

THE EFFECTS OF ATOMIC ELECTRONS

ON NUCLEAR RADIATION

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ABSTRACT

The effects of the atomic electrons on nuclear gamma emission are considered. It is found that the electrons, excited by the nuclear electrostatic field, can emit gamma rays coherently with the nucleus and thus add to the observed intensity of radiation. The correction is computed for K electrons, for electric dipole and quadrupole radiation, and is found to be small, of the order of a few per cent, for energies equal to the K binding energy. It drops rapidly with increasing energy, varying inversely as the square of the gamma ray energy. The Z-dependence of the effect is essentially Z^{-1} . For gamma ray energies corresponding to electron transitions between bound levels large resonances may occur, but they are of narrow width and their observation would be fortuitous.

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INTRODUCTION

The techniques for observing and measuring low intensity gamma rays, such as those emitted in the decay of low-lying nuclear states, have been improved greatly in recent years, so that it is becoming possible to get more precise information than order of magnitudes on the lifetimes of nuclear levels. These lifetimes, in turn, can be compared with calculations based on various assumptions for nuclear wave functions, and information about the nuclear states may be obtained. In addition, less precise measurements of gamma ray intensities are often used to determine the multipolarity of the radiation, and thus to obtain information about the angular momentum and parity of the states involved.

The usual approach to computation of the nuclear gamma ray lifetimes ignores the surrounding electrons in the atom, and gives the lifetime expected for the decay of a bare nucleus. It is the purpose of this paper to investigate what effect, if any, the atomic electrons have on the gamma rays observed during the decay of an excited nucleus.

It is well known that the principal effect of the atomic electrons is to provide an additional mode of decay for the nucleus -- "internal conversion." This occurs when the electrons are in states characteristic of the ground state of the nucleus and the nucleus is in an excited state. The non-spherical distribution of charge in the nucleus acts as a perturbation potential which induces transitions in the atomic electrons. In particular, it may induce a transition

to a continuum state, so that the atom can decay by exciting and emitting one of its electrons. This process competes with the gamma ray decay, so that effectively the excited nuclear lifetime is reduced. Calculations and observations show that for the heavier atoms, where the low-lying nuclear levels are at energies near the electron binding energies, the probability of internal conversion is comparable to that for gamma ray emission. (1)

There are other effects which the atomic electrons can have on the nucleus. It is possible for the nucleus to emit a gamma ray and for this gamma ray then to be scattered by the surrounding electron cloud. An inelastic scattering, which alters the gamma ray energy, would be observationally distinguishable from the original nuclear gamma ray, but might, in extreme cases, be confused with the decay of another close-by nuclear level. This effect, however, is of second order relative to the "bare" nuclear emission; furthermore, it is incoherent with it, since the final states are different. For these reasons, this "internal inelastic scattering" should be essentially negligible in its observed effects.

An elastic scattering ("internal Rayleigh scattering") is also possible. Cormack (2) has recently considered this effect and concluded that it is also very small. His reasoning is questionable, however, since he has made a classical calculation in which the original gamma emission and the scattering are considered separately. It is, of course, incorrect to do this, since the elastic scattering after emission is coherent with the undisturbed emission (same initial and final states), so that the comparison should be one of amplitudes rather than probabilities. Nevertheless, the relative effect is

still second order, so that the ratio of the amplitudes is expected to be of the order of e^2 , rather than the square of this quantity. The effect, then, is small, if not very small. In any case, this elastic scattering could not alter the total gamma ray intensity, but would change the angular distribution.

There is another effect which would alter the total intensity and which is more comparable in size. It is well known that the rates of gamma transitions for excited electronic states (even to the continuum, as in the photoelectric effect) are several orders of magnitude faster than the rates for nuclear transitions. It is possible for the nucleus to decay by exciting an electron, as in internal conversion, and then for the electron to de-excite by emitting a gamma ray, which it can do rather easily. This effect is thus only one order higher than the straight nuclear emission; furthermore, it is coherent with it, since we have (if the electron returns to its original state) a gamma ray of the same energy and multipolarity emerging. The observed gamma ray intensity, then, is due to the sum of the amplitudes for these two processes.

Other investigators, concerning themselves with the higher order effects on internal conversion coefficients, have considered corrections to the gamma ray intensity. In all cases no note seems to have been taken of the coherent nature of the process; that is, for various reasons, they have taken into account only a real photon emitted by the nucleus and then rescattered by the electrons. Taylor and Mott⁽³⁾ cast out the coherent part of their matrix element by arguing that it just represents a refraction, or scattering, of a real photon. This is not true if, as in our case, the major interaction with the electron is due to the electrostatic field of

the nucleus rather than the absorption of a real photon emitted by the nucleus. Tralli and Goertzel⁽⁴⁾ formulate the problem more generally, but in evaluating sums for second-order matrix elements they neglect the principal value (or coherent) terms because this type of term "is usually neglected." In addition, all their matrix elements are taken with energy conserved, so that they effectively neglect all virtual processes (the coherent ones) as opposed to the real (incoherent) terms. Coish⁽⁵⁾, in commenting on this last work, implies the same neglect. In neither of these latter works are any numerical estimates or computations made.

We can estimate the magnitude of this effect by looking at the cross-sections for internal conversion and for the photoelectric effect.

The internal conversion effect is usually expressed by a coefficient which gives the ratio of the number of electrons to the number of photons emitted. Thus

$$\alpha_{IC} = \frac{|IC|^2}{|R_N|^2} \frac{\rho_e}{\rho_\gamma} \quad (1;1)$$

where (IC), (R_N) are the matrix elements of the potentials for internal conversion and for nuclear gamma emission, and ρ_e , ρ_γ are the densities for final states corresponding to an electron or a gamma ray.

The photoelectric effect is expressed as a cross-section, or more conveniently, as the ratio of its cross-section to that for Thompson scattering:

$$\frac{\sigma_{PE}}{\sigma_T} = \frac{2\pi}{hc} \frac{|R_e|^2 \rho_e}{\frac{8\pi}{3} r_o^2} \quad (1;2)$$

where (R_e) is the matrix element for electronic radiation and r_0 is the classical electron radius $= \frac{e^2}{mc^2}$.

The effect we are concerned with is expressible as the product of the amplitudes for the two previous processes. Since it is second order, we should sum over all possible intermediate states and use an appropriate energy denominator. This procedure can be approximated by dividing by some average energy characteristic of the processes involved, which in this case should be of the order of the gamma ray energy. The ratio of the amplitude to that for straight nuclear emission will then be approximately

$$\begin{aligned} \frac{1}{\bar{E}} \frac{(IC) (R_e)}{(R_N)} &= \frac{1}{\rho_e \bar{E}} \left(\frac{\hbar c}{2\pi} \rho_\gamma \alpha_{IC} \sigma_{PE} \right)^{\frac{1}{2}} \\ &= \frac{1}{\rho_e \bar{E}} \frac{1}{(2\pi)^2} \left(\frac{8\pi}{3} \right)^{\frac{1}{2}} \frac{e^2}{\hbar c} \frac{E_\gamma}{mc^2} (\alpha_{IC} \frac{\sigma_{PE}}{\sigma_T})^{\frac{1}{2}}. \quad (1;3) \end{aligned}$$

To estimate the magnitude of this expression, we can take $\rho_e \bar{E} \sim 1$; $E_\gamma/mc^2 \sim 10^{-1}$ for heavy atoms; $\alpha_{IC} \sim 1$, and $\sigma_{PE}/\sigma_T \sim 10^3$ to 10^5 near the K edge. These figures give a result of about one per cent, which could be in error by a factor of ten or twenty in either direction. In particular, if any resonance effect appeared the result might be considerably larger. In any case, this very rough estimate indicates that the effect is not negligibly small, especially at the lower energies; we will proceed to a more accurate evaluation.

BASIC ASSUMPTIONS

In making the detailed computation of this effect we will be concerned mainly with gamma ray energies comparable with the electron K shell binding energy or several times as large. We will consider the electrons as non-relativistic particles and we will neglect retardation effects in computing radiation matrix elements. This latter approximation is certainly justified for the low energies we consider; the gamma ray wave lengths will be many times larger than the atomic dimensions. For the heaviest atoms the K binding energy is roughly 20 per cent of the electron mass; here relativistic effects are no longer completely negligible. They should not, however, change the results significantly.

In computing the internal conversion we will consider only the effects of the electrostatic field and not the transverse electromagnetic field. This is equivalent to neglecting terms of order v/c in electric multipole radiation and is compatible with the neglect of relativistic effects. This approximation is, of course, not possible for the computation of magnetic multipole radiation, which we will not undertake here.

In computing the behavior of the electrons during the process we treat them as independent, and use Coulomb wave functions; this neglects the effect of the other atomic electrons on the one in question, which consists of a screening of the nuclear field as well as some (small) correlation between electrons. We will discuss later the magnitude of this effect and how it may be approximately taken into account. In addition, we neglect the exclusion principle during the calculation, justifying this procedure at a more appropriate point.

We will compute the effect only for those electrons in the K-shell, and adduce arguments that the effect of the L and higher shells is small.

GAMMA RAY ENERGIES GREATER THAN K BINDING ENERGY

Since our effect is of second order in the electromagnetic field, it is appropriate to treat it by perturbation theory in a time-independent manner. Only when this theory diverges, as in the case of resonances, must we go to a more sophisticated treatment. This will be done in a later section. Here we consider only gamma ray energies larger than the K binding energy.

