ON THE THEORY OF RADIATIVE BETA PROCESSES

by

FOREST GENE HESS

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ABSTRACT

This thesis is devoted to some aspects of the theory of the weak continuous gamma radiation (often called 'Internal Bremsstrahlung') which accompanies beta processes, i.e. negative and positive electron emission and orbital electron capture. Whenever a beta process is accompanied by this gamma radiation, it will be called a "radiative" beta process, otherwise "radiationless".

The results presented in this thesis go beyond those obtained by other authors in two respects.

In the first place, the radiative beta emission probability is calculated for an allowed transition taking into account an arbitrary mixture of all the five beta interactions. Previously, only the theory for the case of pure interactions has been carried out. In the calculations, as in previous ones, Coulomb effects have been neglected.

In the second place, the radiative K capture probability is calculated for an allowed transition taking into account again an arbitrary mixture of the five beta interactions, and, in addition, Coulomb effects. Previously, only the case of pure interactions with the neglection of Coulomb effects has been considered. In order to take Coulomb effects into account, a "semi-relativistic" approximation for the solutions to the Dirac equation with a Coulomb potential has been developed. It turns out that taking Coulomb effects into account reduces the probability of radiative K capture by an order of magnitude.

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COMMITTEE IN CHARGE:

H.F. Angus, Chairman

W. Opechowski
G.M. Shrum
J.B. Warren
F.A. Kaempffer
B.C. Binning
D. Derry
T.E. Hull
A.D. Moore

External Examiner - L.E.H. Trainor
Queen's University

LIST OF PUBLICATIONS

Some Directional Correlation Functions for Successive Nuclear Radiations, Canadian Journal of Physics 30, 130, 1952.

Alternative Solution to the Ehrenfest Problem, American Mathematical Monthly, 61, 323, 1954.

THESIS

ON THE THEORY OF RADIATIVE BETA PROCESSES

This thesis is devoted to some aspects of the theory of the weak continuous gamma radiation (often called "Internal Bremsstrahlung") which accompanies beta processes, i.e. negative and positive electron emission and orbital electron capture. Whenever a beta process is accompanied by this gamma radiation, it will be called a "radiative" beta process, otherwise "radiationless".

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GRADUATE STUDIES

Field of Study: Physics

Electromagnetic Theory	W. Opechowski
Theory of Measurement	A.M. Crooker
Nuclear Physics	K.C. Mann
Quantum Mechanics	G.M. Volkoff
Spectroscopy	A.M. Crooker
Special Relativity	W. Opechowski
Theory of Solids	R.W. Maurer
Group Theory	H. Koppe
Low Temperature Physics	J.M. Daniels
Quantum Theory of Radiation	F.A. Kaempffer
Theoretical Nuclear Physics	W. Opechowski
Theoretical Physics Seminar	W. Opechowski

Other Studies:

Network Theory	A.D. Moore
Integral Equations	T.E. Hull
Complex Variable Theory	D. Derry

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INTRODUCTION AND SUMMARY

Every beta process, i.e. electron or positron emission or orbital electron capture, has a certain probability of being accompanied by a weak continuous gamma radiation. This radiation is not due to de-excitation processes in the nucleus before or after the beta process since such processes give rise to monochromatic radiation. Rather, it is attributed to that caused by the changing dipole moment of the atom when the electronic charge, involved in the beta process, is suddenly shifted; it occurs "during" the beta process. Such radiation has been termed "internal bremsstrahlung". Whenever a beta process is accompanied by internal bremsstrahlung, it will here be referred to as a "radiative" beta process, otherwise - "radiationless".

The measurement of internal bremsstrahlung is complicated by the fact that if any deexcitation processes occur, the resulting monochromatic radiation will probably "smother" it. In this connection, internal bremsstrahlung was first observed by Aston (27) in his measurements on the electron emission of $Ra\,E$. The bremsstrahlung from electron capture was first observed by Bradt, et al (46) in Fe^{55}.

Let us first consider radiative electron and positron emission. The theory for these processes has been given by Knipp and Uhlenbeck (36) and Block(36) for an allowed transition and for "pure" interactions only. In what follows, "pure" interaction means any one of the five well-known beta interactions. Chang and Falkoff (49) and Bolgiano, Madansky and Rasetti (53) extended the calculations to first and second forbidden beta transitions. In all these calculations Coulomb effects have been neglected.

Goodrich and Payne (54) measured the internal bremsstrahlung accompanying the electron emission of P^{32}. They found that their results agreed quite well with the theoretical results for an allowed transition mentioned above.

The calculations given in Chapters I and II of this thesis take into account an arbitrary mixture of the five beta interactions and the results show that a non-zero contribution to the probability arising from cross-terms between scalar and vector, tensor and axial interactions, is present. The calculations are carried out for an allowed transition with the neglection of Coulomb effects for electron and positron emission. The results show that the pure interaction terms of the probability are the same for electron and positron emission; on the other hand, the cross-term contribution changes sign from one case to the other. The explicit expression for the photon energy spectrum is given by Eq. (II.16) and the corresponding curves plotted in Graph II.1

Because of the agreement of Goodrich and Payne's results with the theory including only pure interactions, it was felt that an upper limit on the magniture of the interaction constants appearing in the cross-terms could be obtained from the condition that the contribution of these terms does not destroy the agreement.

However, after the calculations were carried out, more accurate experimental results appeared in the paper by Lidén and Starfelt (55), who criticized Goodrich and Payne's result and concluded that there is a considerable discrepancy between theory and experiment. Consequently, the program connected with the upper limit on the cross-terms had to be abandoned because a proper comparison could not be made until Coulomb effects were taken into account. In any case, the results do extend previous calculations and should be of some

use for comparison with calculations including Coulomb effects for small values of Z.

The calculations of the radiative K capture probability were carried out for the following reasons. Prior to the experimental work of Saraf (54), experimental results agreed with the theoretical results of Morrison and Schiff (40) for an allowed transition and pure interactions neglecting, among other things, Coulomb effects. These authors calculated the ratio $w_k\,dk/w_c$ as a fn. of the photon energy, where $w_k\,dk$ is the probability per second that a photon of energy $\hbar ck$ in the range $d(\hbar ck)$ is emitted during the K capture process and w_c is the probability that a radiationless K capture occurs per second. Before Saraf's work this ratio was measured on an arbitrary scale as a fn. of the photon energy. Since the ratio is of the order 10^{-4}, one can say that w_c is practically the same as the total probability for K capture. Saraf, making use of this fact, was able to measure the actual value of this ratio as a fn. of the photon energy. He found that for radiative K capture in ${}_{55}Cs^{131}$ agreement existed between the Morrison and Schiff theory and experiment for high photon energies but that definite disagreement outside of experimental error existed for low photon energies, the disagreement increasing the lower the photon energy.

This disagreement may be due to the neglection of Coulomb effects in Morrison and Schiff's theory or possibly due to the neglection of the radiative p capture from the L shell which may be of considerable magnitude for the second order radiative process.

The theoretical program which was started to explain this discrepancy was to calculate first the radiative K capture for an allowed transition taking into account Coulomb effects and an arbitrary mixture of the five beta interactions; then, to do the same for radiative p capture from an L shell (the results for the radiative s capture from the L shell are expected to be much smaller than those for radiative s capture from the K shell).

Because of the complexities involved in taking Coulomb effects into account, this program has been carried out only for radiative K capture. It turns out that taking Coulomb effects into account reduces the probability by an order of magnitude and hence increases the disagreement mentioned above. It follows that the radiative p capture probability should be investigated.

In this connection, it should be mentioned that Glauber and Martin (54) have published a short note in which they state that they have calculated radiative s and p capture probabilities for an allowed transition taking Coulomb effects into account. They obtain explicit results for Fe^{55} which was studied experimentally by Madansky and Rasetti (54) who also found a disagreement at low photon energies with Morrison and Schiff's theory. Glauber and Martin find that taking radiative p capture into account explains this low energy discrepancy. However, the information in their note is not sufficient to compare their method (which is entirely different from ours) and their results with those presented in this thesis.

An outline of the contents of this thesis on radiative K capture is given below.

In Chapter I, the probability for radiative and radiationless K capture is formulated by means of the Dirac hole theory along with a discussion of the intermediate states involved.

The contents of Chapter II have already been mentioned above in connection with radiative electron and positron emission.

In Chapter III, Section A the results of Morrison and Schiff are obtained in detail. These authors only outlined their calculations verbally without showing explicit details; for this reason, Section A should be

useful if one desires a detailed understanding of the assumption they make. Essentially, they have neglected Coulomb effects entirely, representing the electrons and neutrinos with Dirac plane waves and, in particular, the K electron by a Dirac plane wave with momentum zero and energy mc^2 i.e. a particle at rest.

In Chapter III, Section B, the radiationless K capture probability w_c is calculated for an allowed transition taking into account Coulomb effects and an arbitrary mixture of the five beta interactions. It has been obtained already by other authors but is given in this thesis as a preparation for the more complicated calculation of the radiative K capture probability $w_k dk$. In obtaining w_c the well-known assumption for the electron and neutrino wave fns. at the nucleus:

$$\frac{pR}{\hbar} \ll 1$$

where p is the electron or neutrino momentum, R the nuclear radius, is made. Also, only the components of the wave fns. having an angular dependence given by the zero order spherical harmonic are retained. Both these approximations are common to the allowed transition in the radiationless case.

Also in Chapter III, Section B, the radiative K capture probability $w_k dk$ for an allowed transition with Coulomb effects, is reduced to a 'sum' over all the energies possible for an electron in the intermediate state. In obtaining the wave fns. for the electron and neutrino at the nucleus the same two assumptions as made in the radiationless case above are used. Although these assumptions are valid in the first order radiationless case it does not immediately follow that they are also valid for the second order radiative case. In particular, because of the "sum" over intermediate states for energies up to infinity, the assumption

$$pR/\hbar \ll 1$$

is not always true. Also, contributions from the neglected components of the

wave fns. are possible and it has not been shown that such contributions are negligible. This would require a separate investigation in itself. However, if we define an allowed transition to be the one for which only those components of the Dirac wave fns. are retained which have an angular dependence given by zero order spherical harmonics, then this last objection disappears.

Also in Chapter III, Section C, the "Sum" over intermediate states mentioned above is considered. It reduces to a sum over all discrete energies and an integral over all continuum energies. Arguments are presented to show that the sum over discrete energies should be negligible and it is then omitted. The remaining integral over continuum energies is too complicated as it stands to be evaluated within a reasonable length of time.

In Chapter III, Section D, the integral is carried out for $_{55}Cs^{131}$ by using what we shall call a "semi-relativisitic" approximation for the solutions to the Dirac Equation with a Coulomb potential. This approximation preserves the normalization of the wave fns. and simplifies the integrand to the extent that it can be plotted and evaluated numerically. The integrand is plotted for Cs^{131} for four different photon energies in Graphs III.1 to III.4. The integration results are tabulated in Table III.2 In Graph III.5 the ratio $w_k dk/w_0$ is plotted in comparison to Morrison and Schiff results. For values of Z other than that of Cs graphical evaluation of the integral would again be necessary; however, the most complicated parts of the integrand have been tabulated in Table III.1 for any value of Z.

In Chapter III, Section E, the validity of the "semi-relativisitic" approximation is investigated. It happens that for $Z=119$ the integral over continuum energies can be easily plotted without making a "semi-relativisitic"

approximation. In Graph III.6, the integrand is plotted for Z = 119 and compared with the curves of the integrand for Z = 119 in which "semi-relativistic" and "non-relativistic" approximations have been made. In the "non-relativistic" approximations Schrodinger wave fns. are used. The integrand and the "semi-relativistic" integrand have the same general shape and it is anticipated that for $_{55}Cs^{131}$ these two curves are much closer together; however, the "non-relativistic" integrand does not have even the same shape as the other two - especially at low photon energies where the integrand is largest. In fact, the value of the integral for the "non-relativistic" approximation turns out to be much larger than for the "semi-relativistic" approximation, and, consequently, the value of the ratio $w_k dk/w_c$ is, in the "non-relativistic" approximation, much closer to the experimental one. This is a rather curious result because, from the theoretical point of view, the "semi-relativistic" approximation should give better results than the "non-relativistic" one.

CHAPTER I

Outline of Theory for Allowed Transitions

In this Chapter a brief review of the theory of electron and positron emission and orbital electron capture for an allowed transition is presented, only those essentials necessary for an understanding of this thesis being discussed. For more details, the reader is referred to the longer articles of Rose (55), Konopinski (55), Konopinski and Langer (53), Blatt and Weisskopf (52), De Groot and Tolhoek (50). The radiative processes, i.e. those for which internal bremsstrahlung occurs, are also considered and expressions for their probabilities are formulated along with a discussion of the intermediate states.

A. Non-Radiative Processes

It is the purpose of this Section to show how the matrix elements for the non-radiative electron and positron emission and orbital electron capture processes are obtained. These matrix elements are then used in Section B for the radiative processes.

In the treatment of the non-radiative processes given below, we shall adopt the convention that an anti-neutrino is emitted in electron emission and a neutrino is emitted in positron emission and orbital electron capture. The results for the opposite convention in which a neutrino is emitted in electron emission and an anti-neutrino in positron emission and orbital capture, are the same. We shall also use the word "lepton" when referring to an electron, positron, neutrino or anti-neutrino.

1. Electron Emission

The basis for the theory of beta-decay, as initiated by Fermi (34), is the assumption that the emission of leptons can be treated in a manner

analogous to the emission of electromagnetic radiation, as explained in Fermi's original paper. As a result, the interaction matrix element is assumed to be:

$$(F|H_{-}|O) = \sum_{n=1}^{A} \int (\psi^* \Omega \varphi)_n \, (\Psi_f^* \Omega_n \Psi_i) \, d\tau_n \qquad (I.1)$$

where: ψ is the wave fn. for an electron in a positive energy state,

φ is the wave fn. for a neutrino in a negative energy state,

Ψ_i, Ψ_f are initial and final nuclear states respectively,

* is the symbol for the adjoint (i.e. transpose and complex conjugate) of a matrix,

Ω, Ω_n are operators operating respectively on lepton and nucleon wave fns.,

$(\quad)_n$ means the value of the fn. in the brackets, taken at the position of the n^{th} nucleon,

$\int d\tau_n$ is taken over the volume containing the n^{th} nucleon i.e. the nuclear volume. (I.2)

In order to write the theory of electron emission in a symmetric form, we shall say that the initial state of the system O consists of the initial nucleus and a neutrino in a negative energy state and the final state of the system F consists of the final nucleus and the emitted electron

By restricting the interaction matrix element to be relativistically invariant, it can be shown that on quite general assumptions there are only five possible choices for Ω . In general, some of the components of Ω are "large" or non-relativistic whereas the remaining components are "small" or relativistic of order v/c where v is the nucleon velocity, the "large"

and "small" components giving rise to different selection rules. For an allowed transition, only the "large" components are used, the resulting expression for the interaction matrix element being no longer relativistically invariant. The "large" components are:

β	called the Scalar interaction	(I.3a)
1	" " Vector "	(I.3b)
$\beta\vec{\sigma}$	" " Tensor "	(I.3c)
$\vec{\sigma}$	" " Axial "	(I.3d)
$i\beta\gamma_5$	" " Pseudoscalar "	(I.3e)

where the matrices β , $\vec{\sigma}$, γ_5 are defined in (A.6) , (A.1) . Note, in particular, that all the interactions are Hermitian. The Pseudoscalar interaction (I.3e) is actually a relativistic one of order v/c; however, it is the largest component of its operator Ω because the others are zero and is retained for this reason.

There are nine different matrices given in (I.3). In order to write a linear combination of the five interactions, it is convenient to define the following quanitities.

$$\begin{aligned} r &= 1,\ 2,\ 3,\ 4,\ 5,\ 6,\ 7,\ 8,\ 9 \\ A^r &= \beta,\ 1,\ \beta\sigma_1,\ \beta\sigma_2,\ \beta\sigma_3,\ \sigma_1,\ \sigma_2,\ \sigma_3,\ i\beta\gamma_5 \\ C_r &= C_S,\ C_V,\ C_T,\ C_T,\ C_T,\ C_A,\ C_A,\ C_A,\ C_P, \end{aligned} \qquad (I.4)$$

With these quantities, the interaction matrix element can be expressed as follows:

$$(F|H_-|0) = G \sum_{r=1}^{9} C_r \sum_{m=1}^{A} \int (\psi^* A^r \varphi)_m \, (\Psi_f^* A_m^r \Psi_i) \, d\tau_m \ . \qquad (I.5)$$

It can be shown that the C's are real. In (I.5) we have imposed the restriction

$$C_S^2 + C_V^2 + C_T^2 + C_A^2 + C_P^2 = 1 \qquad (I.6)$$

on the C's, letting G be the coupling constant of the beta interaction.

An allowed transition is characterized not only by the neglection of the "small" terms in obtaining the interactions (I.3) but also by an approximation concerning the matrix element of the emitted leptons at the n^{th} nucleon in (I.5). In this approximation it is assumed that the matrix element involving the lepton wave fns. is slowly varying over the nuclear volume and hence can be taken outside the nuclear volume integral and sum over the nucleons in (I.5); The lepton wave fns. which are largest at the nucleus and the largest terms in the expansion of these wave fns. about the origin are then used in the extricated matrix element. Thus, for an allowed transition,

$$(F|H_-|0) = G\sum_r C_r (\psi^* A^r \varphi)_R \int A^r \qquad (I.7a)$$

where: R is the nuclear radius and

$$\int A^r = \sum_{m=1}^{A} \int (\Psi_f^* \; A_m^r \; \Psi_i) \, d\tau_m \; . \qquad (I.7b)$$

The nuclear matrix element (I.7b) is assumed to be zero unless a neutron changes into a proton.

If we neglect nuclear charge effects and describe the leptons by plane wave solutions to the Dirac Eq. then, for an allowed transition, we approximate $\exp. i\vec{K}\cdot\vec{r}$ by 1 at the nucleus and so (I.7a) becomes

$$(F|H_-|0) = G\sum_r C_r \; (\xi^* A^r \eta) \int A^r \qquad (I.8)$$

where ξ, η are the matrix amplitudes of the electron, neutrino wave fns. respectively. Approximating the exponential by unity at the nucleus is equivalent to expanding it in terms of spherical waves and noting that the largest term of this expansion at the nucleus is the $l = 0$ term or $\frac{\sin kR}{kR} \approx 1$, i.e. that part of the plane wave fn. having zero orbital angular momentum.

If, on the other hand, we neglect relativistic effects and yet take into account nuclear charge effects by describing the leptons by pherical wave solutions to the Schrodinger Eq. with a Coulomb potential, then these solutions (for energies in the continuum) vary as r^l near the origin, the largest one being that for $l = 0$ as in the plane wave case.

We see from the above considerations that an allowed transition is one for which the relativistic terms of the interaction hamiltonian are neglected (excepting pseudoscalar interaction) and one for which the emitted leptons carry off zero orbital angular momentum. Definite selection rules exist for allowed transitions; however "forbidden" transitions obeying different selection rules do occur, their theory being obtained from a study of the terms neglected in the allowed transition. For further details, see the references listed at the beginning of this Chapter.

The nucleons and their wave fns. will be treated non-relativistically. Consequently, for Scalar and Tensor interactions we shall use the relations

$$\int \beta = \int 1 \qquad \text{and} \qquad \int \beta \vec{\sigma} = \int \vec{\sigma} \qquad (I.9)$$

for the nuclear matrix elements, essentially replacing β by unity. Such a replacement is permitted because in the representation used in this thesis, the diagonal terms of β which are $+1$ connect the "large" non-relativistic components of the nucleon wave fns. whereas the diagonal terms which are -1 connect the "small" relativistic components which we are neglecting.

2. Positron Emission and Orbital Electron Capture

In the theory of positron emission or orbital electron capture, an electron in a negative continuum or positive discrete state is captured by the nucleus with the emission of a neutrino. From the theory of second quantization, creation and annihilation operators are the adjoint of each other and so the interaction hamiltonian for the processes under consideration is the adjoint of the hamiltonian for electron emission. As a result, the interaction matrix element for these processes is obtained by taking the complex conjugate of (I.7), giving

$$(F|H_+|0) = G\sum_r C_r\,(\varphi^* A^r \psi)_R \int A^r \qquad \text{(I.10a)}$$

where

$$\int A^r = \sum_{n=1}^{A} \int (\Psi_f^* A^r \Psi_i)\, d\tau_n \qquad \text{(I.10b)}$$

is zero unless a proton changes into a neutron. In (I.10a) φ is the wave fn. for a neutrino in a positive energy state and ψ is that for an electron in a negative continuum or positive discrete state for positron emission or orbital electron capture respectively.

B. Radiative Processes.

In this section, the probabilities for radiative electron and positron emission are formulated for use later on in Chapter II. In the calculations of Chapter II the lepton wave fns. are approximated by plane wave solutions to the Dirac Eq. neglecting nuclear charge effects ($Z = 0$) so that the final formulae and the discussion of intermediate states given in this section will apply only for this approximation.

Also, the formula for the radiative K capture probability is presented. This thesis, from Chapter III on, is devoted to the calculation of this probability, taking into account both relativistic and Coulomb effects i.e. by using solutions to the Dirac Eq. with a Coulomb potential for the lepton wave fns; consequently, the formula developed in this Section for this process is considerably more general than those for the radiative electron and positron emission in which plane wave fns. are used. The intermediate states for this process are also discussed, relations between their matrix elements being used to simplify the radiative K capture formula.

1. Radiative Electron Emission

This process requires an intermediate state. Let us designate the states of the system as follows:

0, Initial state consisting of nucleus of charge Z and neutrino with energy $-E_{\bar{\nu}}$ $(E_{\bar{\nu}} > 0)$,

$E_{\bar{\nu}}$ is the energy of the anti-neutrino,

I, intermediate state consisting of final nucleus of charge $Z+1$ and emitted electron with energy E_s,

F, final state consisting of final nucleus of charge $Z+1$, an electron with energy E, and a photon with energy $E_\gamma = \hbar c k$.

Conservation of energy between 0 and F states tells us that the available nuclear energy, W, is given by

$$W = E + E_\gamma + E_{\bar{\nu}} , \tag{I.11a}$$

and defining

$$W_e = E + E_\gamma \tag{I.11b}$$

we also find that the energy difference between the I and 0 states is given by

$$E_I - E_0 = E_s - W_e \tag{I.12}$$

The probability per sec., $P\delta$ for the emission of an electron with energy E, an anti-neutrino with energy $E_{\bar{\nu}}$, and a photon with energy E_γ is obtained from the formula

$$P(E,E_\gamma,E_{\bar{\nu}})\delta = \delta \frac{2\pi}{\hbar} \sum_\gamma \int d\Omega_\gamma S_{\bar{\nu}} \int d\Omega_{\bar{\nu}} S_e \int d\Omega_e \left| \sum_I \frac{(F|H_\gamma|I)(I|H_{-1}|0)}{E_I - E_0} \right|^2, \tag{I.13a}$$

a well-known result of time dependent second order perturbation theory. Here P is obtained by integrating over the directions of emission of the photon, anti-neutrino and electron, by summing over the polarizations of the photon, and by summing over all possible states of the anti-neutrino and electron having the energies $E_{\bar{\nu}}$ and E. δ is the Dirac delta fn.

$$\delta = \delta(E + E_\gamma + E_{\bar{\nu}} - W), \tag{I.13b}$$

enforcing the conservation of energy (I.11a); it is used here because it prevents any confusion which might arise otherwise in obtaining the density of final states. The matrix elements in (I.13a) are given by

$$(I|H_{-1}|0) = G \sum_r C_r \, (\xi_s^* A^r \eta) \int A^r \tag{I.14a}$$

$$(F|H_\gamma|I) = e\left[\frac{2\pi\hbar c}{k}\right]^{1/2} (\xi^* \vec{\alpha} \cdot \vec{e}_k \, \xi_s), \quad \vec{p}_s = \hbar\vec{k} + \vec{p} \tag{I.14b}$$

where: $-e$ is the electron charge $(e > 0)$,

$\hbar\vec{k}$, $\vec{p}_s$, $\vec{p}$ are the momenta of the photon and electron in its intermediate and final state respectively,

$\vec{e}_k$ is the unit polarization vector for the photon,

ξ, η are the Dirac plane wave amplitudes for an electron in a positive energy state E and a neutrino in a negative

energy state $-E_{\bar{\nu}}$, ξ satisfying the Eq.

$$(c\vec{\alpha}\cdot\vec{p} + \beta mc^2)\xi = E\xi \qquad (I.15)$$

and η satisfying the same Eq. with $m = 0$ and E, $\vec{p}$ replaced by $-E_{\bar{\nu}}$, $-\vec{p}_{\bar{\nu}}$.

(I.14a) is obtained from (I.8), valid for an allowed transition. (I. 14b) is taken from Heitler (54) p. 144, Eqs. (25) and (27).

The momentum conservation in (I.14b) permits only two energies for the electron in the intermediate state; these are

$$E_s = \pm \left[(cp_s)^2 + (mc^2)^2 \right]^{1/2}, \qquad (I. 16)$$

$\vec{p}_s$ being determined by (I.14b). In (I.13a) the sum over intermediate states I, using (I.12), becomes a sum over the energies (I.16) and the spin orientations of the elctron wave amplitude ξ_s satisfying (I.15) with E replaced by E_s and $\vec{p}$ by $\vec{p}_s$

We want to calculate the probability per sec., $S(k)\,dk$ that a photon of energy $\hbar ck$ in the range $d(\hbar ck)$ is emitted during the electron emission. To obtain it, we must multiply (I.13a) by the density of states of the emitted anti-neutrino and electron and integrate over all $E_{\bar{\nu}}$ and E and also just multiply the result by the photon density of states. Thus, carrying out the integral over $E_{\bar{\nu}}$ first and converting the remaining integral over E to one over W_e defined in (I.11b), we find that

$$S(k)dk = \frac{k^2 dk}{(2\pi)^9 (\hbar c)^6} \int_{mc^2+E_\gamma}^{W} dW_e \; cp\,(W_e - E_\gamma)(W - W_e)^2 P(W_e - E_\gamma, E_\gamma, W - W_e) \qquad (I.17a)$$

where

$$cp = \left[(W_e - E_\gamma)^2 - (mc^2)^2 \right]^{1/2}.$$

The formulae (I.13) and (I.17) are used in Chapter II to calculate

the probability for radiative electron emission for an allowed transition, neglecting nuclear charge effects.

2. Radiative Positron Emission

In this subsection it is shown that the probability for radiative positron emission, to the same approximations as in subsection 1 above, can be obtained from the probability for radiative electron emission given in subsection 1 merely by replacing the electron mass m by $-m$ in the results. This fact is used in Ch. II.

