atomic number varies approximately as $Z^{4/3}$ (in agreement with the predictions of the Fermi-Thomas statistical model of the atom, but with a different proportionality constant) for the light atoms, but the binding energy varies as $Z^{12/5}$ for heavy atoms. Consequently, binding energies for atoms near the end of the periodic table will be approximately 15 percent too low when calculated by the Fermi-Thomas expression with a coefficient chosen to give agreement with experimental values for the light elements.

(2) In so far as the charge distribution in heavy atoms can be specified by a single "atomic radius," this atomic radius varies with Z approximately as $Z^{-7/5}$.

(3) On the basis of Dickinson's estimates of the accuracy of the values of eV given by (1), one would estimate that the accuracy of Eq. (3) for atomic binding energies should be 5 percent or better.

Unfortunately, the possibility of a direct experiment test of the foregoing conclusions appears very remote at the present time.

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The Theory of Internal Conversion*

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The theory of the internal conversion process is presented on a firm quantum-mechanical foundation and in a form most convenient for calculations. The question of the correct gauge for the radiation potentials and the effect of the finite size of the nucleus on these potentials are considered.

I. INTRODUCTION

THE theory of the internal conversion process has been developed by Mott[1] and by Taylor and Mott[2] on the basis of correspondence principle arguments. In 1936, Hulme[3] discussed the interaction of two particles in a form applicable to the theory of internal conversion. This paper put the theory on a firm quantum-mechanical foundation so far as the matrix elements used in the calculation of N_e, the number of electrons ejected per second, were involved. Unfortunately, Hulme's explicit introduction of the coulomb direct interaction and his expansion of the radiation field in a series of plane rather than spherical waves made it impossible to compare the theory directly with the prescription followed by the calculators of internal conversion coefficients. Up to the present date, no rigorous quantum-mechanical derivation of the matrix elements used in the calculation of N_q, the number of gamma-quanta emitted per second, has been presented.

In view of the recent exact calculations of internal conversion coefficients,[4–6] it seems that a rigorous quantum-mechanical investigation of the internal conversion process is desirable.

II. THE PROBLEM

It is desired to calculate the transition probability from the initial state in which the nucleus is excited, the electron is in its ground state (bound electron), and no quanta are present to a final state in which the nucleus is in its ground state, the electron is in its excited state (continuum electron), and no quanta are present. The nucleus and the electron interact with each other only through the electromagnetic field coupling. Since no quanta are present initially or finally, the intermediate states are those for which a single quantum is present, and either both nucleus and electron are in their ground states (first intermediate state) or both are excited (second intermediate state). The first intermediate state corresponds to a double process in which the nucleus makes a transition to its ground state and emits a gamma-quantum, and the electron makes a transition to its excited state and absorbs this quantum. Since the intermediate state need not conserve energy, the energy of the gamma-quantum does not have to equal the initial excitation energy of the nucleus. The second intermediate state corresponds to a double process in which the electron makes a transition to its excited state and emits a gamma-quantum, and the nucleus makes a transition to its ground state and absorbs this quantum. In this case it is apparent that the intermediate state cannot conserve energy.

The description of the states is summarized in Table I.

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[1] N. F. Mott, Ann. inst. Henri Poincaré 4, 207 (1933).

[2] H. M. Taylor and N. F. Mott, Proc. Roy. Soc. (London) A142, 215 (1933).

[3] H. R. Hulme, Proc. Roy. Soc. (London) A154, 487 (1926).

[4] Rose, Goertzel, Spinrad, Harr, and Strong, Phys. Rev. 76, 1883 (1949); and privately circulated tables of results.

[5] B. A. Griffith and J. P. Stanley, Phys. Rev. 75, 534 (1949).

[6] J. R. Reitz, Phys. Rev. 77, 10 (1950).

TABLE I. Description of states.

State	Nucleus	Electron	Number of quanta	Energy	Prob. amp.
Initial	excited	ground	0	W	a
First intermediate	ground	ground	1	k	b_k
Second intermediate	excited	excited	1	$W+k+E$	b_k'
Final	ground	excited	0	E	c_E

The equations for the probability amplitudes are[7]

$$i\dot{a}=Wa+\int dkH_{0k}b_k+\int dkH_{0k}'b_k', \tag{2a}$$

$$i\dot{b}_k=kb_k+H_{k0}a+\int dEH_{kE}c_E, \tag{2b}$$

$$i\dot{b}_k'=(k+W+E)b_k'+H_{k0}'a+\int dEH_{kE}'c_E, \tag{2c}$$

$$i\dot{c}_E=Ec_E+\int dkH_{Ek}b_k+\int dkH_{Ek}'b_k', \tag{2d}$$

with the initial conditions

$$a(0)=1,\quad b_k(0)=b_k'(0)=c_E(0)=0. \tag{2e}$$

In the above equations, $\int dk$ denotes integration over all gamma-ray energies and summation over all multipoles in the radiation field, while $\int dE$ denotes integration over all energies of the continuum electron and summation over the spins. The matrix elements are

