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Relativistic Radiative Transitions.

Wilbur Boswell Payne
Louisiana State University and Agricultural & Mechanical College

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RELATIVISTIC RADIATIVE TRANSITIONS

A Thesis
Submitted to the Graduate Faculty of the
Louisiana State University and
Agricultural and Mechanical College
in partial fulfillment of the
requirements for the degree of
Doctor of Philosophy

in

The Department of Physics

by
Wilbur B. ^{well} Payne
M.S., Louisiana State University and
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ABSTRACT

Radiative electric dipole matrix elements have been calculated for a single electron in a Coulomb field. The wave functions used are those determined by the single electron Dirac equation. The Dirac radial eigenfunctions through the $4F_{7/2}$ state are tabulated. In Chapter II these matrix elements are calculated neglecting the effects of retardation. The matrix elements calculated are those leading to the emission of K series characteristic X-rays or absorption by an ion containing one K electron. These matrix elements are evaluated numerically for several elements of atomic number greater than 28, and applied to calculations of the transition probability, rate of energy emission, partial line widths, and relative intensities of the principle lines of the K series of heavy elements.

In Chapter III the effects of retardation are included in calculations of the matrix elements which lead to the $K\alpha$ X-ray lines. It is shown that retardation reduces the magnitude of the squared matrix element for the $2P_{3/2}-1S_{1/2}$ transition about 15 per cent, while not significantly changing the same quantity for the $2P_{1/2}-1S_{1/2}$ transition; the numbers applying to lead, $Z = 82$. This greatly modifies the relative intensity computations of Chapter II. In Chapter III we also estimate the relative intensities of

electric quadrupole transitions to the electric dipole transition of the K series. It is shown that quadrupole transitions are at most a few per cent as probable as electric dipole transitions between the same pair of shells, which is in fair agreement with the non-relativistic results of Jacobsohn.

In Chapter IV the relativistic matrix elements are used, in combination with non-relativistic matrix elements for transitions to bound states of large principle quantum number and with the non-relativistic calculations by Jacobsohn of the electric quadrupole matrix elements, to compute the integrated absorption cross-section for an ion of lead, Pb^{81+} . For transitions to the continuum, the computations of Gladys White of the relativistic photo-electric cross-section for this ion, are used. The numerical value of the integrated photo-electric cross-section is found to be in fair numerical agreement with the result expected from the theoretical work of Gell-Mann et al.

CHAPTER I

INTRODUCTION

The emission and absorption of electromagnetic energy by a quantum mechanical system may be understood, and is usually treated quantitatively, by the method of quantum mechanical perturbation theory. This theory is given here only in outline form, with definitions of the important quantities. A more thorough treatment is found in many of the references in the bibliography. The reference found most useful by this author is "The Quantum Theory of Radiation", by W. Heitler (Heitler, 54).

In this theory one considers two quantum-mechanical systems, for our purposes an atom and the electromagnetic field, with an interaction energy H_{int} . This interaction, regarded as a perturbation, will cause transitions consisting of a change in the quantum mechanical state of the atom and the emission or absorption of one or more photons. The quantity of fundamental importance in this theory is the transition probability W_{ab} which is the probability per unit time that the atomic system will undergo such a transition.

The transition probability is given (Heitler, 54, p 140) by

$$P(E) dE = \frac{2\pi}{\hbar} N(E) dE |H|^2 \quad (1)$$

where $P(E)$ is the probability per second of emission or absorption of a photon of energy between E and $E + dE$, $\hbar$ is Planck's constant divided by 2π , $N(E)dE$ is the statistical density of final states available, and $|H|^2$ is the square of absolute value the interaction matrix element between the two states of the atomic system. If, as is the case for all of the present work, the transition involves the emission or absorption of a single photon, accompanied by a change in the state of a system which obeys the single electron Dirac equation from a state designated by a subscript b to one designated by the subscript a , H is given (Heitler, 54, p 143) for emission by

$$H_{a,b} = -e \left(\frac{2\pi \hbar^2 c^2}{E_{a,b}} \right)^{1/2} (n_\lambda + 1)^{1/2} \int \psi_a^* (\vec{\alpha} \cdot \vec{e}_\lambda) e^{i(\vec{k} \cdot \vec{r})} \psi_b dV \quad (2)$$

and for absorption by

$$H_{a,b} = -e \left(\frac{2\pi \hbar^2 c^2}{E_{a,b}} \right)^{1/2} n_\lambda^{1/2} \int \psi_a^* (\vec{\alpha} \cdot \vec{e}_\lambda) e^{i(\vec{k} \cdot \vec{r})} \psi_b dV \quad (3)$$

in these equations e , $\hbar$, and c have their usual significance; E_{ab} is the energy of the emitted photon, which due to the conservation of energy is equal to $E_b - E_a$ where these are the energies of the two atomic states; n_λ is the number of photons present in the λ 'th radiation oscillator before the transition, the ψ 's are Dirac wave functions; $\vec{\alpha}$ is the Dirac vector, whose components are 4×4 matrices; $\vec{e}_\lambda$ is the unit vector in the direction of polarization of the photon, and $\vec{k}$ is a wave vector in the

direction of propagation of the photon whose magnitude is equal to $\frac{E_{ab}}{hc} \text{ cm}^{-1}$. The integration is to be performed over all the space region occupied by the atomic system. A discussion of the Dirac wave equations, the definition of $\vec{\alpha}$, and a discussion of the properties of the Dirac matrices and wave functions is found in Heitler and many other works. The particular formalism and notation used for this work is to be found in section 9 of Bethe's Handbuch article (Bethe, 33); and some discussion as well as tabulation of the wave functions ψ is given in Appendix A of this work. For the present, use will be made of the properties required without further discussion; justification of this will be left for Appendix A.

For ease of writing in what follows let

$$(a|O|b) = \int \psi_a^* O \psi_b dV \quad (4)$$

whatever sets of quantum numbers a and b are required for the description of the atomic states and whatever the form of the operator O. Then, for emission we have, combining (1) and (2)

$$P_{aL} = \frac{4\pi^2 e^2 \hbar^2 c^2}{E_{aL}} (n_\lambda + 1) \left| (a | (\vec{\alpha} \cdot \vec{e}_\lambda) e^{-i(\vec{k} \cdot \vec{r})} | b) \right|^2 N(E) \quad (5)$$

We shall be concerned with spontaneous emission, i.e. $n_\lambda = 0$

We may assign the photon emitted to one of many radiation oscillators in the range dE , and we have (Heitler, 54, p 176)

$$N(E) = \frac{E^2 d\Omega}{(2\pi\hbar c)^3} \quad (6)$$

where $d\Omega$ is the element of solid angle about the direction of $\vec{k}$. Combining (5) and (6) we have

$$P d\Omega = \frac{e^2}{\hbar c} \frac{E_{ab}}{2\pi\hbar c} d\Omega \left| (a | (\vec{\alpha} \cdot \vec{e}_\lambda) e^{-i(\vec{k} \cdot \vec{r})} | b) \right|^2 \quad (7)$$

where we have used $\eta_\lambda = 0$. This equation represents the probability per second of emission of a photon in a direction $\vec{k}$ in range $d\Omega$ polarized in the direction e_λ . For the total transition probability P must be summed over the direction of polarization and integrated over the direction of emission.

An absorption probability can be obtained in the same manner. If we assume that the average number of quanta initially present in the λ 'th radiation oscillator with a given direction of polarization is $\bar{n}_\lambda$, we get, combining (1), (3), and (6)

$$P d\Omega = \frac{e^2}{\hbar c} \frac{E_{ab}}{2\pi\hbar c} \bar{n}_\lambda d\Omega \left| (a | (\vec{\alpha} \cdot \vec{e}_\lambda) e^{i(\vec{k} \cdot \vec{r})} | b) \right|^2 \quad (8)$$

$N(E)$ is now considered a density of initial states, but (6) still applies. In any actual experiment, an atom would be irradiated by a beam of photons. If we consider such a beam, coming from a given direction within solid angle of intensity $\frac{I(E) dE}{\hbar}$ (energy per $\text{cm}^2 \cdot \text{sec.}$), then

$\bar{n}_\lambda$ is given by (Heitler, 54, p 179)

$$\bar{n}_\lambda = \frac{(2\pi)^3 \hbar^2 c^2 I(E)}{E^3} \quad (9)$$

Combining (8) and (9), and assuming $I(E)$ is a constant $I(E_{ab})$ is a narrow range of energy near E_{ab} , we get

$$P d\Omega = 4\pi^2 \frac{e^2}{\hbar c} \frac{\hbar c^2}{E_{ab}^2} d\Omega I(E_{ab}) \left| (a | (\vec{\alpha} \cdot \vec{e}_\lambda) | e^{i(\vec{k} \cdot \vec{r})} | b) \right|^2 \quad (10)$$

which must be averaged over the orientation of the atom relative to the direction of the beam.

In both emission and absorption it is sometimes preferable to discuss the rate of emission or absorption of energy rather than the transition probability. We shall call this quantity J . It is obtained from the corresponding transition rate by multiplication by E_{ab} , the energy involved in a single transition. In experiments involving absorption, it is also useful to tabulate the results in terms of a quantity which is independent of the incident intensity.

One such quantity is the absorption cross-section σ , defined as the number of photons absorbed from the beam per second per atom, divided by the incident flux in particles per square centimeter per second. The numerator of σ is given by the absorption probability, and for a beam of photons described by the intensity

$l(E_{ab})$ the incident flux is $\frac{I(E_{ab})}{h E_{ab}}$. The cross-section is therefore

$$\sigma_{ab} d\Omega = \frac{4\pi^2 e^2}{hc} \frac{h^2 c^2}{E_{ab}} d\Omega \left| \langle a | (\vec{\alpha} \cdot \vec{e}_\lambda) e^{i(\vec{k} \cdot \vec{r})} | b \rangle \right|^2 \quad (11)$$

After the average over orientations this will be the differential cross-section in that it refers to absorption from a beam from a given direction, but it is the cross-section integrated over the energy range of the absorption line, so its units are ergs cm^2 . This integration is necessary in order to define an absorption probability, and is performed in the derivation leading to (1). A more rigorous derivation of (11) would require that consideration be taken of the fact that the final state of an absorption process is not stationary in time but decays to lower states by one or more processes. The results of such calculations would however be identically (11). This may be seen from the results of section 18.3 of Heitler (Heitler, 54).

In addition to transition probability and cross-section there are two other quantities related to these same matrix elements of some interest. One of these is the natural line breadth which is discussed in detail in section 18 of Heitler's book. (Heitler, 54, p 181). This quantity, which is the full width at half maximum of the spectral line is defined by Heitler in units of angular frequency. It therefore differs by a factor 2π from the more customary definition (Richtmeyer, 37).

By the methods of high resolution spectroscopy this quantity may be determined quite accurately, although some difficulty in theoretical interpretation is occasioned by the fact that this line width is caused in part by several different processes. That part of the line breadth which is caused by radiation damping we shall call Γ_γ . Γ_γ for a spectral line is the sum of two terms, the level width of the initial energy level Γ_b plus the width of the final level Γ_a . The radiative width of a single level is the sum of the widths due to each possible radiative transition to a lower level, and each transition contributes a width $\Gamma_{ab} = W_{ab}$ where W_{ab} is the total spontaneous emission probability (18). The other quantity is the oscillator strength. Oscillator strength has more an heuristic and historic significance than a practical significance as the direct result of an experiment. Much of the important theoretical work in dispersion theory, even including classical dispersion theory (Breit 32a and b) and much of the theory of radiative transitions in atomic (Bethe, 33) and nuclear (Levinger and Bethe, 50) physics utilizes this quantity. The oscillator strength in non-relativistic quantum mechanics is discussed in detail in Bethe's Handbuch article (Bethe, 33, p 429). In terms of the relativistic matrix element the oscillator strength f_{ab} may be defined

$$f_{ab} = \frac{2mc^2}{3E_{ab}} \left| (a | \vec{\alpha} | b) \right|^2 \quad (12)$$

where $|(a|\bar{\alpha}|b)|^2$ is the matrix element which results after averaging over polarizations and summing over the direction of propagation and over the initial states. This procedure will be discussed in some detail later. Since $\bar{\alpha}$ is a dimensionless quantity, it is obvious that f is also dimensionless. It is also easily shown that this reduces to the non-relativistic definition (Bethe, 33, p 435). It will also be obvious that the quantities σ , Γ and W may be expressed in terms of f .

Since the wave functions Ψ_a and Ψ_b are expressed in terms of spherical harmonics, it is customary to expand the plane wave $e^{i(\vec{k} \cdot \vec{r})}$ appearing in the matrix elements in terms of spherical waves. This expansion, the so-called multipole expansion, is discussed in several works (Rose, 55; Blatt, 52; Stech, 52). The form of the expansion we shall use is

$$e^{i(\vec{k} \cdot \vec{r})} = 4\pi \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{+\ell} i^{\ell} j_{\ell}(kr) Y_{\ell,m}^*(\Theta, \Phi) Y_{\ell,m}(\theta, \phi) \quad (13)$$

where j_{ℓ} is the spherical Bessel's function defined by

$$j_{\ell}(kr) = \left(\frac{\pi}{2kr}\right)^{1/2} J_{\ell+1/2}(kr) \quad (14)$$

where $J_{\ell+1/2}(kr)$ is the regular half-integral Bessel's function defined by Jahnke and Emde (Jahnke, 45), i is the usual $\sqrt{-1}$, the $Y_{\ell,m}$ are spherical harmonics (Bethe, 33, p 275), Θ and Φ are the polar and azimuthal angles of the

vector $\vec{k}$ and θ , ϕ the same for the vector $\vec{r}$. The functions j_ℓ for $\ell = 0, 1$, and 2 are given in Schiff (Schiff, 49, p 77), and others are given in Morse and Feshbach (Morse, 53). For kr small compared to 1 , this series converges rapidly, the ℓ 'th term being proportional approximately to $\frac{(kr)^\ell}{\ell!}$, and it is usual to discuss only the first few terms. The term for $\ell = 0$, which is called the electric dipole term reduces to $j_0(kr) = \frac{\sin kr}{kr}$. The next term contains contributions due to the electric quadrupole and magnetic dipole moments of the atom. The emission and absorption of radiation for allowed, i.e. electric dipole, transitions will be discussed in some detail, and the transition probabilities calculated for several atoms in Chapter II. These dipole transition probabilities will be used to calculate the relative intensities of X-ray transitions in several atoms of atomic number greater than 29 , and a discussion of possible experimental comparison will be given. In Chapter III some effort will be made to improve the approximations of Chapter II and an estimate of the importance of quadrupole transitions made.

The average over polarization directions and integration over directions of emission and of the absorbed radiation will be discussed in some detail for dipole transitions. The procedures are similar for quadrupole emission, and will be outlined in Chapter III. The average over polarizations for emission is discussed in Bethe's

article (Bethe, 33, p 430) and in several other places (Heitler, 54, p 177, Condon, 51, p 101). Equation (7) with the substitution of the $\ell = 0$ term of (13) becomes

$$P d\Omega = \frac{\ell^2}{\hbar c} \frac{E_{a\ell}}{2\pi\hbar} d\Omega \left| (a | \vec{\alpha} \cdot \vec{e}_\lambda | j_0(kr) | b) \right|^2 \quad (15)$$

For the sum over polarization we are free to choose a coordinate system in which $\vec{\alpha}$ is fixed in space and measure our angles from this direction. Since $\vec{\alpha}$ is the velocity operator in Dirac theory, $e\vec{\alpha}$ is the current operator where e is the charge of the particle. The direction of polarization of light emitted by this current must be perpendicular to the direction of emission $\vec{k}$ and can have no component in the direction perpendicular to the current. $(\vec{\alpha} \cdot \vec{e}_\lambda)$ is the component of $\vec{\alpha}$ in the direction of polarization and $(\vec{\alpha} \cdot \vec{e}_\lambda) = |\vec{\alpha}| \cos \Theta$ where Θ is the angle between $\vec{\alpha}$ and $\vec{e}_\lambda$ and where

$$|\vec{\alpha}|^2 = \alpha_x^2 + \alpha_y^2 + \alpha_z^2 \quad (16)$$

Since $\vec{e}_\lambda$ is perpendicular to $\vec{k}$ and in the plane containing $\vec{k}$ and $\vec{\alpha}$, and since the integration in the matrix element is not over the angle Θ , we may factor out the $\cos \Theta$ and replace it by $\sin \Theta$ where Θ is the angle between $\vec{k}$ and $\vec{\alpha}$. For the integration over directions of $\vec{k}$ we have therefore

$$W_{a\ell} = \int P_{a\ell} d\Omega = \frac{\ell^2}{\hbar c} \frac{E_{a\ell}}{2\pi\hbar} \left| (a | |\vec{\alpha}| j_0(kr) | b) \right|^2 \int \sin^2 \Theta d\Omega \quad (17)$$

which gives

$$W_{ab} = \frac{4}{3} \frac{\omega^2}{\hbar c} \frac{E_{ab}}{\hbar} \left| (a || \vec{\alpha} || j_0(kr) || b) \right|^2 \quad (18)$$

where W is the total transition probability.

If, as is true in our case, the states a and b are degenerate, so that more than one set of quantum numbers can lead to a transition of energy E_{ab} , it is still necessary (Heitler, 44, p 108) to sum over the initial states and average over the final states. This will be discussed in detail in Chapter 11, where the dipole transition probabilities are calculated.

A similar argument in the case of absorption (Heitler 54, p 179) leads to an expression for the total absorption probability, assuming the incident radiation to be unpolarized,

$$W = \frac{4\pi^2}{3} \frac{\omega^2}{\hbar c} \frac{\hbar^2 c^2}{E_{ab}^2} I(E_{ab}) \left| (a || \vec{\alpha} || j_0(kr) || b) \right|^2 \quad (19)$$

One further simplifying approximation is generally made in computation of these matrix elements. Since

$$j_0(kr) = \frac{\sin kr}{kr} \quad (20)$$

(Schiff, 49, p 77) and since $kr < 1$, it is customary to let $\sin kr$ be approximated by kr so that

$$j_0(kr) \cong 1, \quad kr \ll 1 \quad (21)$$

This is quite a satisfactory approximation in atomic spectra and even in X-ray transitions for elements of low

atomic number. It amounts to the neglect of the effects of retardation due to the finite size of the source. For elements of high atomic number, for example lead, $Z = 82$, it is not very satisfactory. For lead, if we calculate $h = \frac{E_{ph}}{\hbar c}$ for the theoretical transition energy and assume r is of order of magnitude $\frac{a_0}{Z}$ where $\frac{a_0}{Z}$ is the radius at which the K wave function has its maximum value, we get $kr \cong \frac{3}{8} (Z\alpha)^2 \cong .24$. Since for this value of kr , $\sin kr$ differs from kr by only 1 percent it would appear that this is a satisfactory approximation. Since non-relativistic quantum mechanics follows from relativistic by the approximation $\alpha Z = 0$, this is a consistent non-relativistic approximation. The work of Chapter II is done using it also. In this manner it was felt that one could best determine what change in these quantities was due simply to relativistic effects. In Chapter III the two most important transitions for lead are calculated without this approximation, and we find that the approximation is actually quite poor. This is caused by the fact that our estimate of r is much too small for transitions in which the total angular momentum (see Appendix A) changes.

