ON THE THEORY OF RADIATIVE ELECTRON CAPTURE

by

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B.Sc., Université de Montréal, 1951
M.A., University of British Columbia, 1953

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of

GUY PAQUETTE

B.Sc. (Montreal)
M.A. (British Columbia)

MONDAY, SEPTEMBER 10th, 1956, at 10:30 a.m.

IN ROOM 301, PHYSICS BUILDING

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External Examiner: R. T. SHARP
McGill University

ON THE THEORY OF RADIATIVE CAPTURE OF ORBITAL ELECTRONS

Abstract

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The conclusions are: first, approximations used by Hess were partly inconsistent, although the method was in principle correct; second, taking into account retardation effects results in a gamma spectrum whose intensity amounts to 0.8 of the intensity obtained by Glauber and Martin at 135 Kev. and to 0.2 at 675 Kev. (the gamma spectrum limit being 816 Kev.).

The gamma spectrum of A^{37} determined by Lindqvist and Wu (1955) seems to agree quite well with Glauber and Martin's result. However, Lindqvist and Wu measured only relative intensities and had to apply many instrumental corrections so that it is not yet clear whether the measured spectrum would not agree as well with the spectrum computed in this thesis.

PUBLICATIONS

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GRADUATE STUDIES

Field of Study: Physics

Quantum Mechanics	G. M. Volkoff
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Electromagnetic Theory	W. Opechowski
Theoretical Nuclear Physics	W. Opechowski
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The conclusions are: first, approximations used by Hess were partly inconsistent, although the method was in principle correct; second, taking into account retardation effects results in a gamma spectrum whose intensity amounts to 0.8 of the intensity obtained by Glauber and Martin at 135 Kev. and to 0.2 at 675 Kev. (the gamma spectrum limit being 816 Kev.).

The gamma spectrum of A^{37} determined by Lindqvist and Wu (1955) seems to agree quite well with Glauber and Martin's result. However, Lindqvist and Wu measured only relative intensities and had to apply many instrumental corrections so that it is not yet clear whether the measured spectrum would not agree as well with the spectrum computed in this thesis.

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ABSTRACT

The continuous spectrum of gamma radiation which accompanies the capture of orbital electrons has been recently calculated independently by Glauber and Martin (1954), and by Hess (1955). Both calculations take into account the influence of the nuclear charge on the wave functions but otherwise involve different methods and approximations, the conclusions being also quite different: the intensity of the gamma radiation is an order of magnitude lower according to Hess than according to Glauber and Martin. The purpose of the calculations presented in this thesis has been to settle this disagreement and to explain its origin. To this effect the high energy part of the gamma spectrum, which is almost entirely determined by the contributions of the capture of the 1s and 2s electrons, has been computed for the case of A^{37} for which experimental data are available. In view of the low nuclear charge of A^{37} ($Z = 18$), the non-relativistic Coulomb wave functions could be used, and, apart from neglecting screening effects, the calculations are exact although partly numerical. In particular, the retardation effects which were neglected by Glauber and Martin have rigorously been taken into account.

The conclusions are: first, approximations used by Hess were partly inconsistent, although the method was in principle correct; second, taking into account retardation effects results in a gamma spectrum whose intensity amounts to 0.81 of the intensity obtained by Glauber and Martin at 135 Kev, and to 0.24 at 675 KeV (the gamma spectrum limit being 816 KeV).

The gamma spectrum of A^{37} determined by Lindqvist and Wu (1955) seems to agree quite well with Glauber and Martin's result. However, Lindqvist and Wu measured only relative intensities and had to apply many instrumental corrections so that it is not yet clear whether the measured spectrum would not agree as well with the spectrum computed in this thesis.

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Introduction and Summary

This thesis is concerned with the theory of the "radiative capture" of an orbital electron by the nucleus. We call the process of capture "radiative" when it is accompanied by the emission of a gamma radiation. When no gamma emission takes place, the process is called "radiationless".

The radiative capture, although a factor 10^3 less probable than the radiationless capture, has been observed for several elements, and the corresponding continuous gamma spectrum has been determined (See, for instance, Lindqvist and Wu (55), where also references to earlier papers are given). The most important radiative capture process is that accompanying the radiationless capture of a K-electron. The theory for this case has been developed by several authors (Morrison and Schiff (40), Glauber and Martin (54) and Hess (55)). In order to describe briefly what these authors have done, and to indicate the contribution to the theory, presented in this thesis, we shall have first to sketch the common theoretical basis of all these calculations.

The expression for the probability of the radiative capture is given by a standard formula of the second order time-dependent perturbation theory. In the product of the matrix elements entering this formula, one factor arises from the electromagnetic interaction H_γ and the other from the Fermi interaction H_β. The electromagnetic interaction induces a transition between an initial state and an intermediate state. For instance, the initial state may correspond to an electron characterized by

the principal and orbital quantum numbers n and ℓ respectively. The intermediate state then corresponds to an electron with the quantum numbers n^1 and $\ell^1 = 0$ (an s-electron), and to a photon. The Fermi interaction gives rise to the capture of the electron in that intermediate state and to the creation of a neutrino. The assumption that $\ell^1 = 0$ (but n^1 arbitrary) in the intermediate states, or, in other words, that the captured electron is an s-electron, defines the radiative process corresponding to the "allowed" radiationless capture of an s-electron from the K-shell. We shall call this process the "radiative K-capture", although, in view of the remark above, this phrase should not be interpreted in too literal a sense. We denote the probability of radiative K-capture, i.e. the probability per second that a photon of energy $\hbar ck$ in the range $d(\hbar ck)$ is emitted during the K-capture process by $w_R\, dk$, and the probability that a radiationless K-capture occurs per second by w_c. It is the observed ratio $w_R dk / w_c$, as a function of k, that is compared with theory. In principle, all orbital electrons contribute to the experimental value for $w_R\, dk$. This means that $w_R\, dk$ is a sum of the probabilities obtained for all values of n and ℓ that correspond to the occupied orbits. However, it turns out that only the orbits characterized by $n = 1$, $\ell = 0$; $n = 2$, $\ell = 0$ and $\ell = 1$; and $n = 3$, $\ell = 1$, contribute an appreciable amount to the ratio $w_R dk / w_c$.

As is well known, there are five different interactions H_β possible in the Fermi theory of beta decay, giving rise to allowed and forbidden spectra. In this thesis, as well as in the publications quoted above, only allowed transitions have been

considered.

The first theoretical evaluation of $w_K dk$ was made by Morrison and Schiff (40) who considered only the case of the K-shell electrons, i.e. the case in which n = 1 and $\ell = 0$. These authors made, among others, two important simplifying assumptions: first, they represented the final, intermediate and initial states by plane waves, thereby neglecting the Coulomb interaction between the electron and the nucleus; second, they took into account only the vector interaction. They calculated w_c in the same approximation and they finally obtained the following simple formula:

$$\frac{w_K dk}{w_c} = \frac{\alpha}{\pi} \kappa \left(1 - \frac{\kappa}{\kappa_{max}}\right)^2 d\kappa$$

where $\kappa = \kappa_c k / mc^2$ (dimensionless)

and α is the fine structure constant.

This formula more or less agrees with experimental data for photons of large energy (i.e. $1 - \kappa/\kappa_{max} \ll 1$). However, as was first shown by Saraf's experiments (54), the Morrison-Schiff formula fails completely to explain the large ratio $w_K dk / w_c$ that one obtains experimentally for low energies of the emitted photon.

In order to explain this breakdown of the theory at low photon energies, one may extend Morrison and Schiff's calculations in several directions, by taking into account:

1st the Coulomb interaction between the electron and the nucleus,

2nd an arbitrary mixture of the five beta interactions,

3rd the contribution to radiative capture of electrons with higher values of n and l .

Such an extension of the theory has been carried out by Glauber and Martin (54) and by Hess (55) independently, the latter author restricting himself, however, to taking into account the contribution of the 1s electrons only. The calculations are approximate in both cases, but the method applied by Glauber and Martin is quite different from that applied by Hess. The results do not agree: the intensity of gamma radiation is an order of magnitude smaller according to Hess than it is according to Glauber and Martin.

Glauber and Martin's (54) calculation is non-relativistic as far as wave functions of the electrons are concerned; in other words, they used the Schroedinger wave functions of an electron in the Coulomb field of the nucleus. In that approximation, they could find a relatively simple closed expression for the sum over the intermediate energy states, using, in an ingenious way, the properties of the Green's function. However, in order to evaluate the resulting expression for the probability $w_k dk$, they simplified the expression for the matrix element of the electromagnetic interaction by neglecting the retardation factor. On this simplifying assumption they came to the rather startling conclusion that the ($n = 1$, $l = 0$) - contribution to the photon spectrum is exactly the same as that found by Morrison and Schiff (40), who, as will be recalled, completely neglected the Coulomb interaction. This conclusion seems, on the other hand, to be in agreement with the high energy part of the measured spectrum, since this part, as it was mentioned before, is well

represented by the Morrison-Schiff formula. Glauber and Martin also showed (using the same simplifying assumption) that the observed sudden rise in the gamma spectrum at low energies is due to the contribution of p-electrons (i.e. $\ell = 1$, $n = 2, 3 \ldots$) and that this contribution becomes negligible at high photon energies.

Hess's calculations, on the other hand, start from general formulae in which the Dirac relativistic wave functions are used. However, the actual computation of the expression for $w_K dk$ so obtained, turned out to be impracticable even for the simplest case of the 1s electron. Consequently, number of simplifying assumptions were made: the sum over the intermediate discrete states was assumed to be small compared with the sum over the continuous states, then a "semi-relativistic" approximation for the radial part of the intermediate state wave function was introduced, and the subsequent calculation was carried out numerically for the case of $_{55}Cs^{131}$ for which, at that time, the best experimental data were available (Saraf (54)).

In view of the discrepancy between Hess's results and those of Glauber and Martin, and of the neglecting of the retardation effects by the latter authors, it was felt that an evaluation of $w_K dk$, in which the non-relativistic Coulomb wave functions are used, but which is otherwise rigourous[1], would greatly clarify the situation. Such an evaluation of the contribution of $\ell = 0$ and $n = 1$ and 2 (the contribution in case $n \geq 3$ is negligible), i.e. the contribution that determines completely the photon energy spectrum not very far from its limit, is presented in this thesis

1) It is true that the final part of these calculations has been done numerically. However, no arbitrary approximation has been introduced in those numerical calculations. On the other hand, the screening effects are entirely disregarded, which for a light atom like $_{A}37$ is probably not too serious.

for the case of $^{37}_{18}A$ and $^{131}_{55}Cs$ [1].

Our calculations settle the disagreement between Glauber and Martin's results and those of Hess essentially in favour of the former authors.

The discrepancy is traced down to a rather well hidden inconsistency in the argument which leads from the general relativistic formulae to Hess's "semi-relativistic" expressions. This question is discussed in detail in Chapter II, Section C, of this thesis, as it is of some general interest.

Although our results essentially confirm those of Glauber and Martin, the fact that we did not neglect the retardation effects has some important quantitative consequences. It turns out that the taking into account of these effects leads to a decrease of the intensity of gamma radiation accompanying the K-capture in ^{37}A, the decrease increasing with the increasing photon energy, as can be seen in Fig. 5, in Chapter III (the corresponding numerical data are summarized in Table III, in Chapter III).

In an unpublished paper (56) [2], Glauber and Martin discuss, among other things, some relativistic corrections to their earlier results, and also announce that they have applied "a more fully relativistic treatment of the process which takes account of screening". A comparison of the results of this treatment with Lindqvist and Wu's experimental data for ^{37}A is given in a recent

1) Only one value of the energy spectrum for ^{131}Cs is evaluated, to make a comparison with Hess's result possible. On the other hand, the case of ^{37}A, for which we have the most recent and most reliable experimental data, (Lindqvist and Wu (55)) is considered in detail.

2) A copy of the paper has kindly been made available by Professor Glauber to Professor Opechowski.

note by Wu and al. (56). The high energy part of the spectrum does not seem to be affected by these refinements in the calculation; however, it is not clear whether the retardation effects have been taken into account.

The problem of a detailed comparison of our theoretical results with the experimental data of Lindqvist and Wu (55) is briefly discussed in Chapter III, Section B.

Chapter I

General Formalism of the Theory of Electron Capture.

In this Chapter, we shall be concerned with the general theory underlying the calculations of Chapter III. In Chapter II, we consider, in more details, the wave functions to be used, and we discuss the passage from the general theory to the approximation of Hess (55). In Chapter III we present our own calculations and conclusions, and compare them with those of Glauber and Martin (54).

The notation that we use in sketching the general theory of electron capture is essentially that used by De Groot and Tolhoek (50). In Section A of this Chapter, we set up the general expression for the probability λw_c of radiationless K-capture. A more complete treatment of the subject can be found in the review articles of Rose (55), Konopinski (55), and Konopinski and Langer (53). In Section B, we consider the case of the radiative K-capture probability $\lambda w_R dk$. Finally, in Section C, we derive an alternative expression for the electromagnetic interaction matrix element. This expression is equivalent to the standard one, but is more convenient when one carries out the passage to the non-relativistic approximation.

A - Radiationless K-capture

The probability per second of a radiationless K-capture depends on a matrix element describing a transition between an initial and a final state. The initial state (represented by the

symbol O) consists of a nucleus of charge Z in an energy state W_Z . The final state (represented by the symbol F) consists of a nucleus of charge Z-1 in an energy state W_{Z-1}, of an emitted neutrino of energy E_ν and of a hole in the K- shell. Therefore, if E_{1S} is the energy of the electron in the K-shell,

$$W_Z + E_{1S} = W_{Z-1} + E_\nu \qquad \text{I.1}$$

expresses the law of the conservation of energy. $W_Z + E_{1S} - W_{Z-1} = W$ is the energy available to the transition.