$$\left.\begin{aligned}
H_{Ek}&=e(2\pi/k)^{\frac{1}{2}}\int d\tau\Psi_f^*[\boldsymbol{\alpha}\cdot\mathbf{A}_{LM}{}^{(i)}(kr)\\
&\qquad+i\phi_L{}^{M(i)}(kr)]\Psi_0,\\
H_{Ek}'&=e'(2\pi/k)^{\frac{1}{2}}\int d\tau'\Phi_f^*[\boldsymbol{\alpha}'\cdot\mathbf{A}_{LM}{}^{(i)}(kr')\\
&\qquad+i\phi_L{}^{M(i)}(kr')]\Phi_0,\\
H_{k0}&=e'(2\pi/k)^{\frac{1}{2}}\int d\tau'\Phi_f^*[\boldsymbol{\alpha}'\cdot\mathbf{A}_{LM}{}^{(i)*}(kr')\\
&\qquad-i\phi_L{}^{M(i)*}(kr')]\Phi_0,\\
H_{k0}'&=e(2\pi/k)^{\frac{1}{2}}\int d\tau\Psi_f^*[\boldsymbol{\alpha}\cdot\mathbf{A}_{LM}{}^{(i)*}(kr)\\
&\qquad-i\phi_L{}^{M(i)*}(kr)]\Psi_0
\end{aligned}\right\} \tag{2f}$$

in which Ψ and Φ are, respectively, the electronic and nuclear wave functions with the subscripts 0 and f referring to the initial and final states. Here e, r, $d\tau$, and $\boldsymbol{\alpha}$ refer, respectively, to the charge, position, volume element, and Dirac operator for the electron. The corresponding primed quantities refer to the nucleus. And $\mathbf{A}_{LM}{}^{(i)}$ and $i\phi_L{}^{M(i)}$ are, respectively, the vector and scalar potentials for the 2^Lth multipole of the ith type (electric, magnetic, or longitudinal).

III. SOLUTION BY USE OF THE LAPLACE TRANSFORMS

The system of Eqs. (2a–d) is most easily solved by the use of the laplace transformation. In contrast to the direct method of solution,[8] no assumption as to the general form of the solution has to be made.

We denote the laplace transforms by the use of capitals. For example,[9]

$$L\{a\}=A=\int_0^\infty e^{-st}a(t)dt, \tag{3a}$$

where $s=\eta-i\omega$, and $\eta\geqslant 0$. After applying the initial conditions (2e) and making the substitution $\omega_0=W+E-\omega$, the transforms of Eqs. (2a–d) are

$$(W-\omega-i\eta)A=-i-\int dkH_{0k}B_k-\int dkH_{0k}'B_k', \tag{3b}$$

$$(k-\omega-i\eta)B_k=-H_{k0}A-\int dEH_{kE}C_E, \tag{3c}$$

$$(k+\omega_0-i\eta)B_k'=-H_{k0}'A-\int dEK_{kE}'C_E, \tag{3d}$$

$$(E-\omega-i\eta)C_E=-\int dkH_{Ek}B_k-\int dkH_{Ek}'B_k'. \tag{3e}$$

Before proceeding to the solution of these equations, a discussion of the order of approximation required is appropriate. For the radiation processes[10] which we are considering, $|c_E|^2$ is proportional to e^4. Therefore, as will be seen from the mathematics below, A must be determined in fourth approximation. The zeroth approximation of A gives $a(t)$ as a periodic function of the time; the second approximation gives the decay of $a(t)$ with the emission of the gamma-quantum; and the fourth approximation gives the decay of $a(t)$ with both the emission of the gamma-quantum and the ejection of the extra-nuclear electron. Since the first approximation does not include the effect of the presence of the extra-nuclear electron, B_k need be deter-

[7] Relativistic units with $\hbar=m=c=1$ are used throughout. In the usual notation the equations are of the form:

$$i\dot{b}_m=\Sigma_n\int b_n\psi_m{}^{0*}H'\psi_n{}^0\exp\{i(E_n{}^0-E_m{}^0)t\}d\tau.$$

We set $a_m=b_m\exp(-iE_m{}^0t)$ and substitute, obtaining

$$i\dot{a}_m-E_m{}^0a_m=\Sigma_n\int a_n\psi_m{}^{0*}H'\psi_n{}^0d\tau.$$

[8] See, for example, W. Heitler, *The Quantum Theory of Radiation* (Oxford University Press, New York, 1944).

[9] See any book on laplace transforms; for example, R. V. Churchill, *Modern Operational Mathematics in Engineering* (McGraw-Hill Book Company, Inc., New York, 1944).

[10] See, for instance, Heitler, reference 8, p. 97.

mined in third approximation; C_E need be determined in second approximation only.

In zeroth approximation (3b) gives

$$(W-\omega-i\eta)A=-i. \tag{3f}$$

Substitution of (3f) into (3c, d) yields B_k and B_k' in first approximation:

$$(k-\omega-i\eta)B_k=-H_{k0}A, \tag{3g}$$

$$(k+\omega_0-i\eta)B_k'=-H_{k0}'A. \tag{3h}$$

Substitution of (3g, h) into (3e) gives C_E in second approximation:

$$(E-\omega-i\eta)C_E=A\int dk\left[\frac{H_{Ek}H_{k0}}{k-\omega-i\eta}+\frac{H_{Ek}'H_{k0}'}{k+\omega_0-i\eta}\right], \tag{3i}$$

where the integral over k, which we denote by U_{f0}, is evaluated in Appendix B:

$$U_{f0}=-ee'\int d\tau\int d\tau'\Psi_f^*\Phi_f^*(1-\boldsymbol{\alpha}\cdot\boldsymbol{\alpha}')(e^{i\omega X}/X)\Psi_0\Phi_0. \tag{B5}$$

