=8$		
5	97.7	96.7	1.0	98.5	97.0	0.7	6	87.9°	
7	80.7			75.9	75.5		8	74.0	
9	68.5						9	68.2	
							10	63.3	
11	59.3			58.5			11	59.0	
							12	54.9	
							13	51.1	
							14	48.0	
15	44.4			45.0			15	45.0	
							16	42.4	
							17	40.0	
							18	38.0	
19	32.4						19	36.0	34.9°
							20	34.2	
22				31.2			22	31.0	
24	27.8						24	28.3	29.2
							26	26.0	
							28	23.8	
29	21.5			22.2			29		24.6
							30	21.9	
							32	20.2	
							34	18.6	
35				17.9			35		20.1
							36	17.2	
							38	16.0	
							40	14.9	17.2
							45	12.4	14.6
50				10.3			50	10.3	12.6

b. $E=230$ kv

j	D.A. η_j	l	WKB η_l	η_{-l-1}	Δ_l	l	Curve η_l	Δ_l	Born η_l
−1	207.3°								
1	183.2	1	176.7°	155.1°	21.6°	1	183.2°	21.6°	
2	141.5	2	138.8	130.3	8.5	2	141.5	9.0	
3	120.2	3	118.6	113.2	5.3	3	120.2	5.2	
4	106.2	4	105.1	101.6	3.5	4	106.2	3.5	
5	97.7	5	94.8	92.1	2.7	5	97.7	2.7	
						6	87.3	2.2	
						7	80.5	1.9	
		8			1.7	8	75.0	1.63	
						9	70.0	1.41	
						10	65.7	1.22	
11	64.4	11	62.7			11	62.1	1.05	
						12	59.0	0.92	
						13	56.0	0.80	
						14	53.2	0.68	
		15	49.7		0.6	15	50.8	0.60	
						16	48.4		
						17	46.2		
						18	44.2		
						19	42.3		
		20	41.9			20	40.5		35.2°
						21	38.9		
						22	37.3		
						24	34.4		
						26	31.9		
						28	29.7		
		30	28.1			30	27.7		26.4
						35	23.4		
		40	19.3			40	20.2		20.3
						45	17.7		
		50	15.1			50	15.7		15.9
						55	14.1		
						60	12.7		
		65	11.5			65			11.4
						70	10.5		
		80	9.2			80	8.6		8.4
		100	5.9			100			5.8

$\Delta_l = 5.250e^{-0.1446l}$

Combining with (23), and putting

$$(A/B)=\tan\epsilon=b/a, \tag{24}$$

we obtain

$$-\tan\left[\eta_\kappa-\tfrac{1}{2}(l+1)\pi\right]=\left[(A\cos\delta+B\sin\delta)/(B\cos\delta-A\sin\delta)\right]_\infty=\tan(\epsilon+\delta_\infty). \tag{25}$$

Furthermore, if $Q_0^2=k^2-[j(j+1)/r^2]$,

$$-\delta=\xi-kr=\int_{r_i}^{r}(Q-Q_0)dr+\int_{r_i}^{r}Q_0dr-kr$$

$$=\int_{r_i}^{r}(Q-Q_0)dr+rQ_0\Big|_{r_i}^{r}-[j(j+1)]^{\frac{1}{2}}\cos^{-1}\{[j(j+1)]^{\frac{1}{2}}/kr\}\Big|_{r_i}^{r}-kr. \tag{26}$$

The limiting value is

$$-\delta_\infty=\int_{r_i}^{\infty}(Q-Q_0)dr-r_iQ_0^{(i)}-[j(j+1)]^{\frac{1}{2}}\left[\tfrac{1}{2}\pi-\cos^{-1}\left([j(j+1)]^{\frac{1}{2}}/kr_i\right)\right]. \tag{27}$$

ξ was expanded in powers of $s=j(j+1)$ and numerical integrations were performed from $r_i=0.26$ to infinity. The resulting expressions for δ_∞ are

$$\delta_\infty=23.317+0.0211s+3.16\times10^{-6}s^2+\cdots \qquad (E=100\text{ kv})$$
$$\delta_\infty=37.806+0.01312s+0.7565\times10^{-6}s^2+\cdots \qquad (E\geqq230\text{ kv, or } q=0.8).$$

The phase shift η_κ was determined from (22), (24), (25) and (27).