On assuming the standard Fermi theory of beta processes, the matrix element which determines the probability of electron capture can be written in the following form:

$$(F|H_\beta|O) = \sum_{m=1}^{A} \int (\varphi^\dagger \Omega \psi_{1S})_m (\psi_f^\dagger \Omega_m \psi_i)\, d\tau_m \qquad \text{I.2}$$

where H_β is the interaction Hamiltonian

φ is the wave function for the emitted neutrino

ψ_{1S} is the wave function for the electron in the K-shell

ψ_i and ψ_f are the initial and final nuclear states respectively,

$\dagger$ is the symbol for the adjoint, i.e. the complex conjugate and transpose, of a matrix

Ω and Ω_m are the interaction operators operating respectively on the lepton and

the nucleon wave functions

$( )_m$ means that the function in the brackets is evaluated at the position of the n^{th} nucleon

$\int d\tau_m$ means that the integration is carried over the volume containing the n^{th} nucleon, i.e. the whole nuclear volume

$\sum_{m=1}^{A}$ is a summation over all the nucleons

By restricting the interaction matrix elements to be relativistically invariant, one can show that there are only five possible choices for Ω, and this, on very general assumptions. Ω, in general, consists of two components, one of which is "large" or non-relativistic and the other is "small" or relativistic (of order v/c where v is the nucleon velocity). The "large" and "small" components give rise to different selection rules.

In this thesis, we only consider <u>allowed</u> beta transitions. This means, as is well known, <u>1st</u>, that we neglect the "small" components of the five Fermi interactions,[1] and <u>2nd</u>, that we assume that the emitted neutrino carries away zero orbital angular momentum.

The large components of the five interaction operators are the following:

The Scalar interaction	β	I.3a
The Vector interaction	1	I.3b
The Tensor interaction	$\beta\vec{\sigma}$	I.3c
The Axial Vector interaction	$\vec{\sigma}$	I.3d

1) If one neglects the small components, the resulting expression is of course no more relativistically invariant.

The Pseudoscalar interaction $i\beta\gamma_5$ I.3e

$1, \beta, \vec{\sigma}$ and γ_5 are four by four matrices defined as follows:

$$1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \qquad \beta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \qquad \text{I.4a}$$

$$\vec{\sigma} = \vec{i}\,\sigma_1 + \vec{j}\,\sigma_2 + \vec{k}\,\sigma_3 \qquad \text{I.4b}$$

where $\vec{i}$, $\vec{j}$ and $\vec{k}$ are unit vectors and

$$\gamma_5 = i\alpha_1\alpha_2\alpha_3 \; ; \; \sigma_1 = i\alpha_2\alpha_3 \; ; \; \sigma_2 = i\alpha_3\alpha_1 \; ; \; \sigma_3 = i\alpha_1\alpha_2 \qquad \text{I.4c}$$

$\alpha_1, \alpha_2, \alpha_3$ are matrices defined as follows:

$$\alpha_1 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \qquad \alpha_2 = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix} \qquad \alpha_3 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \qquad \text{I.4d}$$

The five interaction operators thus defined are Hermitian. The pseudoscalar interaction $i\beta\gamma_5$ is relativistic of order v/c; there is no "large" component in this case.

Since the operator Ω of the general expression I.2 may contain an arbitrary linear combination of these five interactions, we introduce five corresponding constants

$$C_S \; , \; C_V \; , \; C_T \; , \; C_A \; , \; C_P \qquad \text{I.5}$$

The subscripts refer to the scalar, vector, tensor, axial vector

and pseudoscalar interactions respectively.

However, the five interactions I.3 actually contain nine different matrices $\hat{A}^{\lambda}$, and it is convenient to introduce the nine coefficients C_{λ} defined as follows:

$$\begin{array}{lccccccccc} r = & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \\ \hat{A}^{\lambda} = & \beta & 1 & \beta\sigma_1 & \beta\sigma_2 & \beta\sigma_3 & \sigma_1 & \sigma_2 & \sigma_3 & i\beta\gamma_5 \\ C_{\lambda} = & C_S & C_V & C_T & C_T & C_T & C_A & C_A & C_A & C_P \end{array} \qquad \text{I.6}$$

With the notation I.6, the interaction matrix element I.3 takes the form:

$$(F|H_\beta|0) = G\sum_{\lambda=1}^{9} C_\lambda \sum_{m=1}^{A} \int (\varphi^\dagger \hat{A}^\lambda \psi_{1s})_m (\psi_f^\dagger \hat{A}_m^\lambda \psi_i)\, d\tau_m \qquad \text{I.7}$$

Here we have supposed that the interaction constants are normalized according to

$$C_S^2 + C_V^2 + C_T^2 + C_A^2 + C_P^2 = 1 ,$$

and we have denoted the intensity factor (the "Fermi constant") by G. The C_λ's can always be chosen real. (See Blatt and Weisskopf (52)).

The assumption that the neutrino carries no orbital angular momentum means that the neutrino wave function φ in the expression I.7 is characterised by a total angular momentum quantum number $j = \frac{1}{2}$. One can show that the expression I.7 is much smaller when φ corresponds to values of j higher than $\frac{1}{2}$ ("Forbidden" transitions).

Finally, we make the usual assumption that the lepton part $(\varphi^{\dagger} A^{n} \psi_{1s})_{n}$ of the Fermi interaction matrix element I.7 is a slowly varying function inside the nucleus. Hence, this lepton matrix element can be written outside the integral sign and, also, outside the sign of summation over all the nucleons in the expression I.7. The lepton matrix element is then usually evaluated at a distance R from the origin, R being the nuclear radius. One obtains

$$(F\,|H_{\beta}|\,0) = G \sum_{n=1}^{9} C_{n} (\varphi^{\dagger} A^{n} \psi_{1s})_{R} \cdot (\int A^{n}) \qquad \text{I.8a}$$

where

$$\int A^{n} = \sum_{m=1}^{A} \int (\psi_{f}^{\dagger} A_{m}^{n} \psi_{i})\, d\tau_{m} \qquad \text{I.8b}$$

is a nuclear matrix element that is assumed different from zero only when a proton changes into a neutron. Expression I.8 is therefore the matrix element for an allowed radiationless K-capture. The probability per second of such an event is then given by the following formula:

$$w_{c} = \frac{2\pi}{\hbar} S_{\nu} \int d\Omega_{\nu} S_{0} \left|(F|H_{\beta}|0)\right|^{2} \qquad \text{I.9}$$

where S_{ν} means that we sum over the spins of the emitted neutrino,

$\int d\Omega_{\nu}$, that we integrate over the angles of emission of the neutrino,

and S_{0}, that we sum over the spins of the initial K-electron.

The lepton wave functions that we use in this thesis are normalised per unit energy interval; hence, the neutrino wave function implicitely contains the density of final states that otherwise would appear as a factor in the expression I.9.

In this thesis, we treat the nucleons and their wave functions as non-relativistic. It follows that for the Scalar and Tensor interactions I.3a and I.3b in the nuclear matrix elements I.8b, one can write

$$\int \beta = \int 1 \quad \text{and} \quad \int \beta \vec{\sigma} = \int \vec{\sigma} \qquad \text{I.10}$$

One can thus replace β by the unit matrix, since, in our formalism, the +1 components of β will connect the "large" non-relativistic components of the nucleon wave functions whereas the -1 components of β will connect the "small" components, which we are neglecting.

B - Radiative K - capture

In the case in which the electron capture is accompanied by the emission of a gamma photon, one has to consider all the intermediate states that the system may occupy, in order to evaluate the probability $w_R \, dk$. In accordance with the hole theory, two types of processes are possible in the transition from the initial to the final state. The initial state of the

system consists of the nucleus N_Z in the energy state W_Z ; all the negative energy states are occupied. The final state consists of a nucleus N_{Z-1} in the energy state W_{Z-1} , a hole in place of the electron characterized by the quantum numbers n and ℓ , a photon of energy $\hbar ck$, and a neutrino of energy E_ν ; all the negative energy states are again occupied. The processes that may take place are of the two following types:

I. - The atomic electron (characterized by n and ℓ) 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. Another electron jumps into the remaining hole with the emission of a photon

The conservation of energy (between the initial and the final states) is expressed by the relation

$$W_Z + E_{n\ell} = W_{Z-1} + E_\nu + \hbar ck \qquad \text{I.11}$$

where $E_{n\ell}$ is the energy of the electron in the shell characterized by n. Therefore, $W_Z + E_{n\ell} - W_{Z-1} = E_\nu + \hbar ck$ is the energy available to the transition.

The matrix element entering the expression for the probability $w_k dk$ should involve a sum over all the intermediate states

of type I plus a sum over the intermediate states of type II. However, it can be shown (see, for example, a similar proof in Heitler (50), p. 147) that the two sums can be evaluated together as one sum taken over all the intermediate states, positive and negative, occupied and not occupied. From the well-known formula of time-dependent perturbation theory, the matrix element is of the form

$$\sum_I \frac{(F|H_\beta|I)(I|H_\gamma|0)}{E_I - E_0} \qquad \text{I.12}$$

where F, I and 0 are symbols for the final, intermediate and initial states respectively. $(I \mid H_\gamma \mid 0)$ is the electromagnetic interaction matrix element and $(F \mid H_\beta \mid I)$ is the same beta interaction matrix element as the one used in the radiationless case Eq. I.10 , except that the 1s-electron wave function is replaced by the intermediate state electron wave function ψ_E (which is also an s-function because we suppose the transition to be allowed). E_I and E_0 are the energy values corresponding to the intermediate and the initial states. In terms of the quantities defined previously, and of E, the energy of the electron in the intermediate state, we have

$$E_I - E_0 = E - E_{nl} + \hbar c k \qquad \text{I.13}$$

The expression for $w_k dk$, similar to that for w_c, Eq. I.10, is as follows:

$$w_k dk = \frac{2\pi}{\hbar} \cdot \frac{k^2 dk}{(2\pi)^3} S_\gamma \int d\Omega_\gamma \cdot S_\nu \int d\Omega_\nu \cdot S_0 \left| \sum_I \frac{(F|H_\beta|I)(I|H_\gamma|0)}{E_I - E_0} \right|^2 \qquad \text{I.14}$$

where S_γ indicates summation over the two directions of polarization of the photon

S_ν and S_o indicates summation over the spins of the neutrino and those of the initial electron respectively

$\int d\Omega_\gamma$ and $\int d\Omega_\nu$ mean, that we integrate over the angles of emission of the photon and of the neutrino respectively

$\frac{k^2 dk}{(2\pi)^3}$ is the photon contribution to the density of final states.

The wave functions are supposed to be normalized per unit energy interval. The matrix elements in I.14 are given by:

$$(F|H_\beta|I) = G \sum_n c_n (\varphi^+ A^n \psi_E)_R \left(\int A^n\right) \qquad \text{I.15}$$

(the symbols have the same meaning as in Section A) and by (See Heitler (50), p.95)

$$(I|H_\gamma|0) = C \int \psi_E^+ \vec{\alpha}\cdot\vec{e}_k \, Q \, \psi_{nl} \, d\vec{r} \qquad \text{I.16}$$

where $C = e\left(\frac{2\pi\hbar c}{k}\right)^{1/2}$

$Q = e^{-i\vec{k}\cdot\vec{r}}$, the retardation factor

$\vec{e}_k$ is the polarization vector of the photon whose wave vector is $\vec{k}$; $|\vec{k}| = k$

$\vec{\alpha}$ is the Dirac matrix defined in I.4

e is the charge of the electron

ψ_E and ψ_{nl} are the wave functions for the electron in the intermediate and the

initial states respectively.

$\psi^{\dagger}$ means the Hermitian conjugate of ψ

The integration is over all space.

In the following Section, we derive another expression for the electromagnetic interaction matrix element I.16, the usefulness of which will be apparent in the next Chapter.

C - The Matrix Element of Electromagnetic Interaction

In this Section, we consider the general case of an electromagnetic transition between a state of energy E described by the electron wave function ψ_E and a state of energy E^1 described by $\psi_{E'}$. ψ_E and $\psi_{E'}$ are Dirac eigenfunctions for an electron in the presence of an electromagnetic field characterized by a vector potential $\vec{A}$ and a scalar potential φ .

The matrix element of the electromagnetic interaction introduced in Section B, Eq. I.16 is then a special case of the following matrix element:

$$M = (E|H_r|E') = C \int \psi_E^{\dagger} \vec{\alpha} \cdot \vec{e}_k Q \psi_{E'} d\vec{\tau} \qquad \text{I.17}$$

We are now going to put this matrix element into another form by applying a transformation introduced by Gordon (28) to decompose the Dirac probability current into an "orbital" part

and a "spin" part.

To this purpose it will be convenient to use a covariant tensor notation (in this, we more or less follow Pauli (33) and Sommerfeld in their presentation of Gordon's method).

We first introduce the contravariant four-vector

$$\gamma^{\mu} \qquad \mu = 0,1,2,3 \tag{I.18}$$

of which the components are chosen to be

$$\gamma^{0} = \beta\,,\ \gamma^{1} = \beta\alpha_1\,,\ \gamma^{2} = \beta\alpha_2\,,\ \gamma^{3} = \beta\alpha_3 \tag{I.19}$$

β, α_1, α_2 and α_3 are defined in Eq. I.4. The components γ^1, γ^2 and γ^3 are thus anti-Hermitian: $(\gamma^{K})^{\dagger} = -\gamma^{K}$, $K = 1,2,3$.

The γ^{μ}'s thus chosen obey the following commutation rule:

$$\gamma^{\mu}\gamma^{\nu} + \gamma^{\nu}\gamma^{\mu} = 2\,g^{\mu\nu}\,I \quad ;\ \mu,\nu = 0,1,2,3 \tag{I.20}$$

where $g^{\mu\nu}$ is the well-known contravariant metric tensor:

$$g^{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{I.21}$$

and where I is the unit matrix. The covariant $g_{\mu\nu}$ is defined such that

$$\sum_{\nu=0}^{3} g^{\mu\nu} g_{\nu\sigma} = \delta^{\mu}_{\sigma} \tag{I.22}$$

where δ^{μ}_{σ} is the Kronecker tensor.