The transition probability for the emission of an electric l, m pole gamma ray of energy $h\omega$ from an excited bare nucleus is given by

$$\frac{2\pi}{\hbar} |H_l^m|^2 \frac{\omega^2}{(2\pi c)^3 \hbar} d\Omega \gamma \quad (3;1)$$

where H_l^m contains the angular dependence of the gamma ray as well as the nuclear matrix element. That is,

$$H_{lN}^m = B_l^m(\theta_\gamma) \langle f | Q_l^m | i \rangle, \quad (3;2)$$

where

$$\langle f | Q_l^m | i \rangle = e \sum_{i=1}^Z \langle \Phi_{Nf} | R_i^l Y_l^{m*}(\underline{R}_i) | \Phi_{Ni} \rangle \quad (3;3)$$

is the matrix element between initial and final nuclear states of the l, m electric moment.*

* The spherical harmonics, $Y_l^m(\theta, \phi)$, are used with the normalizations given in Blatt and Weisskopf, Appendix A. (6)

The potential at \underline{r} , exclusive of the central Coulomb field, on an external electron due to the electrostatic field of the nucleus is given by

$$V = - \sum_{i=1}^Z \frac{e^2}{|\underline{R}_i - \underline{r}|} + \frac{Ze^2}{r} \quad (3;4)$$

$$= - 4\pi e^2 \sum_{\ell=1}^{\infty} \sum_{m=-\ell}^{\ell} \sum_{i=1}^Z \frac{R_i^{\ell}}{2\ell+1} r^{-\ell-1} Y_{\ell}^m(\underline{r}) Y_{\ell}^{m*}(\underline{R}_i)$$

$$= - 4\pi e \sum_{\ell,m} \frac{1}{2\ell+1} Q_{\ell}^m(\underline{R}) r^{-\ell-1} Y_{\ell}^m(\underline{r}) \quad (3;5)$$

(This form is valid for $r > R_i$, that is, for the electron outside the nucleus. The effects due to the electron within the nucleus are negligible, and this form for V can be used everywhere.)

Note that this potential is of order e^2 , i.e., is already second order in the electromagnetic field. This is characteristic of any static potential such as this which can also be interpreted as the exchange of a (longitudinal) photon.

The matrix element for emission of a gamma ray from an excited electron is given by the same expression H_{ℓ}^m as for the nucleus, with the necessary modifications for the change in sign of the charge. For an electric ℓ, m -pole gamma ray emitted by an excited electron, then, we have

$$H_{\ell e}^m = - e B_{\ell}^m(\theta_{\gamma}) \langle \psi_{ef} | r^{\ell} Y_{\ell}^{m*}(\underline{r}) | \psi_{ej} \rangle \quad (3;6)$$

The second order process we are considering consists of the excitation of an electron by the potential V , coupled with the de-excitation of the nucleus, followed by the de-excitation of the

electron by emission of a gamma ray. The energy of the intermediate state is given by E_j , the excited electron energy.

The process can also occur in reverse order, in which first the electron radiates and then the potential V acts. Here the intermediate energy is given by $E_j + E_{\omega} + \Omega$, where Ω is the excitation energy of the nucleus. The initial energy is $\Omega + E_g$, the electron ground state energy.

There is another physical picture to explain this process. Because of the static interaction between nucleus and electron, the initial state can be considered as a superposition of states consisting of the basic state - nucleus excited and electron in its ground state - plus those states for which the nucleus is in its ground state and the electron is excited. Then the gamma ray can be emitted either by the excited nucleus or by the excited electron. Since short times are involved in the electronic radiation, it is not necessary for energy to be conserved in the admixture of excited electron states. The mathematics which describes this physical situation is exactly the same as that used in the description as a second order process.

The matrix element for this process is then given by the sum of two terms and is equal to

$$\begin{aligned}
 & + \frac{4\pi e^2}{2l+1} \langle \Phi_{Nf} | Q_l^m | \Phi_{Ni} \rangle B_l^m(\theta_\gamma) \cdot \\
 & \left\{ \sum_j \frac{\langle \psi_g | r^l Y_l^{m*} | \psi_j \rangle \langle \psi_j | r^{-l-1} Y_l^m | \psi_g \rangle}{E_g + \Omega - E_j} \right. \\
 & \left. + \sum_j \frac{\langle \psi_g | r^{-l-1} Y_l^m | \psi_j \rangle \langle \psi_j | r^l Y_l^{m*} | \psi_g \rangle}{E_g + \Omega - E_j - E_{\omega} - \Omega} \right\} \quad (3;7)
 \end{aligned}$$

$$= H_l^m \frac{4\pi e^2}{2l+1} \left\{ \dots \right\} \quad (3;8)$$

Here we have assumed, as is usual, that the excitation state of the nucleus is such that only a pure electric l, m -pole gamma ray can be emitted.

Overall conservation of energy dictates that the gamma ray energy equal the nuclear excitation energy, that is, $E_\omega = \Omega$; thus the only difference in the matrix elements for the two processes is in the sign of E_ω in the denominator of the sums. Note that for very large gamma ray energies, the two terms cancel to first order in $1/E_\omega$. It is convenient, for this reason, to perform an integration by parts and eliminate this first order term.

Before proceeding with this step and with the more detailed computations, we note that the total transition probability for gamma emission involves the square of the sum of the matrix elements for the bare nucleus and for this effect. Further, the matrix element we have just expressed is a (real) multiple of the bare nucleus matrix element. (It is real if the wave functions, ψ_j , involved, are real; we shall see later that the major contribution is due to their real parts.) This means that we have a correction factor of the form $(1 + f)^2$ to apply if we wish to compute the nuclear matrix element from the observed gamma intensity.

Since f is small, the correction is approximately given by $1 + 2f$ for a single electron. Actually, there are two electrons in the K-shell, so that the correction factor has the form $(1 + 2f)^2$, or approximately, $1 + 4f$.

Thus, we must divide the observed gamma intensity by the correction

factor, $1 + 4f_K$, before making comparisons with intensities computed for the nucleus alone.

We return now to the calculation. We have (since for overall energy conservation $\Omega = E_\omega$):

$$f = \frac{4\pi e^2}{2l+1} \left\{ \sum_j \frac{\langle \psi_g | r^l Y_l^{m*} | \psi_j \rangle \langle \psi_j | r^{-l-1} Y_l^m | \psi_g \rangle}{E_g + E_\omega - E_j} + \sum_j \frac{\langle \psi_g | r^{-l-1} Y_l^m | \psi_j \rangle \langle \psi_j | r^l Y_l^{m*} | \psi_g \rangle}{E_g - E_\omega - E_j} \right\} \quad (3;9)$$

$$= \frac{4\pi e^2}{2l+1} \frac{1}{E_\omega} \left\{ \sum_j \frac{(E_j - E_g) \langle g | r^l Y_l^{m*} | j \rangle \langle j | r^{-l-1} Y_l^m | g \rangle}{E_g + E_\omega - E_j} + \sum_j \frac{(E_g - E_j) \langle g | r^{-l-1} Y_l^m | j \rangle \langle j | r^l Y_l^{m*} | g \rangle}{E_g - E_\omega - E_j} \right\} \quad (3;10)$$

$$= \frac{4\pi e^2}{2l+1} \frac{1}{E_\omega} \left\{ \sum_j \frac{\langle g | [r^l Y_l^{m*}, H] | j \rangle \langle j | r^{-l-1} Y_l^m | g \rangle}{E_g + E_\omega - E_j} + \sum_j \frac{\langle g | r^{-l-1} Y_l^m | j \rangle \langle j | [r^l Y_l^{m*}, H] | g \rangle}{E_g - E_\omega - E_j} \right\} \quad (3;11)$$

$$\begin{aligned} \text{Now } [r^l Y_l^{m*}, H] &= \frac{1}{2m} [r^l Y_l^{m*}, p^2] \\ &= \frac{i\hbar}{m} \nabla (r^l Y_l^{m*}) \cdot \underline{p} + \frac{\hbar^2}{2m} \nabla^2 (r^l Y_l^{m*}) \\ &= \frac{i\hbar}{m} \nabla (r^l Y_l^{m*}) \cdot \underline{p} \\ &= \frac{i\hbar}{m} \underline{p} \cdot \nabla (r^l Y_l^{m*}) \end{aligned} \quad (3;12)$$

since $r^l Y_l^{m*}$ is a solution of the homogeneous Laplace's equation.

Thus

$$f = \frac{4\pi e^2}{2l+1} \frac{1}{E_\omega} \frac{i\hbar}{m} \left\{ \sum_j \frac{\langle g | \underline{p} \cdot \nabla (r^l Y_l^{m*}) | j \rangle \langle j | r^{-l-1} Y_l^m | g \rangle}{E_g + E_\omega - E_j} + \sum_j \frac{\langle g | r^{-l-1} Y_l^m | j \rangle \langle j | \nabla (r^l Y_l^{m*}) \cdot \underline{p} | g \rangle}{E_g - E_\omega - E_j} \right\} \quad (3;13)$$

Since ψ_g for the K-shell is spherically symmetric - that is, $\psi_g = (\gamma^3/\pi)^{1/2} e^{-\gamma r}$, where $\gamma = Z/a_0 = Zme^2/\hbar^2$ - \underline{p} operating on ψ_g is just - $i\hbar \frac{d}{dr} \psi_g = i\hbar\gamma \psi_g$. Thus

$$f = \frac{4\pi l}{2l+1} \frac{\gamma e^2}{E_\omega} \frac{\hbar^2}{m} \left\{ \sum_j \frac{\langle g | r^{l-1} Y_l^{m*} | j \rangle \langle j | r^{-l-1} Y_l^m | g \rangle}{E_g + E_\omega - E_j} - \sum_j \frac{\langle g | r^{-l-1} Y_l^m | j \rangle \langle j | r^{l-1} Y_l^{m*} | g \rangle}{E_g - E_\omega - E_j} \right\} \quad (3;14)$$

or

$$f = \frac{8\pi}{Z} \frac{l}{2l+1} \frac{E_K}{E_\omega} \left\{ B_+ - B_- \right\} \quad (3;15)$$

since $\frac{1}{2} Ze^2\gamma = E_K$, the K binding energy.