TABLE III. *Coefficients in numerical summation of (33).*

l	a_l	b_l	l	a_l	b_l	l	a_l	b_l	l	a_l	b_l
		$E=100$ kv						$E=230$ kv			
0	−9.394	0.589	10	−5.985	−5.298	0	2846.37	850.11	16	269.98	149.42
1	−26.216	−0.822	11	−4.039	−4.064	1	5986.47	1864.48	17	192.99	110.21
2	−32.942	−7.707	12	−2.750	−2.930	2	6994.46	2269.13	18	136.50	80.28
3	−31.721	−11.507	13	−1.949	−2.012	3	6860.86	2320.11	19	95.38	57.66
4	−28.265	−12.983	14	−1.154	−1.369	4	6174.71	2176.12	20	65.70	40.75
5	−23.620	−12.585	15	−0.778	−0.877	5	5277.43	1937.48	21	44.61	28.28
6	−19.089	−11.307	16	−0.455	−0.512	6	4356.53	1666.86	22	29.66	19.13
7	−14.906	−10.070	17	−0.315	−0.350	7	3506.36	1396.93	23	19.25	12.54
8	−11.337	−8.367	18	−0.037	−0.111	8	2767.73	1147.08	24	12.07	7.94
9	−8.404	−6.724	19	0	−0.051	9	2150.64	926.89	25	7.45	4.82
						10	1649.03	738.69	26	4.22	2.63
						11	1249.97	581.42	27	2.30	1.25
						12	937.77	452.45	28	1.09	0.43
						13	696.66	348.42	29	0.28	
						14	512.65	265.56	30	0.09	
						15	373.90	200.26			

(2) Phase shifts from the connection formula

From (20) and (23), we find that

$$\xi-\tfrac{1}{4}\pi=kr-\tfrac{1}{2}(l+1)\pi+\eta_\kappa,$$

and hence,[13]

$$\eta_\kappa=\tfrac{1}{2}(l+\tfrac{1}{2})-\delta_\infty(r_i=r_1),$$

$$=\lim_{r\to\infty}\left(\int_{r_1}^{r}Qdr-\int_{r_0}^{r}Q_0dr\right). \tag{28}$$

This is consistent with (27) if $l+\frac{1}{2}$ be substituted for $[j(j+1)]^{\frac{1}{2}}$.

In Table II are listed the phase shifts as determined (1) with differential analyzer and WKB extension, (2) from the connection formula, (3) from a smooth curve through points found by methods (1) and (2), and (4) by the first-order Born approximation.

Method (4) consisted in applying a formula of Mott and Massey.[14] Since this involves the square of the wave function, the region near the origin contributes little, and the potential may be taken as just $2EV/c^2$.

Results from methods (1) and (2) are in excellent agreement with each other, so that the connection formula method is accurate as well as rapid. The Born phase shifts are surprisingly good, even though the expansion parameter q is not small ($q=0.8$ and 1.056).

INTENSITY OF SCATTERING

With the notation changed as in footnote 4, we have, following Mott[15] and Darwin,[4] as the solutions of (1): F_l, G_l, which refer to the state $j'=-l-1$. The asymptotic form of G_l is $r^{-1}\cos(kr+\delta_l)$. The connection with the previous notation[16] is obtained by setting

$$\eta_{-l-1}-\tfrac{1}{2}(l+1)\pi=\delta_l,\quad \eta_l-\tfrac{1}{2}(l+1)\pi=\delta_{-l-1}.$$

[13] M. E. Rose and H. A. Bethe, Phys. Rev. **55**, 286 (1939), Eq. (103).
[14] Reference 11, p. 28, Eq. (27). See Appendices B and C.
[15] N. F. Mott, Proc. Roy. Soc. **135**, 436 (1932).
[16] See Eq. (23). The quantum number κ of Rose and Bethe (reference 7) is equal to $-j'-1$.