Therefore,

$$g_{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{I.23}$$

The position four-vector is defined as

$$x^{\mu} = (ct, \vec{r}) \qquad \text{I.24}$$

such that the energy - momentum four-vector

$$p^{\mu} = \left(\frac{E}{c}, \vec{p}\right) \qquad \text{I.25}$$

is related to the operator

$$p_{\mu} = i\hbar \nabla_{\mu} = i\hbar \frac{\partial}{\partial x^{\mu}} \qquad \text{I.26}$$

by the rule

$$p_{\mu} = \sum_{\nu=0}^{3} g_{\mu\nu} p^{\nu} \qquad \text{I.27}$$

Therefore, from I.23

$$p_{\mu} = \left(\frac{E}{c}, -\vec{p}\right) \qquad \text{I.28}$$

The electromagnetic field can also be expressed as a four-vector

$$A^{\mu} = (\varphi, \vec{A}) \qquad \text{I.29}$$

The covariant four-vector A_{μ} is given by

$$(\varphi, -\vec{A}) \qquad \text{I.30}$$

In the notation introduced above, the equation satisfied by ψ_E and $\psi_{E'}$ is the following

$$\left[\sum_{\mu=0}^{3} \gamma^{\mu}\left(\frac{\partial}{\partial x^{\mu}} - \frac{ie}{\hbar c} A_{\mu}\right) + \frac{imc}{\hbar}\right]\psi = 0 \qquad \text{I.31a}$$

Introducing the bar function $\bar{\psi} = \psi^{+}\gamma^{0}$, we see that ψ_E and $\psi_{E'}$ satisfy the adjoint equation

$$\sum_{\mu=0}^{3}\left(\frac{\partial}{\partial x^{\mu}} + \frac{ie}{\hbar c} A_{\mu}\right)\bar{\psi}\gamma^{\mu} - \frac{imc}{\hbar}\bar{\psi} = 0 \qquad \text{I.31b}$$

Eqs. I.31 a) and b) are equivalent to the equations used by Pauli (33), p.232.

By solving Eqs. I.31a and I.31b for $\psi_{E'}$ and $\bar{\psi}_E$ respectively, one obtains

$$\psi_{E'} = -\frac{\hbar}{imc}\sum_{\mu=0}^{3}\gamma^{\mu}\left(\frac{\partial}{\partial x^{\mu}} - \frac{ie}{\hbar c}A_{\mu}\right)\psi_{E'} \qquad \text{I.32a}$$

$$\bar{\psi}_E = \frac{\hbar}{imc}\sum_{\mu=0}^{3}\left(\frac{\partial}{\partial x^{\mu}} + \frac{ie}{\hbar c}A_{\mu}\right)\bar{\psi}_E\,\gamma^{\mu} \qquad \text{I.32b}$$

If we write for simplicity $\vec{e}_k = \vec{e}$ and introduce the component $e_0 \equiv 0$, the matrix element M, Eq. I.17, can be written in the form

$$M = C\int \bar{\psi}_E(\vec{r})\, Q\, \vec{\gamma}\cdot\vec{e}\;\psi_{E'}\, d\vec{\tau} \qquad \text{I.33}$$

We now replace $\psi_{E'}$ and $\bar{\psi}_E$ in I.33 each in turn by the expression I.32a and I.32b respectively, which yields:

$$M = -\frac{e\hbar}{imc}\sum_{\mu=0}^{3}\int \bar{\psi}_E\, Q\, \vec{e}\cdot\vec{\gamma}\,\gamma^{\mu}\left(\nabla_{\mu} - \frac{ie}{\hbar c}A_{\mu}\right)\psi_{E'}\, d\vec{\tau} \qquad \text{I.34a}$$

and

$$M = \frac{e\hbar}{imc}\sum_{\mu=0}^{3}\int \left(\nabla_{\mu} + \frac{ie}{\hbar c}A_{\mu}\right)\bar{\psi}_E\,\gamma^{\mu}\, Q\, \vec{e}\cdot\vec{\gamma}\;\psi_{E'}\, d\vec{\tau} \qquad \text{I.34b}$$

Writing again $\vec{e}\cdot\vec{\gamma} = \sum_{\nu} e_{\nu}\gamma^{\nu}$, adding the two expressions I.34 and dividing the result by 2, we obtain for M the following expression:

$$M = \frac{e\hbar}{2imc}\sum_{\mu}\sum_{\nu}\int(\nabla_\mu\bar{\psi}_E\gamma^\mu\gamma^\nu\psi_{E'} - \bar{\psi}_E\gamma^\nu\gamma^\mu\nabla_\mu\psi_{E'})\,e_\nu\,Q\,d\vec{r}$$

$$+ \frac{e\hbar}{2imc}\frac{ie}{\hbar c}\sum_{\mu}\sum_{\nu}\int A_\mu\bar{\psi}_E(\gamma^\mu\gamma^\nu+\gamma^\nu\gamma^\mu)\psi_{E'}\,e_\nu\,Q\,d\vec{r} \qquad \text{I.35}$$

where we have separated the field - dependent terms from the others.

Using the fact that $\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2g^{\mu\nu}$ we separate the terms in which $\nu=\mu$ from those in which $\nu\neq\mu$ to obtain

$$M = \frac{e\hbar}{2imc}\sum_{\mu}\int\Big[(\nabla_\mu\bar{\psi}_E)\psi_{E'} - \bar{\psi}_E(\nabla_\mu\psi_{E'})\Big]g^{\mu\mu}e_\mu\,Q\,d\vec{r}$$
$$+\frac{ce}{mc^2}\sum_{\mu}\int A_\mu g^{\mu\mu}e_\mu\bar{\psi}_E\psi_{E'}\,Q\,d\vec{r}\Big]_{\nu=\mu} \qquad \text{I.36}$$
$$+\frac{e\hbar}{2imc}\sum_{\mu\neq\nu}\sum\int\nabla_\mu(\bar{\psi}_E\gamma^\mu\gamma^\nu\psi_{E'})\,e_\nu\,Q\,d\vec{r}\Big]_{\nu\neq\mu}$$

We now use the relations $e_0 = 0$, $g^{\mu\mu} = -1$ and $A_\mu = -\vec{A}$ for $\mu \neq 0$. (See Eqs. I.21 and I.30). Also we note that when $\nu\neq\mu$, $i\gamma^\mu\gamma^\nu = -i\alpha^\mu\alpha^\nu = \sigma^{\mu\nu}$, where $\sigma^{\mu\nu}$ is the Dirac spin operator. We also separate the $\mu=0$ term from the terms in which μ and ν are different from zero in the last line of I.36. In this way, I.36 becomes the sum of four terms:

$$M = M_1 + M_2 + M_3 + M_4 \qquad \text{I.37}$$

where

$$M_1 = -\frac{e\hbar}{2imc}\int\Big[(\vec{\nabla}\bar{\psi}_E)\psi_{E'} - \bar{\psi}_E(\vec{\nabla}\psi_{E'})\Big]\cdot\vec{e}\;Q\,d\vec{r} \qquad \text{I.37a}$$

$$M_2 = \frac{ce}{mc^2}\int\vec{A}\cdot\vec{e}\;Q\,\bar{\psi}_E\psi_{E'}\,d\vec{r} \qquad \text{I.37b}$$

$$M_3 = -\frac{e\hbar}{2mc} \sum_{\substack{l,m=1 \\ l\neq m}}^{3}\sum^{3} \int \nabla_l (\bar{\psi}_E \sigma^{lm} \psi_{E'}) e_m Q \, d\vec{r} \qquad \text{I.37c}$$

$$M_4 = \frac{e\hbar}{2imc} \int \nabla_0 (\bar{\psi}_E \sum_{m=1}^{3} \gamma^0 \gamma^m e_m \psi_{E'}) Q \, d\vec{r} \qquad \text{I.37d}$$

We now make the assumption that one of the energy levels E, E^1 (let us say, E^1) is a discrete level. Then the function $\psi_{E'}$ vanishes at infinity and the first term of M_1, Eq. I.37a. can be integrated by parts to yield:

$$\frac{e\hbar}{2imc} \int \bar{\psi}_E Q \vec{e} \cdot \nabla \psi_{E'} \, d\vec{r} + \frac{e\hbar}{2imc} \int \bar{\psi}_E \psi_{E'} (-i \vec{e} \cdot \vec{k}) Q \, d\vec{r} \qquad \text{I.38}$$

since $Q = e^{-i\vec{k}\cdot\vec{r}}$. The last term of I.38 is zero since the vectors $\vec{e}$ and $\vec{k}$ are perpendicular to each other. Therefore, M_1 becomes

$$M_1 = \frac{e\hbar}{imc} \int \bar{\psi}_E Q \vec{e} \cdot \nabla \psi_{E'} \, d\vec{r} \qquad \text{I.39}$$

The integrand of M_3 Eq. I.37c can be expressed as a curl: writing B^{lm} for the quantity $\bar{\psi}_E \sigma^{lm} \psi_{E'}$, ($B^{ml} = -B^{lm}$), M_3 becomes

$$M_3 = + \frac{e\hbar}{2mc} \int \vec{I} \cdot \operatorname{curl} \vec{B} \, Q \, d\vec{r} \qquad \text{I.40}$$

where $\vec{B} = \bar{\psi}_E \vec{\sigma} \psi_{E'}$, and $\vec{\sigma}$ has the components $\sigma_1 = \sigma^{23}$, $\sigma_2 = \sigma^{31}$, $\sigma_3 = \sigma^{12}$. I.41

Rearranging and integrating I.40 by parts, one obtains

$$M_3 = \frac{e\hbar}{2mc} \int (\vec{e} \times \vec{B}) \cdot \nabla Q \, d\vec{r} \qquad \text{I.42}$$

since $\psi_{E'}$ and consequently $\vec{B}$ become zero on the infinite bounding surface. Since $\nabla Q = -i\vec{R}Q$ I.42 becomes

$$M_3 = \frac{ic\hbar k}{2mc}\int Q\,\bar{\psi}_E\,\vec{u}\cdot\vec{\sigma}\,\psi_{E'}\,d\vec{r} \qquad \text{I.43}$$

In I.43 we have denoted the vector $\vec{e}\times\frac{\vec{R}}{R}$ by $\vec{u}$.

The expression M_4 , Eq. I.37d, can be written as follows

$$M_4 = \frac{e(E-E')}{2mc^2}\int Q\,\bar{\psi}_E\,\vec{\alpha}\cdot\vec{e}\,\psi_{E'}\,d\vec{r} \qquad \text{I.44}$$

since the time-dependence of $\bar{\psi}_E$ and $\psi_{E'}$ is given by the factors $e^{\frac{iEt}{\hbar}}$ and $e^{\frac{-iE't}{\hbar}}$ respectively.

From Eqs. I.37, I.39, I.43 and I.44, the expression for M equivalent to Eq. I.17 is the following:

$$M = e\left(\frac{2\pi\hbar c}{k}\right)^{1/2}\frac{\hbar k}{2mc}\int e^{-i\vec{R}\cdot\vec{n}}\psi_E^{\dagger}\beta\left[-\frac{2i\vec{e}_R\cdot\nabla}{k} + i\vec{u}\cdot\vec{\sigma} + \frac{(E-E')}{\hbar cR}\vec{\alpha}\cdot\vec{e}_R\right]\psi_{E'}\,d\vec{r}$$

$$+ e\left(\frac{2\pi\hbar c}{k}\right)^{1/2}\frac{e}{mc^2}\int e^{-i\vec{R}\cdot\vec{n}}\,\vec{A}\cdot\vec{e}_R\,\psi_E^{\dagger}\beta\,\psi_{E'}\,d\vec{r} \qquad \text{I.45}$$

where $\vec{u} = \vec{e}_R\times\frac{\vec{R}}{R}$

For the case of an electron in Coulomb field ($\vec{A}=0$), I.45 becomes

$$M = e\left(\frac{2\pi\hbar c}{k}\right)^{1/2}\frac{\hbar k}{2mc}\int e^{-i\vec{R}\cdot\vec{n}}\,\psi_E^{\dagger}\quad\times$$

$$\times\ \beta\left[-\frac{2i\vec{e}_R\cdot\nabla}{k} + i\vec{u}\cdot\vec{\sigma} + \frac{(E-E')}{\hbar cR}\vec{\alpha}\cdot\vec{e}_R\right]\psi_{E'}\,d\vec{r} \qquad \text{I.46}$$

If we compare the expression for the electromagnetic interaction matrix element of Section B, Eq. I.16 with the expression just given, we can conclude that the operator $\vec{\alpha}\cdot\vec{\epsilon}_R$ in the matrix element may be replaced by the operator

$$\frac{\hbar k}{2mc}\beta\left[-\frac{2i\vec{\epsilon}_R\cdot\nabla}{k}+i\vec{\mu}\cdot\vec{\sigma}+\left(\frac{E-E_m}{\hbar c k}\right)\vec{\alpha}\cdot\vec{\epsilon}_R\right] \qquad \text{I.47}$$

in this sense, these two operators are equivalent.

In our general expression of Section B, Eq. I.42, we thus replace the electromagnetic interaction matrix element of Eq. I.16 by the expression I.46 with $\psi_{E'}$ replaced by ψ_{nl} and E' replaced by E_{nl}.

Chapter II

The Expression for the Probability of Electron Capture in Terms of Approximate Wave Functions

In Section A of this Chapter, we introduce the wave functions used in our calculations and we give the general resulting expression for $w_R dR / w_C$, when these wave functions are substituted in the expressions I.9 for w_C and I.14 for $w_R dR$. In Section B, this general expression is simplified by introducing the non-relativistic approximation for the electron wave functions), and put into the form which will serve as a starting point in our calculations of Chapter III. In Section C, we discuss the passage from the general expression of Section A to that used by Hess.