Before proceeding, we note that for very large gamma ray energies we can neglect $E_g - E_j$ in the denominators and find

$$f_{E_\omega \rightarrow \infty} = \frac{16\pi}{Z} \frac{l}{2l+1} \frac{\hbar^2 E_K}{mE_\omega^2} \sum_j \langle g | r^{l-1} Y_l^{m*} | j \rangle \langle j | r^{-l-1} Y_l^m | g \rangle$$

$$\begin{aligned}
 &= \frac{16\pi}{Z} \frac{\ell}{2\ell+1} \left(\frac{E_K}{E_\omega} \right)^2 \frac{2\gamma}{\pi} \int_0^\infty dr e^{-2\gamma r} \\
 &= \frac{16}{Z} \frac{\ell}{2\ell+1} \left(\frac{E_K}{E_\omega} \right)^2, \quad E_\omega \gg E_K. \quad (3;16)
 \end{aligned}$$

This agrees with the classical limit computed by treating the motion of the electron as that of a forced oscillator. Note that this represents an increase in the gamma ray intensity. The correction becomes negligibly small for gamma ray energies ten or more times the K binding energy, if we consider atoms with $Z \sim 50$.

We return again to the exact calculation. Since ψ_g is spherically symmetric, we can readily perform the angular integrations.

Defining the "reduced" radial eigenfunctions by

$$u_j^\ell = r^{-\ell} \int d\Omega Y_\ell^{m*} \psi_j(\underline{r}), \quad (3;17)$$

$$B_+ = \frac{\hbar^2}{m} \int dr \int dr' \psi_g(r) r^{2\ell+1} G_\ell(E_+; r, r') \psi_g(r') r' \quad (3;18)$$

and

$$B_- = \frac{\hbar^2}{m} \int dr \int dr' \psi_g(r) r^{2\ell+1} G_\ell(E_-; r, r') \psi_g(r') r' \quad (3;19)$$

where the Green's functions, $G_\ell(E; r, r')$, are for the reduced radial equation and are defined and evaluated in Appendix A. They are:

$$G_\ell(E_\pm; r, r') = -\frac{2m}{\hbar^2} \frac{\Gamma(\ell+1-ia)}{\Gamma(2\ell+2)} (-2ik)^{2\ell+1} e^{ikr} e^{ikr'}$$

$$\Phi(\ell+1-ia; 2\ell+2; -2ikr_<) \Psi(\ell+1-ia; 2\ell+2; -2ikr_>) \quad (3;20)$$

where $\hbar^2 k^2 = 2mE_+$, and $a = \gamma/k$.

Φ and Ψ are the regular and irregular confluent hypergeometric functions as defined by Bateman (Chap. 6). (7)

$r_<$ and $r_>$ are the greater and lesser of r and r' .

$$G_\ell(E_+; r, r') = G_\ell^*(E_+; r, r') = -\frac{2m}{\hbar^2} \frac{\Gamma(\ell+1-b)}{\Gamma(2\ell+2)} (2\kappa)^{2\ell+1} e^{-\kappa r} e^{-\kappa r'}$$

$$\Phi(\ell+1-b; 2\ell+2; 2\kappa r_<) \Psi(\ell+1-b; 2\ell+2; 2\kappa r_>) \quad (3;21)$$

where $\hbar^2 k^2 = -2mE_- = 2m|E_-|$, and $b = \gamma/k$. For $E_+ = 0$, we have

$$G_\ell(0, r, r') = -\frac{2m}{\hbar^2} \pi i (rr')^{-\ell-\frac{1}{2}} J_{2\ell+1}(2\sqrt{2\gamma r_<}) H_{2\ell+1}^{(1)}(2\sqrt{2\gamma r_>})$$

(3;22)

where J_ν and H_ν are Bessel and Hankel functions; $H_\nu^{(1)} = J_\nu + iY_\nu$.

If we substitute these expressions into those for B and re-write in dimensionless form, we have:

$$B_+ = \frac{2}{\pi} 2^{2\ell+1} \frac{\Gamma(\ell+1-ia)}{\Gamma(2\ell+2)} (-)^{\ell} ia^3$$

$$\iint dx dy e^{-(a-i)x} e^{-(a-i)y} x^{2\ell+1} y \Phi(\ell+1-ia; 2\ell+2; -2ix_<)$$

$$\Psi(\ell+1-ia; 2\ell+2; -2ix_>) \quad (3;23)$$

$$B_- = -\frac{2}{\pi} 2^{2\ell+1} \frac{\Gamma(\ell+1-b)}{\Gamma(2\ell+2)} b^3$$

$$\iint dx dy e^{-(1+b)x} e^{-(1+b)y} x^{2\ell+1} y \Phi(\ell+1-b; 2\ell+2; 2x_<)$$

$$\Psi(\ell+1-b; 2\ell+2; 2x_>) \quad (3;24)$$

$$B_0 = -2i \iint dx dy e^{-x} e^{-y} x^{l+\frac{1}{2}} y^{\frac{1}{2}-l} J_{2l+1}(\sqrt{8x}) H_{2l+1}^{(1)}(\sqrt{8y}) \quad (3;25)$$

These expressions for B cannot in general be evaluated exactly analytically, for they involve an integrand of discontinuous form. What is required is a knowledge of the indefinite integral of the confluent hypergeometric function multiplied by an exponential. The use of series and asymptotic expansions for these functions does not help, as too many terms of the resulting double summation are needed for convergence.

B_0 can be evaluated exactly, however, since an integral representation exists for the product of Bessel functions involved.

(Appendix C) Further, the integrand of B_- reduces to a combination of Bessel functions for $b = 0, \frac{1}{2},$ or 1 ; again an integral representation can be found and these points may be evaluated exactly.

(Appendices B, C, D.)

In addition, we can obtain limiting forms for B_+ and B_- for small a and b ; that is, for large gamma energies. As before, this arises because the hypergeometric functions tend to Bessel functions in this limit. (Appendix D.)

We can then plot these exact evaluations of B and draw an interpolated curve with reasonable accuracy (estimated at about ± 10 per cent of the final result.). We have made these calculations for $l = 1$ and $l = 2$; that is, for electric dipole and quadrupole radiation.

The final result is given in fig. 1, where $8fZ/100$ is plotted against E_ω/E_K for $l = 1$ and $l = 2$.

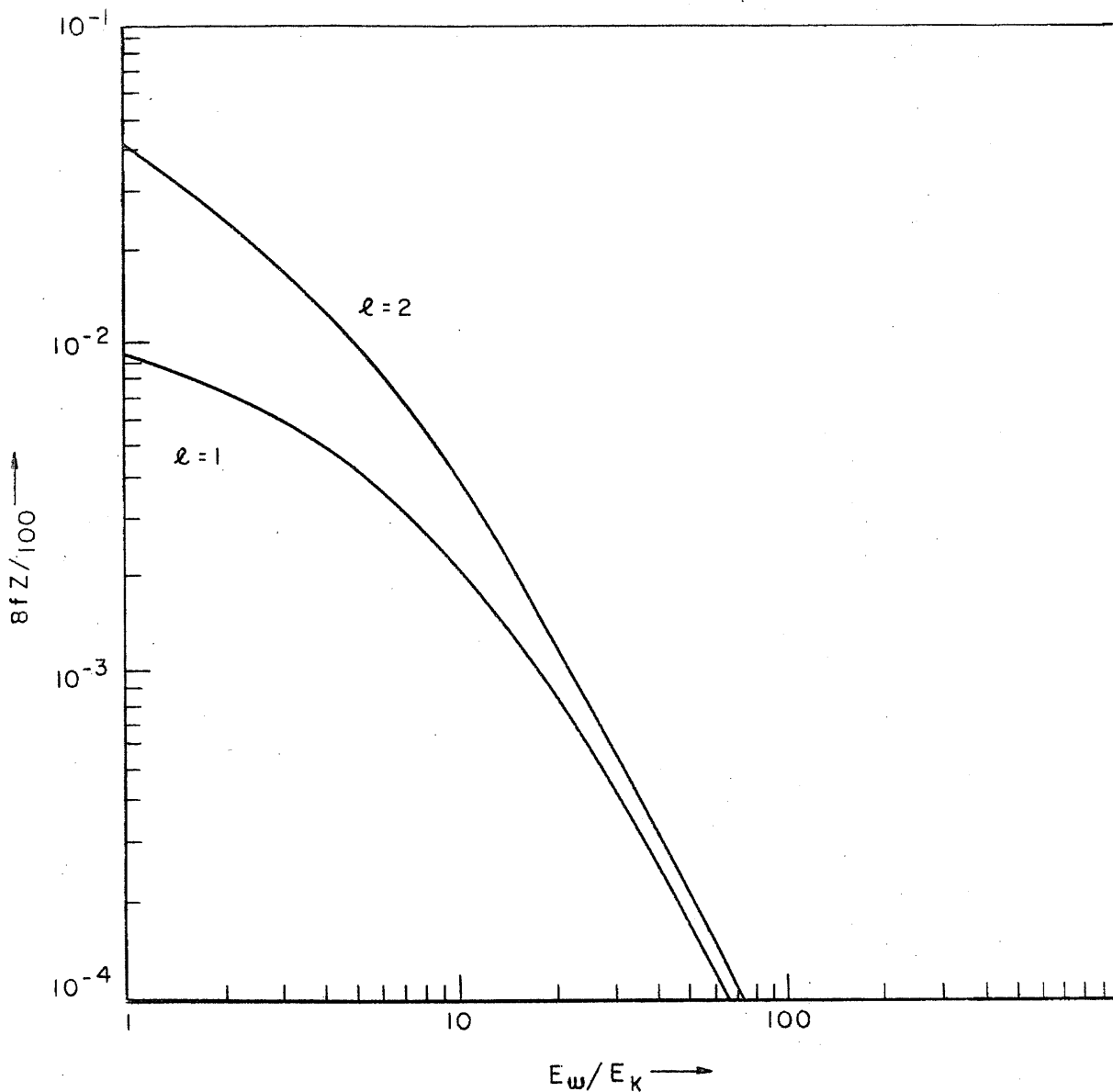


Fig. 1. Correction term for electric dipole and quadrupole radiation. Note that for $Z = 50$, the correction, $4f$, is read directly from the curve.