TABLE IV. *Amplitudes, intensity, and polarization.*

a. $E=100$ kv

θ	f R	f I	g R	g I	r	r_c	δ
2°	−460.0	391.0			0.12		
5°	8.5	150.9			0.30		
10°	41.7	25.3			0.49		
15°	23.68	5.19	0.024	−0.187	0.61	1.02	
30°	−0.66	7.123	−0.089	−0.270	0.82	1.06	
45°	−3.06	2.182	−0.272	−0.208	0.94	1.18	
60°	−2.464	0.174	−0.378	−0.054	1.40	1.36	
75°	−1.55	−0.788	−0.378	0.096	1.56		0.009
90°	−0.762	−1.051	−0.327	0.188	1.64	1.68	0.048
105°	−0.280	−1.065	−0.255	0.222	1.89		0.099
120°	0.008	−0.997	−0.179	0.213	2.16	1.78	0.113
135°	0.280	−0.847	−0.115	0.173	2.19		0.120
150°	0.523	−0.639	−0.065	0.117	2.18	1.83	0.086
165°	0.579	−0.482	−0.027	0.058	(1.98)		0.026
180°	0.492	−0.585	0	0	2.10	1.83	

b. $E=230$ kv ($q=0.8$)

θ	f R	f I	g R	g I	r	r_c	δ
2°	380.1	497.6			0.23		
5°	25.1	150.1			0.52		
10°	−42.5	7.2			0.67		
15°	23.3	11.2			1.22	1.04	
30°	0.94	6.25	−0.03	−0.63	1.13	1.17	
45°	−2.03	2.81			1.65	1.37	
60°	−1.60	1.43	0.40	−0.23	1.88	1.58	
75°	−1.21	0.13			1.43		
90°	−0.91	−0.30	0.39	0.03	1.67	1.82	0.025
105°	−0.87	−0.41			2.58		
120°	−0.73	−0.96	0.26	0.09	(5.46)	1.68	
135°	−0.04	0.59			1.59		
150°	−0.09	0.28	0.13	0.05	0.57	1.43	

Then

$$f(\theta)=\tfrac{1}{2}i\sum_{l=0}^{\infty}\{(l+1)(\exp[i(2\eta_{-l-1}-\pi)]+1)+l(\exp[i(2\eta_l-\pi)]+1)\}P_l(\cos\theta)$$

$$=-\tfrac{1}{2}i\sum_{l=0}^{\infty}\{(l+1)(\exp[2i\eta_{-l-1}]-1)+l(\exp[2i\eta_l]-1)\}P_l(\cos\theta), \tag{29}$$

$$g(\theta)=\tfrac{1}{2}i\sum_{l=1}^{\infty}\{\exp[2i\eta_{-l-1}]-\exp[2i\eta_l]\}P_l^1(\cos\theta),$$

$$(2f/i)=\sum_{l=0}^{\infty}(2l+1)(A_l-iB_l)P_l(\cos\theta), \tag{30}$$

where

$$(2l+1)A_l=(l+1)(1-\cos 2\eta_{-l-1})+l(1-\cos 2\eta_l)$$

$$(2l+1)B_l=(l+1)\sin 2\eta_{-l-1}+l\sin 2\eta_l$$

$$(-2g/i)=\sum_{l=1}^{\infty}2\sin\Delta_l\{-\sin\Sigma_l+i\cos\Sigma_l\}P_l^1(\cos\theta), \tag{31}$$

where

$$\Delta_l=\eta_l-\eta_{-l-1},\quad \Sigma_l=\eta_l+\eta_{-l-1}.$$

For large values of l, the phase shifts decrease in an exponential manner, and so we would expect a similar behavior for A_l and B_l, which is in fact found. Exponential functions $A_\infty(l)$ and $B_\infty(l)$ were fitted in this range, as follows:

$$\left.\begin{aligned}A_\infty(l)&=2.490e^{-0.0733l}+8.342e^{-0.250l}\\B_\infty(l)&=2.082e^{-0.0356l}-1.772e^{-0.148l}\end{aligned}\right\}E=100\text{ kv}$$

$$\left.\begin{aligned}A_\infty(l)&=0.9554e^{-0.0382l}+65.1e^{-0.192l}-2912e^{-0.351l}\\B_\infty(l)&=1.310e^{-0.0186l}+49.4e^{-0.188l}-900e^{-0.304l}\end{aligned}\right\}E=230\text{ kv}. \tag{32}$$

Equation (30) may be written

$$(2f/i)=\sum_{l=0}^{\infty}(2l+1)[A_\infty(l)-iB_\infty(l)]P_l(\cos\theta)+\sum_{l=0}^{\infty}(2l+1)[(A_l-A_\infty(l))-i(B_l-B_\infty(l))]P_l(\cos\theta). \tag{33}$$

The first term on the right-hand side may be evaluated by summing analytically, and the second by summing numerically. The analytical summation is based on the formula

$$\sum_{l=0}^{\infty}(2l+1)x^l P_l(\cos\theta)=(1-x^2)/(1-2x\cos\theta+x^2)^{\frac{3}{2}} \tag{34}$$

and on the substitution $x=e^{-a}$, where a is one of the constants in (32).