A - Wave Functions and the General Expression for $w_k dk/w_c$

We start by considering the spherical wave solution to the Dirac equation for a particle in a Coulomb field. These wave functions are given, for instance, in Rose (37) or in Hess (55). They are normalized per unit energy interval and are characterized by the following quantum numbers: j, the total angular momentum quantum number, which takes half-integral values; μ, which takes all half-integral values from -j to +j; and K, which takes the values $\pm (j + \frac{1}{2})$. Since in this thesis we only need the wave functions for which $j = \frac{1}{2}$ (allowed case: no orbital angular momentum is carried away by the particles), we shall not write the wave functions in their general form. For $j = \frac{1}{2}$, the wave functions are:

$$\underset{\mu=1/2}{\underset{K=1}{\begin{pmatrix} Y_0^0 \dfrac{F^+(r)}{r} \\ 0 \\ \sqrt{\frac{1}{3}}\, Y_1^0 \dfrac{G^+(r)}{r} \\ -\sqrt{\frac{2}{3}}\, Y_1^1 \dfrac{G^+(r)}{r} \end{pmatrix}}} \quad \underset{\mu=-1/2}{\begin{pmatrix} 0 \\ Y_0^0 \dfrac{F^+(r)}{r} \\ \sqrt{\frac{2}{3}}\, Y_1^{-1} \dfrac{G^+(r)}{r} \\ -\sqrt{\frac{1}{3}}\, Y_1^0 \dfrac{G^+(r)}{r} \end{pmatrix}} \quad \underset{\mu=1/2}{\underset{K=-1}{\begin{pmatrix} \sqrt{\frac{1}{3}}\, Y_1^0 \dfrac{F^-(r)}{r} \\ -\sqrt{\frac{2}{3}}\, Y_1^1 \dfrac{F^-(r)}{r} \\ Y_0^0 \dfrac{G^-(r)}{r} \\ 0 \end{pmatrix}}} \quad \underset{\mu=-1/2}{\begin{pmatrix} \sqrt{\frac{2}{3}}\, Y_1^{-1} \dfrac{F^-(r)}{r} \\ -\sqrt{\frac{1}{3}}\, Y_1^0 \dfrac{F^-(r)}{r} \\ 0 \\ Y_0^0 \dfrac{G^-(r)}{r} \end{pmatrix}} \qquad \text{II.1}$$

The functions F^+, F^-, G^+ and G^- are the radial solutions to the Dirac wave equation: we shall not write them explicitly in this thesis. The Y_ℓ^m's are the spherical harmonics defined, for instance, in Blatt and Weisskopf (52), p. 783.

Since we consider only allowed transitions, we set equal to zero the components of the wave function II.1 which contain a spherical harmonics different from Y_0^0. We have therefore, in that approximation,

$$K=1 \qquad\qquad K=-1$$

$$\mu=\tfrac{1}{2} \qquad \mu=-\tfrac{1}{2} \qquad \mu=1/2 \qquad \mu=-1/2$$

$$\begin{pmatrix} Y_0^0 \dfrac{F^+(N)}{\lambda} \\ 0 \\ 0 \\ 0 \end{pmatrix} \qquad \begin{pmatrix} 0 \\ Y_0^0 \dfrac{F^+(N)}{\lambda} \\ 0 \\ 0 \end{pmatrix} \qquad \begin{pmatrix} 0 \\ 0 \\ Y_0^0 \dfrac{G^-(N)}{\lambda} \\ 0 \end{pmatrix} \qquad \begin{pmatrix} 0 \\ 0 \\ 0 \\ Y_0^0 \dfrac{G^-(N)}{\lambda} \end{pmatrix} \qquad \text{II.2}$$

If one sets Z, the nuclear charge, and m, the electron mass, equal to zero in II.2, one obtains the neutrino wave functions φ which will be used in the expressions I.8a and I.45. If one denotes by $\frac{f^+}{R}$ and $\frac{g^-}{R}$ the radial parts of the non zero components of these wave functions, evaluated at the nuclear surface, one easily shows that

$$\left|\frac{f^+}{R}\right| = \left|\frac{g^-}{R}\right| = \frac{E_\nu}{(\pi \hbar^3 c^3)^{1/2}} \qquad \text{II.3}$$

where E_ν is the energy of the emitted neutrino.

In the case of the 1s electron, the two functions with $K=-1$ in II.2 are identically zero. In the case of s electrons in higher discrete levels, these two functions no longer vanish but are small and will be neglected in our calculations. The two remaining wave functions are

$$(\ell=0) \quad \mu=1/2 \qquad K=1 \qquad (\ell=0) \quad \mu=-1/2$$

$$\begin{pmatrix} Y_0^0 \dfrac{F_{n\kappa}^+}{\lambda} \\ 0 \\ 0 \\ 0 \end{pmatrix} \qquad \begin{pmatrix} 0 \\ Y_0^0 \dfrac{F_{n\kappa}^+}{\lambda} \\ 0 \\ 0 \end{pmatrix} \qquad \text{II.4}$$

With the help of II.4 (with n = 1), and of II.3, one readily evaluates the expression I.9 for w_c . The absolute square of

the matrix element in I.9 is

$$\left|(F|H_\beta|0)\right|^2 = G^2 \sum_\lambda \sum_{\lambda'} c_\lambda c_{\lambda'} (SA^\lambda)(SA^{\lambda'})^\dagger (\varphi^\dagger A^\lambda \psi_{1S} \psi_{1S}^\dagger A^{\lambda'} \varphi)_R \qquad \text{II.5}$$

(see Eq. I.8). Operating with S_o on the product $\psi_{1S}\psi_{1S}^\dagger$ yields, because of II.4,

$$S_o \psi_{1S} \psi_{1S}^\dagger = Y_o^{o2} \left| \frac{F_{1S}(R)}{R} \right|^2 \frac{1+\beta}{2} \qquad \text{II.6}$$

where β is defined in I.4. It is also easily seen that the sum S_ν over the four neutrino states yields

$$S_\nu (\varphi^\dagger A^\lambda \tfrac{1+\beta}{2} A^\lambda \varphi)_R = \frac{Y_o^{o2} W^2}{\pi \hbar^3 c^3} \mathrm{Tr} A^\lambda \tfrac{1+\beta}{2} A^{\lambda'} \qquad \text{II.7}$$

where the operator Tr means that we take the trace of the matrix on the right of it. In deriving II.7, we used II.2, II.3 and the fact that $E_\nu = W$, the available energy (See Eq.I.1). Thus, from II.5, 6 and 7,

$$S_\nu S_o \left|(F|H_\beta|0)\right|^2 = Y_o^{o4} \frac{W^2}{\pi \hbar^3 c^3} \left| \frac{F_{1S}(R)}{R} \right|^2 G^2 \times$$

$$\times \sum_\lambda \sum_{\lambda'} c_\lambda c_{\lambda'} (SA^\lambda)(SA^{\lambda'})^\dagger \mathrm{Tr} A^\lambda \tfrac{1+\beta}{2} A^{\lambda'} \qquad \text{II.8}$$

The matrices of which we have to evaluate the traces, in Eq.II.8, are of the form $A^\lambda A^{\lambda'}$ and $A^\lambda \beta A^{\lambda'}$, where the $A^{\lambda'}$s as defined in I.6, are products of the Dirac matrices $\beta, \alpha_1, \alpha_2$ and α_3. Such traces of products of Dirac matrices are given, for instance, in Heitler (50), p.87. When they are evaluated in II.8, the

double sum over r and r^1 becomes

$$\sum_{\lambda}\sum_{\lambda'} C_\lambda C_{\lambda'} (SA^\lambda)(SA^{\lambda'})^\dagger \, T_\lambda A^\lambda \frac{1+\beta}{2} A^{\lambda'}$$

$$= 2\left[(C_S^2 + C_V^2 + 2C_S C_V) \left|SI\right|^2 + (C_T^2 + C_A^2 + 2C_T C_A) \left|S\vec{\sigma}\right|^2 \right. \qquad \text{II.9}$$

$$\left. + C_P^2 \left|S\beta\gamma^5\right|^2 \right]$$

$$= 2T$$

Remembering that the operator $\int d\Omega_\nu$ multiplies the expression I.9 by a factor 4π and that $Y_0^0 = 1/\sqrt{4\pi}$, we obtain from I.9, II.8 and II.9:

$$w_C = \frac{W^2}{\pi \hbar^4 c^3} \left| \frac{F_{1s}^\dagger(R)}{R} \right|^2 G^2 T \qquad \text{II.10}$$

II.10 was used both by Hess and by Glauber and Martin in their calculations.

We now consider the expression for $w_R \, dk$. We first write the sum over the intermediate energy states, Eq. I.12, in a more detailed form, using the electromagnetic interaction matrix element obtained in Section C, Chapter I. Since the wave functions in the intermediate and initial states are s-functions and, consequently, have the same parity, the operator $-\frac{2i\vec{\alpha}_\lambda \cdot \nabla}{R}$ in the expression I.45 for $(F|H_\gamma|I)$ will not contribute to the electromagnetic interaction matrix element. It follows therefore, from I.12, I.13, I.15 and I.45 that

$$\sum_I \frac{(F|H_\beta|I)(I|H_\gamma|0)}{E_I - E_0} = B \sum_\lambda C_\lambda (SA^\lambda) \varphi^\dagger(R) A^\lambda \int d\vec{\pi} \sum_E \frac{\psi_E(R)\, \psi_E^\dagger(\vec{\pi})}{E - E_{ms} + \hbar c k} \times$$

$$\times \beta \left[i\vec{\pi}\cdot\vec{\sigma} + \left(\frac{E - E_{ms}}{\hbar c k}\right) \vec{\alpha}\cdot\vec{\Omega}_R \right] Q \psi_{ms}(\vec{\pi}) \qquad \text{II.11}$$

where

$$B = Ge\left(\frac{2\pi\hbar c}{k}\right)^{1/2}\frac{\hbar k}{2mc} \qquad \text{II.12}$$

Writing $E - E_{ms} = E - E_{ms} + \hbar ck - \hbar ck$, we may put II.11 into the following form

$$\sum_I \frac{(F|H_\beta|I)(I|H_\gamma|0)}{E_I - E_0} = B\sum_\lambda c_\lambda(SA^\lambda)\,\varphi^\dagger(R)\,A^\lambda\int d\vec{r}\, M_{ms}\beta[i\vec{\alpha}\cdot\vec{\sigma} - \vec{\alpha}\cdot\vec{e}_R]Q\psi_{ms}$$

$$+\frac{B}{\hbar ck}\sum_\lambda c_\lambda(SA^\lambda)\,\varphi^\dagger(R)A^\lambda\int d\vec{r}\sum_E \psi_E(R)\psi_E^\dagger(\vec{r})\beta\vec{\alpha}\cdot\vec{e}_R Q\psi_{ms} \qquad \text{II.13a}$$

where

$$M_{ms} = \sum_E \frac{\psi_E(R)\,\psi_E^\dagger(\vec{r})}{E - E_{ms} + \hbar ck} \qquad \text{II.13b}$$

We show in Appendix A that the second line of II.13a may be neglected. We obtain, finally

$$\sum_I \frac{(F|H_\beta|I)(I|H_\gamma|0)}{E_I - E_0} = B\sum_\lambda c_\lambda(SA^\lambda)\,\varphi^\dagger(R)A^\lambda\int d\vec{r}\, M_{ms}\beta[i\vec{\alpha}\cdot\vec{\sigma} - \vec{\alpha}\cdot\vec{e}_R]Q\psi_{ms}(\vec{r}) \qquad \text{II.14}$$

We now form the absolute square of the expression II.14 and apply the operator S_0 on the wave function product $\psi_{ms}\psi_{ms}^\dagger$. Because of II.4 and II.6, we obtain

$$S_0\left|\sum_I \frac{(F|H_\beta|I)(I|H_\gamma|0)}{E_I - E_0}\right|^2 = B^2\sum_\lambda\sum_{\lambda'} c_\lambda c_{\lambda'}(SA^\lambda)(SA^{\lambda'})^\dagger Y_0^2\,\varphi^\dagger(R)\,A^\lambda X$$

$$\times\left[\iint d\vec{r}\,d\vec{r}'\, e^{-i\vec{R}\cdot\vec{r}}\, e^{i\vec{R}\cdot\vec{r}'}\,\underset{\lambda}{F_{ms}(r)}\,\underset{\lambda'}{F_{ms}^*(r')}\, M_{ms}\,P\,M_{ms}'^\dagger\right]A^{\lambda'}\varphi(R) \qquad \text{II.15a}$$

where

$$P = \beta \left[i\vec{u}\cdot\vec{\sigma} - \vec{\alpha}\cdot\vec{e}_R \right]\left[\frac{1+\beta}{2}\right]\left[-i\vec{u}\cdot\vec{\sigma} - \vec{\alpha}\cdot\vec{e}_R \right]\beta \qquad \text{II.15b}$$

and where the prime on M'_{ms} means that we replace r, E by r', E' in II.13. It is shown in Appendix B that

$$P = 1 - \vec{\alpha}\cdot\frac{\vec{R}}{R} \qquad \text{II.16}$$

Because of the form of the wave functions ψ_E, as given by II.2, we may write Eq. II.13b as follows:

$$M_{ms} = Y_0^{0\,2}\left\{ \sum_E \frac{\frac{F_E^+(R)}{R}\,\frac{F_E^{+*}(r)}{r}}{E - E_{ms} + \hbar c k}\left(\frac{1+\beta}{2}\right) + \sum_E \frac{\frac{G_E^-(R)}{R}\,\frac{\vec{G}_E^{*}(r)}{r}}{E - E_{ms} + \hbar c k}\left(\frac{1-\beta}{2}\right)\right\} \qquad \text{II.17}$$