GAMMA RAY ENERGIES SMALLER THAN K BINDING ENERGY

As was noted previously, the Green's function propagators for the Coulomb field are singular for energies corresponding to those of the bound states. The second order perturbation theory employed in the last section thus breaks down and cannot be applied for energies $E_{\omega} < E_K$. To overcome this difficulty we need to look more carefully at the equations governing the reaction and take into account the damping, or interaction of radiation with radiated field. (8)

We are interested, then, in the emission probability for gamma rays of energy less than the K-binding, and near the excitation energy from the K to another shell. As before, states of all energies are in principle available as intermediate states; however, it is clear that the major contribution will come from that single state which is in, or nearly in, resonance with the ground state and gamma ray.

We thus will consider the time-dependent treatment of a problem in which three types of states enter:

The initial state: nucleus excited, electron in ground state, and no gamma ray;

The intermediate state: nucleus in ground state, electron in state n , no gamma ray;

The final state: nucleus in ground state, electron in ground state, a gamma ray of energy $\hbar\omega$.

Let b_0 , b_n , $b_{f\omega}$ be the time dependent amplitudes of these

states in the interaction representation, and Ω , ϵ_n , and ω be the energies of the three types of states (relative to the ground state energy of the unperturbed atom).

The unperturbed Hamiltonian, H_0 , is taken to be that for the electron in a Coulomb field; the perturbing (or additional) parts of the total Hamiltonian are the radiation field for both nucleus and electron, and the electrostatic interaction between nucleus and electron, exclusive of the spherically symmetric Coulomb field.

The exact equations for the amplitudes are then ($\hbar = c = 1$):

$$b'_0 = -i V^* b_n e^{i(\Omega - \epsilon_n)t} - i \sum_{\omega} \sum_{\text{pol}} \sum_{\Delta} A b_{f\omega} e^{i(\Omega - \omega)t} \quad (4;1)$$

$$b'_n = -i V b_0 e^{i(\epsilon_n - \Omega)t} - i \sum_{\omega} \sum_{\text{pol}} \sum_{\Delta} B b_{f\omega} e^{i(\epsilon_n - \omega)t} \quad (4;2)$$

$$b'_{f\omega} = -i A^* b_0 e^{i(\omega - \Omega)t} - i B^* b_n e^{i(\omega - \epsilon_n)t} \quad (4;3)$$

where $A^* = CN$, $B^* = CR$ are respectively the time independent matrix elements for emission of a given multipole gamma ray from the nucleus and from the excited electron. In each case the initial state is the excited, and the final state the ground, level of the nucleus, or electron. C represents the common factors which include the angular dependence of the gamma ray, the various constants, etc. V is the interaction between the nucleus and the electron, by means of which the nucleus is de-excited and the electron is excited. As was seen previously, we may write V as the product of a nuclear and an electron matrix element, $V = NX$.

Further, in the absence of interactions, we have for the rate of emission from the nucleus or from the excited electronic state:

$$\Gamma_N = 2\pi\rho \sum_{\text{pol}} \sum_{\mathbf{A}} |c|^2 |N|^2 \quad (4;4)$$

$$\Gamma_e = 2\pi\rho \sum_{\text{pol}} \sum_{\mathbf{A}} |c|^2 |R|^2$$

where ρ is the density of final states associated with an emitted gamma ray.

We want to solve the time-dependent equations with the initial conditions

$$b_o(0) = 1 \quad ; \quad b_n(0) = b_{fw}(0) = 0 \quad . \quad (4;5)$$

We will look for a solution of the form

$$b_o(t) = e^{-\Gamma t/2} \quad (4;6)$$

$$b_n(t) = \beta \left[e^{-\Gamma t/2} e^{i(\epsilon_n - \Omega)t} - e^{-\gamma t/2} \right]$$

If we can find such a solution, then Γ/Γ_N , we shall see, is the factor $(1 + f)^2$ which we considered previously - the ratio of the number of gamma rays from the atom to that from the bare nucleus.

Substituting the ansatz into the equation for b_{fw} and integrating, we find

$$b_{fw}(t) = \left[A^* + B^* \beta \right] \frac{e^{-\Gamma t/2} e^{i(\omega -)t} - 1}{\Omega - \omega - i\Gamma/2} - B^* \beta \frac{e^{-\gamma t/2} e^{i(\omega - \epsilon_n)t} - 1}{\epsilon_n - \omega - i\gamma/2} \quad . \quad (4;7)$$

To determine Γ , γ , and β , we substitute back into (4;1) and (4;2) and equate coefficients of terms with like time dependence.

We make use of the relation:

$$\sum_{\omega} f(\omega) \frac{e^{-\gamma t/2} - e^{i(\omega_0 - \omega)t}}{\omega_0 - \omega - i\gamma/2} \simeq -i\pi f(\omega_0) \rho(\omega_0) e^{-\gamma t/2} \quad (4;8)$$

when $f(\omega)$ is a slowly varying function of ω (compared to the width of the resonance term).

We find from (4;2) that

$$\gamma = 2\pi\rho \sum \sum |B|^2 = \Gamma_e \quad (4;9)$$

which is as expected; the excited electron decays by emission of a gamma ray as in the unperturbed condition.

Also

$$\beta = \frac{-iV - \pi\rho \sum \sum A^* B}{\frac{\gamma - \Gamma}{2} + i(\epsilon_n - \Omega)} \quad (4;10)$$

and

$$B^* \beta = -A^* \frac{\gamma/2 + iF}{\frac{\gamma - \Gamma}{2} + i(\epsilon_n - \Omega)}, \quad (4;11)$$

where $F = XR$ and we have substituted for A and B from their definitions.

If we now substitute into (1) to determine Γ we find:

$$\begin{aligned} \frac{\Gamma}{2} e^{-\Gamma t/2} &= \left[iV^* \beta + \pi\rho \sum \sum (|A|^2 + AB^* \beta) \right] e^{-\Gamma t/2} \\ &\quad - \left[iV^* \beta + \pi\rho \sum \sum AB^* \beta \right] e^{-\gamma t/2} e^{i(\Omega - \epsilon_n)t} \end{aligned} \quad (4;12)$$

The term in the last bracket is not zero, so that we cannot satisfy this equation exactly; however, we already have found $\gamma = \Gamma_e$. If Γ is of the order of Γ_n , the nuclear width, then $\Gamma \ll \gamma$, so that for times not near zero the second term is negligible compared to the first.

With this qualification, then, we find

$$\Gamma = \Gamma_N \left[\frac{\frac{2F^2}{\gamma} - \frac{\Gamma}{2} + i(\epsilon_n - \Omega - 2F)}{\frac{\gamma - \Gamma}{2} + i(\epsilon_n - \Omega)} \right] \quad (4;13)$$

Calculations of F and γ for particular electron states indicate that our assumption $\Gamma \ll \gamma$ is valid, and that $F^2/\gamma \gg \Gamma$.

Thus we have, approximately:

$$\Gamma \approx \Gamma_N \frac{\frac{2F^2}{\gamma} + i(\epsilon_n - \Omega - 2F)}{\gamma/2 + i(\epsilon_n - \Omega)} \quad (4;14)$$

We see that far away from resonance ($\epsilon_n - \Omega$ large), $\Gamma \rightarrow \Gamma_N$, as is expected.

Separating real and imaginary parts, we find

$$\begin{aligned} \text{Im } \Gamma &= \Gamma_N \frac{(\epsilon_n - \Omega) \left(\frac{\gamma}{2} - \frac{2F^2}{\gamma} \right) - \gamma F}{(\Omega - \epsilon_n)^2 + \gamma^2/4} \\ \text{Re } \Gamma &= \Gamma_N \frac{(F + \Omega - \epsilon_n)^2}{(\Omega - \epsilon_n)^2 + \gamma^2/4} \end{aligned} \quad (4;15)$$

We note that near resonance $\text{Re } \Gamma \gg \text{Im } \Gamma$, which is consistent with our line of thinking.

Further, we are interested primarily in the real part of Γ , which gives the rate of decay of the initial state; the imaginary

part is merely a slight shift in the energy of the line.

To complete the discussion, we note that the distribution of gamma rays is given by

$$\left| b_{F\omega}(\omega) \right|^2 = \frac{|A|^2}{(\Omega - \omega)^2 + \frac{\Gamma^2}{4}} \frac{(\omega - \epsilon_n + F)^2}{(\omega - \epsilon_n)^2 + \frac{\gamma^2}{4}}. \quad (4;16)$$

Since the first factor is a much sharper resonance than the second, we can write

$$\left| b_{F\omega}(\omega) \right|^2 \approx \frac{|A|^2}{(\Omega - \omega)^2 + \frac{\Gamma^2}{4}} \frac{(\Omega - \epsilon_n + F)^2}{(\Omega - \epsilon_n)^2 + \frac{\gamma^2}{4}} = \frac{\Gamma}{\Gamma_N} \frac{|A|^2}{(\Omega - \omega)^2 + \frac{\Gamma^2}{4}} \quad (4;17)$$

near resonance.

This is to be compared with

$$\left| b_{F\omega}^{(0)}(\omega) \right|^2 = \frac{|A|^2}{(\Omega - \omega)^2 + \frac{\Gamma_N^2}{4}} \quad (4;18)$$

in the absence of interaction.