Chapter IV is devoted to examining the applicability to a simple relativistic quantum mechanical system of a dipole sum rule similar to that of non-relativistic quantum mechanics. (Bethe, 33, p 434). This sum rule is easily proven non-relativistically (Bethe, 33, Condon, 51,

p 109), follows directly from the commutation relations of position and momentum. No relativistic proof of this rule has been found possible without the assumption of some extra physical property not clearly determined by the wave equation of the system (Gell-Mann, 54).

It is easy to show, using non-relativistic quantum dispersion theory (Breit 32b, 528), that the existence of a dipole sum rule is equivalent to the statement that the forward scattering of a single bound electron approaches that of a free electron for high photon energies. It is this latter statement which is made as an assumption in the relativistic derivation of this sum rule (Gell-Mann 54 sections 4 and 5). Non-relativistically, the definition of the oscillator strength is (Bethe 33, p 435)

$$f_{aL} = \frac{2m E_{aL}}{3\hbar^2} \left| (a | \vec{r} | b) \right|^2 \quad (22)$$

where $(a | \vec{r} | b)$ is the matrix element

$$(a | \vec{r} | b) = \int \psi_a^* \vec{r} \psi_b dV \quad (23)$$

of the dipole moment of the atom, after summing over the degeneracy of the states a and b. The wave functions appearing in this matrix element are solutions of the Schroedinger equation and the detailed treatment of non-relativistic atomic radiation is given in Bethe's article. The sum rule in terms of this may be stated

$$\sum_a f_{aL} = 1 \quad (24)$$

for a system containing 1 electron. The summation sign means sum over all bound states and integrate over all states of the positive energy continuum. Transitions in which the atom absorbs a photon and the electron is left in a state of positive energy, i.e. the photo electric effect, can also be described in terms of the oscillator strength, or more precisely in terms of an oscillator density per unit energy (Levinger, 50). The details of this are left to Chapter IV. However, if one expresses the cross section for absorption of radiation in terms of the oscillator strength (relativistically or non-relativistically) one gets, using (11), (12), and (19)

$$\sigma = \frac{2\pi^2 e^2 \hbar}{mc} f. \quad (25)$$

using the approximation (21). The integral of σ with respect to the energy of transition corresponds to the summation of f over the final states. That is

$$\int_0^\infty \sigma dE = \frac{2\pi^2 e^2 \hbar}{mc} \sum_a f_{ab} \quad (26)$$

which, if (24) applies relativistically implies

$$\int_0^\infty \sigma dE = \frac{2\pi^2 e^2 \hbar}{mc} \text{ erg cm}^2 \quad (27)$$

In Chapter IV, $\int \sigma dE$ is performed numerically for an ion of $Z = 82$ (lead) which initially contains one electron bound in the lowest energy level. The values of σ for transitions from the ground state to higher bound states are taken from the calculations of transition probability

in Chapter II. For transitions to positive energy states we use the compilation of calculations of the relativistic photo effect which were so generously provided by Gladys White, of the National Bureau of Standards (White, 54).

Excerpts of the Ph.D. Thesis of Boris Jacobsohn (Jacobsohn, 47) have very recently been declassified and made available through the kindness of Dr. Norbert Rosenzweig of Argonne National Laboratory. Dr. Jacobsohn has made calculations of somewhat related processes, including some calculations of Dirac matrix elements. He was primarily concerned with absorption from the L shell of an ion of $Z = 90$ in which all electrons in shells of higher energy than the L shell had been removed. For this fairly simple atomic model he has calculated oscillator strengths using screened Dirac wave functions. He has calculated non-relativistically the quadrupole oscillator strengths, and a correction to the dipole oscillator strength which represents the second term in the expansion of $j_0(kr)$. This is not so complete a correction for the effects of retardation as the calculations of Chapter III of this work. The agreement between his calculation and this work is quite satisfactory in view of the approximations, and his calculation, which was made with non-relativistic wave functions, is applicable to any transition.

In addition to the individual oscillator strengths, Jacobsohn has derived sum-rules similar to the dipole sum-

rule for his quadrupole oscillator strengths and for his retardation correction. Use will be made of these sum-rules to discuss the alteration they would produce in the integrated cross-section. His non-relativistic quadrupole matrix elements will be compared in Chapter III to a preliminary calculation of the magnitude of these terms using relativistic wave functions.

CHAPTER 11

CALCULATION OF DIPOLE MATRIX ELEMENTS

In this section we shall calculate the relativistic matrix elements for radiative transitions to or from the ground state of several atoms, and apply the results to a calculation of relative intensities of lines in the K X-ray spectrum of these elements. We restrict ourselves to elements of atomic number greater than 29, since for smaller atomic number relativistic effects are insignificant. We neglect the effects on the wave functions due to the presence of other electrons in the atom. At $Z = 79$ (gold) the dipole transition probabilities have been calculated relativistically for the $K\alpha_1$, and $K\alpha_2$ lines using Slater screened wave functions (Slater, 30) by Burhop and Massey (Burhop, 36). As might be expected this screening correction results in a strong reduction of the total transition probability, but does not seriously affect the intensity ratios. Since earlier work at Louisiana State University (Tuan, 53) in non-relativistic K transition probabilities has shown the Slater screening constants to be unsatisfactory approximations for this type of calculation, the effects of screening have been completely neglected in this work. The Slater screening constants were chosen to adjust the energy levels of the

atoms as closely as possible to the experimental values. The calculation of transition probabilities would require modification of these constants to adjust that part of the radial wave function which is important in the overlap integrals involved in the matrix element. No prior theoretical basis for this adjustment is available. Again, by neglecting screening we hope to get a better judgment of the importance of relativistic effects. We also show in Chapter III that the inclusion of the retardation term $j_0(kr)$ in the matrix elements makes a more significant change in the relative intensities of X-ray lines than the effects of screening.

For emission we consider an atom with one vacancy in the K shell, with all other states occupied, and calculate transition probabilities from each higher level, using the formulae from Chapter I. Of course, our lightest element, copper, does not normally have the N shell completely occupied, which must be considered before applying these calculations to the results of any experiments. For absorption we calculate the absorption probability for an atom which initially contains one electron in the K shell, all other states being empty. The absorption calculations thus do not correspond to any normally occurring atomic system, and are of no direct experimental interest. They are used only for the sum rule calculation of Chapter IV.

The matrix elements appearing in equations (18) and (19) of Chapter I are the results of summation over

initial and final states, without regard to the state of polarization of the emitted or absorbed radiation, since the average over polarizations has already been done. For this summation we shall need to specify a and b more completely in terms of the four quantum numbers required to distinguish between the two states. In what follows we will always designate quantities referring to the initial state with primes. The only possible confusion in this results from the radial quantum number, which in Appendix A has been designated n' . This quantum number in the initial state we shall call n'_b and in the final state n'_a .

For reasons of algebraic simplicity it is preferable to decompose $\vec{\alpha}$ into components α_z , $\alpha_+ = \frac{\alpha_x + i\alpha_y}{\sqrt{2}}$ and $\alpha_- = \frac{\alpha_x - i\alpha_y}{\sqrt{2}}$, rather than $\alpha_x, \alpha_y, \alpha_z$. In terms of this decomposition (16) is replaced by

$$|\vec{\alpha}|^2 = \alpha_+^2 + \alpha_-^2 + \alpha_z^2 \quad (28)$$

We shall see when we consider the selection rules that only one of these components is effective in producing transitions between any pair of given states, so that the summation above is never necessary, two of the terms being zero.

The sum over initial and average over final levels may be thought of in the following terms. We consider a large number of atoms in the same initial state (or many repetitions of the same experiment on the same atom)

with no forces present which would favor the occupation of any particular state within a level. The total transition probability is then given by the sum of terms representing the probability of a transition from a definite state within the initial level to a definite state of the final level multiplied by the probability that the initial state is occupied, and summed over all initial and final states available within those levels. The absence of forces which can select particular states insures a uniform distribution among initial and final states. In the case usually considered in atomic spectra, i.e. one electron initially in an excited level and finally in a lower level, the probability of occupation of a given state within the initial level is proportional to the reciprocal of the number of such states, or to $(2j+1)^{-1}$. We are thus led to the usual formula for this sum and average (Bethe, 33, p 435; Heitler, 44, p 108). In X-ray spectra we consider all levels filled except one K state. The occupation probabilities for the initial state are therefore identically 1, and since there is only one possible final state we need only compute

$$\sum_{m'} |(n, l, j, m | \vec{r} | n', l', j', m')|^2 \quad (29)$$

For absorption by an atom containing a single electron in the K shell it is obvious that we need to calculate the sum only over the final states. Since the role of initial and final states is reversed between emission and

absorption we conclude that for our two cases the matrix elements appearing in equations (12), (18) and (19) are identical. (This requires in addition to the above argument that

$$\left| \int \psi_a^* (\vec{\alpha}) \psi_b \right|^2 = \left| \int \psi_b^* (\vec{\alpha}) \psi_a dV \right|^2 \quad (30)$$

which follows from the fact that $\vec{\alpha}$ is Hermitean.) We will show that the sum (29) is independent of m , and hence, of the particular K state involved in the transition. For brevity we shall calculate in detail only one of the sums (29). The other necessary ones follow from an exactly similar procedure, and are simply listed. There should be four types of transitions for which such sums are required, depending on the four possible arrangements of the initial and final levels between type A and type B. (See Appendix A). However one of the states involved in our case is always a K state and hence type A, and the argument following equation (29) permits us to consider only two of the four, since we do not care whether the K wave function is for the initial or final state. We shall calculate the sum (29) for the case where both initial and final states are type A. For this we must write out in detail

$$\psi_a^* \alpha_z \psi_b ; \quad \psi_a^* \alpha_+ \psi_b ; \quad \psi_a^* \alpha_- \psi_b \quad (31)$$

If we let

$$\psi_a = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} \quad \text{and} \quad \psi_b = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{pmatrix} \quad (32)$$

and perform the operations (31) according to the procedures of Appendix A, equations (31) become

$$\psi_a^\dagger \alpha_z \psi_b = u_1^\dagger v_3 - u_2^\dagger v_4 + u_3^\dagger v_1 - u_4^\dagger v_2 \quad (33)$$

$$\psi_a^\dagger \alpha_+ \psi_b = \sqrt{2} (u_1^\dagger v_4 + u_3^\dagger v_2) \quad (34)$$

$$\psi_a^\dagger \alpha_- \psi_b = \sqrt{2} (u_2^\dagger v_3 + u_4^\dagger v_1) \quad (35)$$

If we now use for our wave functions u and v , the type A wave functions given by equation (6) of Appendix A, the terms of (33) become

$$\begin{aligned} u_1^\dagger v_3 &= - \left(\frac{l+m+3/2}{2l+3} \cdot \frac{l'+m'+1/2}{2l'+1} \right)^{1/2} i f_a g_b Y_{l+1, m-1/2}^* Y_{l', m'-1/2} \\ - u_2^\dagger v_4 &= - \left(\frac{l+m+3/2}{2l+3} \cdot \frac{l'-m'+1/2}{2l'+1} \right)^{1/2} i f_a g_b Y_{l+1, m+1/2}^* Y_{l', m'+1/2} \\ u_3^\dagger v_1 &= \left(\frac{l+m+1/2}{2l+1} \cdot \frac{l'-m'+3/2}{2l'+3} \right)^{1/2} i g_a f_b Y_{l, m-1/2}^* Y_{l'+1, m'-1/2} \\ - u_4^\dagger v_2 &= \left(\frac{l-m+1/2}{2l+1} \cdot \frac{l'+m'+3/2}{2l'+3} \right)^{1/2} i g_a f_b Y_{l, m+1/2}^* Y_{l'+1, m'+1/2} \end{aligned} \quad (36)$$

where, as usual, the primes and subscript b are associated with the initial state.

The two terms of equation (34) are

$$\begin{aligned} \sqrt{2} u_1^\dagger v_4 &= \sqrt{2} i \left(\frac{l-m+3/2}{2l+3} \cdot \frac{l'-m'+1/2}{2l'+1} \right)^{1/2} f_a g_b Y_{l+1, m-1/2}^* Y_{l', m'+1/2} \\ \sqrt{2} u_3^\dagger v_2 &= \sqrt{2} i \left(\frac{l+m+1/2}{2l+1} \cdot \frac{l'+m'+3/2}{2l'+3} \right)^{1/2} g_a f_b Y_{l, m-1/2}^* Y_{l'+1, m'+1/2} \end{aligned} \quad (37)$$

and for equation (35) we have

$$\begin{aligned}\sqrt{2} \alpha_2^* V_3 &= \sqrt{2} i \left(\frac{l+m+3/2}{2l+3} \cdot \frac{l'+m'+1/2}{2l'+1} \right)^{1/2} f_a g_b Y_{l+1, m+1/2}^* Y_{l', m'-1/2} \\ \sqrt{2} \alpha_4^* V_1 &= \sqrt{2} i \left(\frac{l-m+1/2}{2l+1} \cdot \frac{l'-m'+3/2}{2l'+3} \right)^{1/2} g_a f_b Y_{l, m+1/2}^* Y_{l'+1, m'-1/2}\end{aligned}\quad (38)$$

The parts of these three sets of equations are to be added together and integrated over all space. We will actually perform the angular integration first, then add the terms together, then perform the summation (29) and then evaluate the radial integrals.

For the angular integrations we make use of the orthogonality relations of the spherical harmonics, (Bethe 33, p 432) which may be expressed

$$\int Y_{l,m}^* Y_{l',m'} d\Omega = \delta_{l,l'} \delta_{m,m'} \quad (39)$$

where δ is the Kronecker δ defined by

$$\begin{aligned}\delta_{l,l'} &= 0, \quad l \neq l' \\ &= 1, \quad l = l'\end{aligned}\quad (40)$$

Applying (39) to equations (36) we see that each of the four terms is zero unless $m = m'$, and also the first two terms are zero unless $l' = l - 1$. Since we are calculating transitions to a final K state, i.e. $l = 0$, we can ignore the terms in which $l' = l - 1$. Thus α_2 can contribute only one term to the sum (29), and with the substitution $l' = l + 1, m' = m$, it is

$$\begin{aligned} & \left| (n, \ell, j, m | \alpha_z | n', \ell+1, j', m) \right|^2 = \\ & \frac{4}{(2\ell+3)^2} \left[(\ell-m+3/2)(\ell+m+3/2) \right] \left[\int_0^\infty f_a g_b r^2 dr \right]^2 \end{aligned} \quad (41)$$

Applying (39) to equations (37) we see that both terms are zero unless $m' = m - 1$. The first is zero unless $\ell' = \ell + 1$, and the second unless $\ell' = \ell - 1$. Again we ignore $\ell' = \ell - 1$ and get as our contribution to (29) from (37)

$$\begin{aligned} & \left| (n, \ell, j, m | \alpha_+ | n', \ell+1, j', m-1) \right|^2 = \\ & \frac{2}{(2\ell+3)^2} \left[(\ell-m+3/2)(\ell-m+5/2) \right] \left[\int_0^\infty f_a g_b r^2 dr \right]^2 \end{aligned} \quad (42)$$

Applying (39) to equations (38) we find that both terms are zero unless $m' = m + 1$. The first term is zero unless $\ell' = \ell + 1$ and the second unless $\ell' = \ell - 1$. Thus the contribution to (39) is

$$\begin{aligned} & \left| (n, \ell, j, m | \alpha_- | n', \ell+1, j', m+1) \right|^2 = \\ & \frac{2}{(2\ell+3)^2} \left[(\ell+m+3/2)(\ell+m+5/2) \right] \left[\int_0^\infty f_a g_b r^2 dr \right]^2 \end{aligned} \quad (43)$$

The selection rules contained in equations (41), (42), and (43) are clearly $\Delta\ell = \pm 1$, $\Delta m = \pm 1, 0$.

Performing the summation (29) we obtain

$$\begin{aligned} & \sum_{m'} \left| (n, \ell, j, m | \vec{\alpha} | n', \ell+1, j', m') \right|^2 = \\ & \frac{2j+3}{j+1} \left[\int_0^\infty f_a(r) g_b(r) r^2 dr \right]^2 \end{aligned} \quad (44)$$

Since both states above are type A, $j = \ell + \frac{1}{2}$ and $j' = \ell + 3/2$. An exactly similar calculation for transitions from type B initial states to type A final states leads to

$$\sum_{m'} |(n, l, j, m | \bar{\alpha} | n', l+1, j', m')|^2 = \frac{1}{j(j+1)} \left[\int_0^\infty (j f_a g_b + (j+1) g_a f_b) r^2 dr \right]^2 \quad (45)$$

In this case $j = j' = l + \frac{1}{2}$. In this calculation we find that the angular integrations impose the new selection rule $\Delta j = \pm 1, 0$.

Equations (44) and (45) represent the only two matrix elements which are necessary for our present dipole calculations. The summed matrix elements permitted by the dipole selection rules are listed in Table I. This is the set which appears in equations (12), (18), and (19) with the approximation (21). These same matrix elements have been tabulated by Jacobsohn (Jacobsohn, 47). Since $j_0(kr)$ introduces no new angular dependence in the matrix elements, if we wish to include this term we merely insert it as a multiplying factor to the integrands of equations (44) and (45).

For the radial integrations we insert the functions f and g from our tables of radial wave functions in Appendix A. The details of the integration and of the numerical evaluation of the resultant matrix elements are left to Appendix B. We give in Table II the numerical values of the total matrix elements for each possible dipole transition to the K shell from the L, M, and N shells for several atoms whose atomic numbers range from 29 to 100. It is only necessary to specify the initial level, since the final state is always a K state.

TABLE 1

DIPOLE MATRIX ELEMENTS

This is the complete list of matrix elements allowed by the electric dipole selection rules. The sums over the degeneracy of the states is done for an atom with an initial vacancy in the state designated by the unprimed quantum numbers.

$$\sum_{m'} \left| \langle n, l, j = l + 1/2, m | \vec{a} | n', l+1, j' = l + 3/2, m' \rangle \right|^2 =$$

$$\frac{2j+3}{j+1} \left[\int_0^\infty f_a(r) g_b(r) r^2 dr \right]^2$$

$$\sum_{m'} \left| \langle n, l, j = l + 1/2, m | \vec{a} | n', l-1, j' = l - 1/2, m' \rangle \right|^2 =$$

$$\frac{2(2j-1)}{j} \left[\int_0^\infty f_b(r) g_a(r) r^2 dr \right]^2$$

$$\sum_{m'} \left| \langle n, l, j = l + 1/2, m | \vec{a} | n', l+1, j' = l + 1/2, m' \rangle \right|^2 =$$

$$\frac{1}{j(j+1)} \left[\int_0^\infty (j f_a g_b + (j+1) g_a f_b) r^2 dr \right]^2$$

$$\sum_{m'} \left| \langle n, l, j = l - 1/2, m | \vec{a} | n', l-1, j' = l - 1/2, m' \rangle \right|^2 =$$

$$\frac{1}{j(j+1)} \left[\int_0^\infty ((j+1) f_a g_b + j g_a f_b) r^2 dr \right]^2$$

TABLE 1 - DIPOLE MATRIX ELEMENTS (continued)

$$\sum_{m'} \left| (n, l, j = l - 1/2, m \mid \vec{\alpha} \mid n', l+1, j' = l + 1/2, m') \right|^2 =$$

$$\frac{2j+1}{j} \left[\int_0^\infty g_a f_b r^2 dr \right]^2$$

$$\sum_{m'} \left| (n, l, j = l - 1/2, m \mid \vec{\alpha} \mid n', l-1, j' = l - 3/2, m') \right|^2 =$$

$$\frac{2j-1}{j} \left[\int_0^\infty f_a g_b r^2 dr \right]^2$$

TABLE 11

DIPOLE MATRIX ELEMENTS

These are the numerical evaluations of the formulae of Table XIV of Appendix B, using the numerical value of the parameters also tabulated in Appendix B.

