Connection between the atomic photoeffect and internal conversion*

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It is shown that over an appreciable energy range K-, L-, and M-shell photoeffect total cross sections are proportional to $E1$ internal-conversion coefficients from the same subshell. In the nonrelativistic dipole approximation the ratio $\beta^{E1}/\sigma = (3/8\pi)(Z\alpha)^{-2}$, independent of shell and subshell; numerically, for s waves, this ratio holds to 1 MeV. Screening effects enter only at low energies, reaching several percent at the K-shell threshold.

It is evident that the atomic photoelectric effect and internal conversion are related, differing in the replacement of a real photon of energy k, linear momentum $\vec{k}$ by a virtual photon of energy k corresponding to the nuclear transition. When it was found that the photoeffect matrix element, except near threshold, is determined at Compton-wavelength distances,[1] it was realized the same should apply to internal conversion, and this was explicitly demonstrated by Band *et al.*[2] Nevertheless, the major numerical calculations of the photoeffect in a central potential by Scofield[3] and the corresponding calculation of internal-conversion coefficients by Hager and Seltzer[4] have proceeded entirely independently and apparently have not been compared.

We wish to point out that over an appreciable range in energy the photoeffect total cross sections (for K, L, and M shells) and the corresponding $E1$ internal-conversion coefficients are proportional. Their ratios are summarized in Figs. 1 and 2. The data are, in general, consistent with a simple relation which we shall prove below in the nonrelativistic dipole approximation, namely, $\beta^{E1}/\sigma = (3/8\pi)(Z\alpha)^{-2}$, independent of shell. We do not yet understand why this relation holds to such high energies, particularly for bound s states. We have noted[5] that for the photoeffect, relativistic

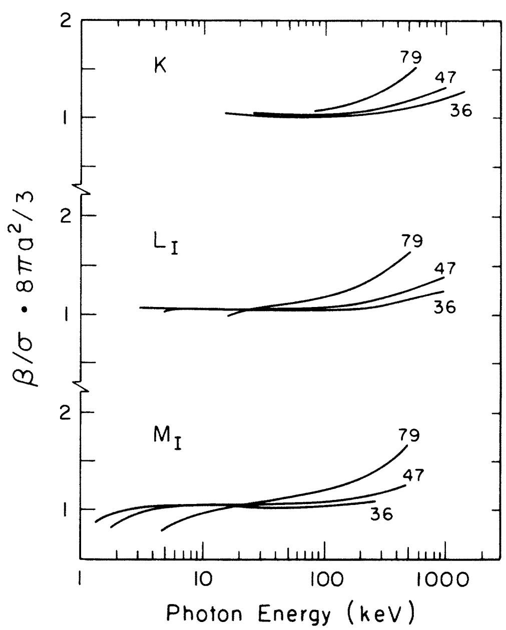

FIG. 1. Ratio $8\pi(Z\alpha)^2 3^{-1}\beta^{E1}/\sigma$ of K, $L_{\rm I}$, and $M_{\rm I}$ $E1$ internal-conversion coefficients β^{E1} to corresponding K, $L_{\rm I}$, and $M_{\rm I}$ photoeffect cross sections σ as a function of transition (or incident photon) energy $\boldsymbol{k}$, for elements $Z=36$, 47, and 79.

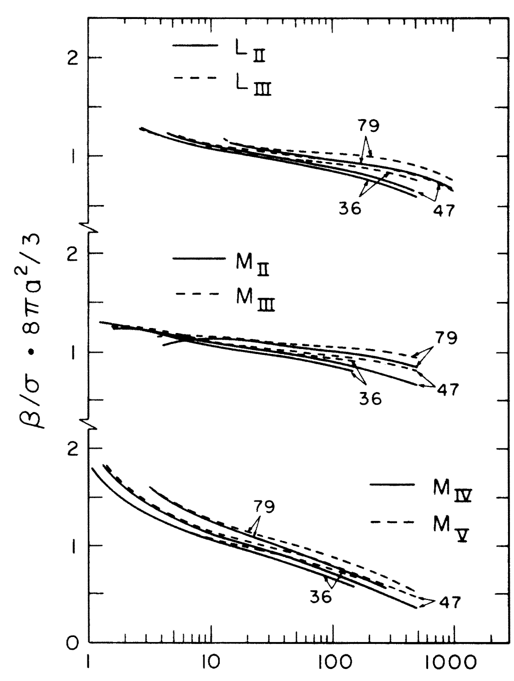

FIG. 2. Same as Fig. 1, but for $L_{\rm II}$ and $L_{\rm III}$, $M_{\rm II}$ and $M_{\rm III}$, $M_{\rm IV}$ and $M_{\rm V}$ subshells.