We see that the main difference in the two expressions near resonance is the substitution of the altered width Γ for the "bare" width Γ_N . This supports our earlier contention that the ratio Γ/Γ_N is the ratio of the gamma emission rates for the atom and bare nucleus.

This can be explained very easily physically. Γ gives the decay rate of the excited nucleus, which decays in two ways - by

emitting photons and by exciting an electron. The electron radiation rate is so much faster than this that essentially all the excited electrons decay by emitting additional photons. Thus the photon emission rate is effectively the same as the nuclear decay rate.

We can compute the ratio Γ/Γ_N for various energies corresponding to electronic transitions between bound levels. We note that the width of the resonances involved is essentially the electronic radiation width, or about $10^{-6} E_\omega$.

At the resonance, our formula gives

$$\frac{\Gamma}{\Gamma_N} = \frac{4F^2}{\hbar^2 \Gamma_e^2} \quad (4;19)$$

where the electronic radiation width

$$\hbar \Gamma_e = \frac{8\pi(l+1)}{l[(2l+1)!!]^2} \left(\frac{\omega}{c}\right)^{2l+1} e^2 |R_l^m|^2, \quad (4;20)$$

with

$$R_l^m = -\left(\frac{\gamma^3}{\pi}\right)^{\frac{1}{2}} \int_0^\infty dr r^{l+2} e^{-\gamma r} \phi_{nl}(r). \quad (4;21)$$

$\phi_{nl}(r)$ is the radial wave function for an electron in the excited state.

$$\begin{aligned} F &= -\frac{4e^2}{2l+1} (\pi\gamma^3)^{\frac{1}{2}} R_l^m \int_0^\infty dr r^{1-l} e^{-\gamma r} \phi_{nl}(r) \\ &= -\frac{4e^2}{2l+1} (\pi\gamma^3)^{\frac{1}{2}} R_l^m X_l^m \end{aligned} \quad (4;22)$$

Thus

$$\frac{\Gamma}{N} = \left(\frac{l}{l+1}\right)^2 \left[(2l+1)!! (2l-1)!! \right]^2 \left(\frac{c}{\omega}\right)^{4l+2} \left(\frac{I_2}{I_1}\right)^2 \quad (4;23)$$

where I_1, I_2 are the radial integrals involved in R and X.

We can easily compute these integrals if we use Coulomb wave functions. We find

$$\frac{\Gamma}{N} = 2^4 \left(\frac{137}{Z}\right)^6 \quad \text{for the } 1S \rightarrow 2P \text{ transition,}$$

and

$$\frac{\Gamma}{N} = 5^4 \left(\frac{137}{2Z}\right)^6 \quad \text{for the } 1S \rightarrow 5P \text{ transition.}$$

Thus, exactly at those energies corresponding to a possible excitation of a K electron, the gamma radiation is very greatly enhanced; however, as noted previously, the spread of this enhancement is very small, so that it would be quite fortuitous if it were ever observed, for this would require a nuclear excited state at precisely the right energy. In addition, we expect no effect from transitions such as the $1S \rightarrow 2P$, since these states are already occupied; the effect will be seen only for transitions to empty levels. Finally, in our theory we considered the effect of only the one level in approximate resonance with the nuclear excitation; clearly, if we had considered all levels we would have some continuous background, probably of the same order of magnitude as the effect computed in the previous section.

EFFECT ON INTERNAL CONVERSION COEFFICIENTS

The internal conversion coefficient is defined as the ratio of the number of electrons emerging from an atom with excited nucleus to the number of quanta observed. This ratio is independent of the specific nuclear properties other than the multipolarity of the radiation, and its measurement is thus a convenient way of determining this quantity. In addition, the L to K branching ratio or the number of electrons ejected from the L shell (with consequent higher energy) compared to the number ejected from the K shell, is a sensitive function of the multipolarity of the transition and again gives a means of determining this quantity. Both of these measurements dealing with total intensities are obviously more susceptible to measurement than an analysis of the angular distribution of the radiation or electrons, which is handicapped by the low intensities involved and the more complicated equipment needed.

Theoretical calculations of the internal conversion coefficients have been made in some detail with progressively increasing accuracy including the effects of screening and relativity. In all these calculations, however, only first order effects have been considered. That is, the gamma ray emission has been expressed for a bare nucleus, and the internal conversion has been computed for a single interaction with the electron.

It is clear that if the atomic electrons affect the rate of gamma emission, they will also affect the internal conversion coefficient. At first glance one might expect the internal conversion

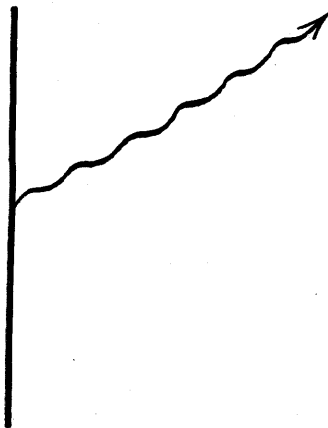
coefficient is altered by just the same factor as the gamma emission rate; however, to be consistent, we should consider effects of the same order in the electron ejection and use the ratio of the two corrections.

We have found that the effect on gamma emission rates is appreciable only at quite low energies, and is due mainly to the direct electrostatic interaction between nucleus and electron. In considering the effect on electron ejection, we will be consistent if we again neglect the effects of transverse fields (which will be of order $(v/c)^2$) except where a real photon is concerned. As before, we will neglect relativistic effects, screening, etc.

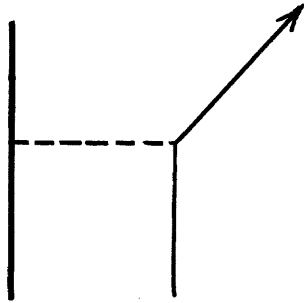
It is convenient in analyzing this problem to consider first a "one electron" atom (that is, an atom in which only one K electron can take part in the interaction) and then consider the case where both K electrons can interact.

The first order effects, as usually computed, correspond to the "one electron" picture.

The gamma emission is represented by the matrix element for the process:

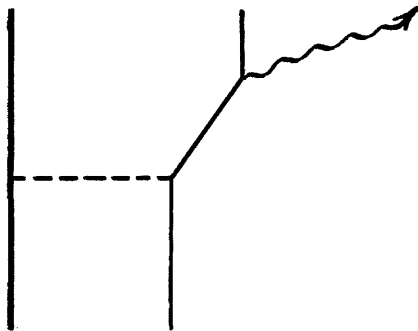


and the internal conversion by the process



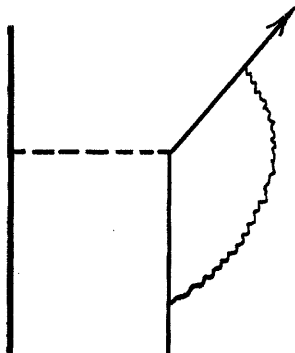
For the energies we are considering, the interaction between nucleus and electron is an instantaneous electrostatic potential.

The correction to the gamma emission rate was represented by the process



and its analogue with the order of interactions on the electron reversed.

To this same order, for the "one electron" atom, there is no correction term for the internal conversion, for radiative corrections of the type



are being neglected as being of order $(v/c)^2 = (Z/137)^2$ relative to the magnitude of the effects considered. (The possibility of a resonance in the energy denominator for this effect does not invalidate this reasoning, for the same resonance occurs in the correction term evaluated above; the fact that we are concerned with the principal part reduces its effect considerably. An estimate similar to that carried out in the introduction confirms this.)

Thus, if f_K is the correction matrix element for the emission rate, and α_0 is the first order internal conversion coefficient, we will have

$$\alpha_{\text{corr}} = \frac{\alpha_0}{|1 + f_K|^2} \approx \alpha_0 (1 - 2f_K) .$$

With both K electrons interacting there are additional correction terms which correspond to the nucleus interacting with one electron and this one in turn interacting with the other. It is not clear how this effect should be taken into account, for it will depend on the degree to which inter-electron interaction has been considered in the calculation of the internal conversion. It is not really a radiative correction at all, but rather one aspect of the problem of using correct atomic wave functions in the computations.

DISCUSSION

Before considering the results we have obtained, we will first discuss some of the approximations we have made - their effect, and how they may be bettered.

Screening

We have considered the electrons as independent, and acting under the influence of the nucleus only. Obviously, there will be some screening of the nuclear field by the other electrons, so that particularly at large distances from the nucleus the electrons sees a much weaker field. This effect is often taken partly into account by using screening coefficients, or effective Z's; that is, we can replace Z by $Z - \sigma$, where σ is often determined empirically. The effect is very small for the K shell, for which σ is approximately 0.3. For higher shells, the correction is increasingly more important. In our problem, however, a major part of the interaction takes place in close to the nucleus; here the distortion of the wave function is expected to be small. Reitz,⁽⁹⁾ in calculating internal conversion coefficients, took screening into account in a different, and perhaps better, way. He used wave functions computed for the Thomas-Fermi-Dirac statistical atom, and found that the correction to the unscreened model was less than 10 per cent; for the low energies with which we are concerned in our problem, the correction was about 3 per cent. This indicates that the screening effect will not change our calculations in any significant way.

Effects of L and Higher Shells

We have considered the effects of K electrons only. Clearly, the other electrons in the atom can also contribute to the increase in intensity, although their effect is expected to be smaller since they are in general less likely to be found near the nucleus. We can estimate this effect in two ways.

Our effect can be considered as a combination of internal conversion and the inverse photo-electric effect. For both of these phenomena the additional effects of higher shells have been considered. For internal conversion, the ratio of the number of electrons ejected from the L shell to the number ejected from the K shell has been calculated to be approximately 10 per cent for dipole, and about 30 per cent for quadrupole, radiation.⁽¹⁾

In the photo-electric effect, Heitler⁽¹⁰⁾ advises that experimental data indicate that the effect of the other shells is to increase the effect by from 20 to 25 per cent. Thus we expect a figure of about 25 per cent to be a fair measure of the additional effect of other shells.