Atomic Number

Initial State	29	47	56	79	82	100
2 P1/2	3.456×10^{-3}	8.905×10^{-3}	1.245×10^{-2}	2.334×10^{-2}	2.487×10^{-2}	3.362×10^{-2}
2 P3/2	6.954×10^{-3}	1.818×10^{-2}	2.551×10^{-2}	4.914×10^{-2}	5.265×10^{-2}	7.492×10^{-2}
3 P1/2	7.646×10^{-4}	1.893×10^{-3}	2.605×10^{-3}	-	4.629×10^{-3}	5.465×10^{-3}
3 P3/2	1.579×10^{-3}	4.180×10^{-3}	5.921×10^{-3}	-	1.273×10^{-2}	1.883×10^{-2}
4 P1/2	2.935×10^{-4}	7.119×10^{-4}	1.050×10^{-3}	-	1.669×10^{-3}	1.846×10^{-3}
4 P3/2	6.111×10^{-4}	1.622×10^{-3}	2.300×10^{-3}	-	4.985×10^{-3}	7.428×10^{-3}

These matrix elements may now be used to calculate the transition probabilities for emission from equation (18) and the rate of emission of energy J defined in Chapter I. These quantities are presented in Table III.

The partial radiative widths Γ_{ab} , as defined in Chapter I are identically equal to the transition probabilities from Table III. There seem to be no accurate experimental measurements of line width in the region of atomic number where relativistic effects would be measurable. In non-relativistic quantum mechanics there is no difference in energy between the $P_{3/2}$ and $P_{1/2}$ levels and no difference in the radial wave functions of electrons in these states. It is therefore customary to calculate non-relativistically the transition probability from a P subshell to the ground state. These transition probabilities are tabulated for hydrogen in Bethe's article (Bethe 33, p 444). For hydrogenic atoms (neglecting screening) of different atomic number one must multiply the values there by Z^4 . The relative intensity of the $P_{3/2}$, $P_{1/2}$ doublet can be simply calculated non-relativistically, and is determined by the ratio of the number of $P_{3/2}$ states (4) to the number of $P_{1/2}$ states (2). Relativistically there is both an energy difference and a radial wave function difference between such levels. The factor of two from the different number of initial states is still present, but is combined with a difference produced by each of the other factors mentioned.

TABLE III

DIPOLE TRANSITION PROBABILITIES

Tabulated are the dipole transition probabilities W of equation (18) in units sec^{-1} and the rate of energy emission J in ergs sec^{-1} for transitions from the indicated initial level to the $1S_{1/2}$ level.

		Atomic Number						
Initial State		29	47	56	79	82	100	
2 P1/2	W	4.43×10^{14}	3.05×10^{15}	6.14×10^{15}	2.40×10^{16}	2.78×10^{16}	5.94×10^{16}	W
	J	6.15×10^6	1.13×10^8	3.28×10^8	2.67×10^9	3.36×10^9	1.13×10^{10}	J
2 P3/2	W	8.95×10^{14}	6.29×10^{15}	1.28×10^{16}	5.21×10^{16}	6.09×10^{16}	1.40×10^{17}	W
	J	1.25×10^7	2.36×10^8	6.91×10^8	5.99×10^9	7.63×10^9	2.83×10^{10}	J
3 P1/2	W	1.14×10^{14}	7.71×10^{14}	1.53×10^{15}	-	6.18×10^{15}	1.16×10^{16}	W
	J	1.87×10^6	3.40×10^7	9.70×10^7	-	8.94×10^8	2.67×10^9	J
3 P3/2	W	2.35×10^{14}	1.71×10^{15}	3.48×10^{15}	-	1.71×10^{16}	4.06×10^{16}	W
	J	3.87×10^6	7.55×10^7	2.22×10^8	-	2.50×10^9	9.47×10^9	J
4 P1/2	W	4.71×10^{13}	3.09×10^{14}	6.08×10^{14}	-	2.35×10^{15}	4.14×10^{15}	W
	J	8.18×10^5	1.44×10^7	4.08×10^7	-	3.59×10^8	1.01×10^9	J
4 P3/2	W	9.81×10^{13}	6.97×10^{14}	1.43×10^{15}	-	7.05×10^{15}	1.68×10^{16}	W
	J	1.70×10^6	3.25×10^7	9.57×10^7	-	1.08×10^9	4.10×10^9	J

Non-relativistically the transition probability (Bethe 33, p 430) depends on the third power of the energy of the emitted radiation. The squared matrix element is proportional to Z^{-2} but independent of the energy. It would therefore be simple to correct the transition probabilities for the difference in energy of the pairs of lines comprising an X-ray doublet. Relativistically this is very difficult because the normalization constants of the wave functions depend on the energy. Hence the matrix elements depend on the transition energy, and it is impossible to separate the differences caused by changed overlap of the wave function from those caused by the differences in energy. It is true, however, that there must be an approximate E^3 dependence of the transition probability, and one could use this fact to correct the relative intensities calculated here for the difference between the experimental energies of the X-ray lines and the ones used in the present work which are predicted from the Dirac equation.

Since in the work of Chapter IV we need probabilities for transitions to shells of greater principle quantum number than four, the limit of our relativistic calculations, it is of some importance to determine the possible error resulting from use of the non-relativistic values for this calculation. Table IV contains the ratios of the total transition probability from each shell to the K shell, to the non-relativistic transition probability given by Bethe.

TABLE IV

TOTAL RELATIVISTIC TRANSITION PROBABILITIES

Given are the ratios of the sum of the transition probabilities of each line of an X-ray doublet to the transition probability from the same subshell from Bethe (Bethe, 33).

Z	Transition		
	2P → 1S	3P → 1S	4P → 1S
29	1.01	1.025	1.006
47	1.02	1.03	1.011
56	1.025	1.04	1.014
79	1.04	-	-
82	1.05	1.05	1.019
100	1.06	1.06	1.025

TABLE V

X-RAY LINE DESIGNATION

Transition	X-ray Line
2 P _{1/2} - 1 S _{1/2}	K α ₂
2 P _{3/2} - 1 S _{1/2}	K α ₁
3 P _{1/2} - 1 S _{1/2}	K β ₃
3 P _{3/2} - 1 S _{1/2}	K β ₁
4 P _{1/2} - 1 S _{1/2}	K β ₂ '
4 P _{3/2} - 1 S _{1/2}	K β ₂

Figure 1. Total relativistic transition probability from the designated sub-shell, divided by the non-relativistic transition probability from the same sub-shell. The points are theoretical.

This total transition probability is the sum of the transition probabilities from the two P levels of a given shell. These ratios are also given graphically in Figure 1. We observe that the total transition probability is nowhere changed as much as ten percent, and in the N shell by less than three percent even for $Z = 100$. Since the relative importance of the contribution from each shell decreases rapidly with n , and since the relativistic effects on this quantity are small, there is obviously very small error involved in using the non-relativistic transition probabilities for $n > 4$. It is interesting to observe the effect of screening on the total transition probability, as calculated for gold ($Z = 79$), by Burhop and Massey (Burhop, 36). Their work indicates that the $2 P_{3/2}$ transition probability is reduced 23.7 percent relative to the non-relativistic value, and the $2 P_{1/2}$ transition probability is reduced 17.1 percent. The total transition probability is thus reduced 21.5 percent.

Since the usual experimental methods of X-ray intensity measurements involve measurement of the energy associated with a given line (Compton, 35), it is the ratio of the J's which should be considered as the relative intensities. For convenience in the discussion of relative intensities we give in Table V the X-ray line designation of each transition. In Table VI and graphically in Figure 2 are given the relative intensities of

TABLE VI

RELATIVE INTENSITIES AND RATIOS OF
TRANSITION PROBABILITY FOR X-RAY DOUBLETS

Relative Intensity

29	2.03	2.07	2.08
47	2.08	2.22	2.25
56	2.11	2.29	2.34
79	2.24	-	-
82	2.27	2.80	3.01
100	2.49	3.55	4.07

Ratio of Transition Probabilities

29	2.02	2.07	2.08
47	2.06	2.21	2.24
56	2.08	2.28	2.34
79	2.17	-	-
82	2.20	2.77	3.00
100	2.36	3.495	4.045

Figure 2. Relative intensities of the K X-ray doublets. The points are theoretical.

the different X-ray doublets for each atom. Non-relativistically each of these numbers would be two, independent of Z and n . We observe that relativistic effects enhance the probability of transitions in which j changes, and decrease those in which j does not change. Part of this is due to the energy dependence of the emission rate. If we assume that the non-relativistic E^4 dependence of J is approximately true, and multiply the relative intensity ratio $K\beta_{2'}/K\beta_2$ for $Z = 100$ by the fourth power of the inverse energy ratios to remove the energy dependence, we get 3.97 which indicates that a large portion of this effect must be due to the changed overlap of the wave functions in the radial integration. The calculation of Chapter III including the retardation factor $j_0(kr)$ in the matrix elements indicates that this term makes a significant change in these relative intensities, and that they should not be expected to conform closely with experiment. They should be considered primarily as a measure of the importance of relativistic effects in such calculations.

Reliable experimental measurements of X-ray relative intensities for atoms of high atomic number are very rare. This is due partly to experimental difficulty when measuring high energy photons with spectroscopic accuracy, and partly to the absence in the literature of suitable theoretical predictions with which to compare the results of any experiment. The very good recent measurements of

K series line widths by Gokhale (Gokhale, 52) using a bent crystal spectrometer extend only to $Z = 50$, and even in this work only total line width is reported, rather than relative intensity. In this region of atomic number the contribution to line widths due to the Auger effect is large enough and uncertain enough to make relative intensity determination from line widths with sufficient accuracy to detect the small relativistic effects very difficult. The much earlier work of J. H. Williams (Williams, 33) measures K series relative intensities, but only for elements of atomic number less than 52. Satisfactory theoretical agreement with this and other experimental measurements in this region of Z has been obtained by Tuan (Tuan, 53) using non-relativistic perturbation theory, but with a somewhat arbitrary adjustment of the Slater screening constants. Recent developments, especially by DuMond, of large bent crystal spectrometers (DuMond, 47) would seem to make possible accurate determinations of relative intensities in elements of high atomic number, although more interest has so far been given to accurate energy determinations of nuclear gamma radiations. DuMond's spectrometer has been used, however, to measure the K spectrum of tungsten ($Z = 74$), (DuMond, 49). The authors were interested primarily in energy determination and do not report relative intensities. In their experiment they completely resolve the $K\alpha_1$, $K\alpha_2$ and $K\beta_1$, $K\beta_3$ doublets and partially resolve the $K\beta_2'$,

$K\beta_2$ doublet.

The necessary corrections to their data for a determination of relative intensities have not been made and any estimates made from their published curves would be only order of magnitude guesses. A few very early experiments at high atomic number are tabulated in Compton & Allison (Compton, 35) and in Bethe's article (Bethe, 33, p 469). A review of the original references given there indicates that the relative intensity figures are not very reliable, and not accurate enough to give a quantitative estimate of relativistic effects.

In Table VII we give the relative intensities of lines originating in different shells. We give the intensity ratios for transitions in which $\Delta j = 0$ to the $K\alpha_2$ line and for transitions in which $\Delta j = 1$ to the $K\alpha_1$ line. Non-relativistically the ratios would be

$$\begin{aligned} K\beta_1 / K\alpha_1 &= K\beta_3 / K\alpha_1 = .309 \\ K\beta_2' / K\alpha_1 &= K\beta_2 / K\alpha_2 = .135 \end{aligned} \tag{47}$$

In both cases we observe relativistically that the ratios of those transitions in which $\Delta j = 1$ are consistently above those non-relativistic ratios, with the difference increasing slowly with increasing Z and the ratios of those transitions in which $\Delta j = 0$ are consistently below the non-relativistic ratios, the difference increasing much more rapidly with Z . This is clearly consistent with our other tabulated relative intensities. We show graphically

TABLE VII

RELATIVE INTENSITIES OF X-RAY
LINES FROM DIFFERENT SHELLS

Relative Intensity	Atomic Number				
	29	47	56	82	100
	.316	.320	.321	.328	.334
	.304	.300	.296	.266	.235
	.137	.138	.138	.142	.145
	.133	.127	.124	.107	.089

These are the ratios of the rates of energy emission of the lines given in the column on the left.

Figure 3. Relative intensities of the K X-ray lines shown. The points are theoretical. The dotted line is the value predicted non-relativistically.

Figure 4. Relative intensities of the K X-ray lines shown. The points are theoretical. The dotted line is the value predicted non-relativistically.

in Figure 3 the ratios $K\beta_1/K\alpha_1$ and $K\beta_3/K\alpha_2$, and in Figure 4 the ratios $K\beta_2'/K\alpha_1$ and $K\beta_2/K\alpha_2$. From Figures 2, 3, and 4 any desired relative intensities may be obtained by simple multiplication or division of the ordinates.

CHAPTER 111

RETARDATION EFFECTS AND QUADRUPOLE EMISSION

As was stated in Chapter I, the omission of the retardation in the dipole matrix element leads to serious errors in determining relative intensities of X-ray transitions for heavy elements. In the derivation of the matrix elements of Chapter II we showed that equations (44) and (45) could be corrected by including the term $j_0(-kr)$ in the radial integrations. If we do this, (44) is replaced by

$$\frac{2j+3}{j+1} \left[\int_0^\infty f_a g_b j_0(-kr) r^2 dr \right]^2 \quad (48)$$

and (45) by

$$\frac{1}{j(j+1)} \left[\int_0^\infty (j f_a g_b + (j+1) g_a f_b) j_0(-kr) r^2 dr \right]^2 \quad (49)$$

We shall evaluate these more exact expressions for the general case of transitions from the two 2P levels of any atom and numerically for lead, $Z = 82$. We choose lead since it is the atom chosen for the work of Chapter IV for calculating the integrated cross-section. Also in this Chapter we shall examine the consequences of omitting higher terms in the expansion (13) and estimate the ratio of the intensity of the most prominent electric quadrupole transitions to the most prominent electric

dipole transitions. We also do this numerically for lead. The relative importance of the higher terms in (13) is of interest in the calculation of Chapter IV, since not only should the integrated non-relativistic cross-section for dipole transitions converge to some limit, but the total integrated relativistic cross-section for all multipoles should converge, if the assumption that scattering by bound electrons approaches that of free electrons (Gell Mann, 54) is valid.

We leave the details of the integrations (48) and (49) to Appendix B, since they are quite similar to the equivalent integrals of Chapter II. We merely state the results here and calculate the transition probabilities and relative intensities for the $K\alpha_1$ and $K\alpha_2$ transitions in lead. From Appendix B we have for the matrix element

$$(48) \quad \frac{8}{3} \left(\frac{2Z}{ka_0} \right)^2 \frac{64 A' \Gamma^2(\gamma_1 + \gamma_2 + 1)}{\Gamma(2\gamma_1 + 1) \Gamma(2\gamma_2 + 1) N_3^{2\gamma_2 + 1} R^{2(\gamma_1 + \gamma_2)}} \frac{1}{R^{2(\gamma_1 + \gamma_2)}} \left[\frac{\sin(\gamma_1 + \gamma_2) \Phi}{\gamma_1 + \gamma_2} \right]^2 \quad (50)$$

with

$$R^2(2P_{3/2}) = \left(\frac{N_3 + 1}{2N_3} \right)^2 + \left(\frac{ka_0}{2Z} \right)^2 \quad (51)$$

and

$$\Phi(2P_{3/2}) = \tan^{-1} \left(\frac{N_3 ka_0}{(N_3 + 1) Z} \right) \quad (52)$$

For the matrix element (49) we have

$$\begin{aligned} & \frac{4}{3} \left(\frac{2Z}{ka_0} \right)^2 \frac{4(2\gamma_1 + 1)}{N_2^{2\gamma_1 + 1} R^{4\gamma_1}} \left[(-2B + N_2(A+B)) \left\{ \frac{\sin 2\gamma_1 \Phi}{2\gamma_1} \right\} \right. \\ & \quad \left. - \frac{(A+B)(N_2 - 1)}{N_2 R} \left\{ \frac{\sin(2\gamma_1 + 1)\Phi}{2\gamma_1 + 1} \right\} \right]^2 \end{aligned} \quad (53)$$

with

$$R^2(2P_{1/2}) = \left(\frac{N_2+1}{2N_2}\right)^2 + \left(\frac{\hbar a_0}{2Z}\right)^2 \quad (54)$$

and

$$\Phi(2P_{1/2}) = \tan^{-1} \left(\frac{N_2 \hbar a_0}{(N_2+1)Z} \right) \quad (55)$$

The parameters N and γ are defined in Appendix A, and their numerical values tabulated in Table XVI of Appendix B. The parameters A' , A , and B are defined and tabulated in Appendix B. The quantity k is defined in Chapter 1 and is given by

$$\hbar a_0 = \frac{E_{ab}}{\hbar c} \quad (56)$$

If we use our values of E_{ab} from Table XVII for Pb we get for the $2P_{3/2}$ transition (equation 50)

$$\hbar(2P_{3/2}) = 3.9616 \times 10^9 \text{ cm}^{-1} \quad (57)$$

and

$$\hbar(2P_{1/2}) = 3.8272 \times 10^9 \text{ cm}^{-1} \quad (58)$$

So, for $Z = 82$

$$\frac{\hbar a_0}{2Z}(2P_{3/2}) = 0.12782 \quad (59)$$

and

$$\frac{\hbar a_0}{2Z}(2P_{1/2}) = 0.12348 \quad (60)$$

Using $N_3 = 2$, and $N_2 = 1.8980$ we get for equation (52)

$$\Phi(2P_{3/2}) = 0.16681 \quad (61)$$

and for (55)

$$\Phi(2P_{1/2}) = 0.16036 \quad (62)$$

Using the tabulated values of γ_1 and γ_2 for lead, we have

$$\begin{aligned} (\gamma_1 + \gamma_2) \Phi(2P_{3/2}) &= 0.45740 \\ \sin(\gamma_1 + \gamma_2) \Phi(2P_{3/2}) &= 0.44462 \end{aligned} \quad (63)$$

and

$$\begin{aligned} 2\gamma_1 \Phi(2P_{1/2}) &= 0.25697 \\ \sin 2\gamma_1 \Phi(2P_{1/2}) &= 0.25415 \end{aligned} \quad (64)$$

and

$$\begin{aligned} (2\gamma_1 + 1) \Phi(2P_{1/2}) &= 0.41733 \\ \sin(2\gamma_1 + 1) \Phi(2P_{1/2}) &= 0.40533 \end{aligned} \quad (65)$$

We observe that in (63) the sine of the angle differs from the angle by about 3.5%. The difference between $R^{-2(\gamma_1 + \gamma_2)}$ and the factors it replaces in the matrix element without retardation is about 1.5%, so the change in the resulting squared matrix element (50) is primarily due to the difference in the $\sin^2$ term. In (64) the difference is only about 1% between the angle and its sine, and although the difference in (65) is larger, we get a cancellation of the effects, which results in almost

no change in the matrix element due to retardation. We omit the further details of the numerical calculation, but the cancellation mentioned above comes about as follows. The first term in the brackets of equation (53) is positive and about twice as large as the second term which is negative. In comparison with the same term without inclusion of retardation, the multiplication by the appropriate sine terms (64) or (65) results in a slight decrease of the first term and a larger decrease of the second. The net effect is an increase in the bracketed quantity, but this is balanced by the increase in the denominator of the quantity R. The total effect on (53) is therefore a small decrease in comparison to the matrix elements used in Chapter 11. For lead the squared averaged matrix elements are numerically

$$|(1S_{1/2} | \vec{\alpha} j_0 | 2P_{3/2})|^2 = 4.469 \times 10^{-2} \quad (66)$$

instead of, from Table 11

$$|(1S_{1/2} | \vec{\alpha} | 2P_{3/2})|^2 = 5.265 \times 10^{-2} \quad (67)$$

which is a 15% decrease in this quantity, and

$$|(1S_{1/2} | \vec{\alpha} j_0 | 2P_{1/2})|^2 = 2.484 \times 10^{-2} \quad (68)$$

instead of, from Table 11

$$|(1S_{1/2} | \vec{\alpha} | 2P_{1/2})|^2 = 2.487 \times 10^{-2} \quad (69)$$

which is an insignificant reduction to our accuracy.