For radiative positron emission an electron in a negative energy state jumps to an intermediate energy state with the emission of a photon and is then captured by the nucleus with the emission of a neutrino. The formulae (I.13) are valid for this case if we replace $\bar{\nu}$ by ν, e by $-e$ and use the matrix elements

$$(F|H_+|I) = G\sum_r C_r \,(\eta'^* A^r \xi'_s)\int A^r \qquad (I.18a)$$

$$(I|H_\gamma|0) = -e\left[\frac{2\pi\hbar c}{k}\right]^{1/2}(\xi'^*_s\,\vec{\alpha}\cdot\vec{e}_k\,\xi'), \quad -\vec{p} = \hbar\vec{k} - \vec{p}_s \qquad (I.18b)$$

where η' is the wave amplitude for a neutrino in a positive energy state E_ν and ξ' is the wave amplitude for an electron with energy $-E$ momentum $-\vec{p}$, E and $\vec{p}$ being the positron energy and momentum. Equation (I.18a) is obtained from (I.10a) (cf (I.8)) and Eq. (I.18b) from Heitler (54), p. 144, Eqs. (25) and (27). Note that the positron and photon momenta are conserved in (I.18b) exactly as in (I.14b). The wave amplitude ξ' satisfies

$$(c\vec{\alpha}\cdot(-\vec{p}) + \beta mc^2)\xi' = -E\xi' \qquad (I.19)$$

$E, \vec{p}$ being positron energy and momentum. Eq. (I.19) is the same as Eq. (I.15) with m replaced by $-$ m. η' satisfies (I.19) with m = 0, the result being the same as Eq. (I.15) with m = 0.

It is easy to see now that, by taking the complex conjugate of the matrix elements (I.18) and replacing m by $-m$, e by $-e$, one obtains the matrix elements (I.14). A glance at (I.13a) shows that it is the square of the absolute value of the sum of the matrix elements over the intermediate states which determines the desired probability and so the fact that the matrix elements (I.18) are the complex conjugate of the matrix elements (I.14) is irrelevant to the probability; also, since e is squared, its sign is irrelevant to the probability; hence, only the replacement of m by $-m$ is relevant to the probability. This is the result which we set out to prove in this subsection.

2. Radiative K Capture

In accordance with the hole theory, two types of process es are possible in the transition from the initial state of the system consisting of the nucleus N_Z and Z atomic electrons to the final state of the system consisting of a nucleus N_{Z-1}, one unoccupied K state and $Z-1$ atomic electrons, a photon and a neutrino. These processes are:

I. The K electron makes a transition to either

(a) an unoccupied discrete state or

(b) an unoccupied positive continuum state

with the emission of a photon. The electron is then captured by the nucleus with the emission of a neutrino.

II. An electron in either

(a) an occupied discrete state or

(b) an occupied negative continuum state

is captured by the nucleus with the emission of a neutrino. The K electron then jumps into the remaining hole with the emission of a photon.

Let us label the initial state of the system by 0, the final

state by F and the intermediate states by I(a), (I)b, II(a), II(b) corresponding to the processes given above.

The conservation of energy between initial and final states tells us that the available energy W is given by:

$$W = W_Z + E_K - W_{Z-1} = E_\nu + \hbar c k , \qquad (I.20)$$

where: W_Z is the energy of the nucleus N_Z,

E_K is the total energy of the K electron,

E_ν is the neutrino energy

$\hbar c k$ is the photon energy.

The probability per sec; $w_k dk$, for the emission of a photon with energy $\hbar c k$ in the range d($\hbar c k$) is given by the formula

$$w_k dk = \frac{2\pi}{\hbar} \frac{k^2 dk}{(2\pi)^3} \sum_\gamma \int d\Omega_\gamma \, S_\nu \int d\Omega_\nu \, \frac{S_0}{2}$$

$$\left| \sum_I \frac{(F|H_+|I)(I|H_\gamma|0)}{E_I - E_0} + \sum_{II} \frac{(F|H_\gamma|II)(II|H_+|0)}{E_{II} - E_0} \right|^2 , \qquad (I.21)$$

a result of second order time dependent perturbation theory. The symbol I represents all the intermediate states for the processes I(a) and I(b) above; similarly II represents the intermediate states for II(a) and II(b). The probability is obtained by summing over the polarizations of the photon and integrating over the directions of emission of the photon and neutrino.

S_ν represents the sum over all possible neutrino states having the energy E_ν and S_0 is the sum over the two K electron states, $S_0/2$ giving the average results for the capture of either K electron. The neutrino density of states does not appear because the neutrino wave fn. will be normalized per unit energy interval, automatically accounting for the density of states.

The matrix elements for the transitions are:

$$(I|H_\gamma|0) = e\left[\frac{2\pi\hbar c}{k}\right]^{1/2} \int \psi_{eI}^{*}\ \vec{\alpha}\cdot\vec{e}_k\ e^{-i\vec{k}\cdot\vec{r}}\ \psi_K\, d\vec{r}\ , \qquad (I.22a)$$

$$(F|H_+|I) = G\sum_r C_r\ (\varphi^*\, A^r\, \psi_{eI})_R\ \int A^r \qquad (I.22b)$$

where: ψ_{eI} = Dirac Coulomb wave fn. for the electron in intermediate states II(a) or I(b),

ψ_K = Dirac Coulomb wave fn. for K electron,

φ = Dirac wave fn. for neutrino with positive energy E_ν,

Dirac Coulomb wave fn. meaning a solution to the Dirac Eq. with a Coulomb potential. $(F|H_\gamma|II)$, $(II|H_+|0)$ are given by (I.22a), (I.22b) respectively with I replaced by II on the right hand side of the Equations. The expression (I.22a) is taken from Heitler (54), Eq. (21b) on p. 143, that for (I.22b) from (I.10a).

The formula (I.21) can be simplified by means of the relation

$$\sum_D \frac{(F|H_+|D)(D|H_\gamma|0)}{E_D - E_0} = \sum_{Ia}' \frac{(F|H_+|Ia)(Ia|H_\gamma|0)}{E_{Ia} - E_0} + \sum_{IIa}' \frac{(F|H_\gamma|IIa)(IIa|H_+|0)}{E_{IIa} - E_0}\ , \qquad (I.23)$$

which we shall now prove. The matrix elements on the left are given by (I.22) with I replaced by D and the sum over D means the sum over all electron wave fns ψ_{eD} belonging to <u>all</u> discrete states. Obviously, the sum over D includes the sum over the intermediate states Ia i.e. over all the unoccupied discrete states, so that in order to prove (I.23), we must prove that the sum over D for discrete states which are occupied by electrons is the same as the sum over the intermediate states IIa. Note that the process represented by D is the same as Ia except that we are now concerned with occupied states. Thus, using

$$E_0 = W_L + E_K$$

for the initial state energy, W_Z being the nuclear energy and E_K the total K electron energy, then for an occupied state we have

$$E_D = W_Z + E_B + \hbar c k ,$$

E_B being the total energy of the occupied discrete state. The corresponding intermediate state in the process II(a) has energy

$$E_{IIa} = E_K + W_{Z-1} - E_B + E_\nu .$$

Now, making use of (I.20), we find that

$$E_D - E_0 = -(E_{IIa} - E_0).$$

Furthermore, the matrix elements of D and IIa for the occupied state under consideration are the same, just interchanged; however, the processes represented by D and IIa are initiated by different electrons. In order to make the process IIa the same as D, the electron initiating IIa must be interchanged with the elctron initiating D, such an interchange producing a minus sign because the wave fn. for the system of electrons is anti-symmetric. This minus sign cancels out the difference in the energy denominators given above and hence (I.23) is proved. An argument similar to this one is given by Heitler (54), bottom of p. 213, in connection with the Compton effect. The argument given here could be made much more straightforward by using the formalism of the second quantization.

In the same way, one can prove that

$$\sum_C \frac{(F|H_+|C)(C|H_\gamma|0)}{E_C - E_0} = \sum_{Ib} \frac{(F|H_+|Ib)(Ib|H_\gamma|0)}{E_{Ib} - E_0} + \sum_{IIb} \frac{(F|H_\gamma|IIb)(IIb|H_+|0)}{E_{IIb} - E_0} \qquad (I.24)$$

where the sum over C on the left is the sum over all continuum energy states for the electron in the intermediate state.

Thus, using (I.23) and (I.24), we may write

$$w_k dk = \frac{2\pi}{\hbar} \frac{k^2 dk}{(2\pi)^3} \sum_\gamma \int d\Omega_\gamma S_\nu \int d\Omega_\nu \frac{S_0}{2} \left| \sum_I \frac{(F|H_+|I)(I|H_\gamma|0)}{E_I - E_0} \right|^2 \qquad (I.25)$$

where we now understand the sum over I to mean the sum over <u>all</u> discrete states and <u>all</u> continuum states for the electron in the intermediate state I, no matter whether these states are occupied or not. The matrix elements in (I.25) are still given by (I.22) and since we no longer need to distinguish between I and II, it is convenient to replace ψ_{eI} by ψ_E and let

$$E_I - E_0 = E - E_K + \hbar c k \qquad (I.26)$$

where E is the energy of the electron in the intermediate state.

$w_k dk$ is calculated approximately in Ch.III taking into account Coulomb effects. The radiationless K capture probability w_c is also calculated there to the same approximation and is used for the ratio $w_k dk / w_c$, such a ratio being a more reliable result than the approximate result for $w_k dk$ alone.

Let us now write down the formula for w_c which is used in Ch. III. It is obtained from first order time dependent perturbation theory, i.e.

$$w_c = \frac{2\pi}{\hbar} \frac{S_0}{2} \int d\Omega_\nu S_\nu |(F|H_+|0)|^2 , \qquad (I.27)$$

the matrix element being given by (I.22b). S_ν and S_0 have been defined already after formula (I.21); also, no neutrino density of states appears for the same reason as in (I.25).

Chapter II

Radiative Electron and Positron Emission

In this Chapter, the calculations for the probabilities of radiative electron and positron emission are shown in detail for an allowed transition. The lepton wave fns. are approximated by Dirac plane waves and hence nuclear charge effects are neglected, i.e. $Z = 0$. We shall take into account a mixture of the five beta interactions and in this sense extend the results of Bloch (36), Knipp and Uhlenbeck (36) and Chang and Falkoff (49), who have calculated these probabilities to the same approximation as mentioned above, but for pure interactions only. The results show that non-zero contributions to the probabilities appear also in the cross terms between scalar and vector interactions and in those between tensor and axial interactions.

The calculations for radiative electron emission are carried out in detail, the results for radiative positron emission being obtained from them by replacing m by -m, as shown in Ch. I.

We shall first calculate $P(E, E_\gamma, E_\nu)$ from the formula (I.13a) using the expressions (I.14) for the matrix elements and (I.12) for the energy denominator.

The sum over the intermediate states I is the same as the sum over the energies $\pm|E_s|$ and the spins of the electron in the intermediate state. It is performed by first rationalizing the energy denominator so

that E_s^2 appears, then by replacing $E_s \xi_s$ in the matrix element by $H_s \xi_s$ where

$$H_s = c\vec{\alpha}\cdot\vec{p}_s + \beta mc^2 \qquad \vec{p}_s = \vec{p} + \hbar\vec{k} \,, \tag{II.1}$$

using (I.14b), H_s being independent of s, and finally by carrying out the sum over the electron spin, i.e. the sum over the four intermediate states ξ_s belonging to $\pm|E_s|$, using the relation

$$\sum_s \xi_s \xi_s^* = 1 \,, \tag{II.2}$$

where 1 is the unit matrix. This last relation is the closure relation for the complete set of column matrices ξ_s. The result is:

$$\sum_s \frac{(\xi^*\vec{\alpha}\cdot\vec{e}_k\,\xi_s)(\xi_s^* A^r \eta)}{E_s - W_e} = \frac{1}{E_s^2 - W_e^2}(\xi^*\vec{\alpha}\cdot\vec{e}_k\,[H_s + W_e]\eta) \tag{II.3a}$$

with $$E_s^2 = c^2(\vec{p} + \hbar\vec{k})^2 + (mc^2)^2 \,. \tag{II.3b}$$

Let us now write down some relations of use in connection with operations and averages of anti-neutrino states. Using the projection operator

$$\frac{H_{\bar\nu} + E_{\bar\nu}}{2E_{\bar\nu}} \qquad H_{\bar\nu} = c\vec{\alpha}\cdot\vec{p}_{\bar\nu}$$

which is 1 for positive energy states and 0 for negative energy states and the closure relation for the η's just as in (II.2), we find the relation

$$\int d\Omega_{\bar\nu}\, S_{\bar\nu}\,(\xi^* X \eta)(\eta^* Y \xi)$$
$$= \int d\Omega_{\bar\nu}\,(\xi^* X \frac{c\vec{\alpha}\cdot\vec{p}_{\bar\nu} + E_{\bar\nu}}{2E_{\bar\nu}} Y \xi)$$
$$= 2\pi\,(\xi^* X Y \xi) \tag{II.5a}$$

for the integral over all directions of emission of the anti-neutrino and the sum over the spins of the anti-neutrino in a positive energy state $E_{\bar{\nu}}$. In obtaining (II.5), we have used the results

$$\int d\Omega_{\bar{\nu}}\ \vec{a}\cdot\vec{p}_{\bar{\nu}} = 0\ , \qquad \vec{a}\ \text{a constant vector}$$

$$\int d\Omega_{\bar{\nu}} = 4\pi \tag{II.5b}$$

In performing the sum over the two spins of the emitted electron in a positive energy state, we shall also make use of the well-known result

$$S_e\ (\xi^* X \xi) = Tr\left[X\ \frac{H+E}{2E}\right], \tag{II.6}$$

(see Heitler (54), p. 108, Eq. (14b)).

Using the relations (II.3), (II.5) and (II.6) in (I.13) and (I.14) we find:

$$S_e \int d\Omega_{\bar{\nu}}\ S_{\bar{\nu}} \left|\sum_I \frac{(F|H_\gamma|I)(I|H_{-10})}{E_I - E_0}\right|^2$$

$$= \frac{\alpha\ (2\pi\hbar c)^2\ G^2}{k\left[E_s^2 - W_e^2\right]^2} \sum_{r r'} C_r\, C_{r'} \int A^r \left(\int A^{r'}\right)^* \cdot$$

$$\cdot\ Tr\left[A^r\, A^{r'}\ (H_s + W_e)\vec{\alpha}\cdot\vec{e}_k\ \left(\frac{H+E}{2E}\right)\vec{\alpha}\cdot\vec{e}_k\ (H_s + W_e)\right], \tag{II.7a}$$

where

$$H_s = c\vec{\alpha}\cdot(\vec{p} + \hbar\vec{k}) + \beta mc^2 \qquad H = c\vec{\alpha}\cdot\vec{p} + \beta mc^2\ . \tag{II.7b}$$

A considerable amount of alegebra is required to simplify the product of the matrices appearing in the square brackets of (II.7a), especially for arbitrary values of r and r'. The algebra is given in App. D.

The result is:

$$(H_s+W_e)\vec{\alpha}\cdot\vec{e}_k\left(\frac{H+E}{2E}\right)\vec{\alpha}\cdot\vec{e}_k(H_s+W_e) =$$

$$\left\{\frac{E^2+2c^2(\vec{p}\cdot\hbar\vec{k})+(\hbar ck)^2+W_e^2}{2} - \frac{W_e}{E}\left[E^2+c^2(\vec{p}\cdot\hbar\vec{k})\right] + \frac{2W_e}{E}(c\vec{p}\cdot\vec{e}_k)^2\right\}1$$

$$+\left\{-\frac{\left[E^2-(\hbar ck)^2\right]}{2E} + \frac{2(c\vec{p}\cdot\vec{e}_k)^2}{E} - \frac{W_e^2}{2E} + W_e\right\}H$$

$$+\left\{-\left[E^2+2c^2(\vec{p}\cdot\hbar\vec{k})+(\hbar ck)^2\right]\frac{(c\vec{p}\cdot\vec{e}_k)}{E} + \frac{W_e^2}{E}(c\vec{p}\cdot\vec{e}_k)\right\}\vec{\alpha}\cdot\vec{e}_k$$

$$+\left\{-\frac{\left[E^2+c^2(\vec{p}\cdot\hbar\vec{k})\right]}{E} + 2\frac{(c\vec{p}\cdot\vec{e}_k)^2}{E} + W_e\right\}c\vec{\alpha}\cdot\hbar\vec{k} \qquad (II.8)$$

We have yet to perform the operations

$$\sum_\gamma \int d\Omega_\gamma \int d\Omega_e \qquad (II.9)$$

to find P of (I.13a). Collecting all the quantities affected by these operations in (II.7a) and (II.8), we may write

$$(II.7a) = \frac{1}{[a_0-(\vec{p}\cdot\vec{k})]^2}\Big\{B_0 + B_1(\vec{p}\cdot\vec{k}) + B_2(\vec{p}\cdot\vec{e}_k)^2 + B_3(\vec{a}_1\cdot\vec{p})$$

$$+ B_4(\vec{a}_2\cdot\vec{p})(\vec{p}\cdot\vec{e}_k)^2 + B_5(\vec{a}_3\cdot\vec{e}_k)(\vec{p}\cdot\vec{e}_k) + B_6(\vec{a}_4\cdot\vec{e}_k)(\vec{p}\cdot\vec{e}_k)(\vec{p}\cdot\vec{k})$$

$$+ B_7(\vec{a}_5\cdot\vec{k}) + B_8(\vec{a}_6\cdot\vec{k})(\vec{p}\cdot\vec{k}) + B_9(\vec{a}_7\cdot\vec{k})(\vec{p}\cdot\vec{e}_k)^2\Big\} \qquad (II.10)$$

Where the B's and a's are unaffected by the operations (II.9).

Summing (II.10) over the polarizations of the photon and integrating over the directions of emission of the electron, we find that (II.10) reduces to

$$\int d\Omega_e \Sigma_\gamma \ (\text{II}.7a) = 2\pi \int_0^\pi \frac{\sin\theta\, d\theta}{(a_0 - pk\cos\theta)^2} \Big\{ 2B_0 + 2B_1 pk\cos\theta + B_2 p^2 \sin^2\theta$$

$$+ 2B_3 \frac{\vec{a}_1\cdot\vec{k}}{k} p\cos\theta + B_4 \frac{\vec{a}_2\cdot\vec{k}}{k} p^3 \sin^2\theta\cos\theta + 2B_7 (\vec{a}_5\cdot\vec{k})$$

$$+ 2B_8 (\vec{a}_6\cdot\vec{k}) pk\cos\theta + B_9 (\vec{a}_7\cdot\vec{k}) p^2 \sin^2\theta \Big\} , \qquad (\text{II}.11)$$

as shown in App. D. In (II.11), θ is the angle between $\vec{p}$ and $\vec{k}$. If we now integrate over all directions of emission of the photon in (II.11) then all terms containing ($\vec{a}\cdot\vec{k}$) disappear and we are left with the result:

$$\int d\Omega_\gamma \int d\Omega_e \Sigma_\gamma \ (\text{II}.7a) = 8\pi^2 \int_0^\pi \frac{\sin\theta\, d\theta}{(a_0 - pk\cos\theta)^2} \Big\{ 2B_0 + 2B_1 pk\cos\theta + B_2 p^2 \sin^2\theta \Big\} \qquad (\text{II}.12)$$

The integrals required to evaluate (II.12) are given below. By substitution one can show that

$$a_0 - pk\cos\theta \propto cp\cos\theta - E \quad ;$$

hence, by expressing the fn. in the curly brackets of (II.12) in powers of $cp\cos\theta - E$ and using the integrals

$$\int_0^\pi \sin\theta\, d\theta = 2 \ , \qquad \int_0^\pi \frac{\sin\theta\, d\theta}{cp\cos\theta - E} = \frac{1}{cp} \ln\left(\frac{E-cp}{E+cp}\right) = -\frac{2}{cp} \ln\left(\frac{E+cp}{mc^2}\right),$$

$$\int_0^\pi \frac{\sin\theta\, d\theta}{(cp\cos\theta - E)^2} = \frac{2}{(mc^2)^2} \ , \qquad (\text{II}.13)$$

we can evaluate (II.12).

In connection with the results (II.13), we must remember that when m is replaced by -m, the second integral, for which the logarithm results, is unaffected.

Collecting (II.7a), (II.8), (II.10), (II.12) and (II.13) together with (I.13a), we obtain

$$P(E, E_\gamma, E_{\bar\nu}) = \frac{2\pi}{\hbar}\ \frac{32\pi^4\alpha G^2}{E\,cp\,k^3}\ \sum_{rr'} C_r C_{r'} \int A^r (\int A^{r'})^* \cdot$$

$$\cdot\Big\{ \Big[(W_e^2+E^2)\ln\Big(\frac{E+cp}{mc^2}\Big) - 2W_e cp\Big] Tr\, A^r A^{r'}$$

$$+2mc^2\Big[E\ln\Big(\frac{E+cp}{mc^2}\Big) - cp\Big] Tr\, A^r A^{r'}\beta\Big\} \qquad (II.14)$$

It is convenient at this point to notice that the corresponding result for positron emission, obtained from (II.14) by replacing m by -m everywhere but in the logarithms, is the same as (II.14) but for a sign change in the term containing $Tr\, A^r A^{r'}\beta$. This term later gives rise to the cross terms between the beta interactions. Another m will appear in the expression for S(k) from the lower limit on the integral in (I.17a) but this m is obviously the same for positron and electron emission. In conclusion, the only difference between the electron and positron emission will be a change in sign for the cross terms for $P(E, E_\gamma, E_{\bar\nu})$ and $S(k)\,dk$.

Let us proceed to calculate $S(k)\,dk$ for electron emission. From the formula (I.17a), it is seen that an integral over W_e has yet to be carried out. The required integrals are given in App. D.

In App. A it is proved that

$$Tr\, A^r A^{r'} = 4\,\delta_{rr'} \qquad (II.15a)$$

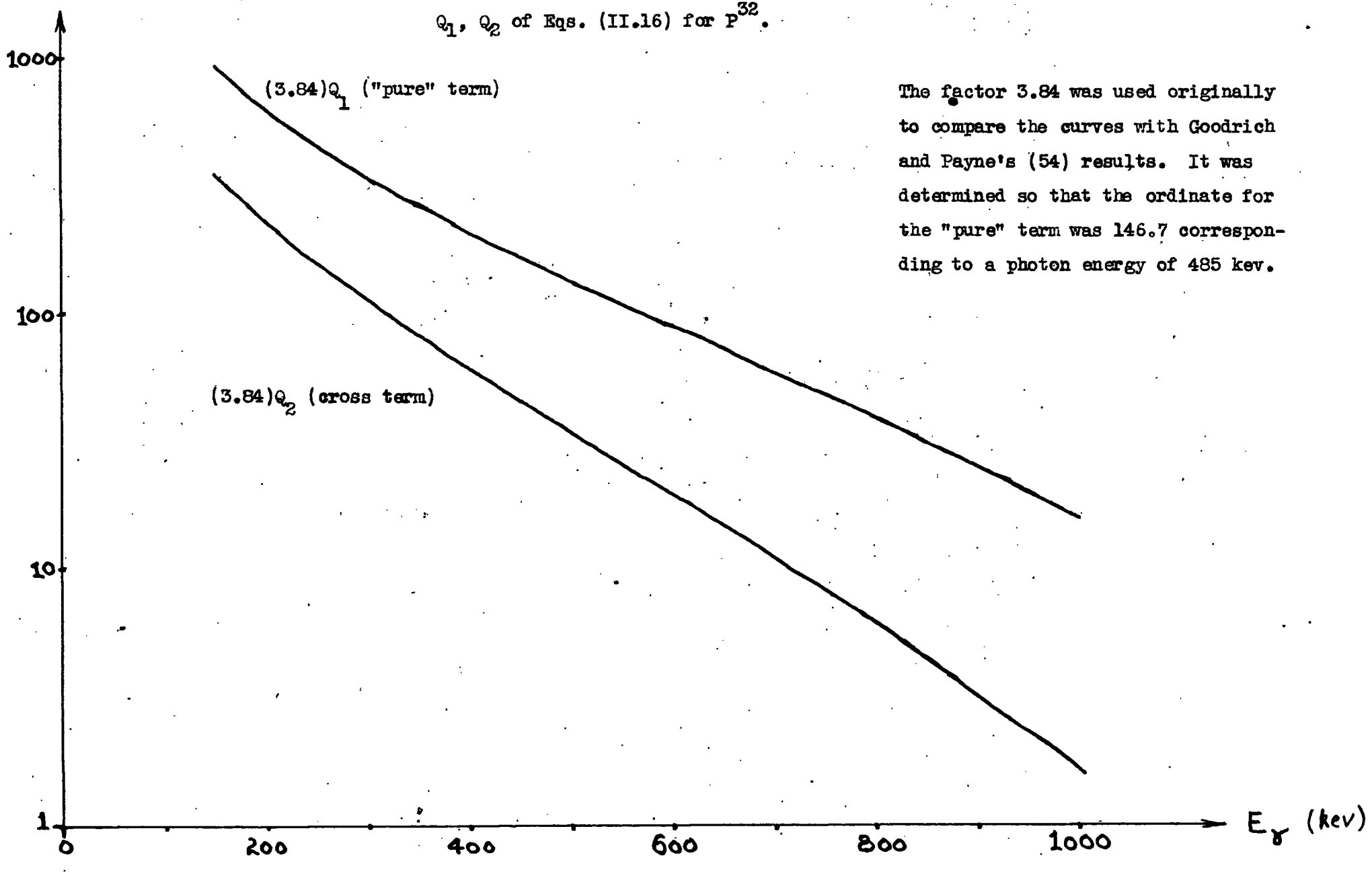
and $Tr\, A^r A^{r'}\beta = 0$ except for the cases:

$$Tr\, A^1 A^2\beta = Tr\, A^2 A^1\beta = 4 \qquad (II.15b)$$

$$Tr\, A^m A^{m+3}\beta = Tr\, A^{m+3} A^m\beta = 4 \qquad m = 3,4,5. \qquad (II.15c)$$

Graph II.1

Q_1, Q_2 of Eqs. (II.16) for P^{32}.



The factor 3.84 was used originally to compare the curves with Goodrich and Payne's (54) results. It was determined so that the ordinate for the "pure" term was 146.7 corresponding to a photon energy of 485 kev.

(II.15b) and (II.15c) show that cross-terms arise between the scalar and vector, tensor and axial interactions respectively as in the well-known case of radiationless electron emission (cf. De Groot and Tolhoek (50)).