We integrate over the angles, using the relation

$$\int d\Omega\, e^{-i\vec{R}\cdot\vec{r}} = 4\pi\,\frac{\sin kr}{kr} \qquad \text{II.18}$$

and introduce the notation

$$L^F_{ms} = \sum_E \frac{\frac{F_E^+(R)}{R}\int_0^\infty \frac{F_E^{+*}(r)}{r}\cdot\frac{\sin kr}{kr}\cdot\frac{F_{ms}(r)}{r}\,r^2\,dr}{E - E_{ms} + \hbar c k} \qquad \text{II.19a}$$

$$L^{G}_{ms} = \sum_{E} \frac{\frac{\bar{G}(R)}{R} \int_0^\infty \frac{\bar{G}_E(r)}{r} \frac{\sin kr}{Rr} \frac{F_{ms}(r)}{r} r^2 dr}{E - E_{ms} + \hbar c k} \qquad \text{II.19b}$$

II.15 becomes

$$S_0 \left| \sum_I \frac{(F|H_\beta|I)(I|H_\gamma|0)}{E_I - E_0} \right|^2 = B \sum_\lambda \sum_{\lambda'} C_\lambda C_{\lambda'} (SA^\lambda)(SA^{\lambda'})^\dagger Y_0^2 \varphi^\dagger(R) A^\lambda \times$$

$$\times \left\{ \left[L^F_{ms}\left(\frac{1+\beta}{2}\right) + L^G_{ms}\left(\frac{1-\beta}{2}\right) \right] \left[1 - \frac{\vec{\alpha}\cdot\vec{R}}{R} \right] \left[L^{*F}_{ms}\left(\frac{1+\beta}{2}\right) + L^{G*}_{ms}\left(\frac{1-\beta}{2}\right) \right] \right\} A^{\lambda'} \varphi(R) \qquad \text{II.20}$$

The summation S_ν over the four neutrino states gives, as in Eq.II.7, the trace of the matrix contained between the two φ 's of Eq. II.20. There also arises, because of II.2 and 3, a factor

$$Y_0^2 \frac{E_\nu^2}{\pi \hbar^3 c^3} = Y_0^2 \frac{(W - \hbar c k + E_{ms} - E_{Is})^2}{\pi \hbar^3 c^3} \qquad \text{II.21}$$

in front of the whole expression. In deriving II.21, we used the equations of energy conservation I.1 and I.11 and the definition I.1 for W. Therefore,

$$S_0 S_\nu \left| \sum_I \right|^2 = B Y_0^2 \frac{(W - \hbar c k + E_{ms} - E_{Is})^2}{\pi \hbar^3 c^3} \sum_\lambda \sum_{\lambda'} C_\lambda C_{\lambda'} (SA^\lambda)(SA^{\lambda'})^\dagger$$

$$\times T_\lambda A^\lambda \left[L^F_{ms}\left(\frac{1+\beta}{2}\right) + L^G_{ms}\left(\frac{1-\beta}{2}\right) \right] \left[1 - \frac{\vec{\alpha}\cdot\vec{R}}{R} \right] \left[L^{F*}_{ms}\left(\frac{1+\beta}{2}\right) + L^{G*}_{ms}\left(\frac{1-\beta}{2}\right) \right] A^{\lambda'} \qquad \text{II.22}$$

It can be seen from the definitions I.6 that the traces of every matrix of the form $A^{\wedge}A^{\wedge\prime}\alpha_i$ and $A^{\wedge}A^{\wedge\prime}\beta\alpha_i$ $(i = 1, 2, 3)$ are zero. Thus, the term $\vec{\alpha}\cdot\frac{\vec{R}}{R}$ of II.22 will not contribute to the trace. Therefore, one has only to evaluate the trace of

$$A^{\wedge}\left[\left|L^{F}_{ms}\right|^{2}\left(\frac{1+\beta}{2}\right)+\left|L^{G}_{ms}\right|^{2}\left(\frac{1-\beta}{2}\right)\right]A^{\wedge\prime} \qquad \text{II.23}$$

in the way explained under Eq. II.8. After this is done, II.22 becomes:

$$S_0 S_\nu \left|\mathcal{E}_I\right|^2 = B Y_0^{o\,4}\,\frac{(W-\hbar c k+E_{ms}-E_{1S})^2}{\pi \hbar^3 c^3}\,X$$

$$X\,2\left[\left(\left|L^{F}_{ms}\right|^2+\left|L^{G}_{ms}\right|^2\right)T_1+\left(\left|L^{F}_{ms}\right|^2-\left|L^{G}_{ms}\right|^2\right)T_2\right] \qquad \text{II.24}$$

with T_1 and T_2 given by

$$T_1=\left(C_S^2+C_V^2\right)\left|S1\right|^2+\left(C_T^2+C_A^2\right)\left|S\vec{\sigma}\right|^2+C_P^2\left|S\beta\gamma_5\right|^2 \qquad \text{II.25a}$$

and

$$T_2=2\,C_S C_V\left|S1\right|^2+2\,C_T C_A\left|S\vec{\sigma}\right|^2 \qquad \text{II.25b}$$

such that $T_1 + T_2 = T$, defined in Eq. II.9. From II.12, II.24 and I.14, we have finally

$$W_R\,dR=\frac{G^2\alpha\,(W-\hbar cR+E_{ms}-E_{1S})^2\,R^3\,dR}{\pi m^2 c^3}\,X \qquad \text{II.26}$$

$$X\,\frac{1}{2}\left[\left(\left|L^{F}_{ms}\right|^2+\left|L^{G}_{ms}\right|^2\right)T_1+\left(\left|L^{F}_{ms}\right|^2-\left|L^{G}_{ms}\right|^2\right)T_2\right]$$

and, from II.10 and II.26

$$\frac{w_R\,dR}{w_c} = \frac{\alpha}{\pi}\,\frac{(\hbar ck)^3\,d(\hbar ck)}{(mc^2)^3}\left(1-\frac{\hbar ck-(E_{ns}-E_{1s})}{W}\right)^2 \times$$

$$\times\left\{\frac{\left(|L^F_{ns}|^2+|L^G_{ns}|^2\right)T_1+\left(|L^F_{ns}|^2-|L^G_{ns}|^2\right)T_2}{2\left|\frac{F_{1s}(R)}{R}\right|^2 T}\right\} \qquad \text{II.27}$$

The above expression for $w_R\,dk/w_c$ will be the basis for the subsequent discussions of this Chapter.

B - Non - Relativistic Expression for $w_R\,dk/w_c$

When Z is small, the expression for the sum over the intermediate energy states, as given by II.17, may be approximated by its non-relativistic form. To this effect,

1^o β is put equal to a unit matrix in II.17, so that the function G^- disappears completely from the expression;

2^o The function $\frac{F^+(\lambda)}{\lambda}$ is replaced by φ_E ; the corresponding solution to Schroedinger's equation;

3^o The sum over all energy states $\sum_E$ becomes a sum over the discrete states and an integral over the positive continuous states.

When the above approximation is made, the expression II.23

becomes

$$|L^F_{ns}|^2 A^2 A'^2 \qquad \text{II.28}$$

and the trace of II.28 gives rise only to the factor T_1 defined in Eq. II.25a. In this approximation, we have, from II.27

$$\frac{w_R dR}{w_C} = \frac{\alpha}{\pi} \frac{(\hbar c k)^3 d(\hbar c k)}{(mc^2)^2} \left(1 - \frac{\hbar c k - (E_{ns} - E_{1s})}{W}\right)^2 \frac{|L^F_{ns}|^2}{\left|\frac{F_{1s}(R)}{R}\right|^2} \frac{T_1}{T} \qquad \text{II.29}$$

If we make use of the fairly well established experimental fact (See, for instance, Konopinski and Langer (53)) that the mixed terms (i.e. those proportional to $C_S C_V$ and $C_T C_A$) are negligible, we may set $T_2 = 0$; and thus $T_1 = T$ in II.29. We also replace the wave function $\frac{F_{1s}(R)}{R}$ for the initial electron by the corresponding solution to Schroedinger's equation $\varphi_{1s}(R)$. Hence, II.29 becomes:

$$\frac{w_R dR}{w_C} = \frac{\alpha}{\pi} \frac{(\hbar c k)^3 d(\hbar c k)}{(mc^2)^2} \left(1 - \frac{\hbar c k - (E_{ns} - E_{1s})}{W}\right)^2 \frac{|L_{ns}|^2}{|\varphi_{1s}(R)|^2} \qquad \text{II.30}$$

where

$$L_{ns} = \sum_E \frac{\varphi_E(R) \int_0^\infty \varphi^*_E(r) \frac{\sin kr}{kr} \varphi_{ns}(r) r^2 dr}{E - E_{ns} + \hbar c k}$$

Expression II.30 is the starting point of our calculations of Chapter III.

C - The Approximation of Hess

Instead of using the approximate electromagnetic interaction matrix element obtained in Chapter I, Section C, which leads to Eq. II.14, Hess used the general relativistic expression I.16 with the operator $\vec{\alpha}\cdot\vec{\ell}_R$. This means that the matrix P of II. 15b was, in his case,

$$P = \vec{\alpha}\cdot\vec{\ell}_R \; \frac{1+\beta}{2} \; \vec{\alpha}\cdot\vec{\ell}_R$$

or

$$P = \frac{1-\beta}{2} \qquad \text{II.31}$$

since $\vec{\alpha}\beta = -\beta\vec{\alpha}$ and $(\vec{\alpha}\cdot\vec{\ell}_R)^2 = 1$

On the other hand, we have seen in Section B that, with the approximate wave functions of the form II.2, the sum M_{ms} over the intermediate energy states takes the form II.17. Since $\left(\frac{1+\beta}{2}\right)\left(\frac{1-\beta}{2}\right) = 0$, it follows from II.17 and II.31 that the factor $M_{ms} P M_{ms}^{1\dagger}$ of II.15a becomes

$$\gamma_0^{04} \sum_E \left(\frac{G_E^-(R)}{R} \frac{G_E^{-*}(r)}{r} \right) \sum_{E'} \left(\frac{G_{E'}^{*}(R)}{R} \frac{G_{E'}^{-}(r')}{r'} \right) \left(\frac{1-\beta}{2} \right) \qquad \text{II.32}$$

$$E - E_{ms} + \hbar c k \qquad\qquad E' - E_{ms} + \hbar c k$$

i.e. that the function F^+ disappears altogether from the sum over the intermediate energy states. Since the functions G for the discrete states are small, Hess was led to neglect the sum over the intermediate discrete states as compared with that over the continuous states; the result obtained was of an order of magnitude smaller than that of Morrison and Schiff. (See Chapter III)

The source of this difficulty resides in the fact that making the approximation II.2 for the wave functions and, at the same time, keeping the operator $\vec{d}\cdot\vec{e}_R$ in its general form in the matrix element of electromagnetic interaction, is inconsistent.

Chapter III

Radiative K-Capture in a Non - Relativistic Approximation

In Section A of this Chapter, we briefly describe the method employed by Glauber and Martin (55) (56), in their derivation of the expression II.30 for $W_R\,dk/W_c$, and we discuss the simplifying assumptions they make in evaluating II.30, and in Section B, we present our own evaluation of that expression for the cases of $^{37}_{18}A$ and $^{131}_{55}Cs$.

A - Method of Glauber and Martin

Let us consider the general form of the matrix element I.12, using the expressions I.15 and I.16 for the beta interaction matrix element and the electromagnetic interaction matrix element respectively:

$$\sum_I \frac{(F|H_\beta|I)(I|H_\gamma|0)}{E_I - E_0} = G\ell\left(\frac{2\pi\hbar c}{k}\right)^{1/2} \sum_\lambda c_\lambda(SA^\lambda)\ \varphi^\dagger(R)A^\lambda \times \cdot \times \int d\vec{r}\ M_{m\ell}\ \vec{\alpha}\cdot\vec{\ell}_k\ e^{-i\vec{k}\cdot\vec{r}}\psi_{m\ell} \qquad \text{III.1a}$$

where $$M_{m\ell} = \sum_E \frac{\psi_E(R)\,\psi_E^\dagger(\vec{r})}{E - E_{m\ell} + \hbar c k R} \qquad \text{III.1b}$$

As pointed out by Glauber and Martin, $M_{m\ell}$ is actually a special case of the Green's function $G_{E_{m\ell}-\hbar ck}(\vec{r}', \vec{r})$ for the wave equation of the electron in a Coulomb field. Since we may set the nuclear radius R equal to zero in III.1a, we have

$$M_{m\ell} = G_{E_{m\ell}-\hbar ck}(0, \vec{r}) \qquad \text{III.2}$$

The reason for the success of this approach is that this one-argument Green's function in its non-relativistic form can be obtained as a solution of the Schroedinger equation for an electron in a Coulomb field. However, Glauber and Martin start

out from the Green's function $\mathcal{G}(E_{n\ell} - \hbar ck)$ of the iterated Dirac equation, and they arrive at a formula which is equivalent to our equation II.27. Only in a later stage of their calculations do they replace $\mathcal{G}$ by the non-relativistic Green's function, and in this way obtain an equation which reduces to our Eq. II.30 in case of s-electrons.

Expression II.30 for L_{ns} cannot be evaluated in a closed form. In order to evaluate $\omega_R \, dR/\omega_c$ in a relatively simple analytical way, Glauber and Martin have set the retardation factor $e^{-i\vec{R}\cdot\vec{r}}$ equal to one. This is equivalent to using an expression for L_{ns} in which $\frac{\sin kr}{kr}$ is replaced by unity for all values of k, i.e. over the whole energy range of the emitted photon. In that manner, and with the help of the analytical expression for the non-relativistic Green's function, they could evaluate $\omega_R \, dR/\omega_c$ almost without numerical calculations.

The argument they present in order to justify the above approximation (i.e. $e^{-i\vec{R}\cdot\vec{r}} \simeq 1$) over the whole energy range is rather lengthy and somewhat unconvincing; it will only be sketched in this thesis.