These changes in the matrix element result in changes in the transition probabilities and emission rates as given below.

For the $K\alpha_1$ line, the transition probability becomes

$$W(2P_{3/2}) = 5.16 \times 10^{16} \text{ sec}^{-1} \quad (70)$$

instead of

$$W(2P_{3/2}) = 6.09 \times 10^{16} \text{ sec}^{-1} \quad (71)$$

from Table III. The rate of emission for this transition becomes

$$J(2P_{3/2}) = 6.46 \times 10^9 \text{ erg sec}^{-1} \quad (72)$$

instead of

$$J(2P_{3/2}) = 7.63 \times 10^9 \text{ erg sec}^{-1} \quad (73)$$

from Table III.

To the same order of accuracy the equivalent quantities for the $K\alpha_2$ line are unchanged.

The relative intensity ratio

$$K\alpha_1 / K\alpha_2 = 1.92 \quad (74)$$

when the effects of retardation are included instead of

$$K\alpha_1 / K\alpha_2 = 2.27 \quad (75)$$

from Table IV.

The ratio of total transition probability to the non-relativistic transition probability becomes

$$\frac{W_{REL}}{W_{N.R.}} = 936 \quad (76)$$

instead of

$$\frac{W_{REL}}{W_{N.R.}} = 1.05 \quad (77)$$

from Table IV.

We conclude from these numbers that the effects of retardation must be included in calculations of X-ray relative intensities of heavy elements, since at least in the one case calculated here, this effect more than compensates for the changes caused by relativistic effects. It is expected that the intensity ratio (74) is more nearly correct than the non-relativistic value for this ratio. Possible influencing effects such as screening and higher order radiative corrections are expected to be small. It is also believed that present experimental techniques may be capable of detecting this 4% difference. The results of such experiments are not available in the literature.

The second term of the expansion (13) can cause radiative transitions between atomic states even if the selection rules of Chapter II forbid electric dipole radiation. This is obvious because of the additional angular dependence of this term. For the processes in

which we are interested, the probability of such transitions is small compared to the electric dipole transition probability. This may be seen from the following argument.. We replace $j_1(kr)$ by its asymptotic expression for small kr (this is the same approximation neglecting retardation as the work of Chapter 11). This asymptotic expression is (Schiff, 49)

$$j_1(kr) \cong \frac{kr}{3} ; kr \ll 1 \quad (78)$$

and we observe that the radial integrals of the matrix elements contain an additional factor kr which is small in the region where the wave functions are large.

If we replace kr in the integrals by some mean value, such as $\frac{\hbar a_0}{2}$, which replaces r by a length of atomic dimensions, we see that these matrix elements are similar to those of Chapter 11 except for the factor $\frac{\hbar a_0}{3^2}$, and the transition probabilities are multiplied by the square of this quantity. This is at best an order of magnitude estimate, since the radial integral for quadrupole emission or absorption contains different wave functions from those of the dipole case.

If, however, this estimate is approximately correct, the inclusion of quadrupole terms in the calculation of the integrated cross-section will result in a small increase in this quantity. In view of this, and the evidence from Chapter 11 that the use of relativistic wave functions results in no order of magnitude changes in total dipole

transition probability, it would seem a reasonable approximation to use non-relativistic wave functions in the quadrupole matrix elements.

To be certain that this approximation is satisfactory, calculations of the quadrupole matrix elements using relativistic wave functions have been made for very simple emission processes which avoid the now very laborious sum over polarizations and integration over directions of emission. The process chosen was emission in the z direction of a photon, by an atom which in the initial state had a single vacancy in the K shell. This restriction of emission to the z direction permits an immediate simplification of the quantity

$$(j_1, k, r) \sum_{M=-\ell}^{\ell} Y_{\ell, M}^*(\theta, \phi) Y_{\ell, M}(\theta, \phi) \quad (79)$$

which is the second term of (13). Using the sum-rule for spherical harmonics (Bethe, 33, p 560)

$$\sum_M Y_{\ell, M}^*(\theta, \phi) Y_{\ell, M}(\theta, \phi) = \sqrt{\frac{2\ell+1}{4\pi}} Y_{\ell, 0}(\sigma) \quad (80)$$

where σ is the angle between the points (θ, ϕ) and (θ, ϕ) , on the unit sphere. Since $\vec{k}$ is in the z direction, $\sigma = \theta$ where θ is the direction of $\vec{r}$, and is one of the variables of integration of the matrix elements.

Use of the decomposition (28) for $\vec{\alpha}$ implies that the 3 possible states of polarization are linear polarization in the z direction and right or left circular polarization in the xy plane. The first of these, which

occurs in transitions in which the effective operator is α_z , cannot accompany emission in the z direction. We restrict our case still further by choosing one of the other two. There will then be a unique initial state (depending, of course, on which K state is vacant) which can be effective in producing radiation of the definite properties we require.

The selection rules for quadrupole emission are well known (Blatt 52, Rose 55) and follow from simple operations with the spherical harmonics in the matrix elements. They may be stated $\Delta \ell = 0, \pm 2$, $\Delta j = 0, \pm 1, \pm 2$, $\Delta m = 0, \pm 1, \pm 2$, with the further restriction that no transitions may occur between two states with $\ell = 0$. The most probable transitions with a final K state are those which originate in the 3D subshell. This is true non-relativistically (Jacobsohn, 47), and must also be true in our case.

The relativistic matrix elements were calculated with retardation neglected, using the expression (78) and were compared to equivalent electric dipole transitions. The matrix elements calculated were

$$\left| \left(1S_{1/2}, m = 1/2 \mid \alpha_- Q \mid 3D_{5/2}, m' = 3/2 \right) \right|^2 \quad (81)$$

and

$$\left| \left(1S_{1/2}, m = 1/2 \mid \alpha_- Q \mid 3D_{3/2}, m' = 3/2 \right) \right|^2 \quad (82)$$

where Q is the operator which results from the simplification

(78) and (80) applied to (79). The results of these calculations, which are now very similar to the calculations needed for Chapter 11, were compared to equivalent simplified electric dipole matrix elements. The comparison showed that the quadrupole transition probability was at most a few percent of the electric dipole from the 3P subshells, in good agreement with the results of the non-relativistic calculations of Jacobsohn (Jacobsohn, 47). The numerical comparisons were made for lead ($Z = 82$). The quadrupole transition probability from the K state to higher discrete states is therefore expected to contribute at most a correction of a few percent to the integrated cross-section, and use of the non-relativistic calculations can be expected to produce no serious error.

The experimental observation of quadrupole lines in the K spectra of heavy elements would seem possible, although difficult. The experimental energy difference between the quadrupole and the nearest dipole lines is considerably larger than the Dirac theory predicts because of the effects of screening, (Hill, 52). The usual spectroscopic difficulties when observing weak lines in the presence of much stronger ones would be encountered. For lead, there is an experimental energy difference of almost 500 electron volts between the $3P_{3/2}$ and $3D_{3/2}$ shell which is very large compared to the resolution of X-ray spectrometers now in use (DuMond, 49), and also large compared to the X-ray line width, which for lead is less than 100

electron volts.

The results of Chapter 11 on relative intensities must not be considered an attempt to determine the relative intensities expected from experiment. At best they are a simple check of the numerical computations. The more refined but less complete calculations of Chapter 111 are probably significantly better estimates of experimental results. The problem of a consistent relativistic treatment of the many electron atomic problem is by no means closed, and calculations similar to those of Chapter 111, together with good experimental measurements of X-ray intensities might aid in distinguishing between simple relativistic effects and the much more complex problem of the interactions of the electrons.

CHAPTER IV

INTEGRATED ABSORPTION CROSS-SECTIONS

The integrated cross-section for absorption with transitions between bound states is given by equation (11). The matrix elements for absorption by an ion with all electrons removed except for one K electron are identical with those for X-ray emission which have been calculated in Chapter II, or in the more accurate calculations of Chapter III. To be consistent with the remainder of the thesis we will calculate the integrated cross-section first using the matrix elements of Table II for electric dipole, without retardation. The effect of further refinements, including retardation corrections and quadrupole transitions on the integrated cross-section will then be discussed.

In terms of the oscillator strength the cross-section is given by (25). This equation is valid for oscillator strengths, when defined relativistically by (12) or non-relativistically by (22) for any radiative matrix element, including the higher multipole terms. As stated in Chapter I, it is also valid for transitions in which the final state of the electron is one of the states of the positive energy continuum. For the photo-electric effect, the derivation of (25) requires that one use in the matrix

element a positive energy wave function which is normalized per energy interval, and, in terms of this matrix element define an oscillator density per energy interval. The summation over final states is then replaced by an integral with respect to the energy of the photon absorbed.

This procedure is not the only method of arriving at a photo-electric cross-section. It is also possible to use positive energy wave functions which have been normalized in some large volume (Heitler 54, Schiff 49). In the photo-electric effect one can discuss the absorption probability for an individual photon, and using equation (1) derive this quantity with $N(E)$ now being the density of final electron states. An absorption cross-section may then be defined in terms of this transition probability. The cross-section so defined must obviously be identical with that given by (25). This second derivation is discussed in some detail in section 21 of Heitler's book (Heitler, 54) with references to several theoretical calculations of this cross-section. The first method, using energy normalized wave functions, is used non-relativistically by Bethe (Bethe, 33) and Jacobsohn (Jacobsohn, 47). A relativistic treatment using this method is given by Hall (Hall, 36). The derivations actually used for the calculations will be discussed in more detail later.

For the calculations of integrated cross-section, it

is convenient to use Mev as the unit of energy and the barn ($1 \text{ barn} = 10^{-24} \text{ cm}^2$) as the unit of cross-section. In these units, and including the factor $1/3$ from the average over polarizations, equation (11) becomes

$$\sigma_{ae} = 37.379 E_{ae}^{-1} |(a|\vec{r}|b)|^2 \text{ Mev-Barns} \quad (83)$$

and equation (25) is

$$\sigma_{ae} = 109.7 f_{ae} \text{ Mev-Barns} \quad (84)$$

In what follows we use (83) to calculate the cross-section for these transitions for which we have calculated the relativistic matrix elements, and (84) for dipole transitions to shells higher than the N shell and to estimate the effects of inclusion of the quadrupole terms and the retardation correction. For the dipole transitions to higher shells the non-relativistic oscillator strengths tabulated by Bethe (Bethe, 33) are used. For the quadrupole terms, the non-relativistic calculations of quadrupole oscillator strengths of Jacobsohn (Jacobsohn, 47) are used. The work of Jacobsohn includes not only the calculation of the oscillator strengths f_{ae}^Q for the most probable transitions, but also a sum rule for all quadrupole transitions. This rule is given by the equation

$$\sum_Q f_{ae}^Q = \frac{7}{15} \frac{(Z\alpha)^2}{n_b} \quad (85)$$

where n_b is the principle quantum number of the initial state. The only quadrupole transitions accompanying

absorption by a K electron are those with final states whose orbital angular momentum is $\ell = 2$. Non-relativistically there is no difference between $D_{3/2}$ and $D_{5/2}$ states, and one therefore combines the transitions to these levels, and calculates, as Jacobsohn has done, the oscillator strengths for transitions from 1S to nD subshells. The values of the oscillator strengths which apply to our problem are given in Table VIII.

TABLE VIII

QUADRUPOLE OSCILLATOR STRENGTHS			
Transition	$\frac{f_{ab}^a}{(Z\alpha)^2} \times 10^3$	$f_{ab}^a \times 10^3$	σ_{ab}^a (Mev-Barns)
1S 3D	8.789	3.150	.346
1S 4D	4.349	1.557	.171
1S 5D	2.342	.838	.092
1S 6D	1.387	.497	.055
1S 7D	.8842	.317	.035
1S 8D	.5970	.214	.023
1S 9D	.4213	.151	.016
1S 10D	.3092	.110	<u>.012</u>

$$\Sigma = .750$$

The values in the second column are the results of the non-relativistic calculation of quadrupole oscillator strengths from Jacobsohn (Jacobsohn, 47). In the third column are the numerical values of f_{ab}^a for lead ($Z = 82$). The fourth column contains cross-section σ_{ab}^a for lead,

given by (84). In Table IX are given the values f_{ab} and σ_{ab} for dipole transitions. For transitions from $1S_{1/2}$ to $nP_{3/2}$ and $1S_{1/2}$ to $nP_{1/2}$ for $n \leq 4$, the numerical values of the matrix elements for lead ($Z = 82$) have been taken from Table II, and σ_{ab} determined from equation (83). For the $1S$ to nP transitions ($n \geq 5$) the non-relativistic oscillator strengths have been taken from Bethe (Bethe, 33). There are tables of these dipole oscillator strengths in Jacobsohn's thesis, with more significant figures given, but these indicate a disagreement of 9 percent in the value of $(1S - 5P)$ between the two tables. Recalculation of this quantity indicate Bethe's value to be correct, and this value has been used here. We also give in Table VIII the value of σ_{ab} for the two transitions for which the relativistic retardation correction is known.

The sum of the numbers in the second column of Table IX represents the cross-sections integrated to the energy required to cause a transition to the $11P$ subshell. Since the $\sigma(E)$ curve in the region of energy where discrete transitions occur is a series of very sharp discrete peaks, whose widths, at least to $n = 5$ are small compared to their separation in energy, the integrated cross-section in this region is a step-function. The steps occur at the energies of the K X-ray lines. It is, however, very difficult to represent these steps on a reasonable scale, so the total effect of discrete transitions will be considered to be an additive constant to the integrated photo-electric

TABLE 1X

DIPOLE ABSORPTION CROSS-SECTION FOR LEAD

Transition	f_{ab}	σ_{ab} Mev-Barns	σ_{ab} (Retarded) Mev-Barns
1S _{1/2} 2P _{1/2}	.1122	12.31	12.30
1S _{1/2} 2P _{3/2}	.2300	25.23	21.37
1S _{1/2} 3P _{1/2}	.01745	1.915	
1S _{1/2} 3P _{3/2}	.0476	5.224	
1S _{1/2} 4P _{1/2}	.00597	.655	
1S _{1/2} 4P _{3/2}	.0175	1.922	
1S 5P	.0139	1.42	
1S 6P	.0078	.856	
1S 7P	.0048	.528	
1S 8P	.0032	.349	
1S 9P	.0022	.243	
1S 10P	.0016	<u>.176</u>	

$$\Sigma = 50.828$$

cross-section.

We have from Table IX

$$\sum_{n=1}^{10} \sigma(1s \rightarrow np) = 50.83 \text{ Mev-Barns} \quad (86)$$

If we wish to include the contributions due to discrete transitions to higher levels, we have in Bethe's work (Bethe, 33) an asymptotic expression for the non-relativistic oscillator strengths for such transitions.

$$f(1s \rightarrow np) \cong 1.6 n^{-3} ; \quad n \text{ large} \quad (87)$$

The Reimann Zeta-function $\zeta(z)$ is defined (Jahnke, 45, p269)

$$\zeta(z) = \sum_{n=1}^{\infty} \frac{1}{n^z} \quad (88)$$

and from the tables,

$$\zeta(3) = 1.202 \quad (89)$$

The formula (87) is quite accurate for $n \geq 10$, and if we subtract from (89) the partial sum

$$\sum_{n=1}^{10} \frac{1}{n^3} \quad (90)$$

we can include the small contribution from all higher discrete states. We get from this

$$1.6 \sum_{n=11}^{\infty} \frac{1}{n^3} = .00716 \quad (91)$$

and use (84) we have

$$\sum_{n=11}^{\infty} \sigma(1s \rightarrow np) = .785 \text{ Mev-Barns} \quad (92)$$

combining (86) and (92) we have

$$\sum_{n=2}^{\infty} \sigma(1S \rightarrow nP) = 51.61 \text{ Mev-Barns} \quad (93)$$

which is the dipole absorption cross-section, integrated to the K series limit, 101.7 kev.

If we use the values of cross-section obtained with inclusion of the effects of retardation in the two strongest transitions, this integrated cross-section is reduced 7.6 percent to

$$\int_0^{101.7} \sigma(E) dE = 47.74 \text{ Mev-Barns} \quad (94)$$

The effects of including retardation in the transition to higher discrete states can at present only be estimated. It is expected that the change in each of the contributing terms will give about the same percentage reduction as was produced in the total contribution from the 1S - 2P transitions. Since the 1S - 2P transitions contribute more than half the integrated cross section to discrete states, we would expect retardation corrections to result in less than 10 percent reduction in the quantity (94). Since the transitions between discrete states make up about half the total integrated cross-section, the total effect of retardation might be as large as 10 percent of $\int_0^{\infty} \sigma dE$. Retardation effects have been included in the photo-electric effect cross-section we will use. The non-relativistic calculation of Jacobsohn (Jacobsohn, 47) tends to support the general conclusion

that retardation corrections are several percent of the total integrated cross-section. He has calculated, and gives a sum-rule for, a correction term which is an approximation to our retardation correction. His calculation was made with non-relativistic wave-functions, and is probably applicable at best to low Z , and transitions to shells of principle quantum number greater than 4 or 5. It is certainly accurate only to terms of order $(Z\alpha)^2$. This sum-rule is given by Jacobsohn as

$$\sum_a f_{aL} (\text{DIPOLE CORRECTION}) = -\frac{2}{15} \frac{(Z\alpha)^2}{n_b^2} \quad (95)$$

For our case, with $Z = 82$ and $n_b = 1$ this would result in a reduction of $\int_0^\infty \sigma dE$ of about 5 percent.