Collecting our results together with the approximation (I.9) for the nuclear matrix elements, one obtains

$$S(k)dk = \frac{\alpha G^2 (mc^2)^4}{4\pi^4 \hbar^6 c^5} dk \cdot x$$

$$\cdot \left\{ \left[(C_S^2 + C_V^2) |\int 1|^2 + (C_T^2 + C_A^2) |\int \vec{\sigma}|^2 + C_S^2 |\int \beta\gamma_5|^2 \right] Q_1(\varepsilon, x, K) \right.$$

$$\left. + \left[2 C_S C_V |\int 1|^2 + 2 C_T C_A |\int \vec{\sigma}|^2 \right] Q_2(\varepsilon, x, K) \right\} \qquad (II.16a)$$

where: $$x = \varepsilon - K \qquad \varepsilon = \frac{W}{mc^2} \qquad K = \frac{\hbar c k}{mc^2} \qquad (II.16b)$$

$$Q_1(\varepsilon, x, K) = \frac{1}{K} \left\{ \left[\varepsilon^2 \left(\tfrac{2}{3} x^3 + x\right) - \varepsilon \left(x^4 + x^2 - \tfrac{1}{8}\right) + \tfrac{7}{15} x^5 - \tfrac{3}{8} x \right] \ln \left[x + \sqrt{x^2 - 1} \right] \right.$$

$$\left. - \left[\varepsilon^2 \left(\tfrac{11}{9} x^2 + \tfrac{4}{9}\right) - \varepsilon \left(\tfrac{7}{4} x^3 + \tfrac{1}{8} x\right) + \tfrac{689}{900} x^4 - \tfrac{1021}{1800} x^2 - \tfrac{8}{75} \right] \sqrt{x^2 - 1} \right\} \qquad (II.16c)$$

$$Q_2(\varepsilon, x, K) = \frac{4}{K} \left\{ \left[\frac{x^4}{12} + \frac{x^2}{4} + \frac{1}{32} \right] \ln \left[x + \sqrt{x^2 - 1} \right] - \left[\tfrac{25}{144} x^3 + \tfrac{55}{288} x \right] \sqrt{x^2 - 1} \right\} \qquad (II.16d)$$

The result (II.16c) agrees with that of Chang and Falkoff (49), who have carried out the integration over W_e to obtain Q_1 only, i.e. they considered pure interactions only.

As before, the results for positron emission are obtained from (II.16) by changing the sign of the cross-terms exactly as in the radiationless

case treated by De Groot and Tolhoek(50).

A graph of the curves Q_1 and Q_2 for P^{32} for which

$$W = 1.71\ mev + mc^2$$

is given in Graph (II.1). The reason for choosing P^{32} is that the radiative electron emission of this element has been the object of several experimental investigations (see the Introduction).

Chapter III

Radiative K Capture

In this Chapter the radiative K capture probability is calculated for an allowed transition taking into account an arbitrary mixture of the five beta interactions and, in addition, Coulomb effects. In order to take Coulomb effects into account, a "semi-relativistic" approximation for the solutions to the Dirac equation with a Coulomb potential is developed.

The calculations are complicated to the extent that, in order to obtain the radiative K capture probability for a given photon energy and nuclear charge Z, it is necessary to evaluate an integral graphically. The most complicated parts of the integrand involved are tabulated, by means of suitably chosen dimensionless quantities, for various photon energies and for any value of Z so that the required integral can be evaluated fairly easily for any value of Z. This integral is then evaluated explicitly to find the radiative K capture probability for $_{55}Cs^{131}$ (neglecting "screening").

Before carrying out the main calculations, we shall first derive Morrison and Schiff's (40) result for $Z=0$. The reason for doing this is that these authors have just outlined their calculations in words without showing any details explicitly. From the derivation, we can see exactly what the assumptions and procedure are.

A. Morrison and Schiff Results.

The main assumption is that the nuclear charge can be neglected; consequently, the leptons can be represented by plane waves. The K electron is represented by a plane wave with zero momentum ($E_K = mc^2$).

The required formulae for the radiative and radiationless K capture probabilities are:

$$W_k\,dk = \frac{2\pi}{\hbar}\,\frac{(W-\hbar c k)^2 k^2 dk}{(2\pi\hbar c)^3\,(2\pi)^3}\sum_\gamma \int d\Omega_\gamma\, S_\nu \int d\Omega_\nu\, \frac{S_o}{2}\left|\sum_I \frac{(F|H_+|I)(I|H_\gamma|0)}{E_I - E_o}\right|^2 \qquad (\text{III.A.1})$$

$$W_c = \frac{2\pi}{\hbar}\,\frac{W^2}{(2\pi\hbar c)^3}\int d\Omega_\nu\, S_\nu\,\frac{S_o}{2}\,|(F|H_+|0)|^2 \qquad (\text{III.A.2})$$

These expressions are taken from (I.25) and (I.27). Since plane waves are used for the leptons, the neutrino density of states has been included. The available energy W is given by

$$W = E_\nu + \hbar c k \qquad (\text{III.A.3})$$

from (I.20). From (I.22), we see that the necessary matrix elements are given by

$$(I|H_\gamma|0) = e\left[\frac{2\pi\hbar c}{k}\right]^{1/2}(\xi^*\vec{\alpha}\cdot\vec{e}_k\,\xi_o) \qquad \vec{p}+\hbar\vec{k}=0 \qquad (\text{III.A.4a})$$

$$(F|H_+|I) = G\int A^r\,(\eta^* A^r \xi), \qquad (\text{III.A.4b})$$

where: A^r is one of the five beta interactions

$\xi, \vec{p}$ are the wave amptitude and momentum for the electron in the intermediate state.

ξ satisfies (I.15), ξ_o the same Eq. with $\vec{p}=0$ and η the same Eq. with $m=0$. From (III.A.4a), the intermediate electron energies possible are

$$E = \pm\sqrt{(\hbar c k)^2 + (mc^2)^2} \qquad (\text{III.A.5})$$

Let us evaluate W_c first using the matrix element (III.A.4b) with ξ replaced by ξ_o. The sum over the two neutrino states belonging to the

energy E_ν , the sum over the two K electron states and the integral over the neutrino directions are carried out by standard procedures (see Heitler (54)). The required relations are:

$$\frac{S_0}{2}\int d\Omega_\nu\, S_\nu\,(\xi_0^* X \eta)(\eta^* Y \xi_0)$$

$$= \frac{S_0}{2}\int d\Omega_\nu\,(\xi_0^* X\, \frac{c\vec{\alpha}\cdot\vec{p}_\nu + E_\nu}{2E_\nu} Y \xi_0)$$

$$= \pi\, S_0\,(\xi_0^* X Y \xi_0)$$

$$= \pi\, Tr\, XY\left(\frac{\beta mc^2 + mc^2}{2mc^2}\right)$$

$$= \frac{\pi}{2}\, Tr\, XY\,(1+\beta). \qquad \text{(III.A.6)}$$

Using this result with

$$A^r A^{r*} = 1 \qquad \text{(III.A.7)}$$

in (III.A.2), (III.A.4), one obtains

$$w_c = \frac{2\pi}{\hbar}\,\frac{G^2 W^2}{(2\pi)^2(\hbar c)^3}\,\left|\int A^r\right|^2 . \qquad \text{(III.A.8)}$$

$w_k dk$ is obtained as follows. The sum over intermediate states in (III.A.1) is carried out first by summing over the two spins of the electron having the two energies (III.A.5). In order to do this the energy denominator, given by (I.26) with $E_K = mc^2$ is rationalized so that E^2 appears i.e. by multiplying numerator and denominator by $E-(\hbar ck - mc^2)$; then, wherever $E\xi$ appears in the numerator, it is replaced with $H\xi$ where

$$H = c\vec{\alpha}\cdot(-\hbar\vec{k}) + \beta mc^2 ,$$

using the momentum conservation in (III.A.4a); finally, the sum is carried out using

$$\sum_{\substack{\text{Energy}\\ \text{spins}}} \xi\xi^* = 1$$

, the unit matrix.

The result is:

$$\sum_I \frac{(F|H_+|I)(I|H_\gamma|0)}{E_I - E_0} = \left[\frac{2\pi\hbar c}{k}\right]^{\frac{1}{2}} \frac{Ge\int A^r}{2\hbar c k\, mc^2} \times$$

$$\times \left\{ (\eta^* A^r H \vec{\alpha}\cdot\vec{e}_k \xi_0) - (\hbar c k - mc^2)(\eta^* A^r \vec{\alpha}\cdot\vec{e}_k \xi_0) \right\} .$$

Squaring this result and performing the K electron and neutrino operations with the help of (III.A.6), one obtains a result independent of photon directions and polarizations so that the photon operations merely introduce a factor $2(4\pi)$. The result is, using (III.A.7),

$$W_k\, dk = \frac{2\pi}{\hbar} \frac{\alpha G^2 \left|\int A^r\right|^2}{\pi (2\pi)^2 (\hbar c)^3} \frac{(W - \hbar c k)^2 \hbar c k\, d(\hbar c k)}{mc^2} \qquad (\text{III.A.9})$$

and so, from (III.A.8) and (III.A.9), we find Morrison and Schiff's result:

$$\frac{W_k\, dk}{W_c} = \frac{\alpha}{\pi}\left(\frac{W}{mc^2}\right)^2 (1-\varepsilon)^2 \varepsilon\, d\varepsilon , \qquad \varepsilon = \frac{\hbar c k}{W} \qquad (\text{III.A.10})$$

This ratio can also be obtained from the results in Section III.B, which take Coulomb effects into account, by setting $Z = 0$.

However, the value of the ratio so obtained is smaller by a factor two than that given by the Morrison and Schiff formula (III.A.10). It would thus appear that the Morrison and Schiff formula is not quite correct even for the case $Z = 0$, owing to the very crude assumptions on which it is based.

B. Radiative and Radiationless K Capture.

In this Section, explicit expressions for the matrix elements appearing in $w_k dk$ and w_c of (I.21) and (I.27) are presented, and the sums over the spins and polarization along with the integrals over the solid angles are performed. As a result, a simpler expression for $w_k dk$ and a final expression for w_c are obtained.

Calculation of W_c

The calculation of W_c is outlined below. Although the procedure followed is essentially the same as that of De Groot and Tolhoek (50), it is presented here mainly as an introduction to the more complicated calculation of $w_k dk$.

From (I.27), the probability for the radiationless electron capture per sec. is given by

$$w_c = \frac{2\pi}{\hbar} S_\nu \int d\Omega_\nu \frac{S_0}{2} |(F|H_+|0)|^2 \qquad (\text{III.B.1})$$

where

$$(F|H_+|0) = G \sum_r C_r (\varphi^* A^r \psi_K)_R \int A^r \qquad (\text{I.10}) \qquad (\text{III.B.2})$$

ψ_K, φ being the wave fns. for the K electron and neutrino, evaluated at the nuclear radius R.

The choice of the electron and neutrino wave fns. is important, the same type of choice being used in the calculation of $w_k dk$. For the K electron, the only wave fns. possible are those from App. C for which $\ell = 0, j = \frac{1}{2}$

and $\mu = \pm \frac{1}{2}$, corresponding to the two spin orientations. The K electron wave fns. will be approximated by setting the small radial component G equal to zero. Thus

$$\psi_K(\vec{R}) = Y_0^0 \frac{F_K^+(R)}{R} \xi_m , \qquad m = 1, 2 \qquad (\text{III.B.3})$$

where:

ξ_m is a four component column vector with unity in its m^{th} row and zeros elsewhere,

$Y_0^0 = \frac{1}{\sqrt{4\pi}}$

$F_K^+(R)/R$ supplies the dependence on the nuclear radius.

The neutrino wave fn. belonging to the continuum is obtained by the following argument. We look for those wave fns. which are largest at the nucleus. The large and small radial components of the neutrino wave fn., denoted by f and g respectively, vary at most as $\left(\frac{pR}{\hbar}\right)^\lambda$ (App. C) where $\lambda = j + \frac{1}{2}$ for the neutrino ($Z = 0$). At the nuclear radius then, the well-known approximation

$$\frac{pR}{\hbar} << 1 , \qquad (\text{III.B.4})$$

tells us that the largest wave fns. are those for which j is smallest i.e. $j = \frac{1}{2}$ and hence $\kappa = \pm 1$. It can be shown (cf. Marshak (42)) that at the nucleus f^+ varies as $\frac{pR}{\hbar}$ whereas g^+ varies as $\left(\frac{pR}{\hbar}\right)^2$ so that g^+ may be neglected with respect to f^+. On the other hand, g^- varies as f^+, and f^- as g^+ so that we can also neglect f^- with respect to g^- . Hence, the neutrino wave fns. used here, taking into account all neglections mentioned, are;

$$\varphi_m(R) = Y_0^0 \, N \, \xi_{m'} \qquad (\text{App. C.}) \qquad (\text{III.B.5})$$

where

$m' = 1, 2, 3, 4$ corresponding to $j = \frac{1}{2}$, $\kappa = +1$, $\mu = \pm \frac{1}{2}$ $(\ell = 0)$

and $j = \frac{1}{2}$, $\kappa = -1$, $\mu = \pm \frac{1}{2}$ $(\ell = 1)$,

$$N = \frac{L}{R}\begin{pmatrix} f^+ & 0 \\ 0 & f^+ \\ & & g^- \\ & & & g^- \end{pmatrix}$$

$$\left|\frac{f^+}{R}\right|^2 = \left|\frac{g^-}{R}\right|^2 = \frac{E_\nu^2}{\pi\hbar^3 c^3}$$

Note that the sum S_ν appearing in (III.B.1) denotes the sum over these four states.

The matrix element appearing in (III.B.2) now has the form,

$$(\varphi^* A^r \psi_K)_R = Y_0^{0\,2}\,\frac{F_K^+(R)}{R}\quad(\xi_{m'}^*, N^* A^r \xi_m),$$

using (III.B.3) and (III.B.5). Substituting this expression into (III.B.2) and (III.B.1.) and carrying out the sums S_0 and S_ν with the help of the relations:

$$\sum_{m=1}^{2} \xi_m \xi_m^* = \frac{1+\beta}{2} \qquad \text{(III.B.6)}$$

$$\sum_{m'=1}^{4} \xi_{m'}^* X \xi_{m'} = Tr\, X\ ,$$

one obtains

$$w_c = \frac{\pi}{\hbar}\int d\Omega_\nu\, Y_0^{0\,4}\left|\frac{F_K^+}{R}\right|^2 G^2 \sum_{rr'} C_r C_{r'} \int A^r (A^{r'})^* \times$$

$$\times\, Tr\; N^* A^r \frac{1+\beta}{2} A^{r'*} N. \qquad \text{(III.B.7)}$$

This result is independent of the neutrino direction of emission, so that the integral over the solid angle merely contributes a factor 4π.

Using the relations

$$A^{r\,*} = A^r$$

$$Tr\, X A^{r'} N = Tr\, A^{r'} N X \qquad \text{(III.B.8)}$$

$$NN^* = \frac{E_\nu^2}{\pi\hbar^3 c^3} \qquad \text{(see (III.B.5))}$$

one can reduce the trace operation in (III.B.7) to the evaluation of

$$Tr\, A^{r'} A^r \left(\frac{1+\beta}{2}\right).$$

Now, from App. A,

$$Tr\ A^{r\prime}A^{r} = 4\delta_{r'r} \qquad (A^{r})^2 = 1$$

(III.B.10a)

and $$Tr\ A^{r\prime}A^{r}\beta = 0$$

except for cross-terms between the scalar and vector, tensor and axial interactions, for which

$$Tr\ A^{1}A^{2}\beta = Tr\ A^{2}A^{1}\beta = 4$$

$$Tr\ A^{n+3}A^{n}\beta = Tr\ A^{n}A^{n+3}\beta = 4 \qquad n = 3,4,5$$

(III.B.10b)

respectively.

Substituting the above results into (III.B.7) and making use of the relations (I.4) and (I.9), one obtains

$$W_C = \frac{E_\nu^2}{2\pi\hbar^4 c^3}\ \frac{|F_K^+(R)|^2}{R^2}\ G^2\left\{(C_S+C_V)^2|\int 1|^2 + (C_T+C_A)^2|\int\vec{\sigma}|^2 + C_P^2|\int\beta\gamma_5|^2\right\} \qquad (III.B.11)$$

This result may be obtained from De Groot and Tolhoek's (50) Eq. (61) by multiplying their result by 4π to include the integral over neutrino directions and by $\frac{1}{2}$ to include the averaging factor for the K electrons.

Calculation of $w_k\,dk$

The radiative K capture probability per second is obtained from the formula

$$w_k\,dk = \frac{2\pi}{\hbar}\,\frac{k^2\,dk}{(2\pi)^3}\sum_{\sigma}\int d\Omega_\gamma \int d\Omega_\nu\, S_\nu\, \frac{S_0}{2}\,\left|\sum_I \frac{(F|H_+|I)(I|H_\gamma|0)}{E_I - E_0}\right|^2 , \qquad (III.B.12)$$

given by Eq. (I.25). The summation over I denotes the sum over all the discrete and positive and negative continuum states corresponding to all the solutions of the Dirac Eq. for the electron in the intermediate state. In (III.B.12) the energy denominator is given by (I.26) and the matrix elements by (I.22). In the following, we shall label the wave fn ψ_{eI}, appearing in (I.22), by ψ_E.

The K electron and neutrino wave fns. are given by (III.B.3) and (III.B.5) respectively.

The wave fns. possible for the electron in the intermediate state are obtained as follows. It is assumed that at the nucleus,

$$\frac{pR}{\hbar} \ll 1 \qquad (III.B.13)$$

as before so that, using a similar argument as in (III.B.4) for the neutrino, we find from App. C that the largest wave fn. is that for which $j = \frac{1}{2}$, $K = \pm 1$. We shall also assume that the largest components of the electron wave fns belonging to these quantum numbers are F^+, G^- and shall neglect G^+, F^-. As in radiationless transitions, the components of the lepton wave fns. which are retained here are those whose angular dependence is given by the spherical harmonic of order zero and those neglected are theones whose angular dependence

is given by the spherical harmonic of order one.

A word about the assumptions is necessary. For radiationless transitions, the above assumptions are valid and give good agreement with experimental results. It must be realized, however, that radiative processes are second order processes, including a summation over the intermediate states of an electron which can have energies up to infinity, so that the assumption (III.B.13) is not always true. In the radiationless case, it can be shown that the components of the wave fns. neglected supply a negligible contribution to the probability. It does not follow that this is still the case for the radiative transitions and a detailed investigation of this point should be made. Of course, the assumptions made may be regarded as defining, by analogy with the radiationless case, an allowed radiative beta transition.

We shall use

$$\psi_E = \frac{Y_0^\circ}{r} \begin{pmatrix} F_E^+ & & 0 & \\ & F_E^+ & & G_E^- \\ 0 & & G_E^- & \end{pmatrix} \xi_s \,, \qquad s = 1, 2, 3, 4 \qquad \text{(III.B.14)}$$

these four wave fns. all belonging to the same energy E in the discrete or continuum case (for the K state $G^- = 0$).

Expressions for the matrix elements appearing in (III. B.12) may now be given. From Eqs. (III.B.3), (III.B.14), (I.22) we find that

$$\int \psi_E^* \, \vec{\alpha} \cdot \vec{e}_k \, e^{-i\vec{k}\cdot\vec{r}} \, \psi_K \, d\vec{r} = \xi_s^* \, M_{EK} \, \vec{\alpha} \cdot \vec{e}_k \, \xi_m \qquad \text{(III.B.15a)}$$

where

$$\left.\begin{aligned} M_{EK} &= \begin{pmatrix} A_{EK} & & 0 & \\ & A_{EK} & & B_{EK} \\ 0 & & B_{EK} & \end{pmatrix} \\ A_{EK} &= \int_0^\infty F_E^{+*} \, \frac{\sin kr}{kr} \, F_K^+ \, dr \\ B_{EK} &= \int_0^\infty G_E^{-*} \, \frac{\sin kr}{kr} \, F_K^+ \, dr \end{aligned}\right\} \qquad \text{(III.B.15b)}$$

use being made of the integral

$$\int e^{-i\vec{k}\cdot\vec{r}}\, d\Omega = 4\pi \frac{\sin kr}{kr} \quad , \quad Y_o^{o\,2} = \frac{1}{4\pi}$$

in obtaining (III.B.15). Similarly, from Eqs. (III.B.5) and (III.B.14)

$$(\varphi^* A^r \psi_E)_R = Y_o^{o\,2}\, \xi_{m'}^*\, N^* A^r T_E\, \xi_s \qquad \text{(III.B.16a)}$$

where

$$T_E = \frac{1}{R} \begin{pmatrix} F_E^+(R) & 0 & 0 & 0 \\ 0 & F_E^+(R) & 0 & 0 \\ 0 & 0 & G_E^-(R) & 0 \\ 0 & 0 & 0 & G_E^-(R) \end{pmatrix} \qquad \text{(III.B.16b)}$$

If we now substitute the results (III.B.16) and (III.B.15) into (III.B.12) and carry out the summation over the four intermediate electron states belonging to the energy E, using

$$\sum_{s=1}^{4} \xi_s\, \xi_s^* = 1 \,,$$

the unit matrix, we get

$$\sum_I \frac{(F|H_+|I)(I|H_\gamma|0)}{E_I - E_0} = e\left[\frac{2\pi\hbar c}{k}\right]^{1/2} Y_o^{o\,2}\, G \sum_r C_r \int A^r \cdot$$

$$\cdot\, \xi_{m'}^*\, N^* A^r Q\, \vec{\alpha}\cdot\vec{e}_k\, \xi_m \,, \qquad \text{(III.B.17a)}$$

where

$$Q = \sum_E \frac{T_E\, M_{EK}}{E - E_K + \hbar c k} \,, \qquad \text{(III.B.17b)}$$

which, from (III.B.16b) and (III.B.15b), is a diagonal matrix.

Squaring the sum of the matrix elements in (III.B.17) and summing over the two K electron states and the four neutrino states with the help of (III.B.6) one obtains

$$S_\nu \frac{S_0}{2} \left| \sum_I \frac{(F|H_1|I)(I|H_2|0)}{E_I - E_0} \right|^2$$

$$= e^2 \frac{2\pi\hbar c}{k} \frac{\gamma_0^{0\,4} G^2}{2} \sum_{rr'} C_r C_{r'} \int A^r \left(\int A^{r'}\right)^* \times$$

$$\times Tr \left[N^* A^r Q \vec{\alpha}\cdot\vec{e}_k \left(\frac{1+\beta}{2}\right) \vec{\alpha}\cdot\vec{e}_k \; Q^* A^{r'*} N \right] \qquad \text{(III.B.18)}$$

Let us now obtain an expression for the trace in (III.B.18). Using the result that α_i anticommutes with β and $(\vec{\alpha}\cdot\vec{e}_k)^2 = 1$, one can show that

$$\vec{\alpha}\cdot\vec{e}_k \left(\frac{1+\beta}{2}\right) \vec{\alpha}\cdot\vec{e}_k = \frac{1-\beta}{2} \qquad \text{(III.B.19)}$$

Also, since

$$\frac{1-\beta}{2} = \begin{pmatrix} 0 & 0 \\ 0 & \begin{matrix} 1 & 0 \\ 0 & 1 \end{matrix} \end{pmatrix}$$

and Q is diagonal,

$$Q \left(\frac{1-\beta}{2}\right) Q^* = |L|^2 \left(\frac{1-\beta}{2}\right) \qquad \text{(III.B.20)}$$

where

$$L = \frac{1}{R} \sum_E \frac{G_E^-(R) \int_0^\infty G_E^-(r)^* \frac{\sin kr}{kr} F_\kappa^+(r)\, dr}{E - E_\mu + \hbar c k} , \qquad \text{(III.B.21)}$$

from (III.B.17b), (III.B.16b) and (III.B.15b). With the help of the relations given in (III.B.8), one can now show that the trace operation in (III.B.18) is reduced to the evaluation of

$$Tr\; A^{r'} A^r \left(\frac{1-\beta}{2}\right),$$

which is obtained from (III.B.10).

The above results are independent of the directions of emission of the photon and neutrino and also independent of the polarization of the photon; hence the remaining operations $\sum_{\gamma} \int d\Omega_{\gamma} \int d\Omega_{\nu}$ to obtain $w_k\, dk$ merely multiply our results by a factor $2(4\pi)^2$.

Collecting all the results together into (III.B.12) and using the substitutions (I.4) and (I.9), one obtains

$$w_k\, dk = \frac{\alpha\, k\, dk}{\pi^2 \hbar^2 c} (W - \hbar c k)^2 |L|^2 G^2 \left\{ (C_S - C_V)^2 |\int 1|^2 + (C_T - C_A)^2 |\int \vec{\sigma}|^2 + C_P^2 |\int \beta\gamma_5|^2 \right\} \quad \text{(III.B.22a)}$$

where,

$$\alpha = \frac{e^2}{\hbar c} \approx \frac{1}{137}$$

$$W - \hbar c k = E_\nu \quad \text{(I.20)} \quad \text{(III.B.22b)}$$

C. EXPRESSION FOR L

The expression for the radiative K capture probability obtained in (III.B.22) contains in one factor the same photon energy dependence as in Morrison and Schiff's expression (III.A.10) and in the remaining factor an additional dependence due to the presence of $|L|^2$, where L, as defined in (III.B.21), is given by

$$L = \frac{1}{R} \sum_E \frac{G_E^-(R)\, B_{EK}}{E - E_K + \hbar c k} \quad , \qquad (\text{III.C.1a})$$

$$B_{EK} = \int_0^\infty G_E^{-*}(r)\, \frac{\sin kr}{kr}\, F_K^+(r)\, dr \quad . \qquad (\text{III.C.1b})$$

The summation dummy E runs over all possible energy values for the intermediate electron, i.e. all negative continuum, discrete, and positive continuum values.

It is the object of this Section to evaluate the radial integral B_{EK} and to write out explicitly the summand of (III.C.1a). In performing the "sum" over E, we shall neglect the contribution of discrete states and approximate $G_E^-(R)$. Several arguments are presented to justify these approximations in the hope that everything up to the end of this Section can be considered acceptable for an allowed transition. A more questionable assumption is then made in Section III.E where L is calculated in what we shall call a semi-relativistic approximation.

We shall neglect the summation over discrete levels for the following reasons. First, the Morrison and Schiff results of Section III.A make use of intermediate electron wave functions belonging to the continuum only. Second, it is shown in App. C that even when the nuclear charge is taken into account, G_E^- is zero for a discrete state in the non-relativistic limit. Thus, we may conclude that the greatest contribution to L should come from the "summation" over the continuum levels.

Our neglection of the discrete sum means that we are disregarding those intermediate states arising when the K electron jumps to an empty discrete level with the emission of a photon and is then captured with the emission of a neutrino and those when a bound electron, other than the K electron is captured with the emission of a neutrino, the remaining hole being filled by the K electron with the emission of a photon. These transitions are labelled I(a) and II(a) in Ch.I.