We give in Table III the coefficients of the second sum,

$$a_l=(2l+1)[A_l-A_\infty(l)] \quad \text{and} \quad b_l=(2l+1)[B_l-B_\infty(l)].$$

This method of summation would be less practical for higher energies, because $P_l(\cos\theta)$ is tabulated[17] only to $l=32$.

At $E=100$ kv, the sum in (31) converges rapidly, and only seven terms were calculated. For $E=230$ kv, however, the convergence is not as good, and one needs about twenty-five terms. One would expect a behavior of this sort, because for higher energies the electrons come closer to the nucleus, and the spin-orbit interaction terms can therefore be of more influence.

After summing the series (30) and (31) for f and g, we have, as in our previous paper, multiplied the values of $|f|^2+|g|^2$ by $(4/q^2)\sin^4\frac{1}{2}\theta$, in order to find the ratio r of our calculated scattering intensity to the "Rutherford" value. Furthermore, the asymmetry 2δ in double scattering, $2\delta=2[(fg^*-gf^*)/(|f|^2+|g|^2)]^2$, has been obtained. The results are given in Table IV, together with r_c, the ratio for a Coulomb field.

Results

The results for 100 kv are what one might expect. At large angles the distribution is practically the same as that obtained for a Coulomb field. (The discrepancies are not large, and are probably caused by small errors in the determination of the phase shifts for small l.) At small angles, in this case angles less than 60°, the effects of shielding become evident, and the intensity of scattering is less than the Coulomb value.

For 230 kv, the calculations are probably not very accurate, since reliance was placed on the WKB method to a great extent. In particular, it would have been desirable to have had data from the differential analyzer for $j=-2$ to $j=-6$, inclusive. (Such runs had been taken, but were later proved to be incorrect.) The values of r in Table IV fluctuate, but it is probably legitimate to conclude that the angular distribution is of the Coulomb character for angles greater than 15°, and that the shielding is only effective for smaller angles.

Summary and Conclusions

For a given value of the Dirac angular momentum quantum number j, one can eliminate one component of the radial wave function, and obtain a single Schroedinger-like equation for the motion of an electron. The electron is influenced by an effective field (we have called it the Dirac field) which is dependent on the energy, and which may be deduced from the Hartree field.

We have calculated the scattering intensity for electrons of 100 kv and 230 kv influenced by mercury atoms. The Hartree field is known, and the Dirac field was found. Phase shifts were determined by three different methods: (1) integration with the aid of the differential analyzer, (2) the WKB method, and (3) with the Born approximation.

The WKB phases are in excellent agreement with the analyzer phases for 100 kv, and in good agreement for 230 kv. This method seems, therefore, to be rather reliable, and our results do not indicate that it should break down for small phase shifts.

The first-order Born approximation results, for large values of l, in phase shifts which agree well with those calculated by the other methods. The first-order wave function is, however, quite different from the unperturbed one, and so the reason for the smallness of higher order corrections to the phase shifts is not known.

[17] H. Tallquist, Soc. Scient. Fennica, Comm. Phys.-Math. **6**, Nos. 3 and 10 (1933).

The angular distribution appears to be Coulombian for large angles, within the limits of error of our calculations. The shielding becomes effective below 60° for 100-kv electrons, and below 15° for 230-kv electrons.

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Appendix A

Differential analyzer procedure

Having obtained $(y'/y)_{r=0.002}$, we integrated Eq. (5) outward, setting $Q^2(r)=\mathfrak{F}(r)+j\mathfrak{G}(r)-[j(j+1)/r^2]$, where

$$\mathfrak{F}(r)=k^2-\frac{2EV}{c^2}+\frac{V^2}{c^2}-\frac{1}{2\Pi c}\frac{d^2V}{dr^2}-\frac{3}{4}\frac{1}{\Pi^2c^2}\left(\frac{dV}{dr}\right)^2,$$

and

$$\mathfrak{G}(r)=\frac{1}{r\Pi c}\frac{dV}{dr}.$$

$\mathfrak{F}(r)$ was fed in from one input table, $\mathfrak{G}(r)$ from another, and $1/r^2$ was usually generated by two integrators.