The argument is of a different nature for each of the following three photon energy ranges:

$$\begin{aligned} &(1) && \hbar ck < \tfrac{1}{2}(Z\alpha)^2 mc^2 \\ &(2) && \tfrac{1}{2}(Z\alpha)^2 mc^2 < \hbar ck < Z\alpha\, mc^2 \\ &(3) && Z\alpha\, mc^2 < \hbar ck \end{aligned} \qquad \text{III.3}$$

In the range (1) of low photon energies, the photons have a wave length at least $(Z\alpha)^{-1}$ times larger than the atomic system. In this case, one may therefore set $\frac{\sin kr}{kr}$ in II.30.

Consequently, only one term in the sum and integral over intermediate states is different from zero because of the orthonormal properties of the φ's, namely the term for which $E = E_{ms}$. Then L_{ms} becomes, simply

$$L_{ms} = \frac{\varphi_{ms}(R)}{\hbar c k} \qquad \text{III.4}$$

and Eq. II.30 becomes <u>identical</u> with the Morrison and Schiff ratio when $n = 1$ and $\ell = 0$. (This is a rather startling consequence, in view of the fact that Morrison and Schiff completely neglected Coulomb effects, while Eq. III.4 is derived from an expression containing (non-relativistic) Coulomb wave functions).

In the intermediate energy range (2) one may not a priori neglect the retardation effects. However, a study of the form of the analytical expression for the Green's function $\mathcal{G}_{E_{ms}-\hbar c k}(0,r)$, which contains a decreasing exponential, shows that its range remains much smaller than the photon wave length so that the retardation effects seem again to be unimportant, i.e. again $e^{i\vec{k}\cdot\vec{r}} \simeq 1$. It follows that in this range also, one obtains the expression of Morrison and Schiff when $n = 1$ and $\ell = 0$.

In the high energy range (3) the retardation must be taken into account. However, in that range, Glauber and Martin used the free particle form of the Green's function and approximated the initial wave function by a constant. These approximations are the same as the one used by Morrison and Schiff in deriving their result: namely, the neglection of all Coulomb effects in the intermediate states wave functions and the assumption that the initial electron may be considered at rest. For the high energy region, Glauber and Martin used therefore the same

expression as that used by Morrison and Schiff.

The neglecting of all retardation effects allowed Glauber and Martin to evaluate the contribution to $w_R dk$ made by the p-electrons of the L and M shells ($n = 1, 2$; $\ell = 1$) in a relatively simple way. This contribution was shown to explain the sudden rise of the photon spectrum at low energies (Glauber and Martin (55)).

In an unpublished paper (56), Glauber and Martin introduced a relativistic correction to the 1s and 2s state spectra by mean of a canonical transformation applied to the Green's function. This correction is seen to apply only to the low and intermediate energy ranges of the photon spectra, as defined in III.3 and it is evaluated again on the assumption that the retardation factor may be put equal to one. These corrected results were compared with the experimental data, for the case of A^{37}, by Lindqvist and Wu (55) and there appears to be an essential agreement between theory and experiment.

As stated in the Introduction, a "more fully relativistic" calculation carried out by Glauber and Martin has not yet been published in details, but the results have been compared with the experimental data for A^{37} (See Wu and al. (56)). From this comparison, it would appear that the correction resulting from these latest calculations does not affect the high energy part of the theoretical spectrum.

Although there can be little doubt that Glauber and Martin's results are essentially correct, we think that a direct non-relativistic calculation of $w_R dk/w_c$ free of additional simplifying assumptions is still of some value. Such a calculation, which we undertake in Section B of this Chapter for the

case of 1s and 2s electrons, makes it, in particular, possible to see more clearly the role played by the retardation effects.

B - Evaluation of $W_k dk / W_c$ in a Non-Relativistic Approximation for the Case of 1s and 2s Electrons.

In evaluating L_{ms} directly, (Eq. II.30) one must consider separately the discrete and the continuous intermediate energy states. The procedure adopted is to first carry out the integration over the space variable r. The exact formulae for the first four terms of the sum over the intermediate discrete energy states are obtained and an approximate expression is derived for the remainder of the sum, which can be transformed into an integral. The integral over the continuous energy states is evaluated numerically between the limits equal to mc^2 and about $1.5\ mc^2$ respectively. The integrand for higher energies can be approximated by a relatively simple analytic expression and the integration carried out analytically. The error involved in that procedure is quite small, as will be apparent from the numerical results.

1^o Discrete States

The space dependence of the general non-relativistic

"s-function" describing a particle in a discrete energy level $E_{ns}=E_n$ is given by (see, for instance, Kramers (38), P.311)

$$\varphi_{E_n}(r) = \frac{F_n}{r} = 2\left(\frac{\mu}{n}\right)^{3/2} e^{-\frac{\mu r}{n}} \mathcal{H}\left(1-n; 2; \frac{2\mu r}{n}\right) \qquad \text{III.5}$$

where $$\mu = \frac{Z\alpha mc}{\hbar}$$

and where $\mathcal{H}\left(1-n; 2; \frac{2\mu r}{n}\right)$ is the confluent hyper-geometric function as defined, for instance, in MacRobert (54), p.346. The function III.5 is normalized such that

$$\int \left[Y_0^0 \varphi_{E_n}(r)\right]^2 d\vec{\tau} = 1 \qquad \text{III.6}$$

When r = R, the nuclear radius, Eq. III.5 becomes

$$\varphi_{E_n}(R) = 2\left(\frac{\mu}{n}\right)^{3/2} e^{-\frac{\mu R}{n}} \mathcal{H}\left(1-n; 2; \frac{2\mu r}{n}\right) \quad ; \qquad \text{III.7}$$

since $$\mu R = \frac{Z\alpha mc}{\hbar\left(\frac{1}{R}\right)} \simeq 10^{-3} \qquad \text{for } R \sim 10^{-13} \text{ cm} \qquad \text{III.8}$$

and since $\mathcal{H}$ is a finite polynomial of the form

$$1 + \frac{1-n}{2}\left(\frac{2\mu r}{n}\right)\frac{1}{1!} + \frac{(1-n)(2-n)}{2\cdot 3}\left(\frac{2\mu r}{n}\right)^2 \frac{1}{2!} + \qquad \text{III.9}$$

one may write approximately

$$\Psi_{E_n}(R) \simeq 2\left(\frac{\mu}{n}\right)^{3/2} \qquad \text{III.10}$$

We call $L_{D_{1S}}$ the part of L_{1S} which contains the sum over the intermediate discrete states. The initial states 1s and 2s that we shall consider are represented by the wave functions (see III.5, III.9):

$$\varphi_{1S} = \varphi_{E_1} = 2\mu^{3/2} e^{-\mu r} \qquad \text{III.11a}$$

$$\varphi_{2S} = \varphi_{E_2} = 2\left(\frac{\mu}{2}\right)^{3/2} e^{-\frac{\mu}{2}r}\left(1 - \frac{\mu}{2}r\right) \qquad \text{III.11b}$$

Replacing φ_E and $\varphi_{m\ell}$ in II.30 by their values III.5, III.10 and III.11, one obtains for the two $L_{D_{nS}}$, n=1,2:

$$L_{D_{1S}} = 8\mu^{9/2} \sum_{n=1}^{\infty} \frac{\int_0^\infty e^{-\mu r - \frac{\mu r}{n}} \frac{\sin kr}{kr} \varphi_1^1(1-n; 2; \frac{2\mu r}{n}) r^2 dr}{n^3 (E_n - E_1 + \hbar c k)} \qquad \text{III.12a}$$

$$L_{D_{2S}} = \frac{8\mu^{9/2}}{2\sqrt{2}} \sum_{n=1}^{\infty} \frac{\int_0^\infty e^{-\frac{\mu}{2}r - \frac{\mu r}{n}} \frac{\sin kr}{kr} \left(1 - \frac{\mu}{2}r\right) \varphi_1^1 r^2 dr}{n^3 (E_n - E_2 + \hbar c k)} \qquad \text{III.12b}$$

where φ_1^1 in 12b is the same hypergeometric function as in 12a. The energy E_n is given by the expression

$$E_n = mc^2\left(1 + \left(\frac{Z\alpha}{\lambda + n - 1}\right)^2\right)^{-1/2} \qquad \text{III.13}$$

If one approximates $\lambda = (1 - (Z\alpha)^2)^{1/2}$ by the expression

$$\lambda \simeq 1 - \tfrac{1}{2}(Z\alpha)^2 \qquad \text{III.14}$$

one obtains

$$E_n - E_1 = \tfrac{1}{2}(z\alpha)^2 mc^2 \left(1 - \frac{1}{n^2}\right) \qquad \text{III.15a}$$

and

$$E_n - E_2 = \tfrac{1}{2}(z\alpha)^2 mc^2 \left(\frac{1}{4} - \frac{1}{n^2}\right. \qquad \text{III.15b}$$

As we have already mentioned, we start by integrating over the space variable r in Eqs. III.12. To this effect we expand the hypergeometric functions into their (finite) polynomial form of equation III.9 and integrate term by term. The space integral of III.12a, for instance, yields

$$\int_0^\infty e^{-\mu r - \frac{\mu\Delta}{m}} \frac{\sin kr}{kr} \mathcal{F} r^2 dr$$

$$= \frac{1}{2ik}\left\{\int_0^\infty dr\, e^{-Ar} r\left[1 + \frac{1-n}{2}\left(\frac{2\mu r}{n}\right)\frac{1}{1!} + \cdots\right] - c.c.\right\} \qquad \text{III.16}$$

where $A = \mu + \frac{\mu}{m} - ik$

This is readily integrated to give

$$\frac{1}{2ik}\cdot\frac{1}{A^2}\left\{\left[1 + \frac{2\cdot(1-n)}{2}\left(\frac{2\mu}{nA}\right) + \frac{2\cdot 3(1-n)(2-n)}{2\cdot 3}\left(\frac{2\mu}{nA}\right)^2\cdot\frac{1}{2!} + \cdots\right] - c.c.\right\} \qquad \text{III.17}$$

The expression in the square bracket of III.17 is the ordinary hypergeometric series of argument $\frac{2\mu}{nA}$. (See Magnus and Oberhettinger, p.7). Hence the integral III.16 can be written:

$$\frac{1}{2ik}\,\frac{1}{\mu^2}\left[\frac{n^2 z^2}{4}\,\mathcal{F}(1-n, 2; 2; z) - c.c.\right] \qquad \text{III.18}$$

in which z stands for

$$\frac{2\mu}{nA} = \frac{2/n}{1+\frac{1}{n}-i\alpha} \qquad \text{III.19}$$

$$\text{where } \alpha = \frac{k}{\mu} = \frac{\hbar k}{Z\alpha mc} \qquad \text{III.20}$$

We next use the relation: (See Magnus and Oberhettinger p.8)

$$\mathcal{F}(\alpha,\beta;\rho;z) = (1-z)^{-\alpha}\mathcal{F}(\alpha,\rho-\alpha;\beta;\tfrac{z}{z-1}) \qquad \text{III.21}$$

Therefore $$\mathcal{F}(1-n,2;2;z) = (1-z)^{n-1} \qquad \text{III.22}$$

With the help of III.22, III.18, III.20 and III.15a, the expression III.12a becomes

$$L_{D_{1s}} = \sum_{n=1}^{\infty} L_{D_{1s}}^{(n)} = \frac{\sqrt{\mu}}{\hbar c}\sum_{n=1}^{\infty}\frac{(-i)\left\{z^2(1-z)^{n-1} - c.c.\right\}}{n\alpha\left\{\frac{1}{2}Z\alpha\left(1-\frac{1}{n^2}\right)+\alpha\right\}} \qquad \text{III.23a}$$

In case of $L_{D_{2s}}$, the second term in the integrand in Eq. III.12b leads to the hypergeometric function

$$\mathcal{F}(1-n,3;2;z) = (1-z)^{n-1}\left[1+\left(\frac{n-1}{2}\right)\left(\frac{z}{z-1}\right)\right]$$

this last formula is easily obtained using again III.21. A calculation similar to that above yields then for $L_{D_{2s}}$ (Eq.III.12b)

$$L_{D_{2s}} = \sum_{n=1}^{\infty} L_{D_{2s}}^{(n)} = \frac{\sqrt{\mu}}{\hbar c}\frac{1}{2\sqrt{2}}\sum_{n=1}^{\infty}\frac{(-i)\left\{z^2(1-z)^{n-1}\left[1-\frac{n}{2}\cdot\frac{z}{1-z}+\frac{n}{2}\cdot\frac{n+1}{2}\cdot\frac{z^2}{1-z}\right]-c.c.\right\}}{n\alpha\left[\frac{1}{2}Z\alpha\left(\frac{1}{4}-\frac{1}{n^2}\right)+\alpha\right]} \qquad \text{III.23b}$$

In III.23b, however, z is

$$z = \frac{2/n}{\frac{1}{2}+\frac{1}{n}-i\alpha} \qquad \left(\alpha = \frac{\hbar k}{Z\alpha mc}\right) \qquad \text{III.23c}$$

In evaluating $L_{D_{1S}}$ and $L_{D_{2S}}$ we calculate the first four terms of the sum over n separately, and we derive an approximate expression for the summand when $n \geq 5$. The numerical values that we obtain later will show that this approximation introduces an error of less than 1% in the expressions for $L_{D_{1S}}$ and $L_{D_{2S}}$. We first consider the case of $L_{D_{1S}}$ and then the case of $L_{D_{2S}}$.

a) Case of $L_{D_{1S}}$

Let us consider, in the summand of Eq. III.23a the factor

$$\mathcal{J}_{1S} = (-i)\left[z^2(1-z)^{n-1} - c.c. \right] \qquad \text{III.24}$$

and write z in the form

$$z = \frac{2/n}{1+\frac{1}{n}-ix} = \frac{2/n}{\rho_+ e^{-i\varphi_+}} \qquad \text{III.25a}$$

$$1-z = \frac{\rho_- e^{-i\varphi_-}}{\rho_+ e^{-i\varphi_+}} \qquad \text{III.25b}$$

where $\rho_\pm = \left[\left(1 \pm \frac{1}{n}\right)^2 + x^2 \right]^{1/2}$ III.25c

and $\varphi_\pm = \tan^{-1} \frac{x}{1 \pm \frac{1}{n}}$ III.25d

If III.25a and b are inserted in III.24, one obtains

$$g_{1S} = \frac{8}{n^2}\left(\frac{\rho_-}{\rho_+}\right)^n \frac{1}{\rho_+\rho_-} \sin\left[(n+1)\varphi_+ - (n-1)\varphi_-\right] \quad \text{III.26}$$ [1)]

Therefore, from III.13a

$$L_{D_{1S}} = \frac{\sqrt{\mu}}{\hbar c}\cdot\frac{8}{\chi}\sum_{n=1}^{\infty} \frac{\rho_-^{n-1}}{\rho_+^{n+1}} \frac{\sin\left[(n+1)\varphi_+ - (n-1)\varphi_-\right]}{n^3\left[\frac{1}{2}\chi\alpha\left(1-\frac{1}{n^2}\right)+\chi\right]} \quad \text{III.27}$$

The first four terms of the sum III.27 are given below

$$1)\quad L^{(1)}_{D_{1S}} = \frac{\sqrt{\mu}}{\hbar c}\frac{32}{(\chi^2+4)^2\chi} \quad \text{III.28}$$

by using the definitions of $\rho_\pm$ and φ_+, Eqs. III.25c and d. When the retardation factor is put equal to one in the expression III.12a, only the term n = 1 in the sum over n contributes to the value of $L_{D_{1S}}$ (because of the orthonormality of the wave functions used in the integrand). $L_{D_{1S}}$, in that case, is given by III.28 in which the x in the factor $(\chi^2+4)^2$ is put equal to zero. Therefore:

$$L_{D_{1S}} = \frac{\sqrt{\mu}}{\hbar c}\frac{2}{\chi} = \frac{2\mu^{3/2}}{\hbar c k} \quad \text{III.28a}$$

and one obtains the Morrison and Schiff expression for $\omega_k dk/\omega_c$.