Let us now evaluate B_{EK} exactly. The integrals required for the electron in intermediate discrete state are evaluated in App. B and will not be discussed further. The radial wave fns. for the electron in an intermediate continuum state and a K electron, as obtained in Appendix C., may be written in the form:

$$F_K^{+}(r) = N_0(Z,E_K)\, r^{\lambda} e^{-\frac{\mu r}{\hbar}} \qquad (III.C.2a)$$

where

$$N_0(Z,E_K) = \left[\frac{Z\alpha(mc^2+E_K)}{\Gamma(2\lambda+1)\,\hbar c}\right]^{1/2}\left(\frac{2\mu}{\hbar}\right)^{\lambda} \qquad (III.C.2b)$$

$$c\mu = \sqrt{(mc^2)^2 - E_K^2} = Z\alpha mc^2 \qquad E_K = mc^2\sqrt{1-(Z\alpha)^2}$$

and $$G_E^{-*}(r) = \delta\sqrt{|E|-\delta mc^2}\; N(Z,E)\, e^{i\chi_-}\, r^{\lambda} \times \qquad (III.C.3a)$$

$$\times\left\{\left(\lambda + i\frac{Z\alpha E}{cp}\right)e^{\frac{ipr}{\hbar}} F\left(\lambda - i\frac{Z\alpha E}{cp}, 2\lambda+1; -\frac{2ipr}{\hbar}\right) - \left(K - i\frac{Z\alpha mc}{p}\right)e^{-\frac{ipr}{\hbar}} F\left(\lambda + i\frac{Z\alpha E}{cp}, 2\lambda+1; \frac{2ipr}{\hbar}\right)\right\}$$

where

$$N(Z,E) = \left[4\pi\hbar c^2 p\right]^{-1/2} \frac{\left|\Gamma\left(\lambda + i\frac{Z\alpha E}{cp}\right)\right|}{\Gamma(2\lambda+1)}\left(\frac{2p}{\hbar}\right)^{\lambda} e^{\frac{\pi Z\alpha E}{2cp}} \qquad (III.C.3b)$$

and $\delta = +1$ for $E \geq mc^2$, $\delta = -1$ for $E \leq -mc^2$.

Substitution of the expressions (III.C.2) and (III.C.3) in (III.C1a) provides one with integrals of the type given in App. B, Eq. (B.20) and evaluated exactly there. Using the result (B.24) along with the definition

$$u(k) = \frac{1}{k}\,\frac{\Gamma(2\lambda+1)\,\hbar^{2\lambda}}{[\mu+i(p-\hbar k)]^{2\lambda}}\,F\left(\lambda+i\frac{Z\alpha E}{cp},\,2\lambda,\,2\lambda+1;\,\frac{2ip}{\mu+i(p-\hbar k)}\right) \qquad (III.C.4a)$$

one finds that

$$B_{EK} = -\delta\sqrt{|E|-\delta mc^2}\;N N_0\, e^{i\chi_-}\,\frac{1}{2i}\left\{(\lambda+i\frac{Z\alpha E}{cp})[u^*(k)+u^*(-k)]+\right.$$

$$\left.+(\kappa-i\frac{Z\alpha mc}{p})[u(k)+u(-k)]\right\}. \qquad (III.C.4b)$$

In order to obtain an expression for G_E^- at the nuclear radius, we shall assume that

$$\frac{pR}{\hbar} \ll 1,$$

as mentioned previously. With this assumption we need retain only the lowest power of $pR/\hbar$ in the expansion of $G_E^-(R)$ in (III.C,3a). Thus

$$\frac{G_E^-(R)}{R} = \delta\sqrt{|E|-\delta mc^2}\;N(Z,E)\,e^{-i\chi_-}\left\{\lambda-\kappa-i\frac{Z\alpha(E+mc^2)}{cp}\right\}R^{\lambda-1}, \qquad (III.C.5)$$

where N is given by (III.C.3b)

Assembling the results (III.C.4) and (III.C.5) into (III.C.1a) with the help of the definition

$$Q(E) = \frac{1}{2i}\left\{\lambda-\kappa-i\frac{Z\alpha}{cp}(E+mc^2)\right\}\left\{(\lambda+i\frac{Z\alpha E}{cp})[u^*(k)+u^*(-k)]+\right.$$

$$\left.+(\kappa-i\frac{Z\alpha mc}{p})[u(k)+u(-k)]\right\} \qquad (III.C.6)$$

one obtains

$$L = -N_0 R^{\lambda-1}\left\{\int_{-\infty}^{-mc^2}+\int_{mc^2}^{\infty}\right\}\frac{dE\;(|E|-\delta mc^2)\,N^2(Z,E)\,Q(E)}{E-E_K+\hbar ck}, \qquad (III.C.7)$$

i.e. the integrand is the same for each integral with the exception that δ is -1 for the first and $\delta=+1$ for the second. Because of the change in the sign of δ, a <u>different</u> fn. of E is integrated over the negative range compared to that over the positive range. This fact makes it difficult to apply contour methods for the evaluation of L. Note also that no density of intermediate states is required in the integrand since our continuum wave fns. are normalized per unit energy interval.

Using the relation

$$\lambda = \sqrt{\kappa^2 - (z\alpha)^2}$$

and the energy-momentum relation, it is easy to show that Q(E) is real.

Let us now write the integral over the negative continuum in (III.C.7) as one over the positive continuum. Using $|E| = \delta E$, one readily obtains

$$L = -N_0 R^{\lambda-1} \int_{mc^2}^{\infty} dE \left[\frac{(E-mc^2)}{E - E_K + \hbar c k} N^2(z,E) Q(E) - \frac{(E+mc^2)}{E + E_K - \hbar c k} N^2(z,E) Q(-E) \right] . \qquad (III.C.8)$$

This is the expression for L which we shall use in the next Section where L is calculated in a semi-relavistic approximation.

The integrand of (III.C.8) is finite everywhere except possibly at those points where the energy denominators vanish. No such zeros will occur over the energy range mc^2 to ∞ provided

$$|E_K - \hbar c k| < mc^2 .$$

This relation restricts the photon energy to the range

$$0 \leq \hbar c k \leq E_K + mc^2 . \qquad (III.C.9a)$$

besides the range

$$0 \leq \hbar c k < W \qquad (III.C.9b)$$

which already exists physically because the photon energy cannot exceed the available energy W for the transition. Since for Cesium,

$$W = 320 \text{ kev},$$

from Saraf (54), the restriction (III.C.9a) is automatically satisfied; hence, no difficulties in the calculation of L for Cesium arise from the energy denominators. If, on the other hand, it happenad that

$$W > E_K + mc^2 ,$$

then poles would be present and the integration over such poles would have to be carried out using the Cauchy principal value for the integral.

D. CALCULATION OF L IN A SEMI-RELATIVISTIC APPROXIMATION

The understanding of this Section and the purpose of the next may be enhanced by the following outline.

The solutions to the Dirac Eq. with a Coulomb potential are given in Appendix C. These solutions consist of four component column matrices where each component has an angular dependent factor given by a spherical harmonic and a radial dependent factor given by either $F(r)/r$ or $G(r)/r$. In the following we shall refer to just F and G as the radial solutions to the Dirac Eq. For positive continuum energy states, the F's are the "large"radial solutions and the G's the "small" in the sense that the G's go to zero as the energy E approaches mc^2 whereas the F's do not. On the other hand, for negative continuum energy states, the G's are the "large" and the F's the "small" radial solutions in the sense that the F's go to zero as E approaches $-mc^2$ whereas the G's do not. We shall also speak of the radial solutions to the Schrodinger Eq. with a Coulomb potential; as above, such solutions, when divided by r, given the complete radial dependence of the Schrodinger wave fns.

Rules are formulated in Appendix C which, when applied to the large normalized radial solutions of the Dirac Eq. give the corresponding normalized radial solutions to the Schrodinger Eq., and when applied to the small radial solutions give zero. The rules are formulated for both discrete and continuum energy values. After a discussion below of the salient features of these rules, it is shown that in a non-relativistic approximation i.e. one in which these rules are applied to the radial solution, only the negative energy continuum levels (positrons) contribute to L in Eq. (III.C.8).

L, as obtained in the last Section, is too complicated to be evaluated by any simple means. It is not even easy to determine roughly how the integrand varies as a fn. of E except that it is finite everywhere. In order to study this question and also to evaluate the integral, it was decided to plot the integrand (for $Z = 55$, i.e. Cesium neglecting screening) up to some value of E large enough so that the remaining area to infinity could be evaluated by a rapidly convergent series, the main area being obtained graphically. However, even to plot the integrand within a reasonable length of time, it is necessary to make some approximations. It appears that the most consistent and simplest way of doing this, at the same time including the positive energy contribution to the integrand, is to make a "semi-relativistic" approximation based on the above mentioned rules and to adopt as a criterion for a good approximation the requirement that the normalization of the wave fns. be not unduly affected. A plausible argument is given in Appendix C to show that this requirement is satisfied for the semi-relativistic approximation used.

A further check on the validity of the semi-relativistic approximation is provided in the next section. It arises from the fact (discussed below) that when λ is $\frac{1}{2}$ - for which value $Z = 119$, a fairly simple <u>exact</u> expression for the integrand of L in (III.C.8) can be obtained. In the next Section, the exact integrand is plotted for this extremely high Z value and compared with graphs of the integrand using:

(a) The semi-relativistic approximation for the same Z value and

(b) A non-relativistic approximation for Z = 119, obtained by applying the rules mentioned above to the radial solutions of the Dirac Eq. which appear in L.

Definite agreement exists between the general shape of the "exact" and "semi-relativistic" curves, but for high energies there is quite a large discrepancy between the ordinates. It would be surprising if this discrepancy still existed to the same extent in the case of Cesium whose nuclear charge is less than half the value considered; however, a proper investigation of this point appears to be quite complicated and has not been carried out. On the other hand, the "non-relativistic" integrand does not have the same general shape as the other two curves and consequently it appears that a considerable error would be present in the results if the "non-relativistic" approximation had been used.

Difficulties in Evaluating L

Let us consider some of the difficulties in evaluation L without making any approximations outside of those made in the previous Section.

The main difficulty is finding some convenient expression for the hypergeometric fns. of the form

$$F(\lambda+iy, 2\lambda, 2\lambda+1 ; z) \qquad (\text{cf. (III.C.4a)}) \qquad (\text{III.D.1a})$$

where

$$y = \frac{Z\alpha E}{cp} \qquad z = \frac{i2p}{\mu + i(p-\hbar k)} \qquad cp = +\sqrt{E^2-(mc^2)^2} \qquad (\text{III.D.1b})$$

The usual expansion of (III.D.1a) in powers of does not converge for $|z|>1$ (see(B.12)), a situation which occurs for large p ; thus, several expansions of (III.D.1a) over the range of p from 0 to ∞ are required if we try to calculate L (or just plot the integrand) by means of series. Whether the resulting series converge rapidly or not, has not been investigated.

Besides the series for the hypergeometric fn. a series is also necessary for the complex gamma fn. appearing in (III.C.3b).

A procedure for evaluating L for <u>small</u> photon energies is to first expand $\sin kr/kr$ appearing in the radial integral B_{EK} (III.C.1b) into a series of powers of k before carrying out the radial integral. Thus, substituting the series

$$\frac{\sin kr}{kr} = \sum_{n=0}^{\infty} (-1)^n \frac{(kr)^{2n}}{(2n+1)!}$$

into the required type of radial integral

$$\int_0^{\infty} r^{2\lambda} e^{-(\mu+i\beta)\frac{r}{\hbar}} \frac{\sin kr}{kr} F\left(\lambda+iy, 2\lambda+1; \frac{2i\beta r}{\hbar}\right) dr \qquad (III.D.2a)$$

(see (B.20)) gives

$$(III.D.2a) = \sum_{n=0}^{\infty} \frac{(-1)^n k^{2n}}{(2n+1)!} \frac{\Gamma(2\lambda+2n+1)}{\left[\frac{\mu+i\beta}{\hbar}\right]^{2\lambda+2n+1}} F\left(\lambda+iy, 2\lambda+2n+1, 2\lambda+1; \frac{2i\beta}{\mu+i\beta}\right) \qquad (III.D.2b)$$

using the same method for evaluating the integral (B.20).

The advantage of this procedure is that, after using the relations (B.14) and (B.15), one finds the second parameter in the hypergeometric fn. to be a negative integer, -2n, or zero and the fn. itself is then represented by a finite series (from (B.12)), containing 2n terms for the coefficient of k^{2n}. The integration over E must then be carried out (probably by means of other expansions or else graphically) to obtain L as a power series in k, the coefficients also being fns. of k since k appears in the energy denominators of L (III.C.1a).

This procedure has not been used in this thesis, but it would have to be used if values of L for photon energies smaller than 100 kev in the case of Cesium were desired; however, such energies are below those occurring in the measurements ofSaraf (54). The reason why the method that is used to evaluate L breaks down for these small energies is that the integrand of L is plotted (after being approximated) and L, which is then obtained graphically, decreases for small photon energies to a value comparable to the errors in plotting. It may well happen that special approximations will be required to overcome this same sort of difficulty in the procedure just outlined.

Before proceeding to the semi-relativistic approximation, let us first note that if the quantity 2λ appearing in the parameters of the hypergeometric fn. (III.D.1a) is an integer, then an explicit finite expression for these fns. can be obtained from the integral representation (B.13) by integration by parts. Now, in our case

$$\lambda = \sqrt{1-(Z\alpha)^2} \quad , \qquad \kappa = \pm 1 \quad ,$$

so that 2λ, considered as a fn. of Z, is an integer only when $Z = 0, 119, 137$ giving $2\lambda = 2, 1, 0$ respectively. The case $Z = 0$ is of no interest to us and neither is $Z = 137$ for which theintegrand becomes infinite, but the case $Z = 119, \lambda = \frac{1}{2}$ is because the integrand of L as given by (III.C.8) can be obtained exactly and plotted in comparison with a graph of the integrand for the same value of Z using the semi-relativistic approximation. Such a comparison provides a check on the validity of the semi-relativistic approximation and is carried out in Section E.

The Semi-Relativistic Approximation

" The rules by which the non-relativistic normalized radial solutions of the Schrodinger Eq. (including the nuclear Coulomb potential) are obtained " from the normalized radial solutions of the Dirac Eq. are listed below for continuous and discrete states. What we call the "semi-relativistic" approximation is then presented and used to evaluate L.

Rule for Positive Continuum States ($E \geq mc^2$):

Consider our "large" radial solutions F for these states in Appendix C and regard them as fns. of the momentum p using

$$E = + \sqrt{(cp)^2 + (mc^2)^2} \ .$$

Then, in order to obtain the radial solutions to the Schrodinger Eq:

(a) Replace E by the first term in its expansion in powers of p i.e. $E \to mc^2$ (III.D.3a)

(b) Set $\lambda = |K|$ everywhere. (III.D.3b)

Wherever E appears, it is divided by cp so that, using the relation

$$\frac{E}{cp} = \frac{cp}{E + mc^2} + \frac{mc}{p} \to \frac{mc}{p} \ ,$$

we can see what is neglected in this ratio when rule (III.D.3a) is applied. In obtaining the radial solutions to the Schrodinger Eq., we also write $K = \ell + 1$ or $K = -\ell$ for $K = +(j + \frac{1}{2})$ or $K = -(j + \frac{1}{2})$ respectively, both cases producing the same radial solution to theSchrodinger Eq. possessing an orbital angular momentum ℓ.

If the rules (III.D.3) are applied to the "small" radial solution G for the positive continuum, one obtains zero.

Rule for Negative Continuum States ($E \leq -mc^2$):

In this case, we again regard the radial solutions as fns. of p using

$$E = -\sqrt{(cp)^2 + (mc^2)^2}$$

Then to obtain the corresponding radial solutions to the Schrodinger Eq:

(a) Replace E by the first term in its expansion in powers of p i.e. $E = -mc^2$ (III.D.4a)

(B) Set $\lambda = |K|$ everywhere. (III.D.4b)

This rule is obtained as follows. It is shown in Appendix C that for the negative continuum, the G's are the "large" solutions and the F's the "small" in contrast to the positive continuum case. In particular, the negative continuum solutions are related to the positive continuum solutions by the relations

$$G^*(-|E|, K, Z) = e^{i\varphi} F(|E|, -K, -Z) \qquad \text{(III.D.5a)}$$

$$F^*(-|E|, K, Z) = e^{i\varphi} G(|E|, -K, -Z) \qquad \text{(III.D.5b)}$$

considering the wave fns. to be fns. of E, K, Z. $e^{i\varphi}$ is some constant phase factor. The R.H.S. of (III.D.5) shows that the negative continuum states on the L.H.S. represent the motion of a positron in a positive energy state (with K replaced by -K) In making a non-relativistic approximation, the R.H.S. of (5a) must give the radial solution to the Schrodinger Eq. for a positron i.e.e from rule (III.D.3) we just put

$$|E| = mc^2 \qquad \lambda = |K|$$

in the appropriate places, either sign of K giving the same non-relativistic result. The relations (III.D.5) then show that the rule (III.D.4) must be used to obtain the non-relativistic radial wave fns. from our negative continuum radial wave fns.

Applying the rule (III.D.4) to our "small" solns F for the negative continuum, the result is zero. This statement also follows from (III.D.5b) and the fact that G for positive continuum states goes to zero in the non-relativistic limit.

Rule for discrete states

The normalized non-relativistic radial solns for the discrete case are obtained from our radial solutions in Appendix C by setting

$$\lambda = |K| \qquad \text{(III.D.6a)}$$

everywhere and

$$E = mc^2 \qquad \text{(III.D.6b)}$$

in just the square root factors $\sqrt{A}$, $\sqrt{B}$ which appear in front of the radial solutions. Thus $\sqrt{A}$ and hence G go to zero. Note however that the quantity $\sqrt{AB}$ appearing in the wave fns. does not go to zero but

$$\sqrt{AB} \rightarrow \frac{Z\alpha mc}{n} \qquad \text{(III.D.6c)}$$

where n is the non-relativistic energy quantum number,

$$n = n' + |K|$$

The result (III.D.6c) is obtained by first writing exactly

$$1 - \left(\frac{E}{mc^2}\right)^2 = \frac{(Z\alpha)^2}{n'^2 + 2\lambda n' + K^2}$$

for a general discrete level; then using (III.D.6a), one obtains (III.D.6c).

Let us now discuss these rules and, in particular, how a non-relativistic approximation would affect L in Eq. (III.C.1a). First of all, the rules were determined in each case so that the "large" radial solutions gave the non-relativistic radial solutions for an electron or positron depending on the energy region. When the same rules are applied to the "small" radial solutions we get zero. Now L depends only on the "small" radial solutions G^- in the positive continuum and the "large" radial solutions G^- in the negative continuum (neglecting the contibution of the discrete states), so that in a complete

non-relativistic approximation only the negative continuum states would contribute to L. It is the purpose of the semi-relativistic approximation to include the positive continuum contribution to L.

Semi Relativistic Approximation

L depends on the wave fns. of the K electron and the electron in the intermediate state, for both of which $|K|=1$. If we set $\lambda=1$ everywhere in these wave fns. the calculation of L is simplified considerably because, as already mentioned, explicit finite expressions for the hypergeometric fns. and gamma fns. can then be obtained.

Setting $\lambda=1$ in the K electron wave fn., one obtains the substitution (III.D.6c) with $n=1$; substituting these results in the electron wave fn. (III.C.2a), we find that the wave fn. contains in one factor the non-relativistic radial dependence and in the other factor the constant N_0 which can be taken outside the integrand of L and which then cancels out in the ratio $w_k\,dk/w_c$ provided the K electron wave fn. is approximated the same way in w_c. Since we are only interested in this ratio, no further approximations are made for the K electron. Note however, that we shall still let

$$E_K = mc^2\sqrt{1-(Z\alpha)^2} \qquad \text{(III.D.7)}$$

relativistically, in the energy denominators of L in (III.C.8) since no simplification is required there.

The semi-relativistic approximation that is applied to the radial solutions for the electron in the intermediate state is carried out as follows. The square root factors

$$\sqrt{|E| \pm \delta mc^2} \qquad \text{(III.D.8a)}$$

which appear in front of F, G (App. C) are left unchanged; in the remaining fns, we set

$$\lambda = 1 \qquad \text{(III.D.8b)}$$

and, considering these remaining fns. as fns. of p using

$$E = \delta\sqrt{(cp)^2 + (mc^2)^2}$$

replace E by the first term in its expansion in powers of p, i.e.

$$E \to \delta mc^2 \qquad (\text{III.D.8c})$$

as in rules (III.D.3) and (III.D.4). If we also approximated E in the square root factors, we would be carrying out a non-relativistic approximation with the resulting neglection of the positive continuum contribution to L. Let us call the radial fns. resulting from the application of this semi-relativistic approximation, semi-relativistic fns.

It is shown in Appendix C, that, if we look for general radial solutions to the Dirac radial Eqs. having $\lambda = |K|$, we find that such solutions are possible if, and only if, the Dirac radial Eqs. themselves are approximated, the semi-relativistic fns. being solutions of these approximated Eqs. which we shall refer to as semi-relativistic radial Eqs. These semi-relativistic Eqs. are given in Appendix C and are used to show, by a plausible argument, that the normalization of the semi-relativistic fns. is not unduly affected. A special advantage of the semi-relativistic fns. is that, by the choice of suitable units, the most complicated fns. appearing in the integrand of L need to be tabulated only once as far as Z is concerned, since the resulting table can be used for any Z.

It should be mentioned that only the approximation $\lambda = 1$ is needed to simplify the integrand of L to the extent where it can be plotted within a reasonable length of time; however, it is not easy to make any statements about the normalization of the resulting wave fns. and also the most complicated parts of the resulting integrand of L must be recalculated for each different value of Z. It would be possible though to check the resulting integrand for $Z=119$, $\lambda = \frac{1}{2}$ with the exact integrand for this case just as we shall do in the next Section for the semi-relativistic approximation, but, because of time

limitations, such a comparison has not been carried out.

The Semi-Relativistic Integrand of L

We shall now write out explicitly the integrand of L as given by (III.C.8) using the semi-relativistic approximation. In the next Subsection this integrand is plotted as a fn. of the energy E for several values of the photon energy $\hbar ck$.

Carrying out the substitutions (III.D.8) one finds

$$L = -N_0 \int_{mc^2}^{\infty} dE \left[\frac{E-mc^2}{E-E_K+\hbar ck} N^2(Z,mc^2)Q(mc^2) - \frac{E+mc^2}{E+E_K-\hbar ck} N^2(Z,-mc^2)Q(-mc^2) \right] \quad \text{(III.D.9a)}$$

where:

$$N^2(Z,\delta mc^2) = \frac{cp}{4\pi(\hbar c)^3} \left|\Gamma(1+i\delta y)\right|^2 e^{\pi\delta y} \quad \text{(III.D.9b)}$$

$$y = \frac{Z\alpha mc}{p} \quad \text{(III.D.9c)}$$

$$Q(\delta mc^2) = \frac{1}{2i}\left\{2-iy(\delta+1)\right\}\left\{(1+i\delta y)\left[u^*(k)+u^*(-k)\right] - (1+iy)\left[u(k)+u(-k)\right]\right\} \quad \text{(III.D.9d)}$$

$$u(k) = \frac{\hbar^2}{k\left[\mu+i(p-\hbar k)\right]^2} F\left(1+i\delta y, 2, 3; \frac{2ip}{\mu+i(p-\hbar k)}\right) \quad \text{(III.D.9e)}$$

$$\mu = Z\alpha mc \qquad \left|\Gamma(1+i\delta y)\right|^2 = \frac{\pi y}{\sinh \pi y} \quad \text{(from (B.3))} \quad \text{(III.D.9f)}$$

and the K electron energy, E_K, is obtained from Eq. (III.D.7).

The most difficult quantitities to obtain explicitly in the integrand are $Q(\pm mc^2)$ of (III.D.9d). $Q(-mc^2)$ cannot be obtained from $Q(+mc^2)$ by replacing m by -m or y by -y in the resulting expressions. This is apparent when one notices that the factor $(1+iy)$ and not $(1+i\delta y)$ appears in the second term of the right factor of Q in (9d). Let us now obtain explicit expressions for the Qis.

Using (B.19), one finds that $u(k)$ in (III.D.9e), for $\delta = +1$ only, can be written in the form:

$$u(k) = \frac{i\hbar^2}{2k\,p^2 y}\left\{\frac{2ip\,[\mu - i(p+\hbar k)]}{[\mu + i(p-\hbar k)]^{1-iy}\,[\mu - i(p+\hbar k)]^{1+iy}} + \right.$$

$$\left. + \frac{1}{1-iy}\left(\frac{[\mu - i(p+\hbar k)]^2}{[\mu + i(p-\hbar k)]^{1-iy}\,[\mu - i(p+\hbar k)]^{1+iy}} - 1\right)\right\} \qquad \text{(III.D.10)}$$

Before proceeding, let us define the dimensionless quantities:

$$x = \frac{\hbar k}{\mu}\ ,\quad q = \frac{p}{\mu}\ \left(= \frac{1}{y}\ \text{from (III.D.9c)}\right),\quad \mu = Z\alpha mc \qquad \text{(III.D.11)}$$

Then, forming $u(k) + u(-k)$ and substituting the result into (III.D.9d) with $\delta = +1$, one obtains

$$Q(+mc^2) = -\frac{2\hbar^2}{k\,p^2}\,Q_+(q,x) \qquad \text{(III.D.12a)}$$

where

$$Q_+(q,x) = \frac{1}{2i}\left\{\frac{3 - q^2 - x^2 + 4ix}{[1 - i(q-x)]^{1+i/q}\,[1 + i(q+x)]^{1-i/q}} - \text{c.c.}\right\} \qquad \text{(III.D.12b)}$$

c.c. meaning complex conjugate. Q so defined turns out to be real and positive.

A simpler procedure is now used to find $Q(-mc^2)$ from (III.D.9d). Using the relation (B. 16), one can prove that

$$(1+iy)\,u(k) - (1-iy)\,u^*(-k) = \frac{2\hbar^2}{k}\left\{[\mu + i(p-\hbar k)]^{1+iy}\,[\mu - i(p+\hbar k)]^{1-iy}\right\}^{-1} \qquad \text{(III.D.13)}$$

from which one can obtain

$$Q(-mc^2) = -\frac{4\hbar^2}{k\,\mu^2}\,Q_-(q,x) \qquad \text{(III.D.14a)}$$

where

$$Q_-(q,x) = \frac{1}{2i}\left\{\frac{1}{[1 + i(q-x)]^{1+i/q}\,[1 - i(q+x)]^{1-i/q}} - \text{c.c.}\right\} \qquad \text{(III.D.14b)}$$

Q - so defined turning out to be real and positive

As seen from the Eqs. (III.D.9), (III.D.12) and (III.D.14), the integrand of L in the semi rel. approximation is quite complicated. In the next subsection we shall plot it up to a certain value of E and then evaluate the "tail" integral by a rapidly convergent series.

Before doing this, let us first write the integrand of L in a more convenient form.

Defining

$$D_{\pm}(q) = \frac{\pi e^{\pm \pi/q}}{\sinh \pi/q} = \pi\left[\coth(\pi/q) \pm 1\right] \qquad (\text{III.D.15a})$$

$$I = \int_1^\infty d\varepsilon \left\{ \frac{2}{\varepsilon + \varepsilon_K - Z\alpha x} \left[\frac{\varepsilon+1}{Z\alpha}\right] D_- Q_- \right.$$

$$\left. - \frac{1}{\varepsilon - \varepsilon_K + Z\alpha x} \left[\frac{Z\alpha}{\varepsilon+1}\right] D_+ Q_+ \right\} \qquad (\text{III.D.15b})$$

$$\varepsilon = \frac{E}{mc^2} \qquad (\text{III.D.15c})$$

we find from (III.D.9), (III.D.12), (III.D.14) that

$$L = -\frac{N_0}{2\pi Z\alpha mc^2} \frac{I}{x} \qquad (\text{III.D.15d})$$

In the formula (15b) the D's, and Q's, and energy denominators are all positive so that I is positive or negative depending on whether the negative or positive continuum states respectively contribute the most to the integral. The calculations performed in the next two subsections show that the negative continuum states contribute the most (as we should expect from a non-relativistic approximation) giving I positive.