The inclusion of the non-relativistic quadrupole cross-sections from Table VII will result in a small (1.4%) increase of (93). We will ignore both quadrupole and retardation corrections, and use (93) as the cross-section integrated to the K series limit.

There are available several theoretical evaluations of the photo-electric cross-section, each having different regions and ranges of usefulness. The simplest is that given by Heitler (Heitler, 54, sec. 21). Using non-relativistic perturbation theory, including the retardation factor $e^{i(\vec{k} \cdot \vec{r})}$, but approximating the final electron wave function by a free electron wave function (the Born approximation), he arrives at a formula for cross-section per K electron

$$\sigma(E) = \sigma_0 \frac{32}{(Z\alpha)^2} \left(\frac{I}{E}\right)^{7/2} \quad (96)$$

In this equation σ_0 is the cross-section for very low energy scattering by free electrons and is given by

$$\sigma_0 = \frac{8\pi}{3} \left(\frac{e^2}{mc^2}\right)^2 = .6651 \text{ BARNs} \quad (97)$$

and I is the non-relativistic binding energy of a K electron. In view of the use of non-relativistic quantum mechanics, it cannot be applied to elements of high Z , or to transitions for which the final energy is comparable to mc^2 . The use of the Born approximation requires that the energy of the ejected electron be large compared to the binding energy.

A calculation by Stobbe (Stobbe, 30), also non-relativistic, used positive energy Coulomb wave functions, but replaces the retardation factor by 1. This calculation is only valid for low atomic number and small photon energies. The result of this calculation is to multiply (96) by the factor $f(\xi)$, where

$$f(\xi) = 2\pi \left(\frac{I}{E}\right)^{1/2} \frac{e^{-4E \arccot \xi}}{1 - e^{-2\pi\xi}} \quad (98)$$

and

$$\xi = \left(\frac{I}{E-1}\right)^{1/2} = \frac{Z\alpha c}{v} \quad (99)$$

where v the velocity of the electron far from the nucleus in the final state.

A relativistic calculation has been made by Sauter

(Sauter, 31). In this paper use has been made of the Born approximation, and $(Z\alpha)^2$ has been neglected where it appears in the parameters of the Dirac wave function. This calculation is therefore valid only for low Z and for final electron energies large compared to I . The result may be expressed by

$$\sigma = \sigma_0 \frac{3Z^5\alpha^4}{4} \left(\frac{mc^2}{E} \right)^5 (\gamma^2 - 1)^{1/2} \left[\frac{4}{3} + \frac{\gamma(\gamma-2)}{\gamma+1} \left(1 - \frac{1}{2\gamma\sqrt{\gamma^2-1}} \log \frac{\gamma + \sqrt{\gamma^2-1}}{\gamma - \sqrt{\gamma^2-1}} \right) \right] \quad (100)$$

where

$$\gamma = \left(1 - \frac{v^2}{c^2} \right)^{-1/2} \quad (101)$$

A relativistic calculation by Hall (Hall, 36) uses an approximation for the final electron wave function which is superior to the Born approximation. Unlike the relativistic Born approximation this approximation does not require that Z be small. This calculation also retains the αZ terms in the bound state wave functions and is valid for all atomic numbers, but only for photon energies such that $E \gg mc^2$. This restriction is probably too strong, since Hall's formula appears to agree fairly well with experiment even in the region $E \sim mc^2$. His formula may be expressed

$$\sigma = \sigma_0 \frac{3}{2} Z^5 \alpha^4 \frac{mc^2}{E} R e^{-\pi Z\alpha + 2(Z\alpha)^2(1 - \log Z\alpha)} \quad (102)$$

where

$$R = 1 + \left[4(1 - Z^2 \alpha^2)^{1/2} - \frac{5}{3} \right] \frac{mc^2}{E} \quad (103)$$

Another relativistic calculation by Hulme and his coworkers (Hulme, 35), consists in expanding into multipoles, calculating the matrix elements including retardation for each multipole making a significant contribution to the cross-section, and adding them together. For large photon energies the multipole expansion does not converge very rapidly, and this makes a great amount of numerical work necessary, which becomes overwhelming for very large photon energies. The exact, unscreened Coulomb relativistic wave functions are used throughout. The calculation has been made for three values of atomic number ($Z = 26, 50, 84$) and for two photon energies at each atom. ($E = .354$ Mev and 1.13 Mev). The effects of screening have been included only to the extent that the potential has been changed by an additive constant to make the binding energies agree with experiment. Combining these numerical values with Sauter's formula (100) for $Z = 0$ and Hall's formula (102) for all Z and very high photon energies, complete curves for all Z may be obtained by interpolation. These results apply to all energies which are larger than the lower limit of the numerical calculation ($.354$ Mev).

In the compilation of the points of the cross-section curve, Miss White (White, 54) used the formula of Hall (102) for the high energy portion of the curve.

In the intermediate region she used the numerical calculation of Hulme, et al. For the lowest energy points, she has used the formula of Sauter (100) multiplied by the function $f(\xi)$ of Stobbe (98). The justification for this mixing of relativistic and non-relativistic formulae is essentially experimental (Segre, 52). The results of her computation are given in Table X and are shown in Figure 5. Segre's book also contains a summary of photo-effect calculations and useful curves of $f(\xi)$ and of Sauter's formula. The principle uncertainties in this curve are unfortunately in the low energy region, where the contribution to the integrated cross-section is greatest. It is very difficult at present to estimate the theoretical validity of the formula used for computing this part of the curve. It is in this region that the effects of screening would be most pronounced, and the experimental agreement which justified the use of the Sauter-Stobbe formula, was obtained with almost neutral lead atoms where the shielding is present. It is thus difficult to justify the use of this formula for a highly ionized atom.

The integrated photo-electric cross-section was obtained by numerical integration of this curve, beginning at 100 kev (the theoretical binding energy of an unscreened K electron in lead is 101.7 kev). To this integral was added the integrated cross-section (93) due to discrete transitions. The results of this integration are given in Table XI, where we give values of

TABLE X

PHOTO-ELECTRIC CROSS-SECTION FOR LEAD

Energy (Mev)	Cross- Section (Barns)	Energy (Mev)	Cross- Section (Barns)
<u>.088</u>	<u>1098</u>	<u>3.0</u>	<u>.518</u>
.100	788	4.0	.364
.150	266	5.0	.280
.200	121	6.0	.228
.30	41.4	8.0	.166
.40	20.0	10	.130
.50	11.8	15	.0849
.60	7.73	20	.0628
.80	4.17	30	.0413
1.00	2.73	40	.0308
1.5	1.35	50	.0246
2.0	.890		

These are the results of Miss White's computations as discussed in the text.

Figure 5. The photo-electric cross-section for an ion of lead Pb^{81} . The points are the theoretical computations of Miss White.

TABLE XI

INTEGRATED PHOTO-ELECTRIC CROSS-SECTION

W (Mev)	$\int_{.100}^W \sigma dE$ (Mev-Barns)	$\int_0^W \sigma dE$ (Mev-Barns)
.100	-	51.6
.200	32.17	83.59
.400	42.18	93.60
.700	45.28	96.70
1.00	46.41	98.56
2.0	47.89	99.31
4.0	48.98	100.4
7.0	49.75	101.2
10.0	50.12	101.5
16.0	50.72	102.1
20.0	51.00	102.4
50.0	52.13	103.5

$$\int_{.100}^W \sigma(E) dE \quad (104)$$

and

$$\int_0^W \sigma(E) dE = \int_{.100}^W \sigma(E) dE + \sum_{n=2}^{\infty} \sigma(1S \rightarrow nP) \quad (105)$$

for several values of W . Figure VI shows graphically the integrated cross-section (105).

If we take the limit of Hall's formula as E grows very large, which may be done by ignoring the term with E^{-1} in R , it would appear that the cross-section has an E^{-1} dependence at large E . If this dependence is correct, the integrated cross-section does not converge. There is considerable theoretical uncertainty concerning this divergence, and we resort to the simple expedient of stopping the integration at some arbitrary upper limit. The numbers of Table XI indicate that the integrated cross-section is insensitive to the choice of this upper limit, so long as it is greater than a few Mev.

It is in just this region of energy that effects other than photo-electric absorption begins to dominate the absorption cross-section. Of these, the most important is the process of pair production, which begins at a threshold of 1.02 Mev and increases rapidly with increasing energy. For an element of high atomic number, the absorption due to pair formation predominates at all energies greater than 4 or 5 Mev. This rapid increase of cross-section with energy is correct to energies of

Figure 6. Integrated relativistic photo-electric cross-section.

300 Mev by actual experimental verification, and if we utilize the evidence of the order of magnitude agreement of cascade theory with phenomena of cosmic ray showers, it appears valid at the highest energies known. There is no evidence that the integrated total cross-section (including pair production) converges.

Since the process of pair production completely masks the small photo-electric cross-section experimentally, we are at least experimentally justified in resorting to choosing an upper limit in the integration of σ . The convergence of the integrated cross-section predicted by the theory of Gell-Mann et al (Gell-Mann, 54) requires the use of a similar cut-off in the energy region where extreme relativistic effects such as pair production become predominant. With our choice of upper limit, or any other reasonable choice, we observe a fairly close but somewhat uncertain numerical agreement between the relativistic and non-relativistic integrated photo-electric cross-sections. For a summed non-relativistic dipole oscillator strength of unity, the expected integrated cross-section is

$$\int_0^{\infty} \sigma(E) dE = 109.7 \text{ Mev-Barns} \quad \text{N.R.} \quad (104)$$

The relativistic result is

$$\int_0^{50} \sigma(E) dE = 103.5 \text{ Mev-Barns} \quad (105)$$

as shown in Table IX, Retardation for Discrete Transitions, would reduce (105) by at least 4 per cent and probably not more than 15 percent. The inclusion of quadrupole and higher multipole orders for discrete transitions would increase it slightly, probably not more than 3 per cent. One other principle uncertainty is caused by lack of knowledge of the accuracy of the cross-section calculations at energies close to the K series limit when applied to this atomic model. Other equally reasonable choices of cross-section calculations (Davisson, 52) might be made which would result in changes of about 10 per cent in this region of energy.

The theoretical reasoning of Gell-Mann et al (Gell-Mann, 54) would require that (104) and (105) be identical. It is difficult to estimate at present whether further refinements of these preliminary calculations would improve the numerical agreement.

APPENDIX A

The formalism and notation of the Dirac equation for relativistic wave mechanics used throughout this work follows with minor exceptions, that of Sections 7 and 9 of Bethe's article in the Handbuch der Physik (Bethe, 33). Reference will be made in this Appendix to specific equations from that work. Equations in this section will be numbered sequentially, followed by the number of the most nearly equivalent equation in Bethe's article.

The exact form of the wave equation used is

$$\left[E + e\phi + \beta E_0 \right] \psi + \sum_{k=1}^3 \alpha_k (c p_k + e A_k) \psi = 0 \quad \begin{matrix} (106) \\ (7.1) \end{matrix}$$

In this equation E is the total energy including the rest energy E_0 , ϕ is the scalar potential, A_k the k 'th component of the vector potential, p_k is the momentum operator, $p_k = -i\hbar \frac{\partial}{\partial x_k}$, and α_k and β are the Dirac matrices. These quantities are 4×4 matrices, and, as is customary, we choose a representation in which β is diagonal. The index k represents a set of Cartesian axes and 1, 2, 3 may also be x, y, z . The explicit form of these matrices is

$$\alpha_x = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \quad \alpha_y = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \alpha_z = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \quad \beta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \quad (107)$$

The function ψ is a 4 component Spinor (Bade, 53) and may be written

$$\psi = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} \quad (108)$$

where the u 's are functions of position, time and momentum (or energy). The operation of a matrix on a spinor, where the matrix must operate to the right, results in another spinor, whose components are given by

$$(\alpha_i \psi)_\rho = \sum_{\sigma=1}^4 (\alpha_i)_{\rho\sigma} \psi_\sigma \quad \rho = 1 \dots 4 \quad (109)$$

ρ being the matrix row index and σ the column index. The asterisk, applied to a spinor means Hermitean conjugate, i. e.

$$\psi^* = \left(\begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} \right)^* = (u_1^*, u_2^*, u_3^*, u_4^*) \quad (110)$$

where the asterisk applied to a function u means simply complex conjugation. The rule for multiplication of a conjugate spinor with a spinor is

$$\psi_a^* \psi_b = \sum_{j=1}^4 u_{aj}^* u_{bj} \quad (111)$$

The quantities $\alpha \psi^*$ and $\psi \psi^*$ are undefined.

For our purposes we desire those solutions of equation (106) which represent a single electron moving in a Coulomb potential about a fixed point nucleus. This implies in (106) that $\phi = \frac{ze}{r}$ and each $A_k = 0$. This problem is solved exactly in Bethe's article, and we omit the details here. For convenience in tabulating the

functions several parameters are introduced. The functions may be tabulated in terms of four quantum numbers: The principle quantum number n , the orbital angular momentum quantum number ℓ , the total angular momentum quantum number j , and the magnetic quantum number m , representing the Z component of the total angular momentum. Other auxiliary parameters are defined in terms of these and the atomic number Z .

We find two distinct types of wave function, depending on the relation between ℓ and j . We shall refer to them as Type A, in which $j = \ell + \frac{1}{2}$ and type B, in which $j = \ell - \frac{1}{2}$. The components for type A wave functions are given in terms of ℓ and m and the radial wave functions f and g by

$$u_1 = \left(\frac{\ell - m + 3/2}{2\ell + 5} \right)^{1/2} i f(r) Y_{\ell+1, m-1/2} \quad (9.4)$$

$$u_2 = \left(\frac{\ell + m + 3/2}{2\ell + 3} \right)^{1/2} i f(r) Y_{\ell+1, m+1/2}$$

$$u_3 = \left(\frac{\ell - m + 1/2}{2\ell + 1} \right)^{1/2} g(r) Y_{\ell, m-1/2} \quad (112)$$

$$u_4 = - \left(\frac{\ell + m + 1/2}{2\ell + 1} \right)^{1/2} g(r) Y_{\ell, m+1/2} \quad (9.3)$$

For type B wave functions they are

$$u_1 = \left(\frac{\ell + m - 1/2}{2\ell - 1} \right)^{1/2} i f(r) Y_{\ell-1, m-1/2}$$

$$u_2 = - \left(\frac{\ell - m - 1/2}{2\ell - 1} \right)^{1/2} i f(r) Y_{\ell-1, m+1/2} \quad (113)$$

$$u_3 = \left(\frac{\ell - m + 1/2}{2\ell + 1} \right)^{1/2} g(r) Y_{\ell, m-1/2} \quad (9.7)$$

$$u_4 = \left(\frac{\ell + m + 1/2}{2\ell + 1} \right)^{1/2} g(r) Y_{\ell, m+1/2}$$

There are no type B wave functions for $\ell = 0$. The Y's appearing are, as usual, spherical harmonics (Bethe, 33, p 275) and f and g will be defined later.

The nomenclature throughout this work will be as follows. An electronic state requires four quantum numbers for its description. A component of a spectral line results from transitions between two states. All states which have the principal quantum number n in common will be considered to make up a shell, and the sub-shells will be divided on the basis of orbital angular momentum and the levels within a shell will be divided on the basis of total angular momentum. An X-ray line results from transitions between two levels. A level will be described by three quantum numbers, as nlj , for example the $2P_{3/2}$ level where $n = 2$, $\ell = 1$, $j = 3/2$. The usual spectroscopic designation for orbital angular momentum, i.e. S, P, D, F, ... for $\ell = 0, 1, 2, 3 \dots$ will be used. X-ray lines will be designated following Compton and Allison (Compton, 35, p 630) with the exception that we shall distinguish the two lines which make up their $K\beta_2$ by using a prime to designate the higher energy line. (See Table V of Chapter II). We shall also follow Compton and Allison in designation of the shells, i.e. K, L, M, and N for $n = 1, 2, 3, 4$.

Since the transition probabilities to the K shell become smaller rapidly as n increases, we shall content ourselves with calculation of the wave functions for the first

four shells only. The parameters required for them are given in Table XII. We shall tabulate in Plates IA through VIA the radial eigenfunctions f and g for all levels of the first four shells. The functions are given in terms of the parameter $\rho = 2Zra_0^{-1}$ where a_0 is the first Bohr orbit for hydrogen and Z is the atomic number. We have used the symbol α with no subscript or vector sign to represent the fine structure constant $\alpha = \frac{e^2}{\hbar c}$. This should not be confused with the Dirac matrices which invariably have subscripts or vector signs.

The radial wave functions are given by

$$f(\rho) = - \frac{\sqrt{\Gamma(2\gamma+n'+1)}}{\Gamma(2\gamma+1)\sqrt{n'}} \sqrt{\frac{1-\epsilon}{4N(N-\kappa)}} \left(\frac{2Z}{Na_0}\right)^{3/2} \left(\frac{\rho}{N}\right)^{\gamma-1} \\ \left[-n' F(-n'+1, 2\gamma+1, \rho) + (N-\kappa) F(-n', 2\gamma+1, \rho) \right] \quad (114)$$

$$g(\rho) = \frac{\sqrt{\Gamma(2\gamma+n'+1)}}{\Gamma(2\gamma+1)\sqrt{n'}} \sqrt{\frac{1+\epsilon}{4N(N-\kappa)}} \left(\frac{2Z}{Na_0}\right)^{3/2} \left(\frac{\rho}{N}\right)^{\gamma-1} \\ \left[-n' F(-n'+1, 2\gamma+1, \rho) + (N-\kappa) F(-n', 2\gamma+1, \rho) \right] \quad (115)$$

The symbol Γ appearing designates the usual Γ function (Jahnke, 45, p 14) and the F designates the confluent hypergeometric function (Jahnke, 45, p 275). For n' a positive integer or zero, which is true in our case, these functions are polynomials in ρ . In the tabulation presented the terms in the brackets have been collected in powers of ρ and written then as a single polynomial. In addition we have used the identity

TABLE XII

THE PARAMETERS APPEARING IN THE DIRAC RADIAL EIGEN-
FUNCTIONS

The symbol designating the parameter, the name where applicable, and the equation defining it are given. The numbers of the equations are from Bethe's Handbuch article.