The result (B5) is in agreement with that of Hulme.[11] Substitution of (3g, h) into (3b) gives A in second approximation:

$$(W-\omega-i\eta)A=-i-A\int dk\left[\frac{H_{0k}H_{k0}}{k-\omega-i\eta}+\frac{H_{0k}'H_{k0}'}{k+\omega_0-i\eta}\right], \tag{3j}$$

where the integral over k, which we denote by $i\gamma_1$, γ_1 being real and positive, is evaluated in Appendix B. Substitution of (3i, j) into (3c, d) gives B_k and B_k' in the third approximation:

$$\begin{aligned}(k-\omega-i\eta)B_k&=-H_{k0}A-U_{f0}A\int dE\{H_{kE}/(E-\omega-i\eta)\}\\&=-A[H_{k0}+i\pi U_{f0}H_{k\omega}],\end{aligned} \tag{3k}$$

and

$$(k+\omega_0-i\eta)B_k'=-A[H_{k0}'+i\pi U_{f0}H_{k\omega}'], \tag{3l}$$

where $H_{k\omega}$ is H_{kE} with E replaced by ω and likewise for $H_{k\omega}'$. The evaluation of the integrals over E is discussed in Appendix B.

Substituting (3k, l) into (3b) gives A to the fourth approximation:

$$(W-\omega-i\eta)A=-i+i\gamma_1A+i\pi U_{f0}A\int dk\left[\frac{H_{0k}H_{k\omega}}{k-\omega-i\eta}+\frac{H_{0k}'H_{k\omega}'}{k+\omega_0-i\eta}\right],$$

where the integral over k, which we denote by $U_{0f}(=U_{f0}^*)$, is evaluated in Appendix B. Then, writing $\gamma_2=\pi|U_{f0}|^2$,

$$A=-i/[W-\omega-i(\eta+\gamma_1+\gamma_2)]. \tag{3m}$$

Substitution of (3m) into (3i, k) gives

$$C_E=\frac{-iU_{f0}}{(E-\omega-i\eta)[W-\omega-i(\eta+\gamma_1+\gamma_2)]}, \tag{3i$'$}$$

$$B_k=\frac{i[H_{k0}+i\pi U_{f0}H_{k\omega}]}{(k-\omega-i\eta)[W-\omega-i(\eta+\gamma_1+\gamma_2)]}. \tag{3k$'$}$$

The inverse transforms of (3m, i′, k′) are easily obtained.[12] They are

$$a(t)=\exp[-iWt-(\gamma_1+\gamma_2)t], \tag{3n}$$

$$b_k(t)=\frac{[H_{k0}+i\pi U_{f0}H_{k\omega}]}{k-W+i(\gamma_1+\gamma_2)}\{e^{-ikt}-a(t)\}, \tag{3o}$$

$$c_E(t)=\frac{-U_{f0}}{E-W+i(\gamma_1+\gamma_2)}\{e^{-iEt}-a(t)\}. \tag{3p}$$

Hence,

$$N_e=\int dE|c_E(\infty)|^2=\frac{\pi}{\gamma_1+\gamma_2}|U_{f0}|^2, \tag{3q}$$

$$N_q=\int dk|b_k(\infty)|^2=\frac{\pi}{\gamma_1+\gamma_2}|H_{k0}+i\pi U_{f0}H_{k\omega}|^2. \tag{3r}$$

Thus, it is seen that N_q is proportional to

$$|H_{k0}+i\pi U_{f0}H_{k\omega}|^2$$

rather than $|H_{k0}|^2$. The correction term $i\pi U_{f0}H_{k\omega}$ will be discussed in the next section.

IV. COMPARISON WITH CORRESPONDENCE PRINCIPAL RESULTS

Equation (3q) states that the number of electrons ejected per second is proportional to $|U_{f0}|^2$. When the radiation field contains all multipoles, U_{f0} is given by (B5). In practice, the radiation field due to an excited nucleus does not contain all multipoles. The selection rules restrict the field to that of a given multipole, say, the 2^Lth, of a particular type (electric, magnetic, or longitudinal). In this case, U_{f0} is given by Eq. (B3′) of Appendix B. It then follows that $|U_{f0}|^2$ is proportional to

$$\left|\int d\tau\Psi_f^*[\boldsymbol{\alpha}\cdot\mathbf{B}_{LM}(\omega r)+i\psi_L{}^M(\omega r)]\Psi_0\right|^2.$$

This result is in agreement with the correspondence principle prescription for the number of electrons ejected per second.

[11] Reference 3, p. 497.

[12] Reference 9, p. 295.