Tabulation of the Integrand of I

I of Eq. (III.D.15b) must further be written as

$$I = I_1 + I_2 \qquad \text{(III.D.16a)}$$

where $$I_1 = \int_{\varepsilon}^{\varepsilon_0} \frac{dI}{d\varepsilon}\, d\varepsilon \qquad I_2 = \int_{\varepsilon_0}^{\infty} \frac{dI}{d\varepsilon}\, d\varepsilon \qquad \text{(III.D.16b)}$$

$\frac{dI}{d\varepsilon}$ being the total integrand in curly brackets in (III.D.15b). I_1 is obtained graphically in this Subsection and I_2, the "tail" integral in the next. It turns out that for Z = 55, the value

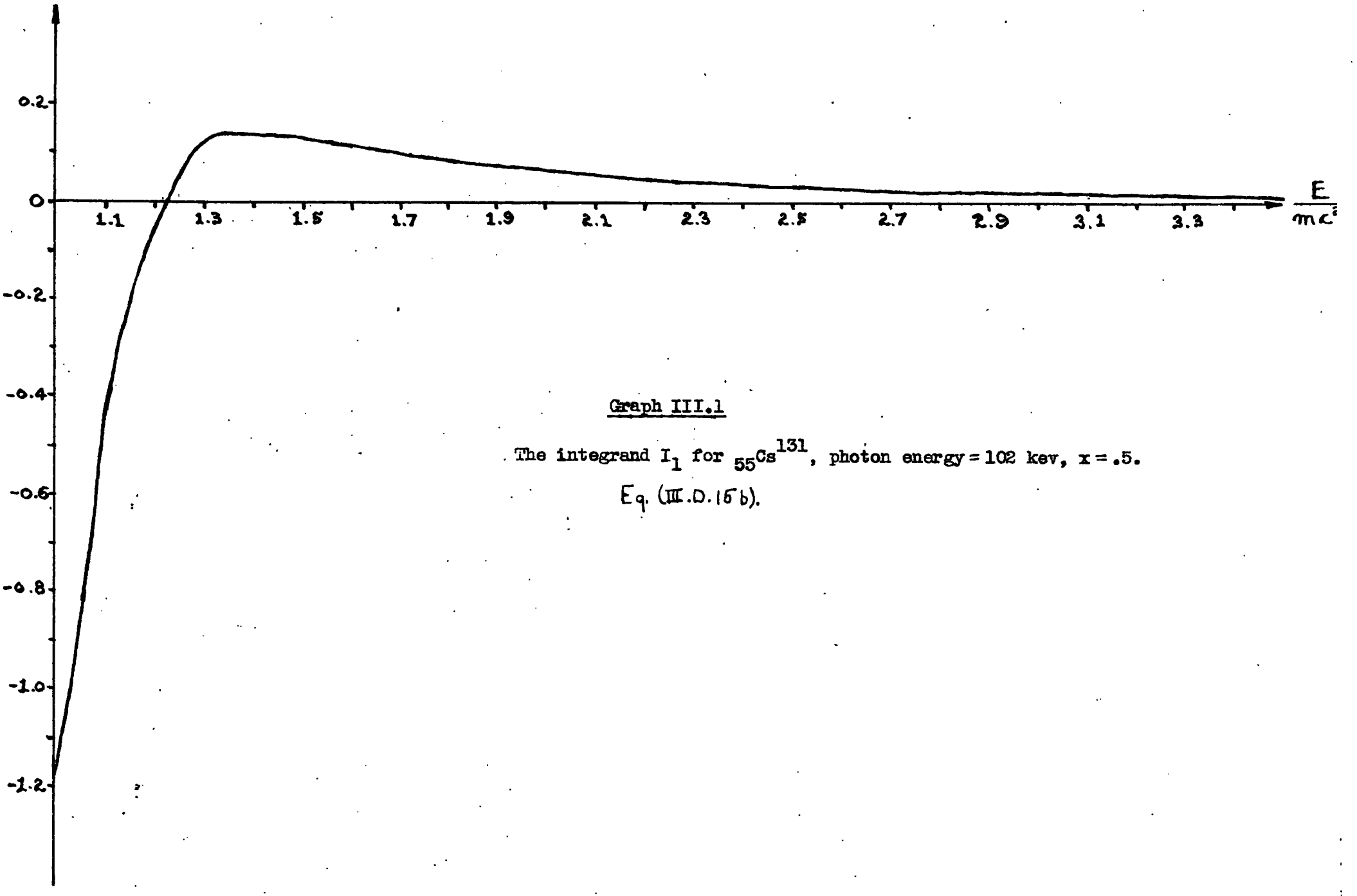
$$\varepsilon_0 = 3.5 \qquad \text{(III.D.17)}$$

is sufficiently large for I_2 to be evaluated analytically, using series expansion of the integrand.

The quantities D and Q appearing in the integrand of I_1 depend on q and x only and are tabulated in terms of these variables in Table III.1. The values of D and Q given in Table III.1, may be used for any value of Z provided one uses the dimensionless units q and x. With these values, the integrand of I_1 for different values of Z can be plotted fairly quickly and I_1 evaluated graphically. The series expression for the "tail" integral I_2 given in this Section is also valid for any value of Z. Consequently, the results given in this Section can be used to calculate the radiative K capture probability for any value of Z, even though just the results for Cesium have been obtained explicitly here.

For Cesium, about 25 values of q were chosen between 0 and 10 for each value of x equal to 0.5, .75, 1, 1.5 in order to obtain enough points to plot the integrand accurately. For large values of the integrand, the accuracy of the calculations was to three significant figures; however, for values of ε near ε_0 the integrand is small in some cases and consequently the accuracy decreases to two significant figures.

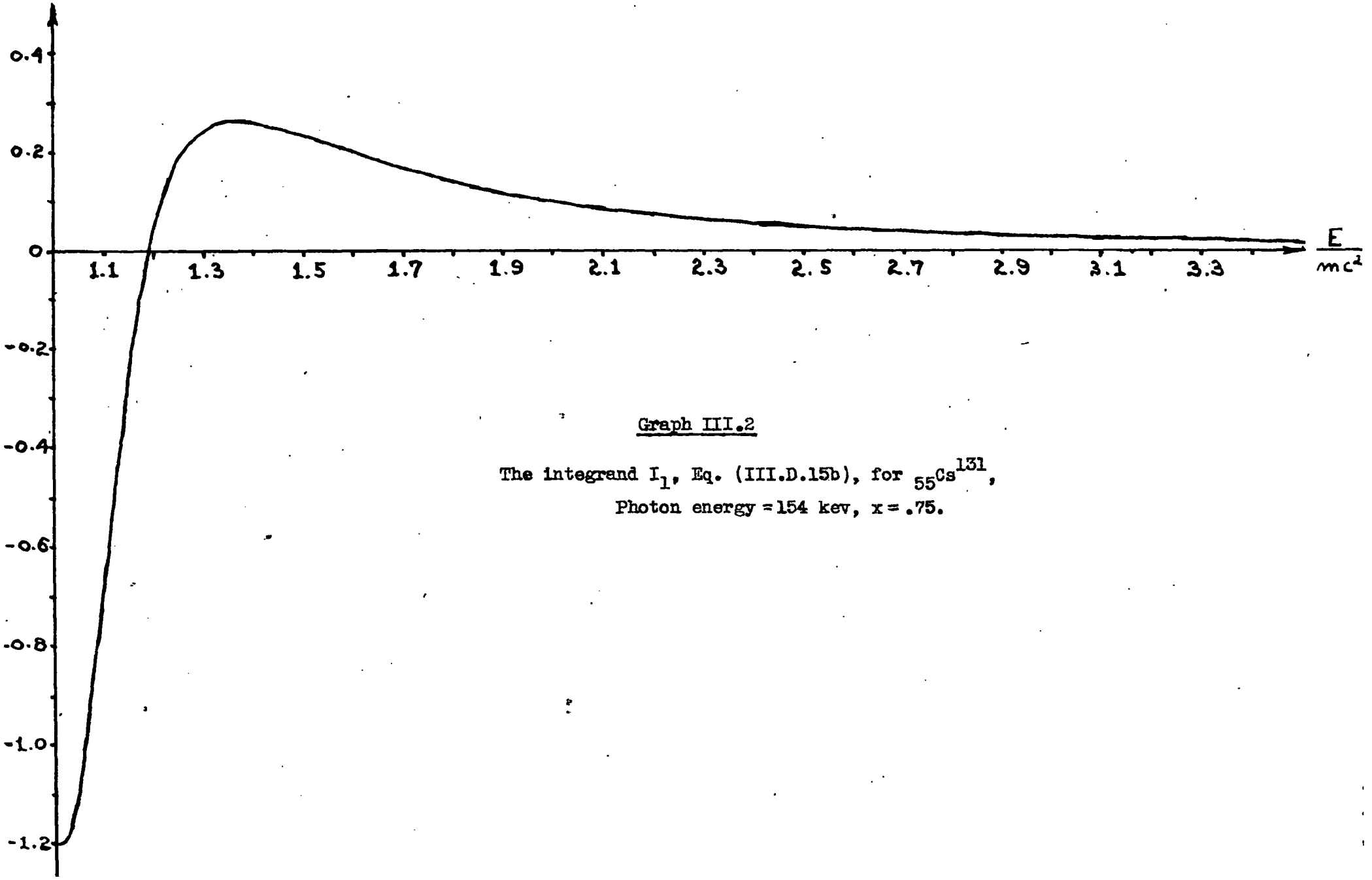
Checks on the calculations were made wherever possible. In particular, the integrand of I_1 for $\varepsilon = 1$ or $q = 0$ must be obtained separately



Graph III.1

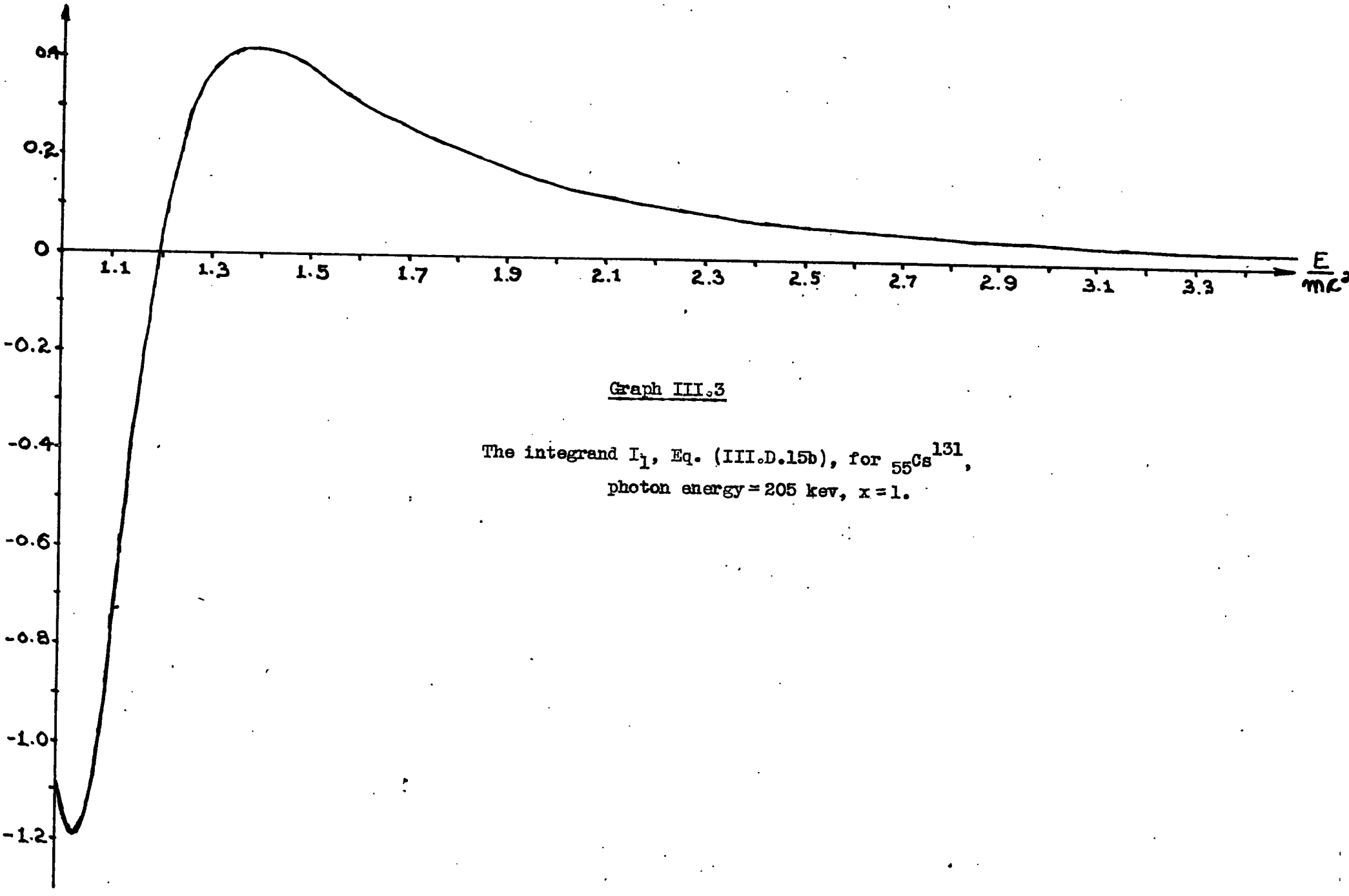
The integrand I_1 for $_{55}Cs^{131}$, photon energy = 102 kev, x = .5.

Eq. (III.D.16b).



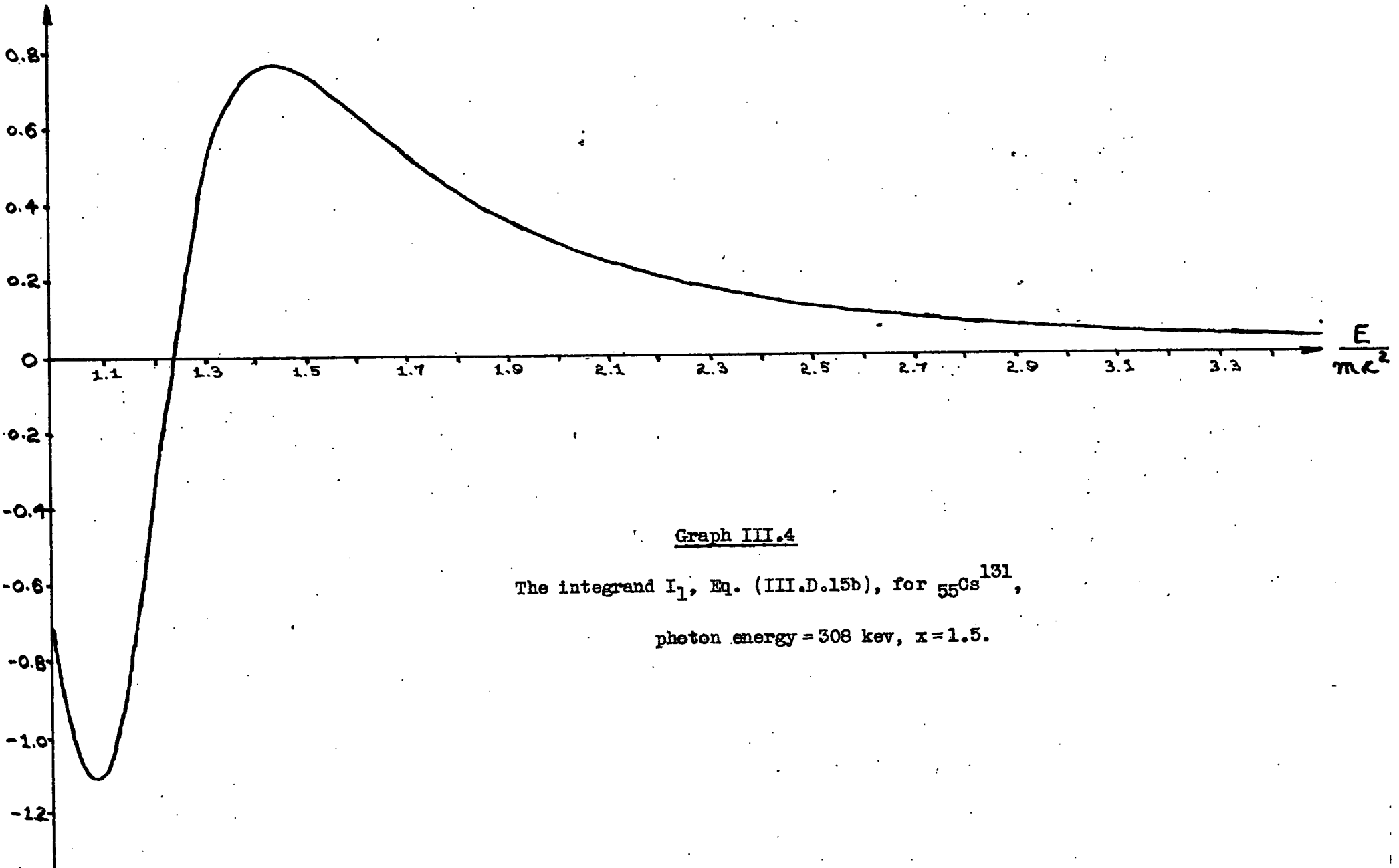
Graph III.2

The integrand I_1, Eq. (III.D.15b), for $_{55}Cs^{131}$,
Photon energy = 154 kev, x = .75.



Graph III.3

The integrand I_1, Eq. (III.D.15b), for $_{55}Cs^{131}$, photon energy = 205 kev, x = 1.



Graph III.4

The integrand I_1, Eq. (III.D.15b), for $_{55}Cs^{131}$,

photon energy = 308 kev, x = 1.5.

from the calculations by a limiting process (the results of which are presented later on in this Subsection), the plotted integrand approaching this point as though it were extrapolated; also, the integrand of I_1 for energies near ε_0 can be checked by the series expression for the integrand of I_2 to an accuracy within 5%.

In Graphs III.1, III.2, III.3, III.4 the integrand of I_1 is presented for x = .5, .75, 1, 1.5. From these Graphs, we see that for small electron energies the positive continuum contribution to the integrand is the significant one even though the largest overall contribution to I comes from the negative energy continuum. As we shall see, the same situation occurs for Z=119 in both the "semi-relativistic" and "exact" curves of the integrand but not for the "non-relativistic" integrand. The values of I_1, obtained graphically, are presented in Table III.2.

Certain precautions are necessary in calculating the Q's because we must stay on the correct sheet of the Riemann surface associated with these complex fns. For this reason, the formulae used to calculate the Q's are given explicitly below.

In order to express the Q's in terms of real quantities, we define

$$\left.\begin{aligned} 1+i(q-x) &= r_- e^{i\theta_-} & 1+i(q+x) &= r_+ e^{i\theta_+} \\ r_- &= \sqrt{1+(q-x)^2} & r_+ &= \sqrt{1+(q+x)^2} \\ \tan\theta_- &= q-x & \tan\theta_+ &= q+x \\ -\tfrac{\pi}{2} \le \theta_- &\le \tfrac{\pi}{2} & 0 \le \theta_+ &\le \tfrac{\pi}{2} \end{aligned}\right\} \quad \text{(III.D.18)}$$

$$\left.\begin{aligned} a &= \ln r_+ r_- + \frac{1}{q}(\theta_+ + \theta_-) & b &= \theta_+ - \theta_- - \frac{1}{q}\ln r_+/r_- \\ a' &= \ln r_+ r_- - \frac{1}{q}(\theta_+ + \theta_-) & b' &= \theta_+ - \theta_- + \frac{1}{q}\ln r_+/r_- \end{aligned}\right\} \quad \text{(III.D.19)}$$

which, when substituted into (III.D.12b) and (III.D.14b) give

$$\left.\begin{aligned} Q_+ &= e^{-a}\left[\, 4x\cos b - (3-x^2-q^2)\sin b\right] \\ Q_- &= e^{-a'}\sin b' \end{aligned}\right\} \quad \text{(III.D.20)}$$

The ranges for the angles θ_+, θ_- given in (III.D.18) are determined as follows. Consider the first term in each of the Q's in (III.D.12b), (III.D.14b) (the c.c. terms are treated in exactly the same way); the multivaluedness arises from those factors in these terms which are raised to pure imaginary powers. As shown in Appendix B, the multivaluedness appears as soon as we make use of the explicit expression (B.19) for the hypergeometric fns. According to the discussion given in Appendix B, we must choose the ranges of θ_+ and θ_- in such a way that

$$\theta_+ + \theta_- \to 0 \qquad \text{as} \qquad q \to 0 ,$$

a requirement satisfied by the ranges in (III.D.18).

When q is zero ($E = mc^2$), one can prove from the definitions (III.D.18) and (III.D.19) (respecting the ranges on the θ's) that:

$$\left.\begin{aligned} a &= \ln(1+x^2) + \frac{2}{1+x^2} & b &= 2\tan^{-1}x - \frac{2x}{1+x^2} \\ a' &= \ln(1+x^2) - \frac{2}{1+x^2} & b' &= 2\tan^{-1}x + \frac{2x}{1+x^2} \end{aligned}\right\} \quad \text{(III.D.21)}$$

By substituting (III.D.21) into (III.D.20), one finds the values of the Q's for $q = 0$.

The "Tail" Integral I_2

The "tail" integral is obtained here as a series in powers of $1/q$. The results (III.D.24) and (III.D.25) are valid for any value of Z.

Let us first expand the expressions (III.D.12b), (III.D.14b) for the Q's. In order that the expansion of the complex binomials in the formulae converge absolutely and uniformly over the range of I_2 ($3.5 \leq \varepsilon \leq \infty$), we must have

$$\left| \frac{1 \pm ix}{q} \right| < 1 .$$

For Cesium, the value of q corresponding to the energy ε_0 is

$$q_0 = 8.36$$

and since $x < 2$, we see that the above relation is satisfied for all $q > q_0$ as required. Expanding these binomials to 4 terms, one finds the Q's, correct to 2 terms, to be given by

$$\left.\begin{aligned} Q_+ &= \frac{4x e^{-\pi/q}}{q^2}\left[1 + \frac{5}{4}\frac{(1+x^2)}{q^2}\right] \\ Q_- &= \frac{4x e^{\pi/q}}{q^4}\left[1 - \frac{(17-7x^2)}{q^2}\right] \end{aligned}\right\} \qquad (III.D.23)$$

Combining these expansions with the D's of (III.D.15a) and making use of the expansion

$$\frac{\pi/q}{\sinh \pi/q} \doteq 1 - \frac{\pi^2}{6q^2} = 1 - \frac{1.65}{q^2}$$

one obtains an absolutely and uniformly convergent series for the products DQ appearing in the integrand of (III.D.15b).

Since also

$$\left|\frac{\varepsilon_k - z\alpha x}{\varepsilon}\right| < 1 \,, \quad \frac{1}{\varepsilon} < 1 \,, \quad \frac{1}{q} < 1 \qquad \text{for} \quad \varepsilon > \varepsilon_0 \text{ or } q > q_0 \,,$$

the other parts of the integrand can be expanded in absolutely and uniformly convergent series of powers of $1/q$. Consequently, all these series can be multiplied and added together to give a convergent result for I_2.

Writing I_2 in the form

$$I_2 = \int_{q_0}^{\infty} \frac{dI}{dq}\, dq \,, \qquad (III.D.24a)$$

one finds

$$\frac{dI}{dq} = \frac{4x}{q^3}\left[1 + \frac{3A_1}{q} - \frac{A_2}{q^2}\right] \qquad (III.D.24b)$$

where

$$\left.\begin{aligned} A_1 &= f - d & A_2 &= \tfrac{3}{4}(13 - 3x^2) + \frac{f^2}{2} + d(f-d) + 1.65 \\ d &= \frac{E_k - \hbar c k}{2\alpha mc^2} & f &= \frac{1}{2\alpha} \,, \end{aligned}\right\} \qquad (III.D.24c)$$

the series (III.D.24b) being correct to the terms shown. Integration of (III.D.24a) gives

$$I_2 = \frac{2x}{q_0^2}\left[1 + \frac{2A_1}{q_0} - \frac{A_2}{2q_0^2}\right], \qquad (III.D.25)$$

the series (III.D.25) converging more rapidly than the series (III.D.24b). Provided E_o or q_o is suitably chosen, this result is quite general.

For Cesium, I_2 is tabulated in Table III.2 using (III.D.22). From the results for I_1 and I_2, $I = I_1 + I_2$ is obtained and tabulated in Table III.2 along with I/x.

Using the relation

$$\frac{dI}{dx} = \frac{\sqrt{q^2 + (1/2\alpha)^2}}{2\alpha mc^2 q} \frac{dI}{dq} , \qquad (III.D.26)$$

with $\frac{dI}{dq}$ given by the series (III.D.24b), one can check the tabulated values of the integrand of I_1 for values of q near $q_o = 8.36$.

The ratio $w_K dk/w_C$

In the radiationless probability w_C, the quantity

$$\frac{F_K(R)}{R} = N_o \qquad \text{from (III.C.22)}$$

for either a semi-relativistic or a non-relativistic approximation, (a different N_o for each case), and also $E_\nu = W$, the available energy, since no photon is emitted.