and multipole effects tend to cancel in the total cross section, so that the nonrelativistic dipole approximation remains valid to near 100 keV; the same is presumably true for internal-conversion coefficients. At these energies and above, screening effects (except for normalization) are unimportant for the photoeffect and presumably also for internal conversion. For s waves, the relation between the two processes appears to remain valid to 1 MeV. We note that the energy dependence of the ratio is nearly independent of principal quantum number for given angular momentum, and that the ratios for states of the same n, l (different j) coincide at low energies.

To prove the relation of the two processes, we begin with the relativistic matrix elements, $M_{\rm ph}$ for photoeffect and $M_{\rm ic}$ for internal conversion. Let p represent the momentum of the continuum electrons and l represent the angular momentum of the initial bound electron. Then

$$M_{\rm ph}=\int \phi_f^\dagger \vec{\alpha}\cdot\vec{\epsilon}\, e^{i\vec{k}\cdot\vec{r}}\,\phi_i\, d\vec{r} \tag{1}$$

for incident photon polarization $\vec{\epsilon}$, which in nonrelativistic dipole approximation becomes

$$M_{\rm ph}^{\rm NR\text{-}dip}=\int \phi_f^*\vec{p}\cdot\vec{\epsilon}\,\phi_i\, d\vec{r} = ik\int \phi_f^*\vec{r}\cdot\vec{\epsilon}\,\phi_i\, d\vec{r}\,. \tag{2}$$

In this approximation, the total cross section is, as is well known,

$$\sigma=\frac{\alpha p k}{2l+1}\,\frac{8\pi^2}{3}\left\{l\left|\int dr P^*_{p,\,l-1}\, rP_{nl}\right|^2 + (l+1)\left|\int dr P^*_{p,\,l+1}\, rP_{nl}\right|^2\right\},$$

where P is related to the solution R of the radial Schrödinger equation by

$$P(r)=\gamma R(r)\,.$$

The internal-conversion matrix element involves the initial and final wave functions of both the nucleus and the electron:

$$M_{ic}=\alpha\int d\vec{r}\int d\vec{R}\,\phi_f^*(\vec{r})\psi_f^*(\vec{R})(1-\vec{\alpha}_r\cdot\vec{\alpha}_R)\times\frac{e^{ik|\vec{R}-\vec{r}|}}{|\vec{R}-\vec{r}|}\phi_i(\vec{r})\psi_i(\vec{R})\,, \tag{3}$$

where $\phi(\vec{r})$ and $\psi(\vec{R})$ are the wave functions of an electron and a nucleus, respectively. One may separate the nuclear variables from the electron variables with the use of the identity

$$\frac{e^{ik|\vec{R}-\vec{r}|}}{|\vec{R}-\vec{r}|}=4\pi ik\sum_L h_L^{(1)}(kr)j_L(kR)Y_{LM}(\hat{r})Y^*_{LM}(\hat{R})\,. \tag{4}$$

Then the nonrelativistic matrix element becomes

$$M_{\rm ic}^{\rm NR}=4\pi ik\alpha\sum_L\int d\vec{r}\,\phi_f^*(\vec{r})h_L^{(1)}(kr)Y_{LM}(\hat{r})\phi_i(\vec{r})\times\int d\vec{R}\,\psi_f^*(\vec{R})j_L(kR)Y_{LM}(\hat{R})\psi_i(\vec{R})\,.$$

In the calculation of the internal-conversion coefficient β, the nuclear integrals cancel:

$$\beta^{(E1)}=2\,\frac{k\alpha}{4}\,\frac{L}{L+1}\int d\Omega_p\left|\int d\vec{r}\,\phi_f^*(\vec{r})h_L^{(1)}(kr)Y_{LM}(\hat{r})\phi_i(\vec{r})\right|^2. \tag{5}$$

The $E1$ internal-conversion coefficient in the nonrelativistic case becomes, expanding for small k,

$$\beta^{(E1)}=\frac{\alpha\pi kp}{2l+1}\left\{l\left|\int drP^*_{p,l-1}h_1^{(1)}(kr)P_{nl}\right|^2+(l+1)\left|\int drP^*_{p,\,l+1}h_1^{(1)}(kr)P_{nl}\right|^2\right\}$$
$$\simeq\frac{\alpha\pi kp}{2l+1}\left\{l\left|\int drP^*_{p,l-1}\frac{1}{(kr)^2}P_{nl}\right|^2+(l+1)\left|\int drP^*_{p,l+1}\frac{1}{(kr)^2}P_{nl}\right|^2\right\}. \tag{6}$$