According to (3r), N_q, the number of gamma-quanta emitted per second, is proportional to $|H_{k0}+i\pi U_{f0}H_{k\omega}|^2$. The second term in this expression represents the effect of the presence of the extra-nuclear electrons. In the case in which the radiation field is restricted to a given multipole,

$$H_{k0}+i\pi U_{f0}H_{k\omega}$$
$$=e'(2\pi/\omega)^{\frac{1}{2}}\int d\tau'\Phi_f^*[\boldsymbol{\alpha}'\cdot\mathbf{A}_{LM}^*(\omega r')-i\phi_L^{M*}(\omega r')]\Phi_0$$
$$\times\Big(1-(2\pi^3e^2/\omega)$$
$$\times\left\{\int d\tau\Psi_f^*[\boldsymbol{\alpha}\cdot\mathbf{B}_{LM}(\omega r)+i\psi_L^M(\omega r)]\Psi_0\right\}$$
$$\times\left\{\int d\tau\Psi_0^*[\boldsymbol{\alpha}\cdot\mathbf{A}_{LM}^*(\omega r)-i\phi_L^{M*}(\omega r)]\Psi_f\right\}\Big). \quad (4a)$$

This result shows that the number of quanta escaping from the atom differs from the number ejected from the bare nucleus only by a factor of order e^2, in agreement with the correspondence principle result of Taylor and Mott.[2]

The physical significance of the correction term is readily seen from (4a). The first bracket in the correction term represents the matrix element for electron transitions from bound to continuum states, i.e., the matrix element for the absorption of a gamma-quantum, while the second bracket represents the matrix element for the emission of a gamma-quantum. The correction term therefore represents an interference between the two radiation fields involved.

Neglecting the factor of order e^2, the internal conversion coefficient for the given multipole radiation is

$$(2\pi^3e^2/\omega)\left|\int d\tau\Psi^*[\boldsymbol{\alpha}\cdot\mathbf{B}_{LM}(\omega r)+i\psi_L^M(\omega r)]\Psi_0\right|^2. \quad (4b)$$

V. THE GAUGE QUESTION

For a given multipole, U_{f0}' is given by (B3') when r is greater than r'. From the method of evaluation of U_{f0} in Appendix B, it is clear that for r less than r'

$$U_{f0}'=(2\pi^2ee'i/\omega)\left\{\int d\tau\Psi_f^*[\boldsymbol{\alpha}\cdot\mathbf{A}_{LM}(\omega r)+i\phi_L^M(\omega r)]\Psi_0\right\}$$
$$\times\left\{\int d\tau'\Phi_f^*[\boldsymbol{\alpha}'\cdot\mathbf{B}_{LM}^*(\omega r')-i\psi_L^{M*}(\omega r')]\Phi_0\right\}.$$

Inside the nucleus, r may be greater or less than r'. Consequently, the complete expression for U_{f0}', including the effect of the finite size of the nucleus, is

$$U_{f0}'=(2\pi^2ee'i/\omega)\Bigg[\left\{\int_R^\infty d\tau\Psi_f^*[\boldsymbol{\alpha}\cdot\mathbf{B}_{LM}(\omega r)+i\psi_L^M(\omega r)]\Psi_0\right\}\left\{\int_0^R d\tau'\Phi_f^*[\boldsymbol{\alpha}'\cdot\mathbf{A}_{LM}^*(\omega r')-i\phi_L^{M*}(\omega r')]\Phi_0\right\}$$
$$+\left\{\int_0^R d\tau\Psi_f^*[\boldsymbol{\alpha}\cdot\mathbf{B}_{LM}(\omega r)+i\psi_L^M(\omega r)]\Psi_0\right\}\left\{\int_0^r d\tau'\Phi_f^*[\boldsymbol{\alpha}'\cdot\mathbf{A}_{LM}^*(\omega r')-i\phi_L^{M*}(\omega r')]\Phi_0\right\}$$
$$+\left\{\int_0^R d\tau\Psi_f^*[\boldsymbol{\alpha}\cdot\mathbf{A}_{LM}(\omega r)+i\phi_L^M(\omega r)]\Psi_0\right\}\left\{\int_r^R d\tau'\Phi_f^*[\boldsymbol{\alpha}'\cdot\mathbf{B}_{LM}^*(\omega r')-i\psi_L^{M*}(\omega r')]\Phi_0\right\}\Bigg], \quad (5a)$$

where the range of r and r' have been indicated on the respective integrals, R denoting the nuclear radius. This result for the effect of the finite size of the nucleus on the radiation potentials is in agreement with that obtained by the correspondence principle method.[13]

If we neglect the contribution from inside the nucleus, (5a) reduces to

$$U_{f0}'=(2\pi^2ee'i/\omega)$$
$$\times\left\{\int_R^\infty d\tau\Psi_f^*[\boldsymbol{\alpha}\cdot\mathbf{B}_{LM}(\omega r)+i\psi_L^M(\omega r)]\Psi_0\right\}$$
$$\times\left\{\int_0^R d\tau'\Phi_f^*[\boldsymbol{\alpha}'\cdot\mathbf{A}_{LM}^*(\omega r')-i\phi_L^{M*}(\omega r')]\Phi_0\right\}. \quad (5b)$$

In the calculations of internal conversion coefficients, however, the range of r has been taken as $0<r<\infty$ rather than as $R<r<\infty$. The question arises as to whether or not this extension of the range of r may be carried out with the radiation potentials expressed in terms of any arbitrary gauge. The answer is in the negative, as has already been pointed out by Dancoff and Morrison.[14] The range may not be extended in the case of electric multipole radiation when the Heitler gauge is employed, because the artificial singularities at the origin introduced in the definition of the multipole potentials make the matrix elements give a finite contribution from an arbitrarily small region. For this same reason, the Heitler gauge may not be used in the investigation of the effect of the finite size of the nucleus on the radiation potentials.

If, by a gauge transformation, we obtain another set of potentials for which the integrand of the matrix element is small at the origin, this latter set can be

[13] N. Tralli and M. E. Rose (unpublished).