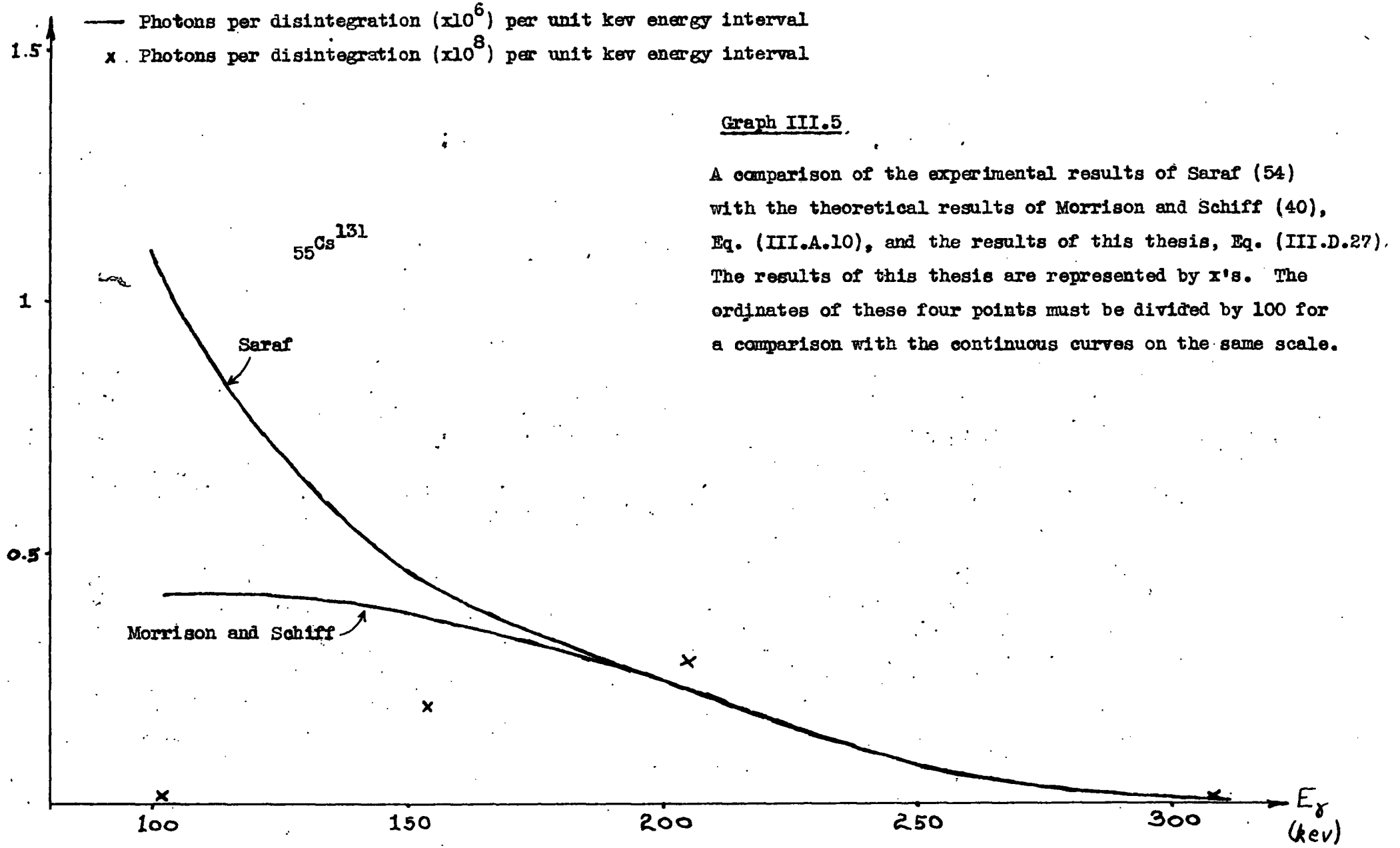
Collecting the formulae (III.B.11), (III.B.22), (III.D.15d) and the above results together, one obtains

$$\frac{w_K dk}{w_C} = Y\left[\frac{I^2}{2\pi^2 (Z\alpha)^2 x^2}\right] \frac{\alpha}{\pi} \left(\frac{W - \hbar c k}{W}\right)^2 \frac{(\hbar c)^2 k\, dk}{(mc^2)^2} \qquad (III.D.27a)$$

where

$$Y = \frac{(C_S - C_V)^2 |\int 1|^2 + (C_T - C_A)^2 |\int \vec{\sigma}|^2 + C_P^2 |\int \beta\gamma_5|^2}{(C_S + C_V)^2 |\int 1|^2 + (C_T + C_A)^2 |\int \vec{\sigma}|^2 + C_P^2 |\int \beta\gamma_5|^2} , \qquad (III.D.27b)$$

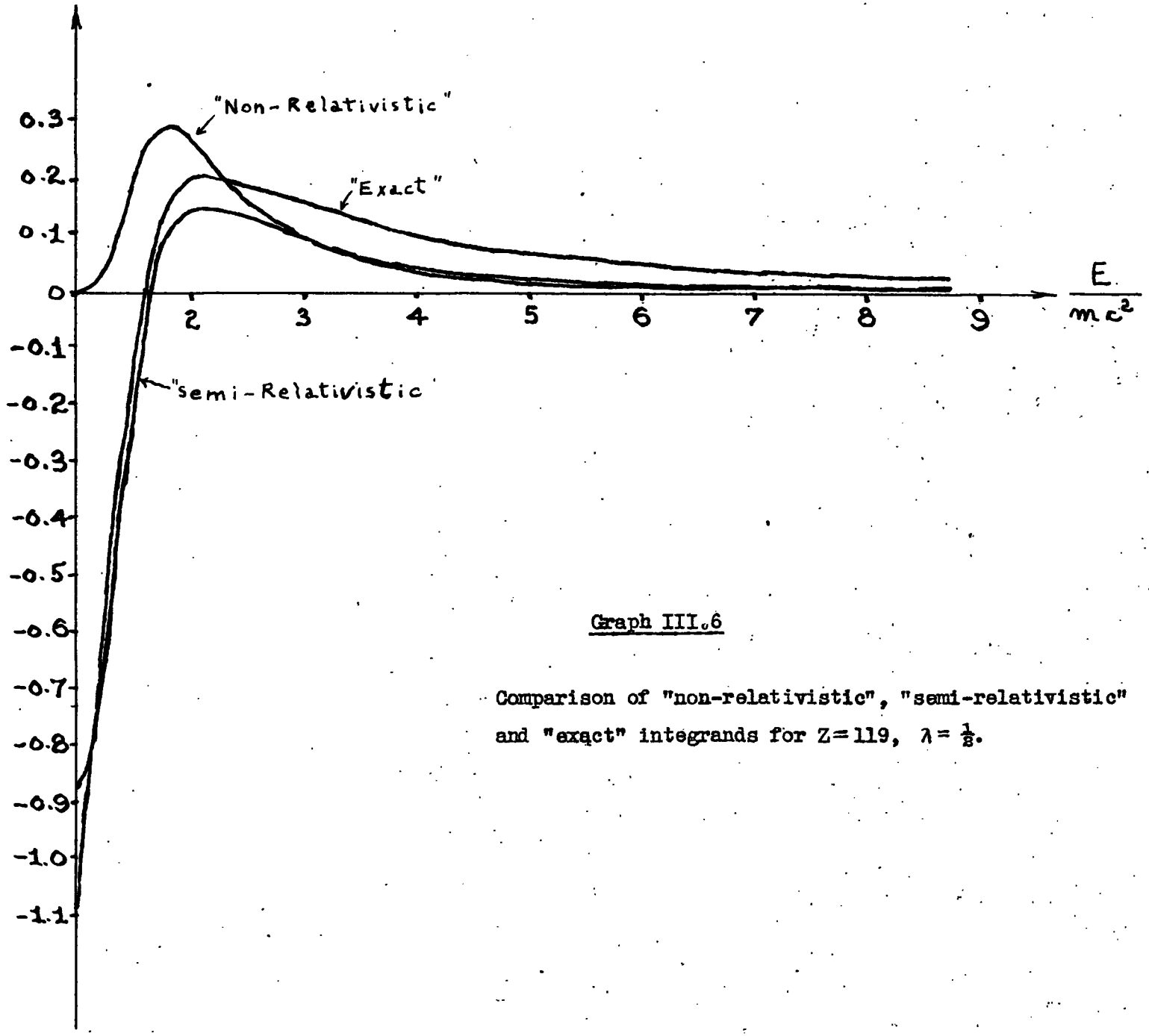
Y being unity if just a "pure" beta interaction is considered. The result (III.D.27a) differs from that of Morrison and Schiff (40), who considered "pure" interactions only, in the quantity appearing in the



Graph III.5.

A comparison of the experimental results of Saraf (54) with the theoretical results of Morrison and Schiff (40), Eq. (III.A.10), and the results of this thesis, Eq. (III.D.27). The results of this thesis are represented by x's. The ordinates of these four points must be divided by 100 for a comparison with the continuous curves on the same scale.

square brackets. In Graph III.5 our results are compared with the Morrison and Schiff formula. Saraf's (54) experimental curve is also shown. A glance at these curves shows that the theory of radiative K capture alone will not explain the experimental results. Also, we see that taking Coulomb effects into account lowers the ratio $w_k dk/w_c$ by an order of magnitude in the low photon energy region.



Graph III.6

Comparison of "non-relativistic", "semi-relativistic" and "exact" integrands for Z=119, $\lambda = \frac{1}{8}$.

E. The Case of $Z = 119$, $\lambda = \frac{1}{2}$

As mentioned previously, the integrand of L as given by (III.C.8) can be obtained exactly for this case. We must remember that the integrand of (III.C.8) has been obtained by neglecting contributions of discrete states and by approximating the electron wave fn. at the nucleus; hence the statement that this integrand can be obtained exactly for $Z = 119$ means that no further approximations are required.

A brief outline showing how the exact integrand is obtained is presented here. The calculation of the integrand in a semi-relativistic approximation presents no difficulties since it is completely similar to that given in the last Section for Cesium except that Z must be changed from 55 to 119. The D's and Q's of the last Section can be used without recalculation.

The exact and semi-relativistic integrand are plotted in Graph III.6 for $x = .75$, i.e. a photon energy of 332 kev. Along with these two curves the non-relativistic integrand is drawn for comparison. It is obtained by replacing the radial solutions to the Dirac Eq. by the corresponding radial solutions to the Schrodinger Eq.; in this non-relativistic approximation, only the negative continuum states contribute to L.

It is perhaps too much to expect very good agreement between any of the approximate curves with the exact one for such a high value of Z. We can see though that the general shape of the exact and semi-relativistic curves is the same, neither one agreeing in shape with the non-relativistic curve; however, there is a discrepancy between the ordinates of the exact and semi-relativistic curves which cannot be overlooked for this value of Z. It is assumed that for Cesium, whose nuclear charge is less than half that for this case, this discrepancy decreases to a much smaller value.

In the semi-relativistic approximation, we have approximated

$$\lambda = \sqrt{1-(z\alpha)^2} \quad \text{by} \quad 1$$

$$E/cp \quad \text{by} \quad mc/p$$

in certain places. As mentioned in the last paragraph of Section III.D before the Subsection on the semi-relativistic integrand of L is presented, it is not necessary to make the above energy approximation although certain advantages in calculating the integrand of L do result from it. If the resulting integrand for just the approximation $\lambda = 1$ were also plotted in Graph III.6 for Z = 119, then we could definitely state that the discrepancy between such a curve and the exact curve must decrease for Z decreasing because the approximation $\lambda = 1$ is so much better for small Z. It does not follow that this approximation would be better than the semi-relativistic one, because the approximation on λ and E might have to be made together. In fact, as shown in Appendix C, if one looks for solutions to the Dirac radial Eqs. for which $\lambda = 1$, then solutions are possible if, and only if, the approximation on E is also made. It appears that the normalization of the semi-relativistic radial solutions is assured (Appendix C); however, nothing can be said about the normalization for the $\lambda = 1$ only approximation since we do not have the Eqs. which the resulting fns. satisfy and the fns. themselves are too complicated to easily evaluate the required normalization integral.

In the remainder of this Section the details involved in calculating the exact integrand for Z = 119 are outlined.

Using (B.18) in (III. C.4a) with $\lambda = \frac{1}{2}$, one obtains

$$u(k) = \frac{\hbar}{2ipk\,(\frac{1}{2} - i\eta)} \left[1 - \left(\frac{1 - i(q+x)}{1 + i(q-x)} \right)^{\frac{1}{2} - i\eta} \right] \qquad (III.E.2a)$$

where

$$\eta = \frac{Z\alpha E}{cp} = y\left(\frac{E}{mc^2}\right) \qquad (III.E.2b)$$

q, x, y being given by (III.D.11) and (III.D.9c). Substituting (III.E.2) into (III.C.6), one obtains

$$Q(E) = \frac{\hbar}{2pk} \left[A(\eta + y) + \tfrac{3}{2} B \right] \qquad (III.E.3a)$$

where

$$\left.\begin{aligned} A &= e^{-\eta(\theta_+ + \theta_-)} \left[\left(\frac{r_+}{r_-}\right)^{-\frac{1}{2}} \sin\alpha - \left(\frac{r_+}{r_-}\right)^{\frac{1}{2}} \sin\beta \right] \\ B &= e^{-\eta(\theta_+ + \theta_-)} \left[\left(\frac{r_+}{r_-}\right)^{-\frac{1}{2}} \cos\alpha - \left(\frac{r_+}{r_-}\right)^{\frac{1}{2}} \cos\beta \right] \end{aligned}\right\} \qquad (III.E.3b)$$

$$\left.\begin{aligned} \alpha &= \frac{\theta_+ + \theta_-}{2} - \eta \ln r_+/r_- \\ \beta &= \frac{\theta_+ + \theta_-}{2} + \eta \ln r_+/r_- \end{aligned}\right\} \quad \text{(III.E.3c)}$$

$$\left.\begin{aligned} &\tan\theta_+ = q + x \qquad \tan\theta_- = q - x \\ &0 \le \theta_+ \le \tfrac{\pi}{2} \qquad -\tfrac{\pi}{2} \le \theta_- \le \tfrac{\pi}{2} \qquad \text{(as in (III.D.18))} \\ &r_+ = \sqrt{1+(q+x)^2} \qquad r_- = \sqrt{1+(q-x)^2} \end{aligned}\right\} \quad \text{(III.E.3d)}$$

Using (B.3), one finds for N in (III.D.3b)

$$N^2(Z,E) = \frac{1}{2\pi(\hbar c)^2} \frac{\pi e^{\pi\eta}}{\cosh \pi\eta} \quad . \qquad \text{(III.E.4)}$$

Substituting (III.E.3) and (III.E.4) into (III.C.8) with the definition

$$Q'(E) = -\frac{2pk}{\hbar} Q(E) \qquad \text{(III.E.5)}$$

one obtains

$$L_{1/2} = -\frac{N_0 R^{-1/2}}{2\pi Z\alpha mc^2} \frac{I_{1/2}}{x} \qquad \text{(III.E.6a)}$$

where

$$I_{1/2} = \frac{1}{2}\int_1^\infty d\varepsilon \left[\frac{1}{\varepsilon + \varepsilon_K - Z\alpha x} \left(\frac{\varepsilon+1}{Z\alpha q}\right) \frac{\pi e^{-\pi\eta}}{\cosh\pi\eta} Q'(-E) \right.$$

$$\left. - \frac{1}{\varepsilon - \varepsilon_K + Z\alpha x} \left(\frac{Z\alpha q}{\varepsilon+1}\right) \frac{\pi e^{\pi\eta}}{\cosh\pi\eta} Q'(E) \right] \qquad \text{(III.E.6b)}$$

It is the integrand of $I_{1/2}$ which is compared in Graph III.6 with the integrand of I (III.D.15b) for Z = 119. The nuclear radial dependence present in (6a) disappears in the ratio $w_k dk/w_c$ for Z = 119, $\lambda = \frac{1}{2}$ and so is not taken into account in the comparison (Cf. (III.D.15d)).

TABLE III.1

A table of the Quantities $D_{\pm}(q)$ $(0 \leq q \leq 10)$ defined by Eq.(III.D.15a) and $Q_{\pm}(q,x)$ $(0 \leq q \leq 10)$ $(x = .5, .75, 1, 1.5, 2)$ defined by Eqs.(III.D.12b) and (III.D.14b).

q	$D_+(q)$	$D_-(q)$	$Q_+(q,.5)$	$Q_-(q,.5)$	E/mc^2
0	6.2832	.....	.2640	3.915	1.0000
.2	6.2832	.....	.2641	3.845	1.0032
.4	6.2832	.....	.2617	3.601	1.0128
.6	6.2834	.00019	.2546	3.114	1.0287
.8	6.2856	.00242	.2419	2.448	1.0505
1.0	6.2948	.01162	.2249	1.770	1.0779
1.2	6.3167	.03355	.2060	1.210	1.1105
1.4	6.3555	.07235			1.1477
1.6	6.4095	.12629	.1697	.4619	1.1893
1.8	6.4807	.19754			1.2347
2.0	6.5670	.28378	.1396	.2423	1.2835
2.2	6.6665	.38331			1.3355
2.4	6.7776	.49442	.1159	.1186	1.3901
2.6	6.8987	.61553			1.4472
2.8	7.0284	.74525	.09738	.06284	1.5064
3.0	7.1656	.88241	.08965	.04699	1.5674
3.5	7.5346	1.25145	.07383	.02434	1.7271
4.0	7.9321	1.64893	.06178	.01365	1.8947
4.5	8.3501	2.06695	.05240	.00820	2.0683
5.0	8.7830	2.49983	.04494	.00519	2.2465
5.5	9.2271	2.94392	.03895	.00343	2.4283
6.0	9.6801	3.39694	.03406	.00236	2.6130
7.0	10.6054	4.32217	.02672	.00121	2.9887
8.0	11.5486	5.26547	.02152	.000688	3.3705
9.0	12.5033	6.22016	.01769	.000420	3.7566
10.0	13.4672	7.18400	.01479	.000268	4.1458

TABLE III.1 (continued)

q	$Q_+(q,.75)$	$Q_-(q,.75)$	$Q_+(q,1)$	$Q_-(q,1)$
0	.3663	1.793	.4204	.7343
.2	.3702	1.843	.4306	.7682
.4	.3805	1.953	.4577	.8723
.6	.3899	2.039	.4914	1.0255
.8	.3828	1.986	.5162	1.1848
1.0	.3655	1.752	.5203	1.2751
1.2	.3383	1.402	.4999	1.2554
1.4	.3082	1.042		
1.6	.2779	.7410	.4180	.8560
1.8	.2498	.5181		
2.0	.2249	.3618	.3327	.4711
2.2	.2039	.2543		
2.4	.1839	.1814	.2664	.2470
2.6	.1673	.1314		
2.8	.1527	.09675	.2174	.1336
3.0	.1399	.07231	.1977	.1001
3.5	.1142	.03740	.1591	.0517
4.0	.09490	.02096	.1311	.0288
4.5	.08014	.01254	.1098	.0172
5.0	.06851	.007920	.0934	.0108
5.5			.0805	.00712
6.0	.05176	.003576	.0701	.00494
7.0	.04054	.001839	.0547	.00256
8.0	.03256	.001033	.0437	.00142
9.0	.02671	.0006232	.0358	.000856
10.0	.02225	.0003981	.0299	.000542

TABLE III.1 (continued)

q	$Q_+(q,1.5)$	$Q_-(q,1.5)$	$Q_+(q,2)$	$Q_-(q,2)$
0	.3947	.1425	.2803	.03794
.2	.4106	.1508	.3128	.03990
.4	.4565	.1764	.3526	.04644
.6	.5286	.2244	.4202	.05828
.8	.6211	.2946	.5167	.07722
1.0	.7165	.3929	.6413	.10587
1.2	.7941	.5100	.7892	.14758
1.4	.8292	.6181	.9449	.20559
1.6	.8121	.6773	1.0817	.28007
1.8	.7535	.6620	1.1697	.35801
2.0	.6737	.5846	1.1772	.42099
2.2	.5921	.4792	1.1072	.44492
2.4	.5180	.3753	.9923	.42269
2.6	.4544	.2870	.8629	.36897
2.8	.4012	.2178	.7436	.30397
3.0	.3567	.1652	.6412	.24201
3.5	.2741	.08573	.4580	.13058
4.0	.2186	.04733	.3456	.07186
4.5	.1792	.02790	.2728	.04170
5.0	.1500	.01735	.2223	.02554
5.5			.1856	.01640
6.0	.1103	.007678	.1578	.01100
7.0	.08486	.003860	.1189	.005452
8.0	.06738	.002154	.0933	.003000
9.0	.05489	.001289	.0754	.001780
10.0	.04566	.0008182	.0624	.001123

TABLE III.2

A tabulation of I (III.D.15b), I_1 (III.D.16b), and I_2(III.D.25).

x	I_1	I_2	$I = I_1 + I_2$	I/x
.5	.0040	.0154	.0194	.0388
.75	.0728	.0244	.0972	.130
1	.163	.034	.197	.197
1.5	.383	.057	.440	.294

APPENDIX A - EVALUATION OF TRACES

Each of the (4 x 4) Dirac matrices and σ_i matrices can be expressed (see A6) as the direct product of any two of the (2 x 2) matrices:

$$S_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad S_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad S_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad S_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{A.1}$$

the last three being the Pauli matrices satisfying the relations

$$S_i S_j = -S_j S_i = i S_k \qquad (i\,j\,k) \text{ cyclic}$$
$$S_i^2 = S_0 \qquad Tr\, S_i = 0 \qquad i,j,k = 1,2,3 \tag{A.2}$$

Using this property along with the properties of the direct products, i.e.

$$(a_1 \times b_1)(a_2 \times b_2) = (a_1 a_2 \times b_1 b_2) \tag{A.3a}$$

$$Tr\,(a \times b) = Tr\, a \; Tr\, b \tag{A.3b}$$

where a's and b's are (2 x 2) matrices, and with the relation

$$Tr\, AB = Tr\, BA \tag{A.4}$$

one can evaluate the required traces in a simple and direct manner. An illustrative example is presented at the end of this Section.

An alternative procedure would be to express the σ matrices as products of α matrices e.g. $\sigma_1 = -i\alpha_2\alpha_3$, and then make use of the general rules given in Heitler (54) for the traces of products of Dirac matrices; however, I prefer the method presented here.

The interaction matrices A^r are:

$$r = 1, 2, 3, 4, 5, 6, 7, 8, 9 \qquad A^{r\,*} = A^r \tag{A.5a}$$

$$A^r = \beta,\ 1,\ \beta\sigma_1,\ \beta\sigma_2,\ \beta\sigma_3,\ \sigma_1,\ \sigma_2,\ \sigma_3,\ i\beta\gamma_5 \qquad (A^{r\,*})^2 = 1 \tag{A.5b}$$

Using (A2) and (A3), one can show that

$$\alpha_i = (s_1 \times s_i) \qquad \beta = (s_3 \times s_0) \qquad \sigma_i = (s_0 \times s_i)$$

$$\gamma_5 = +i\alpha_1\alpha_2\alpha_3 = -(s_1 \times s_0) \tag{A.6}$$

One can also show that β anticommutes with α_i and γ_5 and commutes with σ_i.

By writing down all the products required and using (A.2), (A.3), (A.4), (A.6), one can show that:

$$\left.\begin{aligned} &Tr\ A^r A^{r'} = 4\delta_{rr'} \\ \text{and}\quad &Tr\ A^r A^{r'} \beta = 0 \qquad \text{except for the cases} \\ &Tr\ A' A^2 \beta = Tr\ A^2 A' \beta = 4 \quad \text{(Scalar, Vector interactions)} \\ &Tr\ A^m A^{m+3} \beta = Tr\ A^{m+3} A^m \beta = 4 \quad \text{(Tensor, Axial interactions)} \\ &\qquad m = 3, 4, 5. \end{aligned}\right\} \tag{A.7}$$

Example:

$$Tr\ \alpha_i \sigma_j \beta \gamma_5 = -Tr\ (s_1 \times s_i)(s_0 \times s_j)(s_3 \times s_0)(s_1 \times s_0)$$

$$= -Tr\ (s_1 s_0 s_3 s_1) \times (s_i s_j s_0^2) \qquad \text{(using (A.3a))}$$

$$= -Tr\ (s_1 s_3 s_1)\ Tr\ s_i s_j \qquad \text{(using (A.3b))}$$

$$= Tr\ s_3\ Tr\ s_i s_j \qquad \text{(using (A.2))}$$

$$= 0 \quad \text{since} \quad Tr\ s_3 = 0 \text{ from (A.2).}$$

APPENDIX B

Table of Functions

In the table below, z is a complex number, R(z) is the real part of z, and any other variables are complex numbers unless otherwise specified. The arguments of the hypergeometric fns. will always be shown so that no confusion should arise between them and other fns. denoted by the same letter F.

Gamma Fn.

$$\Gamma(z) = \int_0^\infty e^{-t}\, t^{z-1}\, dt \qquad R(z) > 0$$

$$\frac{\Gamma(\nu+1)}{p^{\nu+1}} = \int_0^\infty t^{\nu}\, e^{-pt}\, dt \qquad R(\nu) > -1 \quad R(p) > 0 \tag{B1}$$

$$\Gamma(z+1) = z\,\Gamma(z)\,, \quad \Gamma(n+1) = n!\,, \quad n \text{ integral or zero} \tag{B.2}$$

$$\Gamma(z)\,\Gamma(1-z) = \frac{\pi}{\sin \pi z}\,, \tag{B.3}$$

Beta Fn.

$$B(\alpha,\beta) = \frac{\Gamma(\alpha)\,\Gamma(\beta)}{\Gamma(\alpha+\beta)} = \int_0^1 t^{\alpha-1}(1-t)^{\beta-1}\, dt \qquad R(\alpha) > 0 \quad R(\beta) > 0 \tag{B.4}$$

Confluent Hypergeometric Fn.

Series expansion:

$$F(\alpha,\beta\,;z) = 1 + \frac{\alpha}{\beta}\frac{z}{1!} + \frac{\alpha(\alpha+1)}{\beta(\beta+1)}\frac{z^2}{2!} + \cdots = \frac{\Gamma(\beta)}{\Gamma(\alpha)}\sum_{m=0}^{\infty}\frac{\Gamma(\alpha+m)}{\Gamma(\beta+m)}\frac{z^m}{m!}\,, \tag{B.5}$$

convergent for finite z.

Integral expression:

$$B(\alpha, \beta-\alpha) F(\alpha, \beta; z) = \int_0^1 e^{zt} t^{\alpha-1} (1-t)^{\beta-\alpha-1} dt \qquad \text{(B,6)}$$

$R(\beta) > R(\alpha) > 0$ (MacRobert (54), p.346, Cf. also Magnus (49), p. 88.)

Useful relations:

$$F(\alpha, \beta; z) = e^z F(\beta-\alpha, \beta; -z) \qquad \text{(B.7)}$$

$$\frac{d}{dz} F(\alpha, \beta; z) = \frac{\alpha}{\beta} F(\alpha+1, \beta+1; z) \qquad \text{(B.8)}$$

$$r \frac{d}{dr} F(\alpha, \beta; \gamma r) = \alpha \left[F(\alpha+1, \beta; \gamma r) - F(\alpha, \beta; \gamma r) \right] \qquad \text{(B.9)}$$

((B.7), (B.8) from Magnus (49), p.87; (B.9) proved by substitution of (B.5).)

$$(\gamma-\alpha) F(\alpha, \gamma+1; z) + \alpha F(\alpha+1, \gamma+1; z) = \gamma F(\alpha, \gamma; z) \qquad \text{(Magnus (49), p.87)} \quad \text{(B.10a)}$$

$$\beta \left[F(\alpha, \beta; z) - F(\alpha+1, \beta; z) \right] = -z F(\alpha+1, \beta+1; z) \qquad \text{(from (B.8),(B.9))} \quad \text{(B.10b)}$$

Asymptotic expressions:

$$F(\alpha, \beta; z) = \frac{1}{2} (G_1 + G_2) \qquad \text{where, for large z,}$$

$$\frac{G_1}{2} = \frac{\Gamma(\beta)}{\Gamma(\beta-\alpha)} (-z)^{-\alpha} \left[1 + O(\tfrac{1}{z}) \right] \qquad \text{(B.11a)}$$

$$\frac{G_2}{2} = \frac{\Gamma(\beta)}{\Gamma(\alpha)} (z)^{\alpha-\beta} e^z \left[1 + O(\tfrac{1}{z}) \right] \qquad \text{(B.11b)}$$

(Sommerfeld p.795-6)

Hypergeometric Fn.