The integration range was divided into three or four sections (0.002−0.016−0.065−0.26−0.65) and dependent variables chosen so as to have the same order of magnitude throughout the section. Near the origin, y behaves as $r^{\rho+\frac{1}{2}}$. We substituted $y=r^{j+1}z$ when $j>0$; $y=r^{|j|}z$ when $j<0$, and used z as the dependent variable. (This made the term in $1/r^2$ vanish.) For large r, y varies sinusoidally, and was used itself. (It might be more accurate to take out the sinusoidal factor, but this was not done for lack of time.) For large values of j, we used the variable $w=yr^{-p}$, where p was some appropriate integer less than j.

Appendix B

Born approximation formulae

The first-order phase shift is to be found from

$$\tan\eta_k=-(\pi/2k)\int_0^\infty(2EV/c^2)[J_{l+\frac{1}{2}}(kr)]^2rdr,$$

where

$$-2rV=2Z_p=33.7e^{-17.376r}+95.9e^{-3.892r}+30.3e^{-1.253r}.$$

The integration and evaluation may be made with the aid of two formulas given by Watson.[18]

$$\int_0^\infty e^{-at}J_\nu(bt)J_\nu(ct)dt=[1/\pi(bc)^{\frac{1}{2}}]Q_{\nu-\frac{1}{2}}\{(a^2+b^2+c^2)/2bc\}.$$

$$Q_l(\cosh\xi)\cong e^{-(l+\frac{1}{2})(\xi-\tanh\xi)}(\operatorname{sech}\xi)^{\frac{1}{2}}K_0[(l+\tfrac{1}{2})\tanh\xi].$$

Appendix C

Note on the Born approximation

Equation (5) may be written in the form

$$y''+\{k^2+[(\tfrac{1}{4}-\rho^2)/r^2]\}y=Uy, \qquad (35)$$

where U has a pole of order one at the origin. A fundamental set of solutions of the homogeneous equation ($U=0$) is

$$v_1=(\tfrac{1}{2}\pi kr)^{\frac{1}{2}}J_\rho(kr); \qquad v_2=(\tfrac{1}{2}\pi kr)^{\frac{1}{2}}J_{-\rho}(kr).$$

For simplicity, consider the Coulomb equation

$$u''+\{-\tfrac{1}{4}+[(\tfrac{1}{4}-\rho^2)/r^2]\}u=-(\lambda\alpha/r)u \qquad (36)$$

where λ is a constant, and ρ will be taken as independent of α.

I. Let $$u=\sum_{s,t=0}^{\infty}u_{s,t}r^{\omega+s}\alpha^t,$$

and require $u_{0,t}=0$ for $t>0$ (normalization condition). The only acceptable exponent is $\omega=\frac{1}{2}+\rho$, and the recursion formula is

$$[(\rho+s+2)^2-\rho^2]u_{s+2,t}=\tfrac{1}{4}u_{s,t}-u_{s+1,t-1}.$$

(All coefficients with negative subscripts are to vanish.) The nonzero coefficients are found to be those with $s\geq0$ and $t=s-2p\geq0$, where

$$p\geq0. \quad \text{That is,} \quad s\geq t. \qquad (37)$$

II. The procedure of I may be modified (*a*) by expanding in powers of α and then (*b*) solving a set of inhomogeneous equations successively. This is convenient for ascertaining the behavior for large r. If $u=\sum_{t=0}^{\infty}u_t\alpha^t$, then

$$u_t''+\{-\tfrac{1}{4}+[(\tfrac{1}{4}-\rho^2)/r^2]\}u_t=-(\lambda u_{t-1}/r), t=1,\cdots\infty. \qquad (38)$$

Since $u_0=v_1$, the solution of (38) with $t=1$ is[19] $u_1=V_1(r)v_1+V_2(r)v_2$, where $V_1=\lambda\int_a^r(v_1v_2/rW)dr$, $V_2=-\lambda\int_b^r(v_1^2/rW)dr$, and W is the Wronskian of v_1 and v_2. The limits a and b must be such that u is regular at $r=0$. At this point, $u_0=v_1=O(r^{\frac{1}{2}+\rho})$ and $v_2=O(r^{\frac{1}{2}-\rho})$. From (37), $s_{\min}=t$, and so $u_1=O(r^{\frac{1}{2}+\rho})$, V_1 must be $O(r)$ and V_2 must be $O(r^{2\rho+1})$. These conditions will be satisfied if and only if $a=0$ and $b=0$.