[14] S. M. Dancoff and P. Morrison, Phys. Rev. 55, 122 (1939).

called correct. This condition is satisfied by the conventional gauge.

APPENDIX A.

EXPANSION OF THE RADIATION FIELD IN SPHERICAL HARMONICS

We introduce the function,

$$\phi_L{}^M(kr)=kf_L(kr)Y_L{}^M(\theta,\phi), \tag{A1}$$

in which $f_L(kr)=(kr)^{-\frac{1}{2}}J_{L+\frac{1}{2}}(kr)$, where J is the bessel function, and $Y_L{}^M(\theta,\phi)$ is the normalized spherical harmonic.[15] Now $\phi_L{}^M$ satisfies the equations

$$\nabla^2\phi_L{}^M-k^2\phi_L{}^M=0, \tag{A2}$$

$$\int d\tau\phi_L{}^M(k)\phi_{L'}{}^{M'*}(k')=\delta_{LL'}\delta_{MM'}\delta(k-k'). \tag{A3}$$

It may then be shown[16] that the radiation potentials can be written

$$\mathbf{A}_{LM}{}^{(l)}=(1/k)\nabla\phi_L{}^M, \tag{A4}$$

$$\mathbf{A}_{LM}{}^{(m)}=[L(L+1)]^{-\frac{1}{2}}(\mathbf{r}\times\nabla)\phi_L{}^M, \tag{A5}$$

$$\mathbf{A}_{LM}{}^{(e)}=[k^2L(L+1)]^{-\frac{1}{2}}\nabla\times(\mathbf{r}\times\nabla)\phi_L{}^M, \tag{A6}$$

in which the superscripts l, m, e on the $\mathbf{A}_{LM}$ refer to longitudinal, magnetic, and electric radiations, respectively.

Using the unit vectors

$$\mathbf{u}_1=-2^{-\frac{1}{2}}(\mathbf{i}+i\mathbf{j}),\quad \mathbf{u}_0=\mathbf{k},\quad \mathbf{u}_{-1}=2^{-\frac{1}{2}}(\mathbf{i}-i\mathbf{j}) \tag{A7}$$

such that all vectors may be written

$$\mathbf{V}=\Sigma_\sigma V_\sigma\mathbf{u}^\sigma=\Sigma_\sigma V^\sigma\mathbf{u}_\sigma, \tag{A8}$$

where $\mathbf{u}^\sigma=\mathbf{u}_\sigma{}^*$ and $V^\sigma=V_\sigma{}^*$ for a real vector, we may express the components of the $\mathbf{A}_{LM}$ as[17]

$$A_{LM\sigma}{}^{(l)}=[(L+1)/(2L+1)]^{\frac{1}{2}}(M+\sigma,-\sigma|LM)_{L+1,1}\phi_{L+1}{}^{M+\sigma}+[L/(2L+1)]^{\frac{1}{2}}(M+\sigma,-\sigma|LM)_{L-1,1}\phi_{L-1}{}^{M+\sigma}, \tag{A9}$$

$$A_{LM\sigma}{}^{(m)}=i(M+\sigma,-\sigma|LM)_{L,1}\phi_L{}^{M+\sigma}, \tag{A10}$$

$$A_{LM\sigma}{}^{(e)}=[L/(2L+1)]^{\frac{1}{2}}(M+\sigma,-\sigma|LM)_{L+1,1}\phi_{L+1}{}^{M+\sigma}-[(L+1)/(2L+1)]^{\frac{1}{2}}(M+\sigma,-\sigma|LM)_{L-1,1}\phi_{L-1}{}^{M+\sigma}. \tag{A11}$$

The relations (A10, 11) are in agreement with those of Heitler.[8]

With the notation

$$\phi_L{}^M(kr')=kJ_L(kr')Y_L{}^M(\theta',\phi'),$$

$$\psi_L{}^M(kr)=kH_L{}^{(1)}(kr)Y_L{}^M(\theta,\phi),$$

$$I=\Sigma_\sigma\mathbf{u}_\sigma\mathbf{u}^\sigma\equiv\mathbf{ii}+\mathbf{jj}+\mathbf{kk},$$

where $J_L(kr')=(kr')^{-\frac{1}{2}}J_{L+\frac{1}{2}}(kr')$, and $H_L{}^{(1)}(kr)=(kr)^{-\frac{1}{2}}H_{L+\frac{1}{2}}{}^{(1)}(kr)$, in which J is the bessel function and $H^{(1)}$ the hankel function of the first kind, the well-known relation[18]

$$e^{ikX}/X=i\pi(4rr')^{-\frac{1}{2}}\Sigma_L(2L+1)J_{L+\frac{1}{2}}(kr')H_{L+\frac{1}{2}}{}^{(1)}(kr)P_L(\cos\Theta),$$

where r is greater than r', $X=|\mathbf{r}-\mathbf{r}'|$, Θ is the angle between $\mathbf{r}$ and $\mathbf{r}'$, and

$$P_L(\cos\Theta)=[4\pi/(2L+1)]\sum_{M=-L}^{L}Y_L{}^{M*}(\theta',\phi')Y_L{}^M(\theta,\phi),$$

may be written

$$(e^{ikX}/X)I=(2\pi^2i/k)\sum_{LM}\psi_L{}^M\phi_L{}^{M*}\Sigma_\sigma\mathbf{u}_\sigma\mathbf{u}^\sigma. \tag{A12}$$