Hypergeometric Fn.

Series expansion:

$$F(\alpha,\beta,\gamma;z) = 1 + \frac{\alpha\beta}{\gamma}\frac{z}{1!} + \frac{\alpha(\alpha+1)\beta(\beta+1)}{\gamma(\gamma+1)}\frac{z^2}{2!} + \dots = \frac{\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\beta)}\sum_{m=0}^{\infty}\frac{\Gamma(\alpha+m)\Gamma(\beta+m)}{\Gamma(\gamma+m)}\frac{z^m}{m!} \quad \text{(B.12)}$$

If α or β is a negative integer or zero, the series is finite.

The infinite series converges for $|z|<1$. (Magnus (49), p.7)

Integral expression:

$$B(\beta,\gamma-\beta)\,F(\alpha,\beta,\gamma;z) = \int_0^1 t^{\beta-1}(1-t)^{\gamma-\beta-1}(1-zt)^{-\alpha}\,dt \quad \text{(B. 13)}$$

$$R(\gamma) > R(\beta) > 0 \qquad \text{(Magnus (49), p.8)}$$

The integral on the right is multivalued; in order to obtain the sereis (B.12), we must stay on the Riemann sheet for which

$$\lim_{z\to 0}\ (1-zt)^{-\alpha} = 1^{-\alpha} = 1 \ .$$

(See the discussion of this point below.) Trouble might arise in the integral for z real and greater than 1; however, this situation does not occur in our calculations.

Useful Relations:

$$F(\alpha,\beta,\gamma;z) = F(\beta,\alpha,\gamma;z) \quad \text{(B.14)}$$

$$F(\alpha,\beta,\gamma;z) = (1-z)^{-\beta}F\left(\beta,\gamma-\alpha,\gamma;\frac{z}{z-1}\right) \quad \text{(Magnus (49), p.8)} \quad \text{(B.15)}$$

$$\frac{(\lambda+iy)\,F(\lambda-iy,2\lambda,2\lambda+1;z(k))}{[\mu+i(p-\hbar k)]^{2\lambda}} + \frac{(\lambda-iy)\,F(\lambda+iy,2\lambda,2\lambda+1;z^*(-k))}{[\mu-i(p+\hbar k)]^{2\lambda}} =$$

$$= \frac{2\lambda}{[\mu+i(p-\hbar k)]^{\lambda+iy}[\mu-i(p+\hbar k)]^{\lambda-iy}}\ , \qquad z(k) = \frac{2ip}{\mu+i(p-\hbar k)} \quad \text{(B.16)}$$

Here λ, y, p, $\hbar k$, and μ are real. (B.16) is obtained from the relation

$$(\beta\pm\alpha)\,F(\alpha,\beta,\gamma;z) - \beta F(\alpha,\beta+1,\gamma;z) + \alpha F(\alpha+1,\beta,\gamma;z) = 0$$

and (B.17), the last relation being obtained by subtracting the 1st

and 2nd relations from the bottom of p.9 in Magnus(49) from each other.

Special Cases: (From (B.13))

$$F(\alpha,\beta,\beta;z) = (1-z)^{-\alpha} \tag{B.17}$$

$$F(\alpha,1,2;z) = \frac{-1}{z(1-\alpha)}\left[(1-z)^{1-\alpha}-1\right] \qquad 0<R(\alpha)<1 \tag{B.18}$$

$$F(1+iy,2,3;z) = -2i\left[\frac{(1-z)^{-iy}}{zy} + \left\{\frac{(1-z)^{1-iy}-1}{z^2y(1-iy)}\right\}\right] \tag{B.19}$$

Evaluation of B_{EK} in (III.C.1b)

To evaluate B_{EK}, it is necessary to evaluate integrals of the type

$$f(k) = \int_0^\infty r^{2\lambda-1} e^{-[\mu+i(\gamma-k)]r} F(\lambda+i\beta, 2\lambda+1; 2i\gamma r)\, dr \tag{B.20}$$

where μ, λ are real and positive and γ, k, β real. In order to integrate (B.20), first substitute the integral expression (B.6) for the confluent hypergeometric fn., then interchange the integrals - possible because of the presence of the decreasing exponential, and carry out the integration over r using (B.1) and finally, compare the result with (B.13) and (B.14) to obtain

$$f(k) = \frac{\Gamma(2\lambda)}{[\mu-i(k-\gamma)]^{2\lambda}} F\left(\lambda+i\beta, 2\lambda, 2\lambda+1; \frac{i2\gamma}{\mu-i(k-\gamma)}\right). \tag{B.21}$$

This result has been obtained previously by Hulme et al (35).

The radial integrals involving the electron in an intermediate discrete state are obtained as follows. Using the relation (B.7), the required integrals can all be expressed in the form:

$$\int_0^\infty r^{2\lambda-1} e^{-(\mu+\gamma-ik)r} F(\alpha, 2\lambda+1; 2\gamma r)\, dr \tag{B.22}$$

where λ, μ, γ are real and positive and α is zero or a negative integer (the special case in which $\alpha = 1$ is not required because of external zero factors). Since α is zero or a negative integer the series for the confluent hypergeomtric fn. is finite; hence, a term by term integration is possible, yielding after comparison with (B.12):

$$(B.22) = \frac{\Gamma(2\lambda)}{[\gamma+\mu-ik]^{2\lambda}} F\left(\alpha, 2\lambda, 2\lambda+1; \frac{2\gamma}{\gamma+\mu-ik}\right) \qquad (B.23)$$

Riemann Surface and Hypergeometric Fn.

Explicit expressions for the hypergeometric fns. used in this thesis are given in (B.17), (B.18), (B.19). Because of the presence of non-integral powers in these expressions, they are multivalued. It is the object of this Subsection to find out which value we must use.

Z in these expressions is of the form

$$Z = \frac{2iq}{1+i(q-x)} \qquad (B.24)$$

from which

$$1-Z = \frac{1-i(q+x)}{1+i(q-x)} \qquad (B.25)$$

Using the definitions (III.D.18) without the restrictions on the ranges of the θ's; we find for (B.25)

$$1-Z = \frac{r_+}{r_-} e^{-i(\theta_+ + \theta_-)} \qquad (B.26)$$

The quantity (B.26) is the only thing in our hypergeometric expressions

which is raised to a non-integral power and hence it causes the multi-valuedness.

In order to obtain the series expansion (B.12) for our hypergeometric fns., we can expand the binomials involving (B.26) provided we take

$$\lim_{z \to 0} (1-z)^{\gamma} = 1^{\gamma} = 1$$

for γ a complex number. This relation defines the sheet of the Riemann surface on which we must remain; thus, using (B.26), we find

$$(1-z)^{\gamma} \to e^{-i\gamma(\theta_+ + \theta_-)}$$

and since the value of this quantity has to be unity as Z (or q) goes to zero, we must have

$$\theta_+ + \theta_- \to 0 \quad \text{for} \quad q \to 0. \tag{B.27}$$

This condition defines a sheet of the Riemann surface and it is satisfied by the range chosen for the θ's in (III.D.18). The same condition (B.27) is obtained again for the complex conjugate of (B.26) which also appears in our Equations in Section III.D.

APPENDIX C.

THE NORMALIZED SOLUTIONS TO THE DIRAC EQUATION WITH A COULOMB POTENTIAL.

The normalized solutions to the Dirac Eq. with a Coulomb potential,

$$\left(-\frac{Ze^2}{r} + c\vec{\alpha}\cdot\vec{p} + \beta mc^2\right)\psi = E\psi \qquad (C.1a)$$

where:

$$\vec{p} = -i\hbar\vec{\nabla} \qquad (C.1b)$$

$$\alpha_1 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \quad \alpha_2 = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix} \quad \alpha_3 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \quad \beta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \qquad (C.1c)$$

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} \qquad (C.1d)$$

are given in the first Subsection below along with the special wave fns. used in the thesis. These solutions have been carried out in detail, although only the details necessary for an understanding of the thesis are presented here.

In the next two Subsections, normalization procedures are discussed along with a comparison of the solutions with those given by others.

In the last Subsection the "semi-relativistic" approximation is presented.

Summary of Normalized Solutions to the Dirac Equation with a Coulomb Potential

Following the procedure given by Kramers (38), one finds that the components of the wave fn. ψ can be separated into angular and radial dependent factors. Their are two independent solutions characterized by the quantum numbers j, m where j represents the total angular momentum and m its z component. These solutions are:

$$\psi_1 = \left[\frac{j+m}{2j}\right]^{1/2} Y^{m-1/2}_{j-1/2}\,\frac{F^+}{r} \qquad \psi_1 = \left[\frac{j-m+1}{2(j+1)}\right]^{1/2} Y^{m-1/2}_{j+1/2}\,\frac{F^-}{r}$$

$$\psi_2 = \left[\frac{j-m}{2j}\right]^{1/2} Y^{m+1/2}_{j-1/2}\,\frac{F^+}{r} \qquad \psi_2 = -\left[\frac{j+m+1}{2(j+1)}\right]^{1/2} Y^{m+1/2}_{j+1/2}\,\frac{F^-}{r}$$

$$\psi_3 = \left[\frac{j-m+1}{2(j+1)}\right]^{1/2} Y^{m-1/2}_{j+1/2}\,\frac{G^+}{r} \qquad \psi_3 = \left[\frac{j+m}{2j}\right]^{1/2} Y^{m-1/2}_{j-1/2}\,\frac{G^-}{r}$$

$$\psi_4 = -\left[\frac{j+m+1}{2(j+1)}\right]^{1/2} Y^{m+1/2}_{j+1/2}\,\frac{G^+}{r} \qquad \psi_4 = \left[\frac{j-m}{2j}\right]^{1/2} Y^{m+1/2}_{j-1/2}\,\frac{G^-}{r} \qquad (C.2)$$

These two solutions are distinguished by the quantity $K = \pm(j+\frac{1}{2})$, the + sign denoting the solution on the left and the - sign the one on the right.

In (C.2), the Y's are spherical harmonics depending on the polar angles θ, φ and are defined by the Equations:

$$Y^m_j(\theta,\varphi) = (-1)^m\left[\frac{2j+1}{4\pi}\,\frac{(j-m)!}{(j+m)!}\right]^{1/2}\frac{\sin^m\theta}{2^j\,j!}\,e^{im\varphi}\left(\frac{d}{d\cos\theta}\right)^{j+m}\left[\cos^2\theta-1\right]^j \qquad (C.3)$$

$$\int Y^{m*}_j\, Y^{m'}_{j'}\, d\Omega = \delta_{jj'}\,\delta_{mm'} \qquad (\Omega = \text{solid angle})$$

The fns. F,G depend on the radius vector r only; their superscripts denote to which sign of K the wave fn. composed of them belongs. These radial fns. satisfy the Eqs.

$$-i\left[\frac{d}{dr} + \frac{K}{r}\right]G = \left[\frac{E-mc^2}{\hbar c} + \frac{Z\alpha}{r}\right]F$$

$$-i\left[\frac{d}{dr} - \frac{K}{r}\right]F = \left[\frac{E+mc^2}{\hbar c} + \frac{Z\alpha}{r}\right]G \quad , \qquad \alpha = \frac{e^2}{\hbar c} \qquad (C.4)$$

the sign of K determining the superscript of F, G.

By setting $E = E_v + mc^2$, one can show from the Eqs. (C.4) that for positive energy states and for either sign of Z, the G's are negligible with respect to the F's in a non-relativistic approximation. Thus, only the first two components of the wave fns. (C.2) are necessary in the non-

relativistic limit so that, if these wave fns., in this limit, describe an electron with orbital angular momentum ℓ, then we must have

$$\left.\begin{aligned} j &= \ell + \tfrac{1}{2} \quad \text{for } K = +(j+\tfrac{1}{2}) \text{ wave fns.} \\ j &= \ell - \tfrac{1}{2} \quad \text{for } K = -(j+\tfrac{1}{2}) \text{ wave fns.} \end{aligned}\right\} \quad (C.5)$$

in the non-relativistic limit.

In solving (C.4) for normalizable solutions, one obtains the following results:

Discrete Solutions ($0 \leq E \leq mc^2$):

$$E(n', K^2) = \frac{mc^2}{\sqrt{1+\left(\frac{Z\alpha}{n'+\lambda}\right)^2}} \qquad n' = 0, 1, 2, \ldots$$

$$\lambda = \sqrt{K^2 - (Z\alpha)^2} \qquad K = \pm(j+\tfrac{1}{2})$$

$$F(r) = N\sqrt{B}\,(2\sqrt{AB}\,r)^{\lambda}\{f_+ + f_-\}$$

$$G(r) = N i\sqrt{A}\,(2\sqrt{AB}\,r)^{\lambda}\{f_+ - f_-\}$$

where: (C.6)

$$f_+ = (\lambda+\Delta)\left[\frac{K+\nabla}{\lambda+\Delta}\right]^{\frac{1}{2}} e^{-\sqrt{AB}\,r}\, F(\lambda-\Delta, 2\lambda+1; 2\sqrt{AB}\,r)$$

$$f_- = (\lambda-\Delta)\left[\frac{K-\nabla}{\lambda-\Delta}\right]^{\frac{1}{2}} e^{\sqrt{AB}\,r}\, F(\lambda+\Delta, 2\lambda+1; -2\sqrt{AB}\,r)$$

$$N = \frac{\hbar}{mc}\,\frac{\sqrt{AB}}{\Gamma(2\lambda+1)}\left[\frac{\Gamma(2\lambda+n')}{n'!\;2Z\alpha}\right]^{\frac{1}{2}}$$

$$\Delta = \lambda + n' \qquad \nabla = \sqrt{n'(n'+2\lambda)+K^2}$$

$$A = \frac{mc^2 - E}{\hbar c} \qquad B = \frac{mc^2 + E}{\hbar c}$$

F, G are normalized so that

$$\int_0^\infty (|F|^2 + |G|^2)\, dr = 1 \tag{C.7}$$

as discussed in the Normalization Subsection below.

In the non-relativistic limit, it can be shown that besides (C.5),

$$n' + |K| = n$$

the non-relativistic total quantum number.

Continuum Solutions ($|E| \geq mc^2$):

$$F(r) = \left[\frac{|E| + \delta mc^2}{4\pi\hbar c^2 p}\right]^{1/2} \frac{\left|\Gamma\left(\lambda + i\frac{Z\alpha E}{cp}\right)\right|}{\Gamma(2\lambda+1)} \left(\frac{2pr}{\hbar}\right)^{\lambda} e^{\pi\frac{Z\alpha E}{2cp}} \left\{f + f^*\right\}$$

$$G(r) = -\delta\left[\frac{|E| - \delta mc^2}{4\pi\hbar c^2 p}\right]^{1/2} \frac{\left|\Gamma\left(\lambda + i\frac{Z\alpha E}{cp}\right)\right|}{\Gamma(2\lambda+1)} \left(\frac{2pr}{\hbar}\right)^{\lambda} e^{\pi\frac{Z\alpha E}{2cp}} \left\{f - f^*\right\} \tag{C.8}$$

where:

$$\delta = +1 \quad \text{if} \quad E \geq mc^2 \qquad \delta = -1 \quad \text{if} \quad E \leq -mc^2$$

$$f = \left(\lambda - i\frac{Z\alpha E}{cp}\right) e^{-i\chi - i\frac{pr}{\hbar}}\, F\left(\lambda + i\frac{Z\alpha E}{cp},\, 2\lambda+1;\, \frac{2ipr}{\hbar}\right)$$

$$cp = +\sqrt{E^2 - (mc^2)^2}, \qquad e^{i\chi} = \left[\frac{K + i\frac{Z\alpha mc}{p}}{\lambda + i\frac{Z\alpha E}{cp}}\right]^{1/2}, \quad \chi \text{ real}.$$

$$\lambda = \sqrt{K^2 - (Z\alpha)^2}$$

Here F, G are normalized per unit energy interval, i.e. if F, G and F', G' belong to the energies E and E' respectively, then

$$\left.\begin{aligned} &\int_0^\infty (F'^* F + G'^* G)\, dr = \delta(E' - E) \\ \text{or} \quad &\int_{\Delta E} dE \int_0^\infty (F'^* F + G'^* G)\, dr = 1 \end{aligned}\right\} \tag{C.9}$$

where ΔE is any small energy interval containing E'.

Wave Fns. Used in the Thesis

K electron: $n' = 0$, $j = \frac{1}{2}$, $K = 1$, $E_K = mc^2(1-(Z\alpha)^2)^{\frac{1}{2}}$.

$$\underset{m=\frac{1}{2}}{\psi} = \begin{pmatrix} Y_0^0\, F^+ \\ 0 \\ \frac{1}{\sqrt{3}}\, Y_1^0\, G^+ \\ -\sqrt{\frac{2}{3}}\, Y_1^1\, G^+ \end{pmatrix} \frac{1}{r} \qquad \underset{m=-\frac{1}{2}}{\psi} = \begin{pmatrix} 0 \\ Y_0^0\, F^+ \\ \sqrt{\frac{2}{3}}\, Y_1^{-1}\, G^+ \\ -\frac{1}{\sqrt{3}}\, Y_1^0\, G^+ \end{pmatrix} \frac{1}{r} \tag{C.10}$$

In obtaining F^+, G^+ one uses $\lambda = \sqrt{1-(Z\alpha)^2}$, $\nabla = 1$, $\lambda - \Delta = 0$ and (B.5) in (C.6).

No solutions for $K = -1$ exist since F^-, G^- are zero.

Continuum Solutions for $K = \pm 1$, $j = \frac{1}{2}$:

For $K = +1$, $j = \frac{1}{2}$, $m = \pm \frac{1}{2}$, these solutions for an electron, have exactly the same form as in (C.10) with F^+, G^+ given by (C.8).

For $K = -1$, $j = \frac{1}{2}$, we have

$$\underset{m=\frac{1}{2}}{\psi} = \begin{pmatrix} \frac{1}{\sqrt{3}}\, Y_1^0\, F^- \\ -\sqrt{\frac{2}{3}}\, Y_1^1\, F^- \\ Y_0^0\, G^- \\ 0 \end{pmatrix} \frac{1}{r} \qquad \underset{m=-\frac{1}{2}}{\psi} = \begin{pmatrix} \sqrt{\frac{2}{3}}\, Y_1^{-1}\, F^- \\ -\frac{1}{\sqrt{3}}\, Y_1^0\, F^- \\ 0 \\ Y_0^0\, G^- \end{pmatrix} \frac{1}{r} \tag{C.11}$$

where F^-, G^- are obtained from (C.8).

The wave fns. of the neutrino have exactly the same form for $K = \pm 1$ as those for the electron wave fns. of the continuum just presented except that the nuclear charge Z and the mass m are set equal to zero in the radial solutions F, G.

Normalization Procedures

In this Subsection, the normalization procedures are outlined and carried out in some detail for continuum states. Essentially, the procedure followed is the one given by Sommerfeld although the method originated with Kramers(38).

For the normalization of discrete and continuum wave fns. the following integrals must be evaluated:

$$\int \psi^* \psi \, d\vec{r} = |N|^2 \int_0^\infty (|F|^2 + |G|^2) dr = 1 \qquad \text{(discrete)} \qquad (C.12)$$

$$\int \psi'^* \psi \, d\vec{r} = |N|^2 \int_0^\infty (F'^* F + G'^* G) dr = \delta(E'-E) \text{(continuum)} \qquad (C.13)$$

where N is the normalization factor. In obtaining the radial integrals (C.12), (C.13), the orthogonality of the spherical harmonics (C.3) has been used. In (C.13) the primed quantities belong to the energy E'.

Instead of using (C.13) to find N, the following integral

$$\int_{\Delta E} dE \int_0^\infty \psi'^* \psi \, d\vec{r} = |N|^2 \int_{\Delta E} dE \int_0^\infty (F'^* F + G'^* G) dr = 1 \qquad (C.14)$$

is used where ΔE is any small energy interval containing E'.

The basic formula used to evaluate these normalization integrals is obtained from (C.4) and its complex conjugate Eqs. for an energy E'. If we call the two Eqs. in (C.4) (a) and (b) and the corresponding complex conjugate Eq's. for an energy E', (c) and (d), and form the quantity

$$(a)F'^* + (b)G'^* + (c)F + (d)G$$

then we can obtain the relation

$$-i\frac{d}{dr}\left(F'^{*}G + G'^{*}F\right) = \left(\frac{E-E'}{\hbar c}\right)\left(F'^{*}F + G'^{*}G\right) \qquad (C.15)$$

from which

$$\int_0^R (F'^{*}F + G'^{*}G)\,dr = \frac{i\hbar c}{E'-E}\left[F'^{*}G + G'^{*}F\right]_R \qquad (C.16)$$

using the fact that $F(0) = G(0) = 0$. The quantity in square brackets on the right is evaluated at the radius R. From the Eq.(C.16), we see that the normalization integral on the left can be evaluated from the asymptotic values of F, G for large R on the right.

(C.16) has been obtained without any restrictions on E and E', so that even for the <u>discrete</u> states we can consider the solutions F, G as fns. of a continuous variable E and make use of a Taylor expansion in powers of (E'-E) to find

$$\int_0^\infty (|F|^2 + |G|^2)\,dr = i\hbar c \lim_{R\to\infty}\left[\frac{\partial F^*}{\partial E}G + \frac{\partial G^*}{\partial E}F\right]_R \qquad (C.17)$$

In obtaining (C.17), we have used the result

$$\lim_{R\to\infty}\left[F^*G + G^*F\right]_R = 0$$

By using the asymptotic solutions for F and G and carrying out the limit on the R.H.S. of (C.17), one can evaluate the discrete normalization integral. For details written in English, see Hill and Landshoff (38).

Let us carry out the normalization of Continuum wave fns. in detail. For convenience, we shall use (in the next few paragraphs only) the quantities:

$$\rho = \frac{r}{\gamma} \qquad \gamma = \frac{\hbar}{mc} \qquad \frac{E}{mc^2} = \delta W \qquad \delta = \pm 1 \quad \text{for} \quad E \gtrless \pm mc^2$$

$$\eta = \sqrt{W^2 - 1} = \frac{p}{mc} \qquad \Delta = \frac{Z\alpha W}{\eta}$$

and the unnormalized solutions:

$$F(\rho) = \sqrt{W+\delta}\ (2\eta\rho)^{\lambda} \left\{ f + f^* \right\}$$

$$G(\rho) = -\delta \sqrt{W-\delta}\ (2\eta\rho)^{\lambda} \left\{ f - f^* \right\} \tag{C.18}$$

$$f = (\lambda - i\delta\Delta)\, e^{-i\chi - i\eta\rho}\, F(\lambda + i\delta\Delta, 2\lambda+1; 2i\eta\rho)$$

$$e^{i\chi} = \left[\frac{K + iZ\alpha/\eta}{\lambda + i\delta\Delta} \right]^{1/2}$$

to evaluate

$$|N_\lambda|^2 \int_{\Delta W} dW \int_0^\infty d\rho \left(F'^* F + G'^* G \right) = |N_\lambda|^2 \int_{\Delta W} dW \lim_{\rho\to\infty} \frac{i}{\delta(W'-W)} \left[F'^* G + G'^* F \right]_\rho = 1 \tag{C.19}$$

where F, G are given by (C.18) and

$$N_\lambda = N (\hbar c)^{\frac{1}{2}} \tag{C.20}$$

In (C.19), W' is contained in the small interval ΔW.

From (B.11) we find, for large ρ,

$$F(\lambda + i\delta\Delta, 2\lambda+1; 2i\eta\rho) \sim \frac{\Gamma(2\lambda+1)}{\Gamma(\lambda+1-i\delta\Delta)} (-2i\eta\rho)^{-\lambda - i\delta\Delta} \tag{C.21a}$$

and defining

$$\frac{\Gamma(2\lambda+1)}{\Gamma(\lambda+1-i\delta\Delta)} = \Gamma e^{-i\xi}, \qquad \lambda - i\delta\Delta = a e^{i\varphi} \tag{C.21b}$$

we obtain, from (C.21) and (C.18),

$$(2\eta\rho)^{\lambda} f \approx a\Gamma e^{-\frac{\delta\pi\Delta}{2}} e^{-i\xi} \qquad (C.22a)$$

where

$$\xi = \eta\rho + \delta\Delta \ln 2\eta\rho + \xi - \frac{\lambda\pi}{2} + \chi - \varphi . \qquad (C.22b)$$

Thus, from (C.18) and (C.22), we have, asymptotically,

$$\left.\begin{aligned} F &\sim 2\sqrt{W+\delta}\; a\Gamma e^{-\frac{\delta\pi\Delta}{2}} \cos\xi \\ G &\sim 2i\delta\sqrt{W-\delta}\; a\Gamma e^{-\frac{\delta\pi\Delta}{2}} \sin\xi \end{aligned}\right\} \qquad (C.23)$$

From (C.23), we find

$$\int_{\Delta W} dW \lim_{\rho\to\infty} \frac{i}{\delta(W'-W)} \left[F'^{*}G + G'^{*}F\right]_{\rho}$$

$$= 4a^2\Gamma^2 e^{-\delta\pi\Delta} \lim_{\rho\to\infty} \int_{\Delta\eta} d\eta\, \eta\, \frac{\sin(\eta-\eta')\rho}{(\eta-\eta')} \qquad (C.24)$$

using $\xi - \xi' \sim (\eta-\eta')\rho$ for large ρ

and $\frac{1}{W-W'} \sim \frac{W}{\eta}\frac{1}{\eta-\eta'}$ for W near W'.

Using

$$\delta(x) = \frac{1}{\pi} \lim_{K\to\infty} \frac{\sin Kx}{x}$$

Heitler (54), Eq. 1, p. 66, we obtain finally

$$(C.24) = 4\pi a^2\Gamma^2 e^{-\delta\pi\Delta}\eta . \qquad (C.25)$$

Thus, from (C.25), (C.21b), (C.19),

$$N_{\eta} = \frac{e^{\frac{\delta\pi\Delta}{2}}}{\sqrt{4\pi\eta}} \frac{|\Gamma(\lambda+i\Delta)|}{\Gamma(2\lambda+1)} \qquad (C.26)$$

and using (C.26), with (C.20) and (C.18), we find the normalized solutions (C.8) for F, G.

Comparison With Normalized Solutions Of Other Authors

Some of the other authors solve the Dirac Eq.:

$$H' \psi' = E \psi' \tag{C.27a}$$

where

$$H' = -\frac{Ze^2}{r} - c\vec{\alpha}\cdot\vec{p} - \beta mc^2 , \tag{C.27b}$$

all quantities appearing in (C.27) being defined in (C.1). Let us investigate how to obtain our solutions ψ from the solutions ψ'.