ϵ : The energy of a level in units of mc^2

$$\epsilon = \left[1 - \left(\frac{\alpha Z}{N} \right)^2 \right]^{1/2} \quad (9.34)$$

N : The apparent principal quantum number

$$N = \left[n^2 - 2n'(k-\gamma) \right]^{1/2} \quad (9.35)$$

n' : The radial quantum number

$$n' = n - k \quad (9.28)$$

κ :

$$\begin{aligned} \kappa &= -(j + 1/2), \quad j = l + 1/2 \\ &= (j + 1/2), \quad j = l - 1/2 \end{aligned} \quad (9.9)$$

k :

$$k = |\kappa| = j + 1/2 \quad (9.28)$$

γ :

$$\gamma = \left[k^2 - (\alpha Z)^2 \right]^{1/2} \quad (9.22)$$

$1S_{1/2}$; $n=1, l=0, j=1/2, u=-1, k=1, n'=0, N=N_1, \gamma=\gamma_1, \epsilon=\epsilon_1$, TYPE A

$$f(\rho) = -\left(\frac{2z}{N_1 a_0}\right)^{3/2} \frac{1}{\sqrt{\Gamma(2\gamma_1+1)}} \sqrt{\frac{1-\epsilon_1}{4N_1(N_1+1)}} e^{-\rho/2N_1} \left(\frac{\rho}{N_1}\right)^{\gamma_1-1} [N_1+1]$$

$$g(\rho) = \left(\frac{2z}{N_1 a_0}\right)^{3/2} \frac{1}{\sqrt{\Gamma(2\gamma_1+1)}} \sqrt{\frac{1+\epsilon_1}{4N_1(N_1+1)}} e^{-\rho/2N_1} \left(\frac{\rho}{N_1}\right)^{\gamma_1-1} [N_1+1]$$

$2S_{1/2}$; $n=2, l=0, j=1/2, u=-1, k=1, n'=1, N=N_2, \gamma=\gamma_1, \epsilon=\epsilon_2$ TYPE A

$$f(\rho) = -\left(\frac{2z}{N_2 a_0}\right)^{3/2} \frac{\sqrt{2\gamma_1+1}}{\sqrt{\Gamma(2\gamma_1+1)}} \sqrt{\frac{1-\epsilon_2}{4N_2(N_2+1)}} e^{-\rho/2N_2} \left(\frac{\rho}{N_2}\right)^{\gamma_1-1} \left[N_2+2 - \frac{(N_2+1)}{2\gamma_1+1} \frac{\rho}{N_2} \right]$$

$$g(\rho) = \left(\frac{2z}{N_2 a_0}\right)^{3/2} \frac{\sqrt{2\gamma_1+1}}{\sqrt{\Gamma(2\gamma_1+1)}} \sqrt{\frac{1+\epsilon_2}{4N_2(N_2+1)}} e^{-\rho/2N_2} \left(\frac{\rho}{N_2}\right)^{\gamma_1-1} \left[N_2 - \frac{(N_2+1)}{(2\gamma_1+1)} \frac{\rho}{N_2} \right]$$

$2P_{1/2}$; $n=2, l=1, j=1/2, u=1, k=1, n'=1, N=N_3, \gamma=\gamma_1, \epsilon=\epsilon_3$, TYPE B

$$f(\rho) = -\left(\frac{2z}{N_2 a_0}\right)^{3/2} \frac{\sqrt{2\gamma_1+1}}{\sqrt{\Gamma(2\gamma_1+1)}} \sqrt{\frac{1-\epsilon_2}{4N_2(N_2-1)}} e^{-\rho/2N_2} \left(\frac{\rho}{N_2}\right)^{\gamma_1-1} \left[N_2 - \frac{(N_2-1)}{(2\gamma_1+1)} \frac{\rho}{N_2} \right]$$

$$g(\rho) = \left(\frac{2z}{N_2 a_0}\right)^{3/2} \frac{\sqrt{2\gamma_1+1}}{\sqrt{\Gamma(2\gamma_1+1)}} \sqrt{\frac{1+\epsilon_2}{4N_2(N_2-1)}} e^{-\rho/2N_2} \left(\frac{\rho}{N_2}\right)^{\gamma_1-1} \left[N_2-2 - \frac{(N_2-1)}{(2\gamma_1+1)} \frac{\rho}{N_2} \right]$$

$2P_{3/2}; n=2, l=1, j=3/2; \kappa=-2, k=2, n'=0, N=N_3, \gamma=\gamma_2, \epsilon=\epsilon_3$ TYPE A

$$f(\rho) = -\left(\frac{2z}{N_3 a_0}\right)^{3/2} \frac{1}{\sqrt{\Gamma(2\gamma_2+1)}} \sqrt{\frac{1-\epsilon_3}{4N_3(N_3+2)}} \rho^{-1/2N_3} \left(\frac{\rho}{N_3}\right)^{\gamma_2-1} [N_3+2]$$

$$g(\rho) = \left(\frac{2z}{N_3 a_0}\right)^{3/2} \frac{1}{\sqrt{\Gamma(2\gamma_2+1)}} \sqrt{\frac{1+\epsilon_3}{4N_3(N_3+2)}} \rho^{-1/2N_3} \left(\frac{\rho}{N_3}\right)^{\gamma_2-1} [N_3+2]$$

$3S_{1/2}; n=3, l=0, j=1/2; \kappa=-1, k=1, n'=2, N=N_4, \gamma=\gamma_1, \epsilon=\epsilon_4$ TYPE A

$$f(\rho) = -\left(\frac{2z}{N_4 a_0}\right)^{3/2} \frac{\sqrt{(2\gamma_1+1)(2\gamma_1+2)}}{\sqrt{\Gamma(2\gamma_1+1)} \sqrt{2}} \sqrt{\frac{1-\epsilon_4}{4N_4(N_4+1)}} \rho^{1/2N_4} \left(\frac{\rho}{N_4}\right)^{\gamma_1-1} \left[N_4+3 - \frac{2\rho}{N_4} \left(\frac{N_4+2}{2\gamma_1+1} \right) + \frac{\rho^2}{N_4^2} \frac{N_4+1}{(2\gamma_1+1)(2\gamma_1+2)} \right]$$

$$g(\rho) = \left(\frac{2z}{N_4 a_0}\right)^{3/2} \frac{\sqrt{(2\gamma_1+1)(2\gamma_1+2)}}{\sqrt{\Gamma(2\gamma_1+1)} \sqrt{2}} \sqrt{\frac{1+\epsilon_4}{4N_4(N_4+1)}} \rho^{1/2N_4} \left(\frac{\rho}{N_4}\right)^{\gamma_1-1} \left[N_4-1 - \frac{2\rho}{N_4} \left(\frac{N_4}{2\gamma_1+1} \right) + \frac{\rho^2}{N_4^2} \frac{N_4+1}{(2\gamma_1+1)(2\gamma_1+2)} \right]$$

$3P_{1/2}; n=3, l=1, j=1/2; \kappa=1, k=1, n'=2, N=N_4, \gamma=\gamma_1, \epsilon=\epsilon_4$ TYPE B

$$f(\rho) = -\left(\frac{2z}{N_4 a_0}\right)^{3/2} \frac{\sqrt{(2\gamma_1+1)(2\gamma_1+2)}}{\sqrt{\Gamma(2\gamma_1+1)} \sqrt{2}} \sqrt{\frac{1-\epsilon_4}{4N_4(N_4-1)}} \rho^{1/2N_4} \left(\frac{\rho}{N_4}\right)^{\gamma_1-1} \left[N_4+1 - \frac{2\rho}{N_4} \left(\frac{N_4}{2\gamma_1+1} \right) + \frac{\rho^2}{N_4^2} \frac{N_4-1}{(2\gamma_1+1)(2\gamma_1+2)} \right]$$

$$g(\rho) = \left(\frac{2z}{N_4 a_0}\right)^{3/2} \frac{\sqrt{(2\gamma_1+1)(2\gamma_1+2)}}{\sqrt{\Gamma(2\gamma_1+1)} \sqrt{2}} \sqrt{\frac{1+\epsilon_4}{4N_4(N_4-1)}} \rho^{1/2N_4} \left(\frac{\rho}{N_4}\right)^{\gamma_1-1} \left[N_4-3 - \frac{2\rho}{N_4} \left(\frac{N_4-1}{2\gamma_1+1} \right) + \frac{\rho^2}{N_4^2} \frac{N_4-1}{(2\gamma_1+1)(2\gamma_1+2)} \right]$$

$3P_{3/2}$; $\kappa=3, l=1, j=3/2, \kappa=-2, k=2, \kappa'=1, N=N_5, Y=Y_2, \epsilon=\epsilon_5$ TYPE A

$$f(\rho) = -\left(\frac{2Z}{N_5 a_0}\right)^{3/2} \frac{\sqrt{2Y_2+1}}{\Gamma(2Y_2+1)} \sqrt{\frac{1-\epsilon_5}{4N_5(N_5+2)}} e^{-\rho/2N_5} \left(\frac{\rho}{N_5}\right)^{Y_2-1} \left[N_5+3 - \frac{N_5+2}{2Y_2+1} \frac{\rho}{N_5}\right]$$

$$g(\rho) = \left(\frac{2Z}{N_5 a_0}\right)^{3/2} \frac{\sqrt{2Y_2+1}}{\Gamma(2Y_2+1)} \sqrt{\frac{1+\epsilon_5}{4N_5(N_5+2)}} e^{-\rho/2N_5} \left(\frac{\rho}{N_5}\right)^{Y_2-1} \left[N_5+1 - \frac{N_5+2}{2Y_2+1} \frac{\rho}{N_5}\right]$$

$3D_{3/2}$; $\kappa=3, l=2, j=3/2, \kappa=2, k=2, \kappa'=1, N=N_5, Y=Y_2, \epsilon=\epsilon_5$ TYPE B

$$f(\rho) = -\left(\frac{2Z}{N_5 a_0}\right)^{3/2} \frac{\sqrt{2Y_2+1}}{\Gamma(2Y_2+1)} \sqrt{\frac{1-\epsilon_5}{4N_5(N_5-2)}} e^{-\rho/2N_5} \left(\frac{\rho}{N_5}\right)^{Y_2-1} \left[N_5-1 - \frac{N_5-2}{2Y_2+1} \frac{\rho}{N_5}\right]$$

$$g(\rho) = \left(\frac{2Z}{N_5 a_0}\right)^{3/2} \frac{\sqrt{2Y_2+1}}{\Gamma(2Y_2+1)} \sqrt{\frac{1+\epsilon_5}{4N_5(N_5-2)}} e^{-\rho/2N_5} \left(\frac{\rho}{N_5}\right)^{Y_2-1} \left[N_5-3 - \frac{N_5-2}{2Y_2+1} \frac{\rho}{N_5}\right]$$

$3D_{5/2}$; $\kappa=3, l=2, j=5/2, \kappa=-3, k=3, \kappa'=0, N=N_6, Y=Y_3, \epsilon=\epsilon_6$ TYPE A

$$f(\rho) = -\left(\frac{2Z}{N_6 a_0}\right)^{3/2} \frac{1}{\Gamma(2Y_3+1)} \sqrt{\frac{1-\epsilon_6}{4N_6(N_6+3)}} e^{-\rho/2N_6} \left(\frac{\rho}{N_6}\right)^{Y_3-1} [N_6+3]$$

$$g(\rho) = \left(\frac{2Z}{N_6 a_0}\right)^{3/2} \frac{1}{\Gamma(2Y_3+1)} \sqrt{\frac{1+\epsilon_6}{4N_6(N_6+3)}} e^{-\rho/2N_6} \left(\frac{\rho}{N_6}\right)^{Y_3-1} [N_6+3]$$

$4S_{1/2}$; $n=4$, $l=0$, $j=1/2$, $u=-1$, $k=1$, $n'=3$, $N=N_1$, $\gamma=\gamma_1$, $\epsilon=\epsilon_1$ TYPE A

$$f(\rho) = - \left(\frac{2z}{N_1 a_0} \right)^{3/2} \frac{\sqrt{(2\gamma_1+1)(2\gamma_1+2)(2\gamma_1+3)}}{\sqrt{\Gamma(2\gamma_1+1)} \sqrt{6}} e^{-\rho/2N_1} \left(\frac{\rho}{N_1} \right)^{\gamma_1-1} \sqrt{\frac{1-\epsilon_1}{4N_1(N_1+1)}} \\ \left[N_1+4 - \frac{3\rho}{N_1} \left(\frac{N_1+3}{2\gamma_1+1} \right) + \frac{3\rho^2}{N_1^2} \frac{N_1+2}{(2\gamma_1+1)(2\gamma_1+2)} - \frac{\rho^3}{N_1^3} \frac{N_1+1}{(2\gamma_1+1)(2\gamma_1+2)(2\gamma_1+3)} \right]$$

$$g(\rho) = \left(\frac{2z}{N_1 a_0} \right)^{3/2} \frac{\sqrt{(2\gamma_1+1)(2\gamma_1+2)(2\gamma_1+3)}}{\sqrt{\Gamma(2\gamma_1+1)} \sqrt{6}} e^{-\rho/2N_1} \left(\frac{\rho}{N_1} \right)^{\gamma_1-1} \sqrt{\frac{1+\epsilon_1}{4N_1(N_1+1)}} \\ \left[N_1-2 - \frac{3\rho}{N_1} \left(\frac{N_1-1}{2\gamma_1+1} \right) + \frac{3\rho^2}{N_1^2} \frac{N_1}{(2\gamma_1+1)(2\gamma_1+2)} - \frac{\rho^3}{N_1^3} \frac{N_1+1}{(2\gamma_1+1)(2\gamma_1+2)(2\gamma_1+3)} \right]$$

$4P_{1/2}$; $n=4$, $l=1$, $j=1/2$, $u=1$, $k=1$, $n'=3$, $N=N_1$, $\gamma=\gamma_1$, $\epsilon=\epsilon_1$ TYPE B

$$f(\rho) = - \left(\frac{2z}{N_1 a_0} \right)^{3/2} \frac{\sqrt{(2\gamma_1+1)(2\gamma_1+2)(2\gamma_1+3)}}{\sqrt{\Gamma(2\gamma_1+1)} \sqrt{6}} e^{-\rho/2N_1} \left(\frac{\rho}{N_1} \right)^{\gamma_1-1} \sqrt{\frac{1-\epsilon_1}{4N_1(N_1-1)}}$$

$$\left[N_1+2 - \frac{3\rho}{N_1} \left(\frac{N_1+1}{2\gamma_1+1} \right) + \frac{3\rho^2}{N_1^2} \frac{N_1}{(2\gamma_1+1)(2\gamma_1+2)} - \frac{\rho^3}{N_1^3} \frac{N_1-1}{(2\gamma_1+1)(2\gamma_1+2)(2\gamma_1+3)} \right]$$

$4P_{1/2}$; CONTINUED

$$g(\rho) = \left(\frac{2z}{N_1 a_0} \right)^{3/2} \frac{\sqrt{(2x_1+1)(2x_1+2)(2x_1+3)}}{\sqrt{\Gamma(2x_1+1)} \sqrt{2}} e^{-\rho/2 N_1 \left(\frac{\rho}{N_1} \right)^{x_1-1}} \sqrt{\frac{1+\epsilon_1}{4N_1(N_1-1)}}$$

$$\left[N_1 - 4 - \frac{3\rho}{N_1} \left(\frac{N_1-3}{2x_1+1} \right) + \frac{3\rho^2}{N_1^2} \left(\frac{N_1-2}{(2x_1+1)(2x_1+2)} \right) - \frac{\rho^3}{N_1^3} \frac{N_1-1}{(2x_1+1)(2x_1+2)(2x_1+3)} \right]$$

$4P_{3/2}$, $n=4$, $l=1$, $j=3/2$, $n=-2$, $k=2$, $n'=2$, $N=N_1$, $x=x_2$, $\epsilon=\epsilon_1$ TYPE A

$$f(\rho) = - \left(\frac{2z}{N_1 a_0} \right)^{3/2} \frac{\sqrt{(2x_2+1)(2x_2+2)}}{\sqrt{\Gamma(2x_2+1)} \sqrt{2}} e^{-\rho/2 N_1 \left(\frac{\rho}{N_1} \right)^{x_2-1}} \sqrt{\frac{1-\epsilon_1}{4N_1(N_1+2)}} \left[N_1 + 4 - \frac{2\rho}{N_1} \left(\frac{N_1+3}{2x_2+1} \right) + \frac{\rho^2}{N_1^2} \frac{N_1+2}{(2x_2+1)(2x_2+2)} \right]$$

$$g(\rho) = \left(\frac{2z}{N_1 a_0} \right)^{3/2} \frac{\sqrt{(2x_2+1)(2x_2+2)}}{\sqrt{\Gamma(2x_2+1)} \sqrt{2}} e^{-\rho/2 N_1 \left(\frac{\rho}{N_1} \right)^{x_2-1}} \sqrt{\frac{1+\epsilon_1}{4N_1(N_1+2)}} \left[N_1 - \frac{2\rho}{N_1} \left(\frac{N_1+1}{2x_2+1} \right) + \frac{\rho^2}{N_1^2} \frac{N_1+2}{(2x_2+1)(2x_2+2)} \right]$$

$4D_{3/2}$; $n=4$, $l=2$, $j=3/2$, $n=2$, $k=2$, $n'=2$, $N=N_1$, $x=x_2$, $\epsilon=\epsilon_1$ TYPE B

$$f(\rho) = - \left(\frac{2z}{N_1 a_0} \right)^{3/2} \frac{\sqrt{(2x_2+1)(2x_2+2)}}{\sqrt{\Gamma(2x_2+1)} \sqrt{2}} e^{-\rho/2 N_1 \left(\frac{\rho}{N_1} \right)^{x_2-1}} \sqrt{\frac{1-\epsilon_1}{4N_1(N_1-2)}} \left[N_1 - \frac{2\rho}{N_1} \left(\frac{N_1-1}{2x_2+1} \right) + \frac{\rho^2}{N_1^2} \frac{N_1-2}{(2x_2+1)(2x_2+2)} \right]$$

$$g(\rho) = \left(\frac{2z}{N_1 a_0} \right)^{3/2} \frac{\sqrt{(2x_2+1)(2x_2+2)}}{\sqrt{\Gamma(2x_2+1)} \sqrt{2}} e^{-\rho/2 N_1 \left(\frac{\rho}{N_1} \right)^{x_2-1}} \sqrt{\frac{1+\epsilon_1}{4N_1(N_1-2)}} \left[N_1 - 4 - \frac{2\rho}{N_1} \left(\frac{N_1-3}{2x_2+1} \right) + \frac{\rho^2}{N_1^2} \frac{N_1-2}{(2x_2+1)(2x_2+2)} \right]$$

$4D_{5/2}; \kappa=4, \ell=2, j=5/2, \kappa=-3, k=3, \kappa'=1, N=N_1, \gamma=\gamma_3, \epsilon=\epsilon_1, \text{ TYPE A}$

$$f(\rho) = -\left(\frac{2z}{N_1 a_0}\right)^{3/2} \frac{\sqrt{2\gamma_3+1}}{\Gamma(2\gamma_3+1)} \sqrt{\frac{1-\epsilon_1}{4N_1(N_1+3)}} e^{-\rho/2N_1} \left(\frac{\rho}{N_1}\right)^{\gamma_3-1} \left[N_1+4 - \frac{\rho}{N_1} \left(\frac{N_1+3}{2\gamma_3+1}\right)\right]$$

$$g(\rho) = \left(\frac{2z}{N_1 a_0}\right)^{3/2} \frac{\sqrt{2\gamma_3+1}}{\Gamma(2\gamma_3+1)} \sqrt{\frac{1+\epsilon_1}{4N_1(N_1+3)}} e^{-\rho/2N_1} \left(\frac{\rho}{N_1}\right)^{\gamma_3-1} \left[N_1+2 - \frac{\rho}{N_1} \left(\frac{N_1+3}{2\gamma_3+1}\right)\right]$$

$4F_{5/2}; \kappa=4, \ell=3, j=5/2, \kappa=3, k=3, \kappa'=1, N=N_1, \gamma=\gamma_3, \epsilon=\epsilon_1, \text{ TYPE B}$

$$f(\rho) = -\left(\frac{2z}{N_1 a_0}\right)^{3/2} \frac{\sqrt{2\gamma_3+1}}{\Gamma(2\gamma_3+1)} \sqrt{\frac{1-\epsilon_1}{4N_1(N_1-3)}} e^{-\rho/2N_1} \left(\frac{\rho}{N_1}\right)^{\gamma_3-1} \left[N_1-2 - \frac{\rho}{N_1} \left(\frac{N_1-3}{2\gamma_3+1}\right)\right]$$

$$g(\rho) = \left(\frac{2z}{N_1 a_0}\right)^{3/2} \frac{\sqrt{2\gamma_3+1}}{\Gamma(2\gamma_3+1)} \sqrt{\frac{1+\epsilon_1}{4N_1(N_1-3)}} e^{-\rho/2N_1} \left(\frac{\rho}{N_1}\right)^{\gamma_3-1} \left[N_1-4 - \frac{\rho}{N_1} \left(\frac{N_1-3}{2\gamma_3+1}\right)\right]$$

$4F_{7/2}; \kappa=4, \ell=3, j=7/2, \kappa=-4, k=4, \kappa'=0, N=N_{10}, \gamma=\gamma_4, \epsilon=\epsilon_{10}, \text{ TYPE A}$

$$f(\rho) = -\left(\frac{2z}{N_{10} a_0}\right)^{3/2} \frac{1}{\Gamma(2\gamma_4+1)} \sqrt{\frac{1-\epsilon_{10}}{4N_{10}(N_{10}+4)}} e^{-\rho/2N_{10}} \left(\frac{\rho}{N_{10}}\right)^{\gamma_4-1} [N_{10}+4]$$

$$g(\rho) = \left(\frac{2z}{N_{10} a_0}\right)^{3/2} \frac{1}{\Gamma(2\gamma_4+1)} \sqrt{\frac{1+\epsilon_{10}}{4N_{10}(N_{10}+4)}} e^{-\rho/2N_{10}} \left(\frac{\rho}{N_{10}}\right)^{\gamma_4-1} [N_{10}+4]$$

$$\Gamma(x+1) = x \Gamma(x) \quad (116)$$

to reduce the number of Γ functions appearing in (114) and (115) to one.