Introducing the vectors $\mathbf{B}_{LM}$ which bear the same relationship to $\psi_L{}^M$ as the $\mathbf{A}_{LM}$ to $\phi_L{}^M$, it may be shown that

$$\sum_{LMi}\mathbf{B}_{LM}{}^{(i)}\mathbf{A}_{LM}{}^{(i)*}=\sum_{LM}\psi_L{}^M\phi_L{}^{M*}\Sigma_\sigma\mathbf{u}_\sigma\mathbf{u}^\sigma,$$

so that[19]

$$(e^{ikX}/X)I=(2\pi^2i/k)\sum_{LMi}\mathbf{B}_{LM}{}^{(i)}\mathbf{A}_{LM}{}^{(i)*}. \tag{A13}$$

Similarly,

$$(e^{-ikX}/X)I=-(2\pi^2i/k)\sum_{LMi}\mathbf{B}_{LM}{}^{(i)*}\mathbf{A}_{LM}{}^{(i)}. \tag{A14}$$

The radiation potentials in the different gauges are easily obtained. The equations of gauge transformation are

$$\phi=\phi'-d\lambda/dt,\quad \mathbf{A}=\mathbf{A}'+\nabla\lambda,$$

where λ is a solution of the wave equation,

$$\nabla^2\lambda-d^2\lambda/dt^2=0. \tag{A15}$$

In the Heitler gauge $\mathrm{div}A'=\phi'=0$. Since the sole condition on λ is that it satisfy Eq. (A15), we may take

$$\lambda=k^{-1}\phi_L{}^Me^{-ikt},$$

so that

$$d\lambda/dt=-i\phi_L{}^Me^{-ikt},\quad \nabla\lambda=\mathbf{A}_{LM}{}^{(l)}e^{-ikt},$$

$$\mathbf{A}'=\mathbf{A}_{LM}{}^{(m)}e^{-ikt}\quad\text{or}\quad\mathbf{A}_{LM}{}^{(e)}e^{-ikt}.$$

In this gauge, therefore, the expressions for ϕ and $\mathbf{A}$ are

Longitudinal:	$i\phi_L{}^M$,	$\mathbf{A}_{LM}{}^{(l)}$,	
Magnetic:	0,	$\mathbf{A}_{LM}{}^{(m)}$,	(A16)
Electric:	0,	$\mathbf{A}_{LM}{}^{(e)}$.	

The expressions for the scalar and vector potentials in the conventional gauge are obtained just as easily. Take

$$\lambda=-[L/k^2(L+1)]^{\frac{1}{2}}\phi_L{}^Me^{-ikt}$$

so that the scalar potential is

$$\phi=-d\lambda/dt=-i[L/(L+1)]^{\frac{1}{2}}\phi_L{}^Me^{-ikt} \tag{A17}$$

and

$$\nabla\lambda=-[L/(L+1)]^{\frac{1}{2}}\mathbf{A}_{LM}{}^{(l)}e^{-ikt}.$$

The electric multipole vector potential is then obtained from the equation of gauge transformation,

$$\mathbf{A}^{(e)}=\mathbf{A}_{LM}{}^{(e)}-[L/(L+1)]^{\frac{1}{2}}\mathbf{A}_{LM}{}^{(l)}. \tag{A18}$$

The magnetic multipole vector potential remains as given by (A5). Hence, in the conventional gauge there are no longitudinal potentials, and the electric multipoles have both scalar and vector potentials.

APPENDIX B.

EVALUATION OF INTEGRALS

In the calculations carried out below, the Heitler gauge (A16), is used.

1. Evaluation of $U_{f0}=\int dk\left[\frac{H_{Ek}H_{k0}}{k-\omega-i\eta}+\frac{H_{Ek}{}'H_{k0}{}'}{k+\omega_0-i\eta}\right]$.

Time-dependent perturbation theory tells us that the transition probability per unit time is appreciable only if energy is conserved between initial and final states.[20] In accordance with the discussion

[15] We use the choice of phase factors of H. Bethe, *et al.*, *Handbuch der Physik* (Verlag. Julius Springer, Berlin, 1933), second edition, 24/1, p. 273; and W. Heitler, Proc. Cambridge Phil. Soc. **32**, 112 (1936).

[16] See, for example, the treatment of P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (M.I.T., Cambridge, Massachusetts, 1946), Chapter IX.

[17] For the properties of the unitary matrices $(m_1m_2|jm)_{j_11}$, see, for example, E. Wigner, *Gruppentheorie* (Braunschweig, Vieweg & Sohn, 1931); or E. U. Condon and G. H. Shortley, *The Theory of Atomic Spectra* (University Press, Cambridge, England, 1935). In the notation of Condon and Shortley, these would be written $(j_11m_1m_2|j_11jm)$.

[18] See, for instance, W. Magnus and F. Oberhettinger, *Special Functions of Mathematical Physics* (Springer-Verlag., Berlin, 1948), p. 21.

[19] See, for instance, Morse and Feshbach, reference 16, p. 486.