Consider the operator

$$O = -i\beta\alpha_1\alpha_2\alpha_3 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \tag{C.28}$$

Making use of the relations

$$\alpha_i \alpha_j + \alpha_j \alpha_i = 2\delta_{ij} \qquad \alpha_i \beta + \beta \alpha_i = 0 \qquad \beta^2 = 1,$$

one can show that $O\alpha_i = -\alpha_i O$, $O\beta = -\beta O$ and hence

$$OH' = HO , \tag{C.29}$$

where H is our Hamiltonian,

$$H = -\frac{Ze^2}{r} + c\vec{\alpha}\cdot\vec{p} + \beta mc^2 ,$$

given in Eq. (C.1). Multiplying (C.27a) by O from the left and using the relation (C.29), one can show that $O\psi'$ is an eigenfunction of H to the eigenvalue E. Thus, assuming ψ', ψ are normalized, we must have:

$$\psi = e^{i\omega} O \psi' \qquad \text{or} \qquad \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} = e^{i\omega} \begin{pmatrix} \psi_3' \\ \psi_4' \\ -\psi_1' \\ -\psi_2' \end{pmatrix} \tag{C.30}$$

where $e^{i\omega}$ is some plase factor which is the same for all four components. The result (C.30) has been used to compare the normalized solutions to the Hamiltonian (C.27b) given by other authors with the solutions given here.

The solutions given in (C.2) and (C.6) for discrete states have been checked with those of Kramers (38), who uses the same Hamiltonian H, and with those of Hill and Landshoff (38), who use H' (C.27b), and agreement has been found except for a common phase factor $e^{i\omega}$ (C.30).

Rose (37) has tabulated the continuum solutions without stating which form of the Hamiltonian he uses; however, if we assume that he used the Hamiltonian H' (C.27b), then agreement exists between the continuum solutions (C.2) and (C.8), for both positive and negative energies, and his solutions except for a common phase factor $e^{i\omega}$ in (C.30).

THE SEMI-RELATIVISTIC APPROXIMATION

We shall first study how to obtain the normalized radial solutions of the Schrodinger Eq. with a Coulomb potential from our "large" radial solutions to the Dirac Eq. For convenience the quantities F, G are called the radial solutions to the Dirac Eq. although the complete radial dependence of the wave fns. is given by these quantities divided by r. Similarly, for the Schrodinger Eq., the complete radial dependence of the wave fns. is given by the "radial solution" divided by r. We shall find that when the rules obtained for the "large" radial solutions, are applied to the "small" radial solutions, the result is zero. A semi-relativistic approximation based on these rules is then formulated and the normalization of the semi-relativistic wave fns. studied.

Discrete States:

Kramers (38), p. 311, states what substitutions are required for discrete states. A restatement in terms of our solutions and notation is as follows:

The normalized discrete radial solutions of the Schrodinger Eq. are given by

$$F_{n\ell}(r) = \left[\frac{Z\alpha}{n^2} \frac{mc}{\hbar} \frac{(n+\ell)!}{(n-\ell-1)!} \right]^{\frac{1}{2}} \frac{e^{-\rho/2}}{(2\ell+1)!} \rho^{\ell+1} F(\ell+1-n, 2\ell+2; \rho) \qquad (C.31a)$$

$$\rho = 2 \frac{Z\alpha mc}{n\hbar} r \qquad (C.31b)$$

the complete radial dependence being $F_{n\ell}/r$. This solution is obtained from either (i.e. for $K = \pm (j + \frac{1}{2})$) of our "large" discrete radial solutions of the form.

$$F = N\sqrt{B}\ (2\sqrt{AB}\,r)^{\lambda}\left\{ f_+ + f_- \right\}$$

by first setting $E = mc^2$ in just the second factor $\sqrt{B}$

$$i.e. \qquad \sqrt{B} = \left[\frac{2mc}{\hbar}\right]^{1/2}$$

then everywhere else setting $\lambda = |K|$ (instead of $\lambda = \sqrt{K^2-(z\alpha)^2}$), and $n = n' + |K|$, where K is either $K = \ell + 1$ or $K = -\ell$ (corresponding to those solutions for which $K = +(j + \frac{1}{2})$ or $K = -(j + \frac{1}{2})$ respectively), either choice producing $(c^{3}_{\lambda}1)$ with orbital angular momentum ℓ.

One may check these statements with the help of the relations (B.10) for the confluent hypergeometric fns. and the exact result

$$1 - \left(\frac{E}{mc^2}\right)^2 = \frac{(z\alpha)^2}{n'^2 + 2\lambda n' + K^2}$$

which, when substituted into $\sqrt{AB}$ with $\lambda = |K|$, $n = n' + |K|$ (Cf. p.86) gives

$$\sqrt{AB} = \frac{z\alpha mc}{n\hbar}$$

Possible minus sign factors may appear in obtaining $(C^{3}_{\lambda}1)$ but these are irrelevant and hence omitted.

Applying the above rules to our "small" radial solutions G in exactly the same way, one obtains zero because the factor $\sqrt{A}$ in front of G goes to zero.

Positive Continuum States

For the case of positive continuum states, the radial solution to the Schrodinger Eq. is given by

$$F_\ell(p,r) = \left[\frac{m}{2\pi\hbar p}\right]^{1/2} \frac{e^{\pi\frac{Z\alpha mc}{2p}}}{(2\ell+1)!} \left|\Gamma\left(\ell+1+i\frac{Z\alpha mc}{p}\right)\right| e^{-\frac{ipr}{\hbar}} \left(\frac{2pr}{\hbar}\right)^{\ell+1} \times$$

$$\times F\left(\ell+1+i\frac{Z\alpha mc}{p}, 2\ell+2; \frac{2ipr}{\hbar}\right) \qquad (C.32)$$

(from Sommerfeld, pp. 115-127) which is normalized per unit energy interval. Again, the complete radial dependence is F_ℓ/r. This expression is obtained from our "large" continuum solutions in a manner somewhat different from that for the discrete states.

The expression (C.32) is a positive energy solution, so we must put $\delta = +1$ in our expression for F. Now, consider the large radial solutions F as fns. of p using

$$E = +\sqrt{(cp)^2 + (mc^2)^2}$$

then, in order to obtain the corresponding radial solution to the Schrodinger Eq: (a) Replace E by the first term in its expansion in powers of p, i.e.

$$E \to mc^2 \qquad (C.33a)$$

(b) Set $\lambda = |K|$ everywhere. (C.33b)

Wherever E appears, it is divided by cp so that, using the relation

$$\frac{E}{cp} = \frac{mc}{p} + \frac{cp}{E+mc^2} \to \frac{mc}{p} ,$$

we can see what is neglected in this ratio when rule (C.33a) is applied. Both values of $K = \ell+1$ or $K = -\ell$ produce the same result (C.32) having orbital angular momentum ℓ.

Again, the relations (B.10) are useful for checking this procedure. Also, possible minus sign factors have been omitted. If these rules are applied to our small solutions G in exactly the same way, one obtains zero

because the factor $(|E|-mc^2)^{1/2}$ in front of G goes to zero.

Negative Continuum States

We shall first show that for negative continuum states the G's are the "large" solutions and the F's the "small".

Let us write our radial solutions as functions of E, K, Z. Then, for negative energy states, $E = -|E|$ and $\delta = -1$, and we have for an electron,

$$F(-|E|, K, Z),\ G(-|E|, K, Z)$$

It is not difficult to prove by direct substitution in F, G (or from the Eqs. (C.4)) that these radial solutions are related to the positive energy radial solutions according to the relations:

$$F(-|E|, K, Z) = e^{i\varphi}\, G^*(|E|, -K, -Z) \qquad \text{(C.34a)}$$

$$G(-|E|, K, Z) = e^{i\varphi}\, F^*(|E|, -K, -Z) \qquad \text{(C.34b)}$$

where φ is real and constant. The parameters on the R.H.S. of (C.34) show that the radial solutions there represent a positron in a positive energy state. Since for a positive energy state, F is large and G is small (independently of the sign of Z), then the relation (C.34) tells us that for an electron in a negative energy state and represented by the radial fns. on the L.H.S. of (C.34), the G's are "large" and the F's are "small".

In order to obtain the non-relativistic radial solution from the large solutions G for the electron in a negative energy state, we see from (C.34) that this is completely equivalent to obtaining the non-relativistic

radial solution for the F's for a positron in a positive energy state. If we replace Z by -Z in the radial Schrodinger solution (C.32), then we obtain the non-relativistic radial solution for a positron in a positive energy state. This solution is then obtained from (C.34b) by setting, just as for the electron in a positive continuum state,

$$|E| = mc^2 \qquad \lambda = |K|$$

both signs of K giving the same result.

The corresponding rule for the "large" radial solution G for an electron in the negative continuum then, from (C.34b), must be to set

$$E = -|E| \to -mc^2 \qquad \text{and} \quad \lambda = |K| \tag{C.35}$$

in exactly the same places as for the positive energy case.

As before, the relations (B.10) can be used to check this procedure and possible minus sign factors have been omitted. If the rule (C.35) is applied to the "small" radial solution F in exactly the same way, one obtains zero because the factor $(|E|-mc^2)^{1/2}$ in front of F goes to zero.

The Semi-Relativistic Approximation for Continuum States.

Let us study the Dirac radial Eqs. to find what effect setting $\lambda = |K|$ and $E = mc^2$ in some of the places mentioned above has on them. The exact radial Eqs. are:

$$-i\left[\frac{d}{dr} + \frac{K}{r}\right]G = \left[\frac{E-mc^2}{\hbar c} + \frac{Z\alpha}{r}\right]F \tag{C.36a}$$

$$-i\left[\frac{d}{dr} - \frac{K}{r}\right]F = \left[\frac{E+mc^2}{\hbar c} + \frac{Z\alpha}{r}\right]G \tag{C.36b}$$

from (C.4).

We shall not approximate the square root energy factors appearing in ffont of F, G because , for the "small" solutions, these factors go to zero in a non-relativistic approximation and we do not want such a result in the approximations which we shall make.

Let
$$\left.\begin{aligned} F &= \sqrt{|E|+\delta mc^2}\; r_1^{\lambda} F_1 \\ G &= -\delta \sqrt{|E|-\delta mc^2}\; r_1^{\lambda} G_1 \\ r_1 &= \frac{pr}{\hbar} \quad , \quad \lambda > 0 \end{aligned}\right\} \qquad (C.37)$$

Substituting (C.37) into (C.36), we find that F_1, G_1 satisfy

$$\left.\begin{aligned} i\left[\frac{d}{dr_1} + \frac{\lambda+K}{r_1}\right] G_1 &= \left[1 + \frac{Z\alpha}{cp}\,\frac{(E+mc^2)}{r_1}\right] F_1 \\ i\left[\frac{d}{dr_1} + \frac{\lambda-K}{r_1}\right] F_1 &= \left[1 + \frac{Z\alpha}{cp}\,\frac{(E-mc^2)}{r_1}\right] G_1 \end{aligned}\right\} \qquad (C.38)$$

these Eqs. still being exact. Comparing (C.37) with our solutions in (C.8), we see what the expressions for F_1, G_1 are and , in particular, from which parts of Eq. (C.38) the quantities λ , K, $Z\alpha E/cp$, $Z\alpha mc/p$ seem to arise.

Let us now force λ to be $|K|$, i.e. the smallest total power of r_1 for series solutions for F, G in (C.37) is $|K|$. This requires that

$$\left.\begin{aligned} F_1 &= \sum_{n=0}^{\infty} a_n\, r_1^n \\ G_1 &= \sum_{n=0}^{\infty} b_n\, r_1^n \end{aligned}\right\} \qquad (C.39)$$

with non-trivial solutions for a_0, b_0. Substituting (C.39) into(C.38) and equating the coefficients of like powers of r_1, we find for r_1^{-1} , the Eqs:

$$\left.\begin{aligned} i(\lambda+K)\, b_0 &= \frac{Z\alpha}{cp}\,(E+mc^2)\, a_0 \\ i(\lambda-K)\, a_0 &= \frac{Z\alpha}{cp}\,(E-mc^2)\, b_0 \end{aligned}\right\} \qquad (C.40)$$

and since we require non-trivial solutions for a_o, b_o in (C.40), we must have

$$(\lambda+K)(\lambda-K) = -\left(\frac{Z\alpha}{cp}\right)^2 (E+mc^2)(E-mc^2) \qquad (C.41)$$

Now, since $\lambda = |K|$, the L.H.S. of (C.41) is zero. In order that (C.41) be satisfied we must have either $Z=0$ (irrelevant) or $E=\delta mc^2$. Conversely, if $E=\delta mc^2$, we must have $\lambda=|K|$ (since $\lambda \to 0$ from (C.37)). These substitutions constitute the semi-relativistic approximation.

If we set in (C.38) $\lambda=|K|$ and $E=\delta mc^2$, we find the approximate Eqs.

$$\left.\begin{aligned} i\left[\frac{d}{dr_1} + \frac{|K|+K}{r_1}\right]\mathcal{G}_1 &= \left[1 + \frac{Z\alpha mc}{p}\frac{(\delta+1)}{r_1}\right]\mathcal{F}_1 \\ i\left[\frac{d}{dr_1} + \frac{|K|-K}{r_1}\right]\mathcal{F}_1 &= \left[1 + \frac{Z\alpha mc}{p}\frac{(\delta-1)}{r_1}\right]\mathcal{G}_1 \end{aligned}\right\} \qquad (C.42)$$

and, from the definitions (C.37), we find our semi-relativistic solutions $\mathcal{F}$, $\mathcal{G}$ given by

$$\left.\begin{aligned} \mathcal{F} &= \sqrt{|E|+\delta mc^2}\; r_1^{|K|} \mathcal{F}_1 \\ \mathcal{G} &= -\delta\sqrt{|E|-\delta mc^2}\; r_1^{|K|} \mathcal{G}_1 \end{aligned}\right\} \qquad (C.43)$$

and satisfying the Eqs:

$$\left.\begin{aligned} -i\left[\frac{d}{dr} + \frac{K}{r}\right]\mathcal{G} &= \left[\frac{E-mc^2}{\hbar c} + \frac{Z\alpha}{r}\left\{1 - \frac{E-\delta mc^2}{E+mc^2}\right\}\right]\mathcal{F} \\ -i\left[\frac{d}{dr} - \frac{K}{r}\right]\mathcal{F} &= \left[\frac{E+mc^2}{\hbar c} + \frac{Z\alpha}{r}\left\{1 - \frac{E-\delta mc^2}{E-mc^2}\right\}\right]\mathcal{G}, \end{aligned}\right\} \qquad (C.44)$$

the "unnormalized" solutions $\mathcal{F}$, $\mathcal{G}$ to these Eqs. being the semi-relativistic fns. obtained from our exact normalized solutions F, G by setting $\lambda=|K|$ and $E = mc^2$ everywhere but in the square root energy factors in front of the solutions.

From these considerations, we see that in order to find the radial solutions to the Dirac Eqs. for $\lambda = |K|$ we must approximate the Eqs. by setting $E = \delta mc^2$ in appropriate places and conversely, the solutions to the approximated Eqs. being the semi-relativistic radial solutions.

Normalization of the Semi-Relativistic Radial Solutions

For E near δmc^2, our semi-relativistic "large" radial solutions become almost equal to the normalized Schrodinger radial solution, the "small" solutions going to zero, and consequently, the semi-relativistic fns. $\mathcal{F}, \mathcal{G}$ are normalized in this limit. This statement is obvious when one realizes that the only difference between the "large" semi-relativistic radial solution and the normalized Schrodinger radial solution lies in the square root energy factor in front of these solutions.

If we use Eqs.(C.44) in exactly the same way as in the Normalization Subsection of this Appendix, we find that the exact normalization of $\mathcal{F}, \mathcal{G}$ can be obtained from the relation

$$-i\frac{d}{dr}\left[\mathcal{F}'^{*}\mathcal{G} + \mathcal{G}^{*}\mathcal{F}\right] = \frac{(E-E')}{\hbar c}\left[\mathcal{F}'^{*}\mathcal{F} + \mathcal{G}'^{*}\mathcal{G}\right]$$

$$+\frac{Z\alpha mc^2}{r}(E-E')\left[\frac{-(1+\delta)\,\mathcal{F}'^{*}\mathcal{F}}{(E'+mc^2)(E+mc^2)} + \frac{(1-\delta)\,\mathcal{G}'^{*}\mathcal{G}}{(E'-mc^2)(E-mc^2)}\right] \qquad (C.45)$$

the primed quantities belonging to the energy E'.

Considering only the positive energy case, the negative energy case being similar, we find for the normalization integral:

$$\lim_{R\to\infty}\int_{\Delta E}dE\int_0^R\left[\mathcal{F}'^{*}\mathcal{F}+\mathcal{G}'^{*}\mathcal{G}\right]dr=-i\hbar c\lim_{R\to\infty}\int_{\Delta E}dE\left[\mathcal{F}'^{*}\mathcal{G}+\mathcal{G}'^{*}\mathcal{F}\right]_R$$

$$+\frac{2Z\alpha\,\hbar c\,mc^2}{(E+mc^2)^2}\lim_{R\to\infty}\int_{\Delta E}dE\int_0^R\frac{\mathcal{F}'^{*}\mathcal{F}}{r}dr \qquad (C.46)$$

taking $E'+mc^2$ outside the last integral (permissible because ΔE is small). The first integral on the R.H.S. is unity as one may check by following through the normalization procedures in this Appendix for the exact Dirac radial solutions in the continuum setting $\lambda=|K|$ and $E=mc^2$ everywhere but in the square root energy factors.

The second integral on the R.H.S. is too complicated to obtain even an order of magnitude for it; however, the following argument seems to show that it is negligible. Remember that when E is near mc^2, $\mathcal{F}$ becomes the normalized Schrodinger radial solution and $\mathcal{G}$ goes to zero. This means the second integral on the R.H.S. of (C.46) is negligible when E is near mc^2.

Let us now compare the integrals involving the $\mathcal{F}$'s only, and show that the one on the R.H.S. of (C.46) is negligible with respect to the one on the L.H.S. The factor in front of the R.H.S. integral is of the order

$$2Z\alpha\frac{\hbar}{mc}\sim 2Z\alpha\,10^{-10}$$

for E near mc^2, this factor decreasing as E increases. The R.H.S. integrand

is finite everywhere as a fn. of r since the radial dependence $\mathcal{F}/r$ varies with r as the non-relativistic Schrodinger radial solution divided by r does. If we carried out the energy integral first in both the integrals under consideration, the resulting integrands would have exactly the same energy dependence but would differ in their radial dependence by the factor r. For this reason, the variation of the integrals with respect to the energy would be the same and since the second integral on the R.H.S. is negligible for E near mc^2, it must still be negligible for higher energies especially since the factor (C.47) multiplying it decreases as $1/E^2$.

Appendix D

Derivation of Eq. (II.8)

The object is to simplify the expression

$$(H_s + W_e)\vec{\alpha}\cdot\vec{e}_k\left(\frac{H+E}{2E}\right)\vec{\alpha}\cdot\vec{e}_k\,(H_s + W_e). \tag{D.1}$$

For convenience, the following definitions and units are used in this appendix only:

$$\vec{e}_k = \vec{m} \qquad \hbar = 1 \qquad c = 1$$
$$H = \vec{\alpha}\cdot\vec{p} + \beta m \qquad H_s = \vec{\alpha}\cdot(\vec{p}+\vec{k}) + \beta m \tag{D.2}$$

Also, the following relations will be used:

$$(\vec{\alpha}\cdot\vec{a})^2 = a^2 \tag{D.3a}$$
$$(\vec{\alpha}\cdot\vec{a})(\vec{\alpha}\cdot\vec{b}) + (\vec{\alpha}\cdot\vec{b})(\vec{\alpha}\cdot\vec{a}) = 2(\vec{a}\cdot\vec{b}) \tag{D.3b}$$
$$H(\vec{\alpha}\cdot\vec{a}) + (\vec{\alpha}\cdot\vec{a})H = 2(\vec{p}\cdot\vec{a}) \tag{D.3c}$$
$$H_s(\vec{\alpha}\cdot\vec{a}) + (\vec{\alpha}\cdot\vec{a})H_s = 2(\vec{p}\cdot\vec{a}) + 2(\vec{k}\cdot\vec{a}) \tag{D.3d}$$
$$H^2 = E^2 \tag{D.3e}$$
$$H_s = H + \vec{\alpha}\cdot\vec{k} \tag{D.3f}$$
$$H_s H + H H_s = 2(E^2 + \vec{p}\cdot\vec{k}) \tag{D.3g}$$
$$\vec{k}\cdot\vec{m} = 0 \tag{D.3h}$$

$\vec{a}, \vec{b}$ being any vectors. All these relations but the last follow from the commutation relations for the Dirac matrices.

Expanding (D.1) in powers of W_e, one obtains

$$(H_s + W_e)X(H_s + W_e) = H_s X H_s + W_e(H_s X + X H_s) + W_e^2 X \tag{D.4a}$$

where

$$X = \vec{\alpha}\cdot\vec{m}\left(\frac{H+E}{2E}\right)\vec{\alpha}\cdot\vec{m} \tag{D.4b}$$

$$X = -\frac{H}{2E} + \frac{(\vec{p}\cdot\vec{m})(\vec{\alpha}\cdot\vec{m})}{E} + \frac{1}{2} \qquad (D.4b)$$

using (D.3a), (D.3c). Simplifying the coefficient of W_e by the use of (D.3e), (D.3f), (D.3g), D.3d), (D.3h), one finds

$$H_s X + X H_s = -\frac{(E^2 + \vec{p}\cdot\vec{k})}{E} + 2\frac{(\vec{p}\cdot\vec{m})^2}{E} + H + \vec{\alpha}\cdot\vec{k} \,. \qquad (D.5)$$

The first term in (D.4a) can be written in the form

$$\begin{aligned} H_s X H_s = & -\frac{1}{2E}(H + \vec{\alpha}\cdot\vec{k})H(H + \vec{\alpha}\cdot\vec{k}) \\ & + \frac{(\vec{p}\cdot\vec{m})}{E}(H + \vec{\alpha}\cdot\vec{k})(\vec{\alpha}\cdot\vec{m})(H + \vec{\alpha}\cdot\vec{k}) \\ & + \frac{1}{2}(H + \vec{\alpha}\cdot\vec{k})^2 \end{aligned} \qquad (D.6)$$

using (D.3f), (D.4b). The terms of (D.6) are simplified as follows: the first term reduces to

$$(H + \vec{\alpha}\cdot\vec{k})H(H + \vec{\alpha}\cdot\vec{k}) = (E^2 - k^2)H + 2(E^2 + \vec{p}\cdot\vec{k})(\vec{\alpha}\cdot\vec{k}). \qquad (D.7a)$$

using (D.2), (D.3c), (D.3e) [illegible]; the second term reduces to

$$(H + \vec{\alpha}\cdot\vec{k})\vec{\alpha}\cdot\vec{m}(H + \vec{\alpha}\cdot\vec{k}) =$$

$$= -\left[E^2 + 2\vec{p}\cdot\vec{k} + k^2\right]\vec{\alpha}\cdot\vec{m} + 2\vec{p}\cdot\vec{m}H + 2(\vec{p}\cdot\vec{m})(\vec{\alpha}\cdot\vec{k}) \qquad (D.7b)$$

using (D.3a), (D.3b), (D.3c) and (D.3h); and the last term reduces to

$$(H + \vec{\alpha}\cdot\vec{k})^2 = E^2 + 2\vec{p}\cdot\vec{k} + k^2 \,, \qquad (D.7c)$$

using (D.3a), (D.3e) and (D.3c).

Collecting the formulae (D.4), (D.5), (D.6) and (D.7) together and changing back to the original units (D.2), one obtains (II.8).

Integrals involved in obtaining Eq. (II.11)

In order to carry out the operations $\int d\Omega_e \sum_\gamma$, we shall let $\vec{k}$ be fixed in direction along one axis $\vec{u}_3$ of an orthogonal set of unit vectors $\vec{u}_1$, $\vec{u}_2$, $\vec{u}_3$. The momentum $\vec{p}$ will be in a direction subtending the angle θ with the $\vec{u}_3$ axis and an azimuthal angle φ to the $\vec{u}_1$ axis. $\vec{e}_k$ can be either $\vec{u}_1$ or $\vec{u}_2$. Subscripts 1, 2, and 3, will refer to the components of a vector along the corresponding axes.

The sum over the photon polarizations is carried out first, then the integral over just the angle φ for the directions of emission of the electron,

$$\int d\Omega_e = \int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta \, d\theta$$

The integrand turns out to be either independent of φ , in which case a non-zero result occurs, or linear in $\sin\varphi$ or $\cos\varphi$, in which case the integration over φ is zero.

Two examples are sufficient to understand the procedure. The expression,

$$\sum_\gamma (\vec{a}\cdot\vec{e}_k)(\vec{p}\cdot\vec{e}_k) = a_1 p_1 + a_2 p_2$$

$$= p\left[a_1 \sin\theta\cos\varphi + a_2 \sin\theta\sin\varphi\right] \quad , \quad \vec{a} \text{ a constant vector,}$$

when integrated over φ gives zero. Also, using

$$\sum_\gamma (\vec{p}\cdot\vec{e}_k)^2 = p_1^2 + p_2^2 = p^2 \sin^2\theta$$

in the expression

$$\sum_\gamma (\vec{a}\cdot\vec{p})(\vec{p}\cdot\vec{e}_k)^2 = p^3 \sin^2\theta\left[a_1 \sin\theta\cos\varphi + a_2 \sin\theta\sin\varphi + a_3\cos\theta\right],$$

one finds

$$\int_0^{2\pi} d\varphi \sum_\gamma (\vec{a}\cdot\vec{p})(\vec{p}\cdot\vec{e}_k)^2 = 2\pi a_3 p^3 \sin^2\theta\cos\theta = 2\pi \frac{\vec{a}\cdot\vec{k}}{k} p^3 \sin^2\theta\cos\theta$$

since $\vec{k}$ is along the $\vec{u}_3$ axis.

Integrals connected with Eq. (II.16)

The integrals over W_e which are required can be written in either of the forms

$$\int_1^x dy\,(y-x)^2\, y \ln\left[y+\sqrt{y^2-1}\right] \tag{D.8a}$$

$$\int_1^x dy\,(y-x)^2\,\sqrt{y^2-1} \tag{D.8b}$$

by means of the substitutions

$$y = \frac{W_e - E_\gamma}{mc^2} \qquad x = \frac{W - E_\gamma}{mc^2} \tag{D.8c}$$

The change of variable

$$y = \cosh u \qquad u = \ln\left[y+\sqrt{y^2-1}\right] \tag{D.9}$$

is enough to express the integrands of (D.8) in a recognizable form, i.e. as a product of **U** and a polynomial in $\cosh u$ and $\sinh u$. An integration by parts gets rid of the **U** term, leaving an integration of a polynomial in $\cosh u$ and $\sinh u$ which can be evaluated by standard procedures. The results are:

$$(D.8a) = \left[\frac{x^4}{12} - \frac{x^2}{4} - \frac{3}{32}\right] \ln\left[x+\sqrt{x^2-1}\right] - \left[\frac{13}{144}x^3 - \frac{101}{288}x\right]\sqrt{x^2-1} \tag{D.10a}$$

$$(D.8b) = -\frac{1}{2}\left[x^2+\frac{1}{4}\right] \ln\left[x+\sqrt{x^2-1}\right] + \frac{1}{12}\left[x^3+\frac{13}{2}x\right]\sqrt{x^2-1} \tag{D.10b}$$

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