Since ϵ is a number close to one and somewhat smaller than one, it is clear that f is much smaller than g . We follow Bethe and call those components of the wave function containing f the small components, and those containing g the large components. In the limit as $\alpha z \rightarrow 0$, the functions $g(r)$ must approach the non-relativistic radial wave functions. The tabulated functions have been checked in this manner against the equations (3.18) in Bethe.

The complete wave functions are obtained by combining the tabulated wave functions with whichever of equations (112) or (113) applies. For tabulating the wave functions of the first four shells we need four different parameters γ . We denote them by subscripts. Since

$$\gamma = \sqrt{k^2 - (\alpha z)^2} \quad \begin{matrix} (117) \\ (9.22) \end{matrix}$$

and

$$k = j + 1/2 \quad \begin{matrix} (118) \\ (9.28) \end{matrix}$$

all states with equal j have equal values of γ . The applicable values of j are $1/2$, $3/2$, $5/2$, $7/2$, and

$$\gamma_k = \sqrt{k^2 - (\alpha z)^2} \quad k = 1, 2, 3, 4 \quad (119)$$

The wave functions require 10 values of N and E , also

designated by subscripts. The equations used for computation of N and ϵ , and the states to which each applies is given in Table XIII. The numerical values for the various atoms of those quantities necessary in the computation of the transition probabilities are given in Appendix B.

TABLE XIII

THE PARAMETERS N AND ϵ

The defining equations, and the ten values of N are given. To each N corresponds an ϵ . The states to which each N apply are also given. The numbers of the equations refer to Bethe's article.

$$N = \left[n^2 - 2n'(h-\gamma) \right]^{1/2} \quad (9.35)$$

$$\epsilon = \left[1 - \left(\frac{\alpha Z}{N} \right)^2 \right]^{1/2} \quad (9.34)$$

$N_1 = 1$	$1S_{1/2}$
$N_2 = \left[2(1+\gamma_1) \right]^{1/2}$	$2S_{1/2}, 2P_{1/2}$
$N_3 = 2$	$2P_{3/2}$
$N_4 = \left[5 + 4\gamma_1 \right]^{1/2}$	$3S_{1/2}, 3P_{1/2}$
$N_5 = \left[5 + 2\gamma_2 \right]^{1/2}$	$3P_{3/2}, 3D_{3/2}$
$N_6 = 3$	$3D_{5/2}$
$N_7 = \left[10 + 6\gamma_1 \right]^{1/2}$	$4S_{1/2}, 4P_{1/2}$
$N_8 = \left[9 + 4\gamma_2 \right]^{1/2}$	$4P_{3/2}, 4D_{3/2}$
$N_9 = \left[10 + 2\gamma_3 \right]^{1/2}$	$4D_{5/2}, 4F_{5/2}$
$N_{10} = 4$	$4F_{7/2}$

APPENDIX B

MATHEMATICAL ADDENDA

The first part of this section contains the evaluation of the radial integrals appearing in the dipole matrix elements of Chapter II, and the numerical values of the parameters involved in these matrix elements. We restrict ourselves to the case where the final state is a K state. The matrix elements we require are those of equations (44) and (45) and the integrals to be performed are

$$\int_0^{\infty} f_a(r) g_b(r) r^2 dr \quad (120)$$

and

$$\int_0^{\infty} [j f_a(r) g_b(r) + (j+1) g_a(r) f_b(r)] r^2 dr \quad (121)$$

The radial wave functions are tabulated in Appendix A. In each of these integrals the wave functions with subscript a are K wave functions. Equation (120) applies to transitions from type A initial states, so the wave functions g_b in it are restricted by the selection rules to those for $nP_{3/2}$ levels. We shall evaluate this integral for $n = 2, 3$ and 4 . Equation (121) applies to transitions from Type B initial states, and the selection rules restrict these states to $nP_{1/2}$ states. We also evaluate this integral for $n = 2, 3$ and 4 .

We will then use the integrals in equations (44) and (45) to determine the matrix elements and tabulate these matrix elements in terms of the parameters given in Table XII and others which we introduce in this section. We tabulate also the numerical values of these parameters. The numerical values of the matrix elements are found in Table II. We will also describe a method for checking the relativistic matrix elements against the equivalent non-relativistic matrix elements. Each matrix element derived in this section has been checked in this fashion.

Since the radial wave functions are tabulated in terms of the parameter $\rho = \frac{2Zr}{a_0}$, it is easiest to transform the integrals (120) and (121) into this form. This may be done by the relation

$$r^2 dr = \left(\frac{a_0}{2Z}\right)^3 \rho^2 d\rho \quad (122)$$

The limits of integration remain unchanged.

Since the hypergeometric functions which appear in the wave functions are so similar, no confusion results if we let

$$F(-n', 2\gamma+1, \rho) = F(-n') \quad (123)$$

This results in considerable shortening of the equations which follow. The K wave functions have a particularly simple form, in that the hypergeometric functions in them reduce to constants; and using $N_1 = 1$ we have from Plate IA for the $1S_{1/2}$ states

$$f_a(\rho) = - \left(\frac{2Z}{a_0} \right)^{3/2} \frac{1}{\sqrt{\Gamma(2\gamma_1+1)}} \sqrt{\frac{1-\epsilon_1}{8}} e^{-\rho/2} \rho^{\gamma_1-1} [2] \quad (124)$$

$$g_a(\rho) = \left(\frac{2Z}{a_0} \right)^{3/2} \frac{1}{\sqrt{\Gamma(2\gamma_1+1)}} \sqrt{\frac{1+\epsilon_1}{8}} e^{-\rho/2} \rho^{\gamma_1-1} [2] \quad (125)$$

Equation (120) may then be written in general form, using equation (115) and the fact that all $P_{3/2}$ levels have $\gamma = \gamma_2$ and $\mathcal{N} = -2$.

$$\left(\frac{a_0}{2Z} \right)^3 \int_0^\infty f_a g_b \rho^2 d\rho =$$

$$K \int_0^\infty e^{-\rho \left(\frac{N'+1}{2N'} \right)} \rho^{\gamma_1+\gamma_2} \left[-\eta'_b F(-\eta'_b+1) + (N'+2) F(-\eta'_b) \right] d\rho \quad (126)$$

with

$$K = \frac{-2}{\sqrt{\Gamma(2\gamma_1+1)}} \frac{\sqrt{\Gamma(2\gamma_1+\eta'_b+1)}}{\Gamma(2\gamma_2+1) \sqrt{\eta'_b!}} \sqrt{\frac{(1-\epsilon_1)(1+\epsilon_1)}{32N'(N'+2)}} \left(\frac{1}{N'} \right)^{\gamma_2+1/2} \quad (127)$$

The brackets in (126) are polynomials in ρ , and may be extracted from the $P_{3/2}$ wave functions in Plates IA to VIA of Appendix A.

In the same manner, we may write equation (121), using the fact that all $P_{1/2}$ wave functions have $\mathcal{N} = 1$ and the fact that $j = 1/2$, as

$$\left(\frac{a_0}{2Z} \right)^3 \int_0^\infty \left(\frac{1}{2} f_a g_b + \frac{3}{2} g_a f_b \right) \rho^2 d\rho =$$

$$\frac{-2 \sqrt{\Gamma(2\gamma_1+\eta'_b+1)}}{[\Gamma(2\gamma_1+1)]^{3/2} \sqrt{\eta'_b!}} \left(\frac{1}{N'} \right)^{\gamma_1+1/2} \int_0^\infty \rho^{2\gamma_1} e^{-\rho \left(\frac{N'+1}{2N'} \right)} \quad (128)$$

$$\left[(A-B) F(-\eta'_b+1) + (A+B)(N'-1) F(-\eta'_b) \right] d\rho$$

Where for convenience we have introduced the parameters

$$A = \frac{3}{2} \left[\frac{(1+\epsilon_1)(1-\epsilon')}{32 N' (N'-1)} \right]^{1/2} \quad (129)$$

and

$$B = \frac{1}{2} \left[\frac{(1-\epsilon_1)(1+\epsilon')}{32 N' (N'-1)} \right]^{1/2} \quad (130)$$

The brackets appearing in (128) may be calculated from the defining equation of the hypergeometric function (Jahnke, 45, p 275) or may be obtained with some simple algebraic manipulation from the wave functions of Appendix A. It also may be written as a polynomial in ρ , involving the parameters A , B , N' and γ_1 .

The two equations (126) and (128) are very similar in nature, and consist of a sum of terms of the general form

$$C \int_0^\infty e^{-a\rho} \rho^x d\rho \quad (131)$$

They may be integrated, using the definition of the Γ function (Jahnke, 45, p 20)

$$\int_0^\infty e^{-a\rho} \rho^x d\rho = a^{-(x+1)} \Gamma(x+1) \quad (132)$$

In equation (126) the highest power of ρ which appears in any of the brackets is the second, and the only values of x which must be considered are

$$x = \gamma_1 + \gamma_2 + n, \quad n = 0, 1, 2 \quad (133)$$

The integration may be performed term by term, and the

identity (116) used to reduce the argument of each Γ function to $(\gamma_1 + \gamma_2 + 1)$. Each term will then have the common factor

$$\left(\frac{N'+1}{2N'}\right)^{-(\gamma_1+\gamma_2+1)} \Gamma(\gamma_1+\gamma_2+1) \quad (134)$$

which may be factored and combined with the constant K. The resulting equations are to be squared and multiplied by

$$\frac{2j+3}{j+1} = \frac{8}{3} \quad (135)$$

to obtain the matrix elements (44). The algebraic details are omitted. The results of this computation are given in Table XIV.

The integration of equation (128) is done in a similar manner. Equation (133) is replaced by

$$x = 2\gamma_1 + n \quad n = 0, 1, 2, 3 \quad (136)$$

and equation (134) by

$$\left(\frac{N'+1}{2N'}\right)^{-(2\gamma_1+1)} \Gamma(2\gamma_1+1) \quad (137)$$

When we apply (116) to the quantity

$$\frac{\sqrt{\Gamma(2\gamma_1+n'_b+1)}}{[\Gamma(2\gamma_1+1)]^{3/2}} \quad (138)$$

of equation (128) we obtain an exact cancellation of the Γ functions from these integrals. The results of this calculation are squared and multiplied by $\frac{1}{j(j+1)} = \frac{4}{3}$ to give the matrix elements of (45). These are tabulated in Table XV.

TABLE XIV

DIPOLE MATRIX ELEMENTS

These are the dipole matrix elements as given by equation (44). They are given for each $nP_{3/2}$ initial state in terms of parameters defined in Appendix A and the auxiliary parameter.

$$A' = \frac{(1 - \epsilon_1)(1 + \epsilon')}{32 N' (N' + 2)}$$

$$2P_{3/2} \rightarrow 1S_{1/2} ; \quad \epsilon' = \epsilon_3, \quad N' = N_3 = 2$$

$$\frac{8}{3} 2^{2(\gamma_1 + \gamma_2 + 2)} \frac{A' \Gamma^2(\gamma_1 + \gamma_2 + 1)}{\Gamma(2\gamma_1 + 1) \Gamma(2\gamma_2 + 1)} \frac{N_3^{2\gamma_1 + 1}}{(N_3 + 1)^{2(\gamma_1 + \gamma_2 + 1)}} \left[16 \right]$$

$$3P_{3/2} \rightarrow 1S_{1/2} ; \quad \epsilon' = \epsilon^5, \quad N' = N_5$$

$$\frac{8}{3} 2^{2(\gamma_1 + \gamma_2 + 2)} (2\gamma_2 + 1) A' \frac{\Gamma^2(\gamma_1 + \gamma_2 + 1)}{\Gamma(2\gamma_1 + 1) \Gamma(2\gamma_2 + 1)} \frac{N_5^{2\gamma_1 + 1}}{(N_5 + 1)^{2(\gamma_1 + \gamma_2 + 1)}} \left[N_5 + 1 - \frac{2(N_5 + 2)}{(N_5 + 1)} \frac{(\gamma_1 + \gamma_2 + 1)}{2\gamma_2 + 1} \right]^2$$

$$4P_{3/2} \rightarrow 1S_{1/2} ; \quad \epsilon = \epsilon_7, \quad N' = N_8$$

$$\frac{8}{3} 2^{2(\gamma_1 + \gamma_2 + 2)} \frac{(2\gamma_2 + 1)(2\gamma_2 + 2)}{2} \frac{A' \Gamma^2(\gamma_1 + \gamma_2 + 1)}{\Gamma(2\gamma_1 + 1) \Gamma(2\gamma_2 + 1)} \frac{N_8^{2\gamma_1 + 1}}{(N_8 + 1)^{2(\gamma_1 + \gamma_2 + 1)}} \left[N_8 + \frac{4(\gamma_1 + \gamma_2 + 1)}{2\gamma_2 + 1} \left(\frac{N_8 + 2}{(N_8 + 1)^2} \frac{(\gamma_1 + \gamma_2 + 2)}{(2\gamma_2 + 2)} - 1 \right) \right]^2$$

TABLE XV

DIPOLE MATRIX ELEMENTS

These are the matrix elements given by equation (45). They are given for each $nP_{1/2}$ initial state in terms of parameters defined in Appendix A and the auxiliary quantities A and B (equations (17) and (18) Appendix B).

$$2P_{1/2} \rightarrow 1S_{1/2} ; \quad \epsilon' = \epsilon_2, \quad N' = N_2$$

$$\frac{4}{3} \frac{(2\gamma_1+1) 2^{4\gamma_1+4} N_2^{2\gamma_1+1}}{(N_2+1)^{4\gamma_1+2}} \left[-2B + N_2(A+B) - \frac{2(N_2-1)(A+B)}{N_2+1} \right]^2$$

$$3P_{1/2} \rightarrow 1S_{1/2} ; \quad \epsilon' = \epsilon_4, \quad N' = N_4$$

$$\frac{4}{3} \frac{(2\gamma_1+1)(2\gamma_1+2) 2^{4\gamma_1+4} N_4^{2\gamma_1+1}}{2(N_4+1)^{4\gamma_1+2}} \left[2(A-B) + (N_4-1)(A+B) \right. \\ \left. - 4 \frac{(A-B) + (N_4-1)(A+B)}{(N_4+1)} + 4 \frac{(N_4-1)(A+B)}{(N_4+1)^2} \right]^2$$

$$4P_{1/2} \rightarrow 1S_{1/2} ; \quad \epsilon = \epsilon_7, \quad N' = N_7$$

$$\frac{4}{3} \frac{(2\gamma_1+1)(2\gamma_1+2)(2\gamma_1+3) 2^{4\gamma_1+4} N_7^{2\gamma_1+1}}{6(N_7+1)^{4\gamma_1+2}} \left[3(A-B) + (N_7-1)(A+B) \right. \\ \left. - 6 \frac{2(A-B) + (N_7-1)(A+B)}{(N_7+1)} + 12 \frac{(A-B) + (N_7-1)(A+B)}{(N_7+1)^2} - 8 \frac{(N_7-1)(A+B)}{(N_7+1)^3} \right]^2$$

The equivalent non-relativistic matrix elements for a transition from an nP subshell to the 1S shell are given (Bethe, 33) by the relation

$$\left| \left(a \left| \frac{\vec{V}}{c} \right| b \right) \right|^2 = \frac{(Z\alpha)^2 2^6 n^3 (n-1)^{2n-3}}{(n+1)^{2n+3}} \quad (139)$$

The P3/2 transitions make up 2/3 of this and the P1/2 make up 1/3. We would therefore expect our matrix elements to approach 2/3 of (139) for P3/2 and 1/3 of (139) for P1/2 transitions in the non-relativistic limit. We may take this limit for most of the parameters by simply letting $\alpha Z \rightarrow 0$. The only exceptions to this rule are the quantities A, B, and A'. This may be seen by writing each parameter of Table XII using the binomial expansion in powers of αZ . In each case there is a leading term large compared to αZ in the limit $\alpha Z \rightarrow 0$. We get the following limiting expressions for our parameters.

$$\left. \begin{array}{l} \gamma_1 \rightarrow 1 \\ \gamma_2 \rightarrow 2 \\ N_1, N_3 \rightarrow 2 \\ N_4, N_5 \rightarrow 3 \\ N_7, N_8 \rightarrow 4 \end{array} \right\} \lim, \alpha Z \rightarrow 0 \quad (140)$$

Since in this limit, each ϵ tends to 1, and the quantities A, B, and A' contain factors $1 - \epsilon$, it is necessary to retain the first term containing αZ , but we drop higher powers of this quantity. In this manner we get for our non-relativistic limits

$$\begin{aligned}
 A &\rightarrow \frac{3\alpha z}{2N'(32N'(N'-1))} \\
 B &\rightarrow \frac{\alpha z}{2\sqrt{32N'(N'-1)}} \\
 A' &\rightarrow \frac{(\alpha z)^2}{32N'(N'+2)}
 \end{aligned}
 \quad \lim, \alpha z \rightarrow 0 \quad (141)$$

Also, using the fact that

$$\Gamma(n+1) = n! , \quad n \text{ integral} \quad (142)$$

we get in this limit

$$\frac{\Gamma^2(\gamma_1 + \gamma_2 + 1)}{\Gamma(2\gamma_1 + 1)\Gamma(2\gamma_2 + 1)} \rightarrow \frac{3}{4} , \quad \lim \alpha z \rightarrow 0 \quad (143)$$

Using these limiting values, it is easy to show that the tabulated matrix elements converge to (130) with $n = \lim N'$ in (139).