[20] See, for instance, L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1949), Sec. 29.

in Schiff[20] and in Hulme,[21] the second term in the integrand cannot be ignored. It is taken into account by integrating the first term from $-\infty$ to $+\infty$ instead of from 0 to $+\infty$. Then

$$U_{f0}=\int_{-\infty}^{+\infty} dk\frac{H_{Ek}H_{k0}}{k-\omega-i\eta}$$
$$=2\pi ee'\sum_{LMi}\int_{-\infty}^{+\infty}\frac{dk}{k(k-\omega-i\eta)}\times\left\{\int d\tau\Psi_f^*[\boldsymbol{\alpha}\cdot\mathbf{A}_{LM}^{(i)}(kr)+i\phi_L^{M(i)}(kr)]\Psi_0\right\}\times\left\{\int d\tau'\Phi_f^*[\boldsymbol{\alpha}'\cdot\mathbf{A}_{LM}^{(i)*}(kr')-i\phi_L^{M(i)*}(kr')]\Phi_0\right\}, \quad \text{(B1)}$$

in which the superscript (i) refers to the longitudinal, magnetic, or electric 2^L multipole, and $\phi_L^{M(i)}=0$ for $i=m$, e, and $\phi_L^{M(l)}=\phi_L^M$. The Σ_{LMi} of the bracketed terms may be written

$$\sum_{LMi}\int d\tau\int d\tau'\Psi_f^*\Phi_f^*[\boldsymbol{\alpha}\cdot\mathbf{A}_{LM}^{(i)}(kr)\boldsymbol{\alpha}'\cdot\mathbf{A}_{LM}^{(i)*}(kr')+i\phi_L^M(kr)\boldsymbol{\alpha}'\cdot\mathbf{A}_{LM}^{(l)*}(kr')-i\phi_L^{M*}(kr')\boldsymbol{\alpha}\cdot\mathbf{A}_{LM}^{(l)}(kr)+\phi_L^M(kr)\phi_L^{M*}(kr')]\Psi_0\Phi_0. \quad \text{(B2)}$$

Since the hamiltonians have the form,

$$H=-\boldsymbol{\alpha}\cdot\mathbf{p}-\beta m-\boldsymbol{\alpha}\cdot\mathbf{A}_{LM}^{(i)}(kr)-i\phi_L^{M(i)}(kr),$$
$$H'=-\boldsymbol{\alpha}'\cdot\mathbf{p}'-\beta'm'-\boldsymbol{\alpha}'\cdot\mathbf{A}_{LM}^{(i)*}(kr')+i\phi_L^{M(i)*}(kr'),$$

we obtain

$$\boldsymbol{\alpha}\cdot\mathbf{A}_{LM}^{(l)}(kr)=(1/k)\boldsymbol{\alpha}\cdot\nabla\phi_L^M(kr)=(i/k)\boldsymbol{\alpha}\cdot\mathbf{p}\phi_L^M(kr)=(i/k)[\phi_L^M(kr)H-H\phi_L^M(kr)]$$

and

$$\boldsymbol{\alpha}'\cdot\mathbf{A}_{LM}^{(l)*}(kr')=(i/k)[\phi_L^{M*}(kr')H'-H'\phi_L^{M*}(kr')].$$

Then (B2) reduces to

$$\int d\tau\int d\tau'\Psi_f^*\Phi_f^*\left\{\sum_{LMi}\boldsymbol{\alpha}\cdot\mathbf{A}_{LM}^{(i)}(kr)\boldsymbol{\alpha}'\cdot\mathbf{A}_{LM}^{(i)*}(kr')+[1-(W+E)/k]\sum_{LM}\phi_L^M(kr)\phi_L^{M*}(kr')\right\}\Psi_0\Phi_0.$$

Hence,

$$U_{f0}=2\pi ee'\int d\tau\int d\tau'\Psi_f^*\Phi_f^*\left[\int_{-\infty}^{+\infty}\frac{dk}{k(k-\omega-i\eta)}\times\left\{\sum_{LMi}\boldsymbol{\alpha}\cdot\mathbf{A}_{LM}^{(i)}(kr)\boldsymbol{\alpha}'\cdot\mathbf{A}_{LM}^{(i)*}(kr')+\sum_{LM}[1-(W+E)/k]\phi_L^M(kr)\phi_L^{M*}(kr')\right\}\right]\Psi_0\Phi_0.$$

Now, the dependence of $\phi_L^M(kx)$ and $\mathbf{A}_{LM}^{(i)}(kx)$ on k is confined to the (spherical) bessel function $J_L(kx)$ which each contains. We consider the case where r is greater than r' and make the substitution,

$$2J_L(kr)=H_L^{(1)}(kr)+H_L^{(2)}(kr).$$

As has been remarked above, the integral is to be evaluated for conservation of energy, $W=E=k=\omega$. Then, from the location of the pole, it is clear that only the $H_L^{(1)}(kr)$ part of $J_L(kr)$ will contribute to the integral. Therefore,

$$U_{f0}=(2\pi^2ee'i/\omega)\int d\tau\int d\tau'\Psi_f^*\Phi_f^*\left\{\sum_{LMi}\boldsymbol{\alpha}\cdot\mathbf{B}_{LM}^{(i)}(\omega r)\times\boldsymbol{\alpha}'\cdot\mathbf{A}_{LM}^{(i)*}(\omega r')-\sum_{LM}\psi_L^M(\omega r)\phi_L^{M*}(\omega r')\right\}\Psi_0\Phi_0, \quad \text{(B3)}$$

where the $\mathbf{B}_{LM}$ differs from the $\mathbf{A}_{LM}$ only in the replacement of J_L by $H_L^{(1)}$.