Alternatively, we can estimate the effects of the L and higher shells by looking at the form of our expression for f . We note that it depends inversely on Z ; this dependence is due to a direct dependence on the radius of the K shell. In addition, it depends inversely (at high energies) on the square of the ratio of gamma ray to K shell energy. For the L shell, the radius is 4 times as large, but the energy is $\frac{1}{4}$ as great; thus, again we are led to the conclusion that the L shell effect is roughly 25 per cent of the K shell effect.

The Exclusion Principle

In our calculation, we assumed that all intermediate states were available to the interacting electron; that is, we ignored the exclusion principle in that certain of these states will be occupied by other electrons in the atom. It can be easily shown that if we consider the possible interactions of all the atomic electrons and ignore the exclusion principle with reference to intermediate states we arrive at the same result as if we had taken it into account. This is generally true; as long as the initial and final wave functions are properly anti-symmetrized, we may use any complete set of intermediate wave functions. (This is true as long as the interactions considered are symmetric; all physical terms are of this type.)

Discussion of Results

We turn finally to a consideration of the results we have obtained. We noted that previous investigators, by neglecting the possibility of coherence, had concluded that the atomic electrons had a negligible effect on nuclear radiation. Our numerical results indicate that while the effect is not completely negligible, it is practically so. For electric dipole radiation, the additional intensity is less than one per cent (for $Z = 50$) for all energies greater than the K binding energy, and drops very rapidly. Although decreasing Z tends to increase the correction, this is more than overbalanced by the lack of low energy nuclear transitions in the light elements. For electric quadrupole radiation,

which is far more prevalent in nuclei, the correction is approximately 4 per cent (for $Z = 50$) at the K binding energy and again drops very rapidly. Neither of these figures really represents a significant correction when one considers the experimental accuracy involved; in addition, any nuclear models cannot be expected to predict with anything approaching this degree of accuracy.

The effect on the internal conversion coefficients is similarly essentially negligible, since here again the experimental accuracy is not yet refined to this degree.

Finally, we noted that for gamma energies corresponding to transitions between electronic bound states there would be a large enhancement; here, however, we argue that because of the narrow width of these resonances it would be quite fortuitous if they were observed.

APPENDIX A

GREEN'S FUNCTIONS

We wish to compute the Green's function propagators for the "reduced" radial electron wave functions. That is, we want to evaluate the sum:

$$\sum_j \frac{u_j^l(r') u_j^{*l}(r)}{E - E_j} = G_l(E; r', r) \quad (A;1)$$

where

$$u_j^l(r) = r^{-l} \int d\Omega Y_l^{m*} \psi_j(\underline{r}) \quad , \quad (A;2)$$

for $\psi_j(\underline{r})$ the normalized eigenfunction for an electron of energy E_j in the field of a nucleus of charge Ze .

u_j^l satisfies the reduced radial Schrodinger equation

$$\left[\frac{d^2}{dr^2} + \frac{2l+2}{r} \frac{d}{dr} + \frac{2\gamma}{r} + k_j^2 \right] u_j^l = \left[L_r + k_j^2 \right] u_j^l = 0. \quad (A;3)$$

Here $\gamma = \frac{Z}{a_0} = \frac{Zme^2}{\hbar^2}$

and $k_j^2 = \frac{2m}{\hbar^2} E_j$.

Applying the operator L_r to the Green's function, we find

$$\begin{aligned} L_r G_l(E_j, r, r') &= -\frac{2m}{\hbar^2} \sum_j \frac{k_j^2 u_j^l(r') u_j^{*l}(r)}{k^2 - k_j^2} \\ &= -k^2 G_l + \frac{2m}{\hbar^2} \sum_j u_j^l(r') u_j^{*l}(r) \quad . \end{aligned} \quad (A;4)$$

Now, the complete eigenfunctions are normalized by

$$\sum_j \psi_j(\underline{r}') \psi_j^*(\underline{r}) = \delta(\underline{r} - \underline{r}') \quad , \quad (\text{A;5})$$

so that

$$\begin{aligned} \sum_j u_j^l(\underline{r}') u_j^{*l}(\underline{r}) &= (rr')^{-l} \int d\Omega \int d\Omega' Y_l^{m*}(\underline{r}') Y_l^m(\underline{r}) \delta(\underline{r} - \underline{r}') \\ &= (rr')^{-l-1} [\delta(r - r') + \delta(r + r')] \\ &= r^{-2l-2} [\delta(r - r') + \delta(r + r')] \quad . \quad (\text{A;6}) \end{aligned}$$

Thus G_l satisfies the equation:

$$(L_r + k^2) G_l(r, r') = \frac{2m}{\hbar^2} r^{-2l-2} [\delta(r - r') + \delta(r + r')] \quad (\text{A;7})$$

and similarly,

$$(L_{r'} + k^2) G_l(r, r') = \frac{2m}{\hbar^2} r'^{-2l-2} [\delta(r' - r) + \delta(r + r')] \quad . \quad (\text{A;8})$$

So G can be expressed in the form

$$\begin{aligned} G(r, r') &= C f(r) g(r') & r < r' \\ &= C f(r') g(r) & r > r' \end{aligned} \quad (\text{A;9})$$

where f and g are respectively the regular and irregular (at the origin) solutions of the homogeneous equation.

The constant C is determined by the conditions at the discontinuity $r = r'$; one integration of the differential equation gives

$$\frac{d}{dr} G(r, r') \Bigg|_{r'-\epsilon}^{r'+\epsilon} = \frac{2m}{\hbar^2} r^{-2l-2} \quad (\text{A;10})$$

or

$$C = \frac{2m}{\hbar^2} r^{-2l-2} [g'f - f'g]^{-1} \quad . \quad (\text{A;11})$$

The equation $(L + k^2) u = 0$ is of the form treated by Bateman 6.2(1).

It has as solutions

$$u = e^{-\kappa r} C\left(\ell + 1 - \frac{\gamma}{\kappa}; 2\ell + 2; \mp 2\kappa r\right) \quad (\text{A};12)$$

where $\kappa^2 = -k^2$, and C is a confluent hypergeometric function.

For negative energies, $E < 0$, $\kappa^2 > 0$, we impose the boundary condition that G be finite (vanishing) at infinity. This requires that

$$\begin{aligned} f &= e^{-\kappa r} \Phi\left(\ell + 1 - \frac{\gamma}{\kappa}; 2\ell + 2; 2\kappa r\right) \\ g &= e^{-\kappa r} \Psi\left(\ell + 1 - \frac{\gamma}{\kappa}; 2\ell + 2; 2\kappa r\right) . \end{aligned} \quad (\text{A};13)$$

where Φ is the ordinary confluent hypergeometric function known otherwise as ${}_1F_1$, and Ψ is the other solution of this equation defined by Bateman and closely related to the Whittaker functions.

Making use of the Wronskian for these two solutions of the equation we find, finally, that for negative energies

$$\begin{aligned} G_\ell(E; r, r') &= \\ &= -\frac{2m}{\hbar^2} \frac{\Gamma\left(\ell + 1 - \frac{\gamma}{\kappa}\right)}{\Gamma(2\ell + 2)} (2\kappa)^{2\ell+1} e^{-\kappa r} e^{-\kappa r'} \Phi\left(\ell + 1 - \frac{\gamma}{\kappa}; 2\ell + 2; 2\kappa r_{<}\right) \\ &\quad \Psi\left(\ell + 1 - \frac{\gamma}{\kappa}; 2\ell + 2; 2\kappa r_{>}\right) \end{aligned} \quad (\text{A};14)$$

where $r_{<}$, $r_{>}$ refer to the smaller and larger of r , r' .

We note in passing that G becomes infinite (i.e., is not defined) wherever $\ell + 1 - \frac{\gamma}{\kappa}$ is a non-positive integer. This occurs whenever the energy E corresponds to that of a bound state, and is to be expected.

In addition, we note that the confluent hypergeometric functions $\Phi(a, c, x)$ or $\Psi(a, c, x)$ are readily related (by means of derivatives, etc.) to the functions with a and/or c increased or decreased by some integer. Further, whenever $c = 2a$, they reduce to Bessel functions. This last feature will prove valuable in making exact calculations.

In an exactly analogous manner, we can find the Green's functions for positive energy and for zero energy. In these cases the solutions at infinity are oscillatory; a careful consideration of the perturbation theory treatment of the problem shows that we wish to take that solution which corresponds to outgoing waves at infinity. (11)

For positive energies, $E > 0$, then, we find:

$$G_l(E; r, r') = -\frac{2m}{\hbar^2} \frac{\Gamma(l+1-i\frac{\gamma}{k})}{\Gamma(2l+2)} (-2ik)^{2l+1} e^{ikr} e^{ikr'}$$

$$\Phi(l+1-i\frac{\gamma}{k}; 2l+2; -2ikr_{<}) \Psi(l+1-i\frac{\gamma}{k}; 2l+2; -2ikr_{>}) .$$

(A;15)

For zero energy, $E = 0$, the solutions reduce to Bessel functions and we have:

$$G_l(0; r, r') = -\frac{2m}{\hbar^2} \pi i (rr')^{-l-\frac{1}{2}} J_{2l+1}(2\sqrt{2\gamma r_{<}}) H_{2l+1}^{(1)}(2\sqrt{2\gamma r_{>}}) \quad (A;16)$$

where $H_\nu^{(1)}$ is the Hankel function = $J_\nu + iY_\nu$.