In order to evaluate these matrix elements, it is necessary to evaluate for each atom the various parameters appearing. The defining equations are in Table XII. For several atoms ranging in atomic number from 29 to 100 the values of these parameters are given in Table XVI.

In addition to the energies ϵ we need the transition energies, which are the energy differences between the levels involved in the transition. In Table XVII we give these energies in kev for each X-ray line for which we have calculated the matrix elements. Also given are the non-relativistic values for these energies. We identify the non-relativistic transition by indicating the initial

TABLE XVI

PARAMETERS APPEARING IN THE DIPOLE MATRIX ELEMENTS

	ATOMIC NUMBER					
	29	47	56	79	82	100
γ_1	.977354	.939351	.912700	.817124	.801233	.683770
γ_2	1.986774	1.970376	1.957810	1.915122	1.908396	1.862133
N_2	1.986645	1.969442	1.955863	1.906371	1.898016	1.835086
N_4	2.984864	2.959291	2.941224	-	2.864425	2.781201
N_5	2.996256	2.990109	2.985904	-	2.969308	2.953687
N_7	3.982979	3.954251	3.933980	-	3.848038	3.755345
N_8	3.994383	3.985160	3.978819	-	3.953933	3.930462
ϵ_1	.977354	.939351	.912700	.817124	.801233	.683770
ϵ_2	.994322	.984721	.977931	.953185	.949008	.917543
ϵ_3	.994387	.985188	.978905	.957561	.954198	.931067
ϵ_4	.997481	.993262	.990302	-	.977939	.964968
ϵ_5	.997503	.993400	.990591	-	.979486	.969004
ϵ_7	.998588	.996232	.994591	-	.987837	.980940
ϵ_8	.998596	.996290	.994712	-	.988483	.982616

TABLE XVII

X-RAY TRANSITION ENERGIES

In the first part of the table are the X-ray line energies predicted by the Dirac equation, without screening. In the second part are the energies of the equivalent transitions from the Schrodinger equation. In both parts the units are kev.

X-ray line	Atomic Number					
	29	47	56	79	82	100
$K\alpha_1$	8.703	23.421	33.829	71.659	78.160	126.361
$K\alpha_2$	8.670	23.183	33.331	69.523	75.508	119.451
$K\beta_1$	10.296	27.618	39.800	-	91.082	145.746
$K\beta_3$	10.286	27.547	39.652	-	90.291	143.683
$K\beta_2'$	10.854	29.094	41.906	-	95.679	152.701
$K\beta_2$	10.850	29.064	41.844	-	95.349	151.845
Transition						
2P-1S	8.580	22.537	31.994	-	68.602	102.011
3P-1S	10.169	26.711	37.888	-	81.306	120.902
4P-1S	10.725	28.172	39.961	-	85.753	127.515

subshell. In Table XVIII we show the ratios of the relativistic energies to the equivalent non-relativistic energies. In both table and figures we have used the energies predicted from the relevant wave equation, neglecting screening. In Table XIX we give for convenience the experimental transition energies (where these are known) taken from Hill, et al (Hill, 52). These energies make possible estimates of the relative importance of the energy dependence of the transition probabilities of Chapter II compared to the changes caused by the use of the relativistic wave functions.

In the first part of Chapter III we correct for the effects of retardation by including the term $j_0(kr)$ in the radial integration. This results simply in a change in equations (120) and (121) and (126) and (128) to include this term. The integrations of equations (126) and (128) are, however, changed by the extra radial dependence. Since we do the integration with respect to the variable

ρ , and $\rho = \frac{Zr}{a_0}$, we observe that

$$j_0(kr) = j_0\left(\frac{ka_0}{2Z} \rho\right) \quad (144)$$

Since we shall do only the $K\alpha_1$, and $K\alpha_2$ transitions, we can write equations (126) and (128) in detail, including the retardation term, and express the brackets as functions of ρ . For the $K\alpha_1$ term we have from (126) and (127)

TABLE XVIII

RATIO OF RELATIVISTIC UNSCREENED X-RAY ENERGIES
TO NON-RELATIVISTIC EQUIVALENT ENERGY

In this table are the ratios of the energy of the most energetic line of an X-ray doublet predicted by the Dirac equation to the non-relativistic difference in energy between the same two shells. Both energies are computed without screening.

Energy Ratio	Atomic Number				
	29	47	56	82	100
$\frac{K\alpha_1}{2P-15}$	1.014	1.039	1.057	1.139	1.239
$\frac{K\beta_1}{3P-15}$	1.012	1.034	1.050	1.120	1.205
$\frac{K\beta_2^r}{4R-15}$	1.012	1.033	1.049	1.116	1.198

TABLE XIX

EXPERIMENTAL X-RAY ENERGIES

The values in this table are taken from the tables of Hill, et al (Hill, 52). The units are kev.

X-Ray Line	Atomic Number					
	29	47	56	79	82	100*
$K\alpha_1$	8.047	22.160	32.182	68.754	74.917	118.97
$K\alpha_2$	8.028	21.988	31.803	66.939	72.750	113.33
$K\beta_1$	8.905	24.942	36.364	-	84.883	134.48
$K\beta_3$	-	24.909	36.289	-	84.392	133.09
$K\beta_{2'}$	-	25.455	37.246	-	87.308	138.48
$K\beta_2$	-	-	37.234	-	87.190	138.11

* The values for $Z = 100$ are obtained by extrapolation.

$$\int_0^\infty f_a g_b j_0(-kr) r^2 dr = \frac{8(A')^{1/2}}{[\Gamma(2\gamma_1+1)\Gamma(2\gamma_2+1)]^{1/2}} \left(\frac{1}{N_3}\right)^{\gamma_2+1/2}$$

$$\int_0^\infty \rho^{\gamma_1+\gamma_2} j_0\left(-\frac{ka_0}{2z}\rho\right) e^{-\rho\left(\frac{N_3+1}{2N_3}\right)} d\rho \quad (145)$$

The minus sign appears by virtue of the minus sign in equation (2) of Chapter 1. In the same fashion equation (128) is replaced by

$$\int_0^\infty \left(\frac{1}{2} f_a g_b + \frac{3}{2} g_a f_b\right) j_0(-kr) r^2 dr =$$

$$\frac{2(2\gamma_1+1)}{\Gamma(2\gamma_1+1)N_2^{\gamma_1+1/2}} \int_0^\infty \rho^{2\gamma_1} j_0\left(-\frac{ka_0}{2z}\rho\right) e^{-\rho\left(\frac{N_2+1}{2N_2}\right)} d\rho \quad (146)$$

$$\left[-2B + N_2(A+B) - \frac{(N_2-1)(A+B)}{N_2(2\gamma_1+1)}\rho\right] d\rho$$

In order to evaluate these integrals we use the well known trigonometric identity

$$e^{-i kr} = \cos kr + i \sin(-kr) \quad (147)$$

Since, from equation (20)

$$j_0(kr) = \frac{\sin kr}{kr} \quad (148)$$

we observe that

$$j_0\left(-\frac{ka_0}{2z}\rho\right) = -\frac{2z}{ka_0\rho} \operatorname{Im} \left[e^{-i \frac{ka_0}{2z}\rho} \right] \quad (149)$$

where Im means imaginary part.

If we apply (149) to (145) we see that we wish to evaluate

$$= \frac{2z}{\hbar a_0} \cdot \frac{g(A')^{1/2}}{[\Gamma(2\gamma_1+1)\Gamma(2\gamma_2+1)]^{1/2}} \left(\frac{1}{N_3}\right)^{\gamma_2+1/2} \quad (150)$$

$$\text{Im} \int_0^\infty \rho^{\gamma_1+\gamma_2+1} e^{-\rho \left[\frac{N_3+1}{2N_3} + i \frac{\hbar a_0}{2z} \right]} d\rho$$

This integral is clearly of the form (131), so the integration results in an expression similar to (132).

Writing just the integral of (150) we have

$$\text{Im} \int_0^\infty \rho^x e^{-a\rho} d\rho \quad (151)$$

with

$$x = \gamma_1 + \gamma_2 - 1 \quad (152)$$

and

$$a = \left[\frac{N_3+1}{2N_3} + i \frac{\hbar a_0}{2z} \right] \quad (153)$$

for simplicity we rewrite a , with obvious definitions for u and v

$$a = u + iv \quad (154)$$

Applying (132) to (151) yields

$$\text{Im} \left[a^{\Gamma(x+1)} \Gamma(x+1) \right] \quad (155)$$

Since x is real, $\Gamma(x+1)$ is real, so (155) becomes

$$\Gamma(x+1) \text{Im} \left[\frac{1}{a^{(x+1)}} \right] \quad (156)$$

In order to perform the operation Im in (156) we observe the following properties of complex numbers

$$u + iv = R e^{i\Phi}, \text{ with}$$

$$R^2 = u^2 + v^2 \quad \text{and} \quad \Phi = \tan^{-1} \frac{v}{u} \quad (157)$$

and if we express a by (154),

$$\frac{1}{a^{(x+1)}} = R^{-(x+1)} e^{-i(x+1)\Phi} \quad (158)$$

Now, using (147) we may write (156) as

$$R^{-(x+1)} \Gamma(x+1) \sin^{-(x+1)} \Phi \quad (159)$$

since

$$\sin^{-x} = -\sin^x \quad (160)$$

(159) becomes, identifying x from (152)

$$- \Gamma(\gamma_1 + \gamma_2) R^{-(\gamma_1 + \gamma_2)} \sin^{(\gamma_1 + \gamma_2)} \Phi \quad (161)$$

and (150) may be written

$$\frac{2Z}{\hbar a_0} \frac{g(A')^{1/2}}{[\Gamma(2\gamma_1+1) \Gamma(2\gamma_2+1)]^{1/2}} \left(\frac{1}{N_3} \right)^{\gamma_2+1/2} \frac{\Gamma(\gamma_1+\gamma_2) \sin^{(\gamma_1+\gamma_2)} \Phi}{R^{(\gamma_1+\gamma_2)}} \quad (162)$$

Using the identity (116) to get a form more suitable for comparison with the other matrix elements, we see that

$$\Gamma(\gamma_1 + \gamma_2) = \frac{\Gamma(\gamma_1 + \gamma_2 + 1)}{\gamma_1 + \gamma_2} \quad (163)$$

If we square (162) and multiply by

$$\frac{2j+3}{j+1} = \frac{8}{3} \quad (164)$$

we obtain for the squared averaged matrix element (48) the following expression, which is written also as equation (50) of Chapter III:

$$\frac{8}{3} \left(\frac{2Z}{A a_0} \right)^2 \frac{64 A' \Gamma^2(\gamma_1 + \gamma_2 + 1) R^{-2(\gamma_1 + \gamma_2)}}{\Gamma(2\gamma_1 + 1) \Gamma(2\gamma_2 + 1) N_3^{2\gamma_2 + 1}} \left[\frac{\sin(\gamma_1 + \gamma_2) \Phi}{\gamma_1 + \gamma_2} \right]^2 \quad (165)$$

with

$$R^2(2P_{3/2}) = \left(\frac{N_3 + 1}{2N_3} \right) + \left(\frac{h(2P_{3/2}) a_0}{2Z} \right)^2 \quad (166)$$

and

$$\Phi(2P_{3/2}) = \tan^{-1} \left(\frac{N_3 a_0}{(N_3 + 1) Z} h(2P_{3/2}) \right) \quad (167)$$

A very similar calculation of the squared average matrix element (49) leads to the following expression, which is also given as equation (53) of Chapter III.

$$\frac{4}{3} \left(\frac{2Z}{A a_0} \right)^2 \frac{4(2\gamma_1 + 1)}{N_2^{2\gamma_1 + 1} R^{4\gamma_1}} \left[\left(-2B + \frac{N_2(A+B)}{N_2(A+B)} \right) \left\{ \frac{\sin 2\gamma_1 \Phi}{2\gamma_1} \right\} - \frac{(A+B)(N_2 - 1)}{N_2 R} \left\{ \frac{\sin(2\gamma_1 + 1) \Phi}{2\gamma_1 + 1} \right\} \right]^2 \quad (168)$$

where

$$R^2(2P_{1/2}) = \left(\frac{N_2 + 1}{2N_2} \right)^2 + \left(\frac{N_2 a_0}{(N_2 + 1) Z} h(2P_{1/2}) \right)^2 \quad (169)$$

and

$$\Phi(2P_{1/2}) = \tan^{-1} \left(\frac{N_2 a_0}{(N_2 + 1) Z} h(2P_{1/2}) \right) \quad (170)$$

Equation (165) should be contrasted with the first equation of Table XIV, which it replaces, and equation (168) with the first equation of Table XV. Since the

equations of Table XIV and XV are the results of the approximation for long wave length, that is

$$\frac{ka_0}{2z} \ll 1 \quad (171)$$

The more exact expressions should reduce to the simpler forms in this limit. That this is so may be easily seen by applying the following limits to (165) and (168)

$$\begin{aligned} \sin(\gamma_1 + \gamma_2) \bar{\phi} &\cong (\gamma_1 + \gamma_2) \bar{\phi} \cong (\gamma_1 + \gamma_2) \tan \bar{\phi} \\ &\cong \frac{(\gamma_1 + \gamma_2) N_2 ka_0}{(N_2 + 1) z} \quad \text{if } \frac{ka_0}{2z} \ll 1 \end{aligned} \quad (172)$$

with equivalent expressions for $\sin(2\gamma_1 \bar{\phi})$ and $\sin((2\gamma_1 + 1) \bar{\phi})$, and

$$R^2 = \left(\frac{N'+1}{2N'} \right)^2 \quad \frac{ka_0}{2z} \ll 1 \quad (173)$$

Numerical evaluation of these matrix elements and the transition probabilities associated with them for lead is discussed in Chapter III.

The values of all fundamental physical constants used in the calculation of this work are taken from DuMond and Cohen (DuMond, 51).

BIBLIOGRAPHY

- (Bade, 53) W. L. Bade and H. Jehle, Rev. Mod. Phys., 25, 714 (1953).
- (Bethe, 33) H. A. Bethe, Handbuch der Physik, Vol. XXIV, 1 Chapter III Berlin: Julius Springer, (1933).
- (Blatt, 52) J. M. Blatt and V. F. Weisskopf, Theoretical Nuclear Physics New York: John Wiley and Sons (1952).
- (Breit, 32a) S. A. Korff and G. Breit, Rev. Mod. Phys. 4, 471 (1932).
- (Breit, 32b) G. Breit, Rev. Mod. Phys. 4, 504 (1932).
- (Burhop, 36) H. S. W. Massey and E. H. S. Burhop, Proc. Roy. Soc. London, 153 A, 661 (1936).
- (Compton, 35) A. H. Compton and S. K. Allison X-rays in Theory and Experiment Second Edition, New York: D. Van Nostrand (1935).
- (Condon, 51) E. U. Condon and G. H. Shortley The Theory of Atomic Spectra Cambridge: The University Press (1951).
- (Davisson, 52) C. M. Davisson and R. D. Evans, Rev. Mod. Phys. 24, 79 (1952).
- (DuMond, 47) J. W. M. DuMond, Rev. Sci. Inst. 18, 626 (1947).
- (DuMond, 49) B. B. Watson, W. J. West, D. A. Lind, and J. W. M. DuMond Phys. Rev. 75, 505 (1949)

- (DuMond, 51) J. W. M. DuMond and E. R. Cohen Phys. Rev. 82, 555 (1951).
- (Gell-Mann, 54) M. Gell-Mann, M. L. Goldberger, and W. E. Thirring Phys. Rev. 95, 1612 (1954).
- (Gokhale, 52) B. G. Gokhale, Anal. de Phys. (Paris) 7, 852 (1952).
- (Hall, 36) H. Hall Rev. Mod. Phys. 8, 358 (1936).
- (Heitler, 44) W. Heitler, The Quantum Theory of Radiation, Second Edition, London, Oxford University Press (1944).
- (Heitler, 54) *ibid*, Third Edition.
- (Hill, 52) R. D. Hill, E. L. Church and J. W. Mihelich, Rev. Sci. Inst. 23, 523, (1952).
- (Hulme, 35) H. R. Hulme, J. McDougall, R. A. Buckingham and R. H. Fowler Proc. Roy. Soc., London, A149, 131 (1935).
- (Jacobsohn, 47) B. Jacobsohn, Thesis: University of Chicago (1947) Unpublished.
- (Jahnke, 45) E. Jahnke and F. Emde, Tables of Functions Fourth Edition, New York, Dover Press (1945).
- (Levinger, 50) J. S. Levinger and H. A. Bethe Phys. Rev. 78, 115 (1950).
- (Morse, 53) P. M. Morse and H. Feshbach Methods of Theoretical Physics, Parts 1 and 11, New York, McGraw-Hill, (1953).
- (Richtmeyer, 37) E. G. Ramberg and F. K. Richtmeyer Phys. Rev., 51, 913 (1937).

- (Rose, 55) M. E. Rose, Multipole Fields, New York, John Wiley and Sons, (1955).
- (Sauter, 31) F. Sauter Ann. d. Phys. 11, 454, (1931).
- (Schiff, 49) L. I. Schiff, Quantum Mechanics, New York; McGraw Hill, (1949).
- (Slater, 30) J. C. Slater, Phys. Rev. 36, 57, (1930).
- (Stech, 52) B. Stech, Zeits fur Naturforschung 7a, 401, (1952).
- (Stobbe, 30) M. Stobbe, Ann. d. Phys. 7, 661, (1930).
- (Tuan, 53) T. F. Tuan, Thesis: Louisiana State University, (1953) Unpublished.
- (White, 54) Gladys White, Private Communication.

VITA

Wilbur B. Payne was born in Pittsburgh, Pennsylvania, in 1926. He attended public schools in Kingsport, Tennessee, and Covington, Virginia. He was graduated from Covington High School in 1944 and entered the Army of the United States, serving until 1947. He entered Tulane University in February, 1948, and was granted the Bachelor of Science degree by that institution in 1951. He began graduate studies at Louisiana State University in September, 1951, and received the degree of Master of Science in June, 1953. He is now a candidate for the Doctor of Philosophy degree in the department of physics.

EXAMINATION AND THESIS REPORT

Candidate: Wilbur B. Payne

Major Field: Physics

Title of Thesis: Relativistic Radiative Transitions

Approved:

J. S. Levin

Major Professor and Chairman

Howard Hix

Dean of the Graduate School

EXAMINING COMMITTEE:

Max Goodrich

Ralph C. Mobley

Sloyd W. Morris

W. M. Mendenhall

Richard C. Keen

Date of Examination:

July 27, 1955