[21] See reference 3, p. 494.

We note here that, in general, the radiation field does not contain all the multipoles. Selection rules usually restrict the radiation field to a given multipole, say the 2^Lth, of a particular type (l, m, or e). In this case, (B1) reduces to

$$U_{f0}'=2\pi ee'\int_{-\infty}^{+\infty}\frac{dk}{k(k-\omega-i\eta)}\int d\tau\Psi_f^*[\boldsymbol{\alpha}\cdot\mathbf{A}_{LM}(kr)+i\phi_L^M(kr)]\Psi_0\times\left\{\int d\tau'\Phi_f^*[\boldsymbol{\alpha}'\cdot\mathbf{A}_{LM}^*(kr')-i\phi_L^{M*}(kr')]\Phi_0\right\}, \quad \text{(B1')}$$

where it is to be remembered that $\phi_L^M=0$ for electric and magnetic radiation. Carrying out the integration over k as indicated above, (B1′) becomes

$$U_{f0}'=(2\pi^2ee'i/\omega)\left\{\int d\tau\Psi_f^*[\boldsymbol{\alpha}\cdot\mathbf{B}_{LM}(\omega r)+i\psi_L^M(\omega r)]\Psi_0\right\}\times\left\{\int d\tau'\Phi_f^*[\boldsymbol{\alpha}'\cdot\mathbf{A}_{LM}^*(\omega r')-i\phi_L^{M*}(\omega r')]\Phi_0\right\}. \quad \text{(B3')}$$

Returning to (B3) we note that, from (A12),

$$\sum_{LM}\psi_L^M(\omega r)\phi_L^{M*}(\omega r')=(\omega/2\pi^2 i)(e^{i\omega X}/X),$$

and

$$\sum_{LMi}\boldsymbol{\alpha}\cdot\mathbf{B}_{LM}^{(i)}(\omega r)\boldsymbol{\alpha}'\cdot\mathbf{A}_{LM}^{(i)*}(\omega r')=\sum\boldsymbol{\alpha}\cdot\mathbf{B}_{LM}^{(i)}(\omega r)\mathbf{A}_{LM}^{(i)*}(\omega r')\cdot\boldsymbol{\alpha}'=\boldsymbol{\alpha}\cdot(\omega/2\pi^2i)(e^{i\omega X}/X)I\cdot\boldsymbol{\alpha}'=(\omega/2\pi^2i)(e^{i\omega X}/X)(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha}'). \quad \text{(B4)}$$

Substitution of these results into (B3) gives

$$U_{f0}=-ee'\int d\tau\int d\tau'\Psi_f^*\Phi_f^*(1-\boldsymbol{\alpha}\cdot\boldsymbol{\alpha}')(e^{i\omega X}/X)\Psi_0\Phi_0. \quad \text{(B5)}$$

The same result is obtained for U_{f0} when r is less than r'.

2. Evaluation of $\int dk\frac{H_{0k}H_{k0}}{k-\omega-i\eta}+\frac{H_{0k}'H_{k0}'}{k+\omega_0-i\eta}$.

Proceeding as above, the integral reduces to

$$\int_{-\infty}^{+\infty}dk\frac{|H_{0k}|^2}{k-\omega-i\eta}=\int_{-\infty}^{+\infty}dk\frac{(k-\omega)|H_{0k}|^2}{(k-\omega)^2+\eta^2}+i\int_{-\infty}^{+\infty}dk\frac{\eta|H_{0k}|^2}{(k-\omega)^2+\eta^2}.$$

The first integral on the right represents the principal value part of the original integral and is usually neglected. In the second integral, $|H_{0k}|^2$ is a slowly varying function of k. For small η, the denominator has a sharp minimum for $k=\omega$, so that the integrand has a sharp maximum. We may therefore take $|H_{0k}|^2$ outside the integral sign and replace it by its value at $k=\omega$, $|H_{0\omega}|^2$. Hence,

$$\int_{-\infty}^{+\infty}dk\frac{|H_{0k}|^2}{k-\omega-i\eta}=i|H_{0\omega}|^2\int_{-\infty}^{+\infty}dk\frac{\eta}{(k-\omega)^2+\eta^2}=i\pi|H_{0\omega}|^2=i\gamma_1,$$

where

$$|H_{0\omega}|^2=(2\pi e'^2/\omega)\left|\int d\tau'\Phi_f^*[\boldsymbol{\alpha}'\cdot\mathbf{A}_{LM}^{(i)*}(\omega r')-i\phi_L^{M*}(\omega r')]\Phi_0\right|^2.$$

3. Evaluation of $\int dE[H_{kE}/(E-\omega-i\eta)]$ **and** $\int dE[H_{kE}'/(E-\omega-i\eta)]$.

Proceeding as above, we obtain

$$\int dE[H_{kE}/(E-\omega-i\eta)]=i\pi H_{k\omega}$$

and

$$\int dE[H_{kE}'(E-\omega-i\eta)]=i\pi H_{k\omega}'.$$

4. Evaluation of $\int dk\left[\frac{H_{0k}H_{k\omega}}{k-\omega-i\eta}+\frac{H_{0k}'H_{k\omega}'}{k+\omega_0-i\eta}\right]$.

Comparison of this integral with that denoted by U_{f0}, and noting (A14), shows that this integral is $U_{0f}=U_{f0}^*$.