We thus need to establish a connection between the radial matrix elements I_1 and I_{-2}, where

$$I_s=\int drP^*_{p,\,l\pm1}r^sP_{nl}\,. \tag{7}$$

For this purpose we evaluate the commutator relation

$$[H,[H,\vec{r}\,]]=\vec{\nabla}V\,, \tag{8}$$

between states i and f to obtain

$$(E_f-E_i)^2\langle f\,|\,\vec{r}\,|\,i\rangle=\langle f\,|\vec{\nabla}V\,|\,i\rangle\,. \tag{9}$$

If i and f are angular momentum eigenstates $r^{-1}PY_{lm}$ in a spherically symmetric potential V, so that $\vec{\nabla}V=\hat{r}\,dV/dr$, and $\int d\Omega\, Y^*_{l_fm_f}\,\hat{r}Y_{l_im_i}$ does not vanish, then

$$(E_f-E_i)^2\int drP_f^*rP_i=\int drP_f^*\frac{dV}{dr}P_i\,. \tag{10}$$

In the case of a point Coulomb potential $V=-a/r$, we thus obtain the simple relationship

$$k^2 I_1 = a I_{-2} \ . \tag{11}$$

Inserting this into Eqs. (3) and (6) gives simply

$$\beta^{E1}/\sigma = 3/8\pi a^2 \ , \tag{12}$$

the result which we have compared with the numerical calculations of the two processes.

We have elsewhere shown[6] that the screened central potential $V(r)$ within the interior of the atom is well represented in the form

$$V(r) = -(a/r)[1 + V_1(\lambda r) + V_2(\lambda r)^2 + V_3(\lambda r)^3 + \cdots] , \tag{13}$$

where $\lambda \simeq Z^{1/3}\alpha$ is a small parameter characterizing the screening and the coefficients V_i are of order unity, decreasing, and generally alternating in sign. We have obtained expressions for wave functions as expansions in λ, good within the interior of the atom, and we have used these[5] to obtain expressions for the dipole photoeffect cross section, as a series in λ, good within 0.5%. However, to compare photoeffect and internal conversion, we do not need to calculate either. Inserting (13) into (10) gives

$$k^2 I_1 = a[I_{-2} - V_2\lambda^2 I_0 - 2V_3\lambda^3 I_1 + \cdots] \ . \tag{14}$$

We will show that there is a simple exact relation between I_0 and I_{-2} in a screened potential, and, consequently, it is easy to obtain an approximate relation between I_1 and I_{-2} in a screened potential valid through order λ^3. To do this we now make use of the fact that angular momentum changes by one in these transitions. In terms of the radial Hamiltonian $H(l)$ satisfying

$$H(l)P_{q,l}(r) \equiv \left(-\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} + V(r) \right) P_{q,l}(r) = E_{q,l}P_{q,l}(r) \ , \tag{15}$$

we have

$$\begin{aligned} kI_0 &= (E_{p,l\pm1} - E_{nl})I_0 \\ &= \int dr\{[H(l\pm1)P_{p,l\pm1}]^* P_{nl} - P_{p,l\pm1}[H(l)P_{nl}]\} \\ &= \int dr P^*_{p,l\pm1}[H(l\pm1) - H(l)]P_{n,l} = \pm(l + \tfrac{1}{2} \pm \tfrac{1}{2})I_{-2} \ . \end{aligned} \tag{16}$$

Thus through λ^3

$$[k^2 + 2aV_3\lambda^3] I_1 = a[1 \mp (V_2\lambda^2/k)(l + \tfrac{1}{2} \pm \tfrac{1}{2})]I_{-2} \ . \tag{17}$$

These screening corrections to Eqs. (11) and (12) thus vanish for high energies. Inserting Eq. (17) into Eqs. (3) and (6) gives, for initial s waves ($l=0$), the simple result

$$\frac{\beta^{E1}}{\sigma} = \frac{3}{8\pi a^2}\left(1 + \frac{2V_2\lambda^2}{K} + \frac{4aV_3\lambda^3}{K^2} + \cdots\right). \tag{18}$$

The screening correction increases at low energies, and by the K-shell threshold is of order $4Z^{-4/3}$, i.e., a few percent.

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