---

1) There are an infinite number of choices for the values of $\varphi_\pm$, Eq. III.25d. However, if one writes $\varphi_\pm = \varphi'_\pm + m\pi$ where m = ... -2, -1, 0, 1, 2, ... and $0 \leq \varphi'_\pm \leq \frac{\pi}{2}$, one sees that the expression III. remains the same for any choice of m.

Similarly

$$2)\quad \Delta^{(2)}_{D_{1S}} = \frac{\sqrt{\mu}}{\hbar c}\,\frac{4x^2}{\left[\left(\frac{3}{2}\right)^2 + x^2\right]^3\left[\frac{3}{8}z\alpha + x\right]} \qquad \text{III.29}$$

$$3)\quad \Delta^{(3)}_{D_{1S}} = \frac{\sqrt{\mu}}{\hbar c}\,\frac{128\,x^2\left[\left(\frac{2}{3}\right)^2 + x^2\right]}{81\left[\frac{4}{9}z\alpha + x\right]\left[\left(\frac{4}{3}\right)^2 + x^2\right]^4} \qquad \text{III.30}$$

$$4)\quad \Delta^{(4)}_{D_{1S}} = \frac{\sqrt{\mu}}{\hbar c}\,\frac{x^2\left[x^4 + \frac{22}{16}x^2 + \frac{5}{16}\left(\frac{5}{4}\right)^2\right]}{2\left(\frac{15}{32}z\alpha + x\right)\left[\left(\frac{5}{4}\right)^2 + x^2\right]^5} \qquad \text{III.31}$$

The terms for $n \geq 5$ may be approximated in the following way. Let us consider the expression δ_{1S}, Eq. III.26 and expand it in powers of $\frac{1}{n}$. We neglect all terms of powers equal to and smaller than n^{-2} in the expansion. We consider first the argument of the sine function in III.26; we have

$$n(\varphi_+ - \varphi_-) + \varphi_+ + \varphi_- \qquad \text{III.32}$$

From III.25d, and from the rule for the tangents of sums and differences of angles, we obtain

$$\varphi_+ - \varphi_- = \tan^{-1}\left(\frac{-\frac{2x}{n}/1-\frac{1}{n^2}}{1+\frac{x^2}{1-\frac{1}{n^2}}}\right) \qquad \text{III.33a}$$

and $$\varphi_+ + \varphi_- = \tan^{-1}\left(\frac{\frac{2x}{1-\frac{1}{n^2}}}{1-\frac{x^2}{1-\frac{1}{n^2}}}\right) \qquad \text{III.33b}$$

If one neglects the terms in $1/n^2$ in III.33, one obtains

$$n(\varphi_+ - \varphi_-) + \varphi_+ + \varphi_- \simeq -\frac{2x}{1+x^2} + 2\tan^{-1}x \qquad \text{III.34}$$

In deriving III.34, we used the series expansion for the function $\tan^{-1}$ with $\left(\left|\frac{2x}{n}/1+x^2\right|^2 < 1\right)$ and neglected the powers equal to or smaller than n^{-2}.

We approximate φ_+ and φ_- in the same manner; from III.25d,

$$\rho_\pm \simeq (1+x^2)^{1/2}\left(1 \pm \frac{1/n}{1+x^2}\right) \qquad \text{III.35}$$

Therefore, from III.35

$$\rho_+ \rho_- \simeq (1+x^2) \qquad \text{III.36}$$

and

$$\left(\frac{\rho_-}{\rho_+}\right)^n \simeq \left(\frac{1 - 1/n/1+x^2}{1 + 1/n/1+x^2}\right)^n$$

$$\simeq e^{-\left(2/1+x^2\right)} \qquad \text{III.37}$$

To derive III.37, we made use of the relation

$$\left(1 \pm \frac{a}{n}\right)^n \simeq e^{\pm a}\left(1 - \frac{a^2}{2n} + \theta\left(\frac{1}{n^2}\right) + \cdots\right) \qquad \text{III.38}$$

With the help of III.35, III.36, III.34 and III.27, one may write as an approximate expression for $L_{D_1S}^{(n)}$ when n is large:

$$L_{D_1S}^{(n)} \simeq \frac{\sqrt{\mu}}{\hbar c} \frac{8\ell^{-\left(2/1+x^2\right)} \sin 2\left[\tan^{-1}x - \frac{x}{1+x^2}\right] \frac{1}{n^3}}{x(x^2+1)\left(x + \frac{z\alpha}{2}\right)} \qquad \text{III.39}$$

It follows therefore that

$$\sum_{n=5}^{\infty} L_{D_1S}^{(n)} \simeq L_{D_1S}^{\sim} = \frac{\sqrt{\mu}}{\hbar c} \frac{8\ell^{-\left(2/1+x^2\right)} \sin 2\left[\tan^{-1}x - \frac{x}{1+x^2}\right]}{50\, x(x^2+1)\left(x + \frac{z\alpha}{2}\right)} \qquad \text{III.40}$$

We shall evaluate L_{D_1S}, Eq. III.27, as follows

$$L_{D_1S} = L_{D_1S}^{(1)} + L_{D_1S}^{(2)} + L_{D_1S}^{(3)} + L_{D_1S}^{(4)} + L_{D_1S}^{\sim} \qquad \text{III.41}$$

with the terms in the sum given respectively by III.28a, 29, 30, 31 and 40.

b) Case of L_{D2S}

The case of L_{D2S} is treated like the one of L_{D1S}. We consider the expression III.23b for L_{2S} and write

$$f_{2S} = (-i)\left[z^2(1-z)^{n-1}\left(1 - \frac{\alpha}{2}\frac{z}{1-z} + \frac{n}{2}\cdot\frac{n+1}{2}\cdot\frac{z^2}{1-z}\right) - c.c.\right] \qquad \text{III.42}$$

where z is given by III.23c. One can show that

$$f_{2S} = \frac{8}{n^2}\left(\frac{3}{4} - x^2 - \frac{1}{n^2}\right)\frac{(\rho'_-)^{n-2}}{(\rho'_+)^{n+2}}\sin\left[(n+2)\varphi'_+ - (n-2)\varphi'_-\right] \qquad \text{III.43a}$$

in analogy with Eq. III.26, with

$$\rho'_\pm = \left[\left(\frac{1}{2} \pm \frac{1}{n}\right)^2 + x^2\right]^{1/2} \qquad \text{III.43b}$$

and

$$\varphi'_\pm = \tan^{-1}\left(\frac{x}{\frac{1}{2} \pm \frac{1}{n}}\right) \qquad \text{III.43c}$$

It follows from III.43a and III.23b that

$$L_{D2S} = \sum_n L^{(n)}_{D2S} = \frac{2\sqrt{2}}{\alpha}\sum_{n=1}^{\infty}\frac{\left(\frac{3}{4} - x^2 - \frac{1}{n^2}\right)\frac{(\rho'_-)^{n-2}}{(\rho'_+)^{n+2}}\sin\left[(n+2)\varphi'_+ - (n-2)\varphi'_-\right]}{n^3\left[\frac{1}{2}z\alpha\left(\frac{1}{4} - \frac{1}{n^2}\right) + x\right]} \qquad \text{III.44}$$

$$\times \frac{\sqrt{\mu}}{\hbar c}$$

The first four terms of the sum III.44 are the following:

$$L^{(1)}_{D2S} = \frac{\sqrt{\mu}}{\hbar c}\cdot\frac{\left(-x^2 - \frac{1}{4}\right)\sin\left[3\tan^{-1}\frac{2\alpha}{3} + \tan^{-1}2x\right]}{\left(x - \frac{3}{8}z\alpha\right)\left(x^2 + \frac{9}{4}\right)^{3/2}\left(x^2 + \frac{1}{4}\right)^{1/2}} \qquad \text{III.45a}$$

$$L^{(2)}_{D_{2S}} = \frac{2\sqrt{2}}{x}\frac{\sqrt{\mu}}{kc}\frac{\left(\frac{1}{2}-x^2\right)\sin\left(4\tan^{-1}x\right)}{8x\left(x^2+1\right)^2} \qquad \text{III.45b}$$

$$L^{(3)}_{D_{2S}} = \frac{2\sqrt{2}}{x}\frac{\sqrt{\mu}}{kc}\frac{\left(\frac{23}{16}-x^2\right)\left(x^2+1/36\right)^{1/2}\sin\left[5\tan^{-1}6x - \tan^{-1}6x\right]}{27\left(x+\frac{5}{72}z\alpha\right)\left(x^2+\frac{25}{36}\right)^{5/2}} \qquad \text{III.45c}$$

$$L^{(4)}_{D_{2S}} = \frac{2\sqrt{2}}{x}\frac{\sqrt{\mu}}{kc}\frac{\left(\frac{11}{16}-x^2\right)\left(x^2+\frac{1}{16}\right)\sin\left[6\tan^{-1}4x - 2\tan^{-1}4x\right]}{64\left(x+\frac{3}{32}z\alpha\right)\left(x^2+\frac{9}{16}\right)^3} \qquad \text{III.45d}$$

and for $n \geq 5$

$$L^{(n)}_{D_{2S}} \simeq \frac{2\sqrt{2}}{x}\frac{\sqrt{\mu}}{kc}\frac{\left(\frac{3}{4}-x^2\right)e^{-\left(1/x^2+\frac{1}{4}\right)}\sin\left[4\tan^{-1}2x - \frac{2x}{x^2+1/4}\right]}{\left(x+\frac{1}{8}z\alpha\right)\left(x^2+\frac{1}{4}\right)^2}\cdot\frac{1}{n^3} \qquad \text{III.45e}$$

In III.45e we have neglected the powers equal to or smaller than n^{-2} when compared to unity. From III.45e, it follows that

$$\sum_{n=5}^{\infty} L^{(n)}_{D_{2S}} \simeq L^{\sim}_{D_{2S}} = \frac{2\sqrt{2}\sqrt{\mu}}{x\,kc}\frac{\left(\frac{3}{4}-x^2\right)e^{-\left(1/x^2+\frac{1}{4}\right)}\sin\left[4\tan^{-1}2x - \frac{2x}{x^2+1/4}\right]}{\left(x+\frac{1}{8}z\alpha\right)\left(x^2+\frac{1}{4}\right)^2}\cdot\frac{1}{50} \qquad \text{III.46}$$

$L_{D_{2S}}$ will be evaluated as follows

$$L_{D_{2S}} = L^{(1)}_{D_{2S}} + L^{(2)}_{D_{2S}} + L^{(3)}_{D_{2S}} + L^{(4)}_{D_{2S}} + L^{\sim}_{D_{2S}} \qquad \text{III.47}$$

where the terms are given by Eqs. III.45 and III.46.