APPENDIX B

REDUCTION OF CONFLUENT HYPERGEOMETRIC FUNCTIONS
TO BESSEL FUNCTIONS

The confluent hypergeometric functions (a, c, x) and (a, c, x) reduce to Bessel functions whenever $c = 2a$. The relationships are:

$$\begin{aligned} \Phi(a, 2a, 2x) &= \Gamma(a + \frac{1}{2}) (\frac{1}{2} x)^{-a + \frac{1}{2}} e^x I_{a - \frac{1}{2}}(x) \\ \Psi(a, 2a, 2x) &= \frac{1}{\sqrt{\pi}} (2x)^{-a + \frac{1}{2}} e^x K_{a - \frac{1}{2}}(x) \end{aligned} \tag{B;1}$$

$$\begin{aligned} \Phi(a, 2a, -2ix) &= \Gamma(a + \frac{1}{2}) (\frac{1}{2} x)^{-a + \frac{1}{2}} e^{-ix} J_{a - \frac{1}{2}}(x) \\ \Psi(a, 2a, -2ix) &= \frac{\sqrt{\pi}}{2} i e^{i(a - \frac{1}{2})\pi} (2x)^{-a + \frac{1}{2}} e^{-ix} H_{a - \frac{1}{2}}^{(1)}(x) \end{aligned} \tag{B;2}$$

Further, the confluent hypergeometric functions with parameters a, c are readily related to those with parameters $a + n, c + n$ (n any integer) by means of simple derivatives. Of particular interest to us are the relations:

$$\begin{aligned} \Phi(a, c, x) &= \frac{1}{c - a - 1} e^x x^{2 + a - c} \frac{d}{dx} \left[e^{-x} x^{c - a - 1} \Phi(a + 1, c, x) \right] \\ \Psi(a, c, x) &= - e^x x^{2 + a - c} \frac{d}{dx} \left[e^{-x} x^{c - a - 1} \Psi(a + 1, c, x) \right] \end{aligned} \tag{B;3}$$

and

$$\begin{aligned} \Phi(a, c, x) &= - \frac{c - 1}{c - a - 1} e^x \frac{d}{dx} \left[e^{-x} \Phi(a, c - 1, x) \right] \\ \Psi(a, c, x) &= - e^x \frac{d}{dx} \left[e^{-x} \Psi(a, c - 1, x) \right] \end{aligned} \tag{B;4}$$

We can use these relations to evaluate the limiting form of B_+ as $a \rightarrow 0$ and of B_- as $b \rightarrow 0$. Also, we can evaluate B_- at the points

$$b = \frac{1}{2}, \quad b = 1.$$

We find the following forms for B:

$$B_+(a \rightarrow 0) = -a^3 i \iint dx dy e^{-ax} e^{-ay} x^{\ell+\frac{1}{2}} y^{\frac{1}{2}-\ell} J_{\ell+\frac{1}{2}}(x_{<}) H_{\ell+\frac{1}{2}}^{(1)}(x_{>}) \quad (B;5)$$

$$B_-(b \rightarrow 0) = -\frac{2}{\pi} b^3 \iint dx dy e^{-bx} e^{-by} x^{\ell+\frac{1}{2}} y^{\frac{1}{2}-\ell} I_{\ell+\frac{1}{2}}(x_{<}) K_{\ell+\frac{1}{2}}(x_{>}) \quad (B;6)$$

$$B_-(b=1) = \frac{2}{\pi} \frac{1}{\ell(\ell+1)} \iint dx dy x^{\ell+1} y^{1-\ell} \left[\frac{d}{dx} \left(e^{-x} x^{\frac{1}{2}} I_{\ell+\frac{1}{2}}(x) \right) \right]_{x_{<}} \left[\frac{d}{dx} \left(e^{-x} x^{\frac{1}{2}} K_{\ell+\frac{1}{2}}(x) \right) \right]_{x_{>}} \quad (B;7)$$

$$B_-(b=\frac{1}{2}) = -\frac{1}{4\pi} \frac{1}{2\ell+1} \iint dx dy e^{-\frac{1}{2}x} e^{-\frac{1}{2}y} x^{\ell+1} y^{1-\ell} \left[I_{\ell}(x_{<}) - I_{\ell+1}(x_{<}) \right] \left[K_{\ell}(x_{>}) + K_{\ell+1}(x_{>}) \right] \quad (B;8)$$

APPENDIX C

INTEGRAL REPRESENTATIONS OF BESSEL FUNCTIONS

We are interested in finding a representation for the discontinuous forms $I_\nu(x_<) K_\nu(x_>)$ and $J_\nu(x_<) H_\nu^{(1)}(x_>)$. In particular, we would like a form symmetrical in $x_<$ and $x_>$, for then double integrals could be carried out independently, greatly simplifying the calculation.

In Bateman 7.14.2(57) we find the formula

$$I_\mu(\beta b) K_\nu(\beta a) = \beta^{\mu-\nu} \int_0^\infty \frac{t^{\nu-\mu+1}}{t^2 + b^2} J_\nu(at) J_\mu(bt) dt \quad (C;1)$$

for $\text{Re} \beta > 0$; $\text{Re} \nu > -1$, $a \geq b$, $\text{Re}(\nu - \mu) < 2$.

This is just the form we desire, if we set $\beta = 1$; that is:

$$I_\mu(x_<) K_\nu(x_>) = \int_0^\infty dt \frac{t^{\nu-\mu+1}}{1+t^2} J_\mu(x_<t) J_\nu(x_>t) \quad (C;2)$$

We can prove a similar formula for the Bessel function J_ν and H_ν .

Consider the integral

$$\int_C dz \frac{J_\nu(bz) H_\nu^{(1)}(az) z}{z^2 - \beta^2}$$

where $\text{Im} \beta > 0$. Let the contour C be the infinite semi-circle in the upper half-plane and the real axis.

If a, b real, and $a \geq b$, the integral vanishes over the semi-circle as its radius gets very large. Therefore, we have for the integral

$$\int_{-\infty}^{\infty} dt \frac{t}{t^2 - \beta^2} J_\nu(bt) H_\nu^{(1)}(at)$$

$$= \int_0^{\infty} dt \frac{t}{t^2 - \beta^2} \left[J_\nu(bt) H_\nu^{(1)}(at) - J_\nu(e^{i\pi}bt) H_\nu^{(1)}(e^{i\pi}at) \right]$$

(C;3)

$$= \int_0^{\infty} dt \frac{t}{t^2 - \beta^2} J_\nu(bt) \left[H_\nu^{(1)}(at) - e^{i\pi\nu} H_\nu^{(1)}(e^{i\pi}at) \right]$$

since

$$J_\nu(e^{i\pi}x) = e^{i\pi\nu} J_\nu(x) .$$

But $H_\nu^{(1)}(x) = \frac{i}{\sin \pi\nu} \left[J_\nu(x)e^{-i\nu\pi} - J_{-\nu}(x) \right]$, so that

$$H_\nu^{(1)}(x) - e^{i\pi\nu} H_\nu^{(1)}(e^{i\pi}x) = \frac{i}{\sin \nu\pi} \left[e^{-i\pi\nu} J_\nu(x) - e^{i\pi\nu} J_\nu(x) \right]$$

$$= 2 J_\nu(x) .$$

(C;4)

Thus the integral is equal to

$$2 \int_0^{\infty} dt \frac{t}{t^2 - \beta^2} J_\nu(at) J_\nu(bt) .$$

We can also evaluate the integral by residues, and find, for

$\text{Im } \beta > 0$, that its value is

$$\pi i J_\nu(\beta b) H_\nu^{(1)}(\beta a)$$

Thus we have the formula

$$J_\nu(\beta b) H_\nu^{(1)}(\beta a) = \frac{2}{\pi i} \int_0^{\infty} dt \frac{t}{t^2 - \beta^2} J_\nu(at) J_\nu(bt)$$

(C;5)

for a, b real; $a \geq b$, $\text{Im } \beta > 0$.

In particular, if we set $\beta = 1$, and deform the contour so as to pass below the pole at $t = 1$, we have

$$J_\nu(x_<)H_\nu^{(1)}(x_>) = \frac{2}{\pi i} \int_0^\infty dt \frac{t}{t^2-1} J_\nu(tx_<) J_\nu(tx_>) \quad (C;6)$$

where \int_0^∞ signifies the change in the path of integration.

APPENDIX D

EVALUATION OF INTEGRALS

1. The B_0 Integral

We wish to compute

$$B_0 = -2i \iint du dv e^{-u} e^{-v} u^{l+\frac{1}{2}} v^{\frac{1}{2}-l} J_{2l+1}(\sqrt{8u}) H_{2l+1}^{(1)}(\sqrt{8v}) \quad (D;1.1)$$

$$= -8i \iint dx dy e^{-x^2} e^{-y^2} x^{2l+2} y^{2-2l} J_{2l+1}(\sqrt{8}x) H_{2l+1}^{(1)}(\sqrt{8}y). \quad (D;1.2)$$

If we use the integral representation for this product of Bessel functions (Appendix C, (C;5)) and interchange the order of integration, we have

$$B_0 = -\frac{16}{\pi} \int_0^\infty dt \frac{t}{t^2-8} \int_0^\infty dx e^{-x^2} x^{2l+2} J_{2l+1}(xt) \int_0^\infty dy e^{-y^2} y^{2-2l} J_{2l+1}(yt), \quad (D;1.3)$$

where the integral is taken along a contour which passes below the pole at $t = \sqrt{8}$.

We can perform the integrations on x and y and find

$$B_0 = -\frac{2^{-4l}}{\pi} \frac{1}{\Gamma(2l+2)} \int_0^\infty dt \frac{t^{4l+3}}{t^2-8} e^{-t^2/4} \Phi(2; 2l+2; -t^2/4) \quad (D;1.4)$$

where Φ is the regular confluent hypergeometric function.