[18] Watson, *Bessel Functions* (Cambridge University Press, 1922), pp. 389 and 158.

[19] E. L. Ince, *Ordinary Differential Equations* (Longmans, 1927), p. 122.

Evidently the above conclusions will be true when U still has a pole of order one at $r=0$, but is non-Coulomb. With V_1 and V_2 modified accordingly, the first-order wave function will be

$$u=\{1+\alpha V_1(r)\}v_1+\alpha V_2(r)v_2. \quad (39)$$

At large r, $v_1\sim\sin(kr-\frac{1}{2}\rho\pi)$ and $v_2\sim\cos(kr+\frac{1}{2}\rho\pi)$. Hence $u\sim$const $\{\cos(kr-\frac{1}{2}l\pi)\sin\eta_\kappa+\sin(kr-\frac{1}{2}l\pi)\cos\eta_\kappa\}$ where

$$\tan\eta_\kappa=\frac{\{1+\alpha V_1(\infty)\}\sin\frac{1}{2}(l-\rho)\pi+\alpha V_2(\infty)\cos(l+\rho)\pi}{\{1+\alpha V_1(\infty)\}\cos\frac{1}{2}(l-\rho)\pi-\alpha V_2(\infty)\sin(l+\rho)\pi}$$
$$=\alpha V_2(\infty) \text{ to first order in } \alpha.$$

At $r=\infty$, the first-order wave function contains $\alpha V_1(\infty)$, which is of order unity,[20] and so the function has been greatly modified by the perturbation. Nevertheless, as seen above, this is without effect[21] on the *first-order* phase shift.

[20] We calculated $\alpha V_1(\infty)$ for $l=22$, $E=100$ kv assuming the potential to be $-2EV/c^2$, and integrating numerically with the aid of a Gegenbauer formula (reference 18, p. 390). The result, which should be roughly correct, was near unity.

[21] This became clear during a discussion with Drs. Lamb and Nordsieck of Columbia University, to whom thanks are due for their interest and help.

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A Note on the Analysis of Liquid X-Ray Diffraction Patterns

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The corrected intensity curve given by Eisenstein and Gingrich for the diffraction of x-rays by liquid argon has been subjected to four different fittings, one of them including a weak fourth peak, to determine how sensitive the atomic distribution curve is, to errors in fitting. An analysis has been made for these four cases. The first peak of the atomic distribution curve has about the same shape in each case, the area under this peak varies by less than ten percent, and the position of its maximum remains constant to within about one and one-half percent. The small secondary peak becomes a plateau by the introduction of a weak fourth peak in the intensity curve.

THE method of the Fourier integral analysis of x-ray diffraction patterns[1] is reasonably straightforward in principle, but, in practice, difficulties sometimes arise which make the conclusions from this analysis somewhat uncertain. Thus, for example, it is assumed that at large angle, the scattered x-rays are wholly made up of incoherent and independent coherent radiation, and in this way, the experimental intensity curve is placed on the same scale as the Nf^2 curve. Experimentally, one chooses a point in the diffraction curve beyond which no interference effects can be observed and then makes a fitting of the curves at this point. With weak radiation at large angles, it is difficult to be sure that this point is chosen at large enough angle, and hence uncertainty in the results and conclusions is introduced. Since there is no obvious general approach to the discussion of the effect of different fitting of curves, a few special cases have been worked out to illustrate the effect upon the atomic distribution curve in the case of liquid argon of different fittings in the experimental intensity curve for liquid argon.

In previous work[2] with liquid argon, the experimental curves obtained in several trials consistently showed three maxima, at values of $\sin\theta/\lambda$ of 0.154, 0.280 and 0.415, respectively. One, or possibly two films, showed a faint trace of a fourth maximum, but the films with apparently the best patterns did not show convincing evidence of the existence of the fourth peak, for if it existed on them, it must have had a height no greater than the fluctuations of the microphotometer. With a small camera, of 5.08 cm radius, two overexposed pictures were taken to investigate the region where slight indications of a fourth peak occurred. Superimposed on the dense background, there appeared a weak fourth

[1] B. E. Warren and N. S. Gingrich, Phys. Rev. **46**, 368 (1934).

[2] A. Eisenstein and N. S. Gingrich, Phys. Rev. **58**, 307 (1940).