2° Continuous States

To evaluate the contribution to L_{1s} and L_{2s} , Eq. II.30, involving the integration over the continuous energy states, one must consider the following integral

$$L_{C_{ns}} = \int_{mc^2}^{\infty} \frac{dE\, \varphi_E(R) \int_0^{\infty} \varphi_E^*(r) \frac{\sin kr}{kr} \varphi_{ns}(r)\, r^2 dr}{E - E_n + \hbar c k} \qquad \text{III.48}$$

The non-relativistic wave functions describing an electron in the continuum is the following (See Sommerfeld p.115 & ff.)

$$\varphi_E(r) = \left(\frac{m}{2\pi\hbar p}\right)^{1/2} \frac{2p}{\hbar} \left|\Gamma(1+i\gamma)\right| e^{(\pi\gamma/2)} e^{-\frac{ipr}{\hbar}} \mathcal{F} \qquad \text{III.49}$$

where $\mathcal{F} = \mathcal{F}(1+i\gamma;\, 2;\, \frac{2ipr}{\hbar})$ $\qquad \gamma = \frac{Z\alpha mc}{p}$

This wave function, which is real, is normalized per unit energy interval: this means that

$$\int_{\Delta E} dE \int_0^{\infty} dr\, r^2 \varphi_{E'}^*(r)\, \varphi_E(r) = 1 \qquad \text{III.50}$$

where ΔE is any energy interval containing E^1. The energy E is related to the momentum p of III.49 through the relation

$$E = \left[c^2p^2 + (mc^2)^2\right]^{1/2} \simeq mc^2 + \frac{p^2}{2m} \qquad \text{III.51}$$

When r = R, one cannot set equal to one the factor

$$e^{-\frac{ipR}{\hbar}} \mathcal{F}\left(1+i\gamma, 2; \frac{2ipR}{\hbar}\right) \qquad \text{III.52}$$

as readily as in the case of $L_{D_{1S}}$ (See Eqs. III.7 to III.10) because, in III.48, p becomes infinite at the upper limit of integration. This factor is shortly considered in Appendix C where we conclude that setting it equal to unity does not affect the value of III.48. Therefore, we may write, when r = R

$$\varphi_E(R) = \left[\frac{m}{4\pi\hbar p}\right]^{1/2} \frac{2p}{\hbar} \left|\Gamma(1+i\gamma)\right| e^{\pi\gamma/2} \qquad \text{III.53}$$

The wave functions φ_{1s} and φ_{2s} for the electron in the initial state are given by Eqs. III.11a and III.11b respectively. We consider first the case of $L_{C_{1s}}$ and then that of $L_{C_{2s}}$

a) Evaluation of $L_{C_{1s}}$

With the use of III.49, III.53 and III.11a, III.48 becomes

$$L_{C_{1s}} = 2\mu^{3/2} \int_{mc^2}^{\infty} \frac{dE \; \frac{2pm}{\hbar^2\pi} \left|\Gamma(1+i\gamma)\right|^2 e^{\pi\gamma} \int_0^{\infty} e^{-\mu r - \frac{ipr}{\hbar}} \frac{\sin kr}{kr} \mathcal{F} \, r^2 dr}{E - E_1 + \hbar c k} \qquad \text{III.54}$$

where E_1 is given by Eq. III.13 with n = 1.

$$E_1 = mc^2 \lambda = mc^2\left(1 - \frac{(z\alpha)^2}{2}\right) \qquad \text{III.55}$$

To evaluate III.54, we first express the confluent hypergeometric function in an integral form (See, for instance MacRobert (54) p. 346).

$$\mathcal{F}\left(1+i\gamma;2;\frac{2ikr}{\hbar}\right)=\frac{\Gamma(2)}{\Gamma(1+i\gamma)\Gamma(1-i\gamma)}\int_0^1 e^{\frac{2ikrt}{\hbar}}t^{i\gamma}(1-t)^{-i\gamma}dt \qquad \text{III.56}$$

Then we interchange the order of the integrations over r and t in III.54; this is allowed because of the presence of the decreasing exponential factor $e^{-\mu r}$ in the integrand. Integrating over r first, and then over t, one obtains

$$L_{c_{1S}}=\frac{4\mu^{3/2}m}{\pi\hbar^3 R}\int_{mc^2}^{\infty}\frac{dE\,p\,e^{\pi\gamma}\left|\Gamma(1+i\gamma)\right|^2}{E-E_1+\hbar cR}\,\mathcal{K}_{1S} \qquad \text{III.57}$$

where $$\mathcal{K}_{1S}=\frac{1}{2i}\left(\frac{\hbar}{2ip}\right)^2\left[Z_-^2\mathcal{F}(2,1+i\gamma;2;Z_-)-Z_+^2\mathcal{F}(2,1+i\gamma;2;Z_+)\right] \qquad \text{III.58}$$

$\mathcal{F}$ is the hypergeometric function and

$$Z_\pm=\frac{2ip}{\hbar\mu+ip\pm i\hbar R} \qquad \text{III.59}$$

One arrives at Eqs. III.57, 58 and 59 by making use of the integral representation of the hypergeometric function (See MacRobert (54), p.297):

$$\mathcal{F}(2,1+i\gamma;2;Z)=\frac{\Gamma(2)}{\Gamma(1+i\gamma)\Gamma(1-i\gamma)}\int_0^1 t^{i\gamma}(1-t)^{-i\gamma}(1-Zt)^{-2}dt \qquad \text{III.60}$$

From III.21, it follows that

$$\mathcal{F}(2,1+i\gamma;2;Z)=(1-Z)^{-1-i\gamma} \qquad \text{III.61}$$

For computational purposes, it is convenient to introduce the following dimensionless quantities:

$$q = \frac{p}{\hbar\mu} = \frac{1}{\gamma} \quad ; \quad \chi = \frac{k}{\mu} = \frac{\hbar k}{2\alpha mc} \quad ; \quad \varepsilon = \frac{E}{mc^2} \qquad \text{III.62}$$

$$\varepsilon = \left[1 + (2\alpha q)^2\right]^{1/2}$$

With these notations, III.59 becomes

$$z_\pm = \frac{2iq}{1 + i(q \pm \chi)} \qquad \text{III.63}$$

With the help of III.61, one shows that III.58 yields

$$\mathcal{K}_{1S} = \frac{1}{2i\mu^2}\left[\frac{1}{\left[1+i(q-\chi)\right]^{1-i/q}\left[1-i(q+\chi)\right]^{1+i/q}} - c.c.\right] \qquad \text{III.64}$$

$$= \frac{1}{\mu^2}\, e^{-a} \sin b$$

where $\qquad$ III.65a

$$a = \ln r_+ r_- + \frac{1}{q}(\theta_+ + \theta_-) \qquad \text{III.65b}$$

$$b = \theta_+ - \theta_- - \frac{1}{q} \ln \frac{r_+}{r_-} \qquad \text{III.65c}$$

$$r_\pm = \left[1 + (q \pm \chi)^2\right]^{1/2} \; ; \; \theta_\pm = \tan^{-1}(q \pm \chi), \qquad \text{III.65d}$$

and $\qquad 0 \leq \theta_+ \leq \pi/2 \qquad$ III.66a

$$-\frac{\pi}{2} \leq \theta_- \leq \frac{\pi}{2} \qquad \text{III.66b}$$

These inequalities are essential for avoiding difficulties connected with the multi-valued character of the function III.64.

Using the relation $\Gamma(z)\,\Gamma(1-z) = \pi/\sin \pi z$ we obtain

$$e^{\pi\gamma}\left|\Gamma(1+i\gamma)\right|^2 = \pi\gamma(\coth\pi\gamma+1) \qquad \text{III.67}$$

It follows from III.55, 62, 64 and 67 that

$$L_{c1s} = \frac{\sqrt{\mu}}{\hbar c}\frac{4}{2\alpha\chi}\int_1^\infty I_{1s}\,d\varepsilon \qquad \text{III.68a}$$

where

$$I_{1s} = \frac{(\coth\pi\gamma+1)\,e^{-a}\sin b}{\varepsilon-\lambda+2\alpha\chi} \qquad \text{III.68b}$$

The integrand I_{1s} has been plotted as a function of q, and the integral III.68a evaluated numerically for the lowest values of q(i.e. for q between 0 and q_0 where q_0 corresponds to an energy E of about 1.5 mc^2 in the case of A^{37} and of about $2mc^2$ in the case of Cs^{131}). For the higher energies $(q > q_0)$ an approximate integrand (which is derived below) is used in place of I_{1s} and the resulting integral is performed analytically. Let us write L_{c1s} as the sum of two terms:

$$L_{c1s} = L^{(1)}_{c1s} + L^{(2)}_{c1s} \qquad \text{III.69}$$

where $L^{(1)}_{c1s}$ is the part of L_{c1s} evaluated numerically and $L^{(2)}_{c1s}$ the part of L_{c1s} evaluated analytically. If ε_0 is the energy corresponding to q_0, we have

$$L^{(1)}_{c1s} = \frac{\sqrt{\mu}}{\hbar c}\frac{4}{2\alpha\chi}\int_1^{\varepsilon_0} I_{1s}\,d\varepsilon \qquad \text{III.70a}$$

and

$$L^{(2)}_{c1s} = \frac{\sqrt{\mu}}{\hbar c}\frac{4}{2\alpha\chi}\int_{\varepsilon_0}^\infty \tilde{I}_{1s}\,d\varepsilon \qquad \text{III.70b}$$

We approximate I_{1S} by expanding it in powers of $1/q$ and by taking the first two terms. The expansion of the binomials of Eq. III.64 in powers of $1/q$ is allowed when

$$\left|\frac{1 \pm i\alpha}{q_0}\right| < 1 \qquad q > q_0 \qquad \text{III.71}$$

The upper limit ε_0 of the numerical integration III.70a is chosen such that the corresponding q_0 satisfies III.71. We give below, as an example, the first few terms of the expansion for one of the binomials in III.64:

$$\begin{aligned}[(1-i\alpha)+iq]^{-1+i/q} = {} & (iq)^{-1+i/q} \\ & + (-1+i/q)(1-i\alpha)(iq)^{-2+i/q} \\ & + \frac{(-1+i/q)(-2+i/q)(1-i\alpha)^2}{2}(iq)^{-3+i/q}\end{aligned} \qquad \text{III.72}$$

When the expansions are carried out up to the power $(iq)^{-5}$, it is seen that

$$\mathcal{K}_{1S} \simeq \frac{1}{\mu^2}\,\frac{4\alpha^3 e^{-\pi/q}}{3q^6} + O\left(\frac{1}{q^8}\right) \qquad (q > q_0) \qquad \text{III.73}$$

In the same approximation, one has, for the remaining factors of the integrand I_{1S}, (Eq. III.68b)

$$\coth\frac{\pi}{q} + 1 \simeq \frac{e^{\pi/q}}{\pi/q} \qquad \text{III.74a}$$

$$\varepsilon \simeq 2\alpha q + \frac{1}{2\alpha q} \qquad \text{III.74b}$$

$$d\varepsilon \simeq 2\alpha\, dq \qquad \text{III.74c}$$

$$[\epsilon - (\lambda - Z\alpha\varkappa)]^{-1} \simeq \frac{1}{Z\alpha q} + \frac{\lambda - Z\alpha\varkappa}{(Z\alpha q)^2} \qquad \text{III.74d}$$

Therefore, from III.74, 73, 62, 68b and 70b:

$$\tilde{I}_{1S} = \frac{4\varkappa^3}{3\pi q^5}\left(\frac{1}{Z\alpha q} + \frac{\lambda - Z\alpha\varkappa}{(Z\alpha q)^2}\right) \qquad \text{III.75a}$$

and

$$L^{(2)}_{C_{1S}} = \frac{\sqrt{\mu}}{\hbar c}\,\frac{16\varkappa^2}{15\pi Z\alpha q_0^5}\left(1 + \frac{5}{6}\,\frac{\lambda - Z\alpha\varkappa}{Z\alpha q_0}\right) \qquad \text{III.75b}$$

We have finally, for L_{1S} :

$$L_{1S} = L_{D_{1S}} + L_{C_{1S}} \qquad \text{III.76}$$

with $L_{D_{1S}}$ given by III.41 and $L_{C_{1S}}$ given by III.69

b) Evaluation of $L_{C_{2S}}$

The evaluation of $L_{C_{2S}}$ is carried out along very similar lines. With the aid of III.11b, 49, and 53, III.48 becomes

$$L_{C_{2S}} = 2\left(\frac{\mu}{2}\right)^{3/2}\int_{mc^2}^{\infty} \frac{dE\ \frac{2pm}{\hbar^2\pi}\left|\Gamma(1+i\gamma)\right|^2 e^{\pi\gamma}\int_0^{\infty} e^{-\frac{\mu}{2}r - \frac{ipr}{\hbar}}\frac{\sin kr}{kr}\left(1 - \frac{\mu}{2}r\right)\frac{\partial\varphi}{\partial r}\,r^2\,dr}{E - E_2 + \hbar c k} \qquad \text{III.77}$$

with E_2 given by Eq. III.13 with n = 2:

$$E_2 = mc^2\lambda' \simeq mc^2\left(1 - \frac{1}{8}(Z\alpha)^2\right) \qquad \text{III.78}$$

With the help of III.56 and III.60, one integrates III.77 over r first, and then over t; to obtain:

$$L_{C_{2S}} = \frac{\sqrt{2}\,\mu^{3/2} m}{\pi \hbar^3 R} \int_{mc^2}^{\infty} \frac{dE\, p\, e^{\pi\gamma} \left|\Gamma(1+i\gamma)\right|^2 \mathcal{K}_{2S}}{E - E_2 + \hbar c R} \qquad \text{III.79}$$

where $$\mathcal{K}_{2S} = \frac{1}{2i}\left(\frac{\hbar}{2ip}\right)^2 \left[z_-'^2 \mathcal{F}(2, 1+i\gamma; 2; z_-') - z_-'^3 \left(\frac{\hbar\mu}{2ip}\right) \mathcal{F}(3, 1+i\gamma; 2; z_-') - i d(z_+') \right] \qquad \text{III.80}$$

and

$$z_\pm' = \frac{2ip}{\hbar\frac{\mu}{2} + ip \pm \lambda \hbar R} \qquad \text{III.81}$$

In the notation of III.62, we have

$$z_\pm' = \frac{2iq}{\frac{1}{2} + iq \pm ix} \qquad \text{III.82}$$

and, from III.21,

$$\mathcal{K}_{2S} = \frac{1}{2i\mu^2}\left[\frac{1}{\left[\frac{1}{2} + i(q-x)\right]^{1-i/q}\left[\frac{1}{2} - i(q+x)\right]^{1+i/q}} \left(1 + \frac{1/2 + ix}{(\frac{1}{2}+iq-ix)(\frac{1}{2}-iq-ix)}\right) - c.c. \right]$$

$$= \frac{1}{\mu^2}\left[e^{-a'} \sin b' + e^{-a''}\left(\tfrac{1}{2}\sin b'' + x\cos b''\right)\right] \qquad \text{III.83}$$

where we introduced a notation similar to the one in III.65a

$$a' = \ln r_+' r_-' + \frac{1}{q}(\theta_+' + \theta_-')$$

$$b' = \theta_+' - \theta_-' - \frac{1}{q}\ln\frac{r_+'}{r_-'}$$

$$a'' = a' + \ln r_+' r_-' \qquad \text{III.