This can be simplified by a change of variable to

$$B_0 = -\frac{2}{\pi} \frac{1}{\Gamma(2l+2)} \int_0^\infty dx \frac{x^{2l+1}}{x-2} e^{-x} \Phi(2; 2l+2; -x) \quad (D;1.5)$$

But

$$\begin{aligned} \bar{\Phi}(a; 2l+2; -x) &= e^{-x} \bar{\Phi}(2l; 2l+2; x) \\ &= e^{-x} \frac{\Gamma(2l+2)}{\Gamma(2l)} \int_0^1 du e^{xu} u^{2l-1} (1-u) du \end{aligned} \quad (D;1.6)$$

which can be readily integrated into elementary functions.

Thus

$$B_0 = -\frac{2}{\pi} \frac{1}{\Gamma(2l)} \int_0^\infty dx \frac{x^{2l+1}}{x-2} e^{-2x} \int_0^1 du e^{xu} u^{2l-1} (1-u). \quad (D;1.7)$$

For $l = 1$ this becomes

$$B_0 = -\frac{2}{\pi} \int_0^\infty dx \frac{1}{x-2} \left[e^{-2x}(x+2) + e^{-x}(x-2) \right]. \quad (D;1.8)$$

The integral along the contour passing beneath the pole at $x = 2$ can be evaluated by taking the Cauchy principal value plus πi times the residue at the pole.

Thus

$$B_0 = -\frac{1}{\pi} \left[3 + 8 \int_0^\infty dx \frac{e^{-2x}}{x-2} + 8\pi i e^{-4} \right]. \quad (D;1.9)$$

The principal value integral is readily expressed in terms of the exponential integral.

$$P \int_0^\infty dx \frac{e^{-x}}{x-a} = e^{-a} \int_{-a}^\infty dt \frac{e^{-t}}{t} = -e^{-a} E^*(a), \quad (D;1.10)$$

where $E^*(a)$ is denoted by $\bar{E}i(a)$ in Jahnke-Emde. Thus, for $l = 1$,

$$B_0 = -\frac{1}{\pi} \left[3 - 8e^{-4} E^*(4) + 8\pi i e^{-4} \right] = -\frac{0.1229}{\pi} - 8ie^{-4}. \quad (D;1.11)$$

We note that the imaginary part is small enough so that it can be neglected, since we compare its square with twice the real part.

The computations for $l = 2$ have been carried out in an analogous manner.

2. The B_- Integral for $b = \frac{1}{2}$

We noted that for $b = \frac{1}{2}$

$$B_- = -\frac{1}{4\pi} \frac{1}{2l+1} \iint dx dy e^{-\frac{1}{2}x} e^{-\frac{1}{2}y} x^{l+1} y^{1-l} (I_l - I_{l+1})_{x<} (K_l + K_{l+1})_{x>}. \quad (D;2.1)$$

Using the integral representation (C;1), we have, after interchanging the order of integration:

$$B_- = -\frac{1}{4\pi} \frac{1}{2l+1} \int_0^\infty dt \frac{1}{1+t^2} \iint dx dy e^{-\frac{1}{2}x} e^{-\frac{1}{2}y} x^{l+1} y^{1-l} \left\{ t \left[J_l(xt) J_l(yt) - J_{l+1}(xt) J_{l+1}(yt) \right] + t^2 J_l(x_{<}t) J_{l+1}(x_{>}t) - J_{l+1}(x_{<}t) J_l(x_{>}t) \right\} \quad (D;2.2)$$

$$= -\frac{1}{4\pi} \frac{1}{2l+1} \left\{ \iint dx dy e^{-\frac{1}{2}x} e^{-\frac{1}{2}y} x^{l+1} y^{1-l} \int_0^\infty dt J_l(x_{<}t) J_{l+1}(x_{>}t) + \int_0^\infty dt \frac{1}{1+t^2} \iint dx dy e^{-\frac{1}{2}x} e^{-\frac{1}{2}y} x^{l+1} y^{1-l} \left[t J_l(xt) J_l(yt) - t J_{l+1}(xt) J_{l+1}(yt) - J_l(xt) J_{l+1}(yt) - J_{l+1}(xt) J_l(yt) \right] \right\}. \quad (D;2.3)$$

The first integral of Bessel functions is easily evaluated to give

$$\int_0^{\infty} dt J_{\ell}(x_{<}t) J_{\ell+1}(x_{>}t) = \frac{x_{<}^{\ell}}{x_{>}^{\ell+1}} \quad (D;2.3)$$

Then the integrals on x and y can be readily performed, since we deal with elementary functions. The other integrals containing Bessel functions are first integrated over x and y; they result in rational functions and radicals involving $(1 + 4t^2)$. The final integral over t is then elementary and can be easily evaluated.

As an example, for $\ell = 1$, it reduces to the form

$$B_{-} = -\frac{2}{\pi} \left\{ \frac{3}{2} - 2 \log 2 + \int_0^{\infty} dx \frac{1}{x} \left[(1 + 4x)^{-5/2} - (1 + 4x)^{-3} \right] - 4 \int_0^{\infty} dx (1 + 4x)^{-3} + 2 \int_0^{\infty} dx (1 + x)^{-1} (1 + 4x)^{-3} \right\} \quad (D;2.5)$$

$$= -\frac{1}{27} \frac{1}{\pi} (8 \log 2 - 3) = -\frac{.9421}{\pi} \quad (D;2.6)$$

3. The B_{-} Integral for $b = 1$

For $b = 1$, we found that

$$B_{-} = \frac{2}{\pi} \frac{1}{\ell(\ell+1)} \iint dx dy x^{\ell+1} y^{1-\ell} \left[\frac{d}{dx} \left(e^{-x} x^{\frac{1}{2}} I_{\ell+\frac{1}{2}}(x) \right) \right]_{x_{<}} \left[\frac{d}{dx} \left(e^{-x} x^{\frac{1}{2}} K_{\ell+\frac{1}{2}}(x) \right) \right]_{x_{>}} \quad (D;3.1)$$

Now

$$x^{\frac{1}{2}} I_{\ell+\frac{1}{2}}(x) = \left(\frac{2}{\pi}\right)^{\frac{1}{2}} (-)^{\ell} x^{\ell+1} \left(\frac{d}{x dx}\right)^{\ell} \frac{\sinh x}{x}$$

$$x^{\frac{1}{2}} K_{\ell+\frac{1}{2}}(x) = \left(\frac{\pi}{2}\right)^{\frac{1}{2}} (-)^{\ell} x^{\ell+1} \left(\frac{d}{x dx}\right)^{\ell} \frac{e^{-x}}{x}, \quad (D;3.2)$$

so that the integrals involved are elementary and can be readily computed.

For example, for $\ell = 1$, we find

$$B_- = -\frac{1}{2\pi} \int_0^{\infty} \int_0^{\infty} dx dy y^{-2} \left[1 - e^{-2x}(2x^2 + 2x + 1) \right]_{x <} \\ \left[e^{-2x}(2x^2 + 2x + 1) \right]_{x >} \quad (D;3.3)$$

$$= -\frac{1}{4\pi} \quad (D;3.4)$$

4. The B_- and B_+ Integrals as $E_{\omega} \rightarrow \infty$

We found in equation (3;16) that for very large gamma ray energies,

$$f = \frac{8\pi}{Z} \frac{\ell}{2\ell+1} \frac{E_K}{E_{\omega}} (B_+ - B_-) > \frac{16}{Z} \frac{\ell}{2\ell+1} \left(\frac{E_K}{E_{\omega}}\right)^2 \quad (D;4.1)$$

Since for large E_{ω} , $a^2 \approx b^2 \approx E_K/E_{\omega}$, we note that this implies that in the limit of small a and b we should have

$$B_+ \rightarrow \frac{1}{\pi} a^2$$

$$B_- \rightarrow -\frac{1}{\pi} b^2. \quad (D;4.2)$$

It is a convenient check on the calculations to compute

this limiting form.

We saw (B;6) that as $b \rightarrow 0$

$$B_- = -\frac{2}{\pi} b^3 \int \int dx dy e^{-bx} e^{-by} x^{\ell+\frac{1}{2}} y^{\frac{1}{2}-\ell} I_{\ell+\frac{1}{2}}(x_{<}) K_{\ell+\frac{1}{2}}(x_{>}) . \quad (D;4.3)$$

Using the integral representation (C;1), we have, after interchanging the order of integration:

$$B_- = -\frac{2}{\pi} b^3 \int_0^{\infty} dt \frac{1}{1+t^2} \int_0^{\infty} dx e^{-bx} x^{\ell+\frac{1}{2}} J_{\ell+\frac{1}{2}}(xt) \int_0^{\infty} dy e^{-by} y^{\frac{1}{2}-\ell} J_{\ell+\frac{1}{2}}(yt) \quad (D;4.4)$$

$$= -\frac{2}{\pi} b^2 \frac{\Gamma(\ell+1)}{\Gamma(\frac{1}{2})\Gamma(\ell+\frac{3}{2})} \int_0^{\infty} du \frac{u^{2\ell+2}}{(1+b^2u^2)(1+u^2)^{\ell+1}} F(1, \frac{3}{2}; \ell+\frac{3}{2}; -u^2) . \quad (D;4.5)$$

The hypergeometric function is expressible in terms of elementary functions. As an example, for $\ell = 1$, the lowest order terms in b become, with the substitution $z = u^2/1+u^2$:

$$B_- = -\frac{4}{\pi^2} b^2 \int_0^1 dz \left[\left(\frac{z}{1-z} \right)^{\frac{1}{2}} - \sin^{-1} z \right] \quad (D;4.6)$$

$$= -\frac{8}{\pi^2} b^2 \int_0^{\infty} du \frac{u}{(1+u^2)^2} (u - \tan^{-1} u) \quad (D;4.7)$$

$$= -\frac{1}{\pi} b^2 ,$$

This checks, as it should, with the previous result. Exactly analogous calculations for B_+ as $a \rightarrow 0$, and for higher values of l , yield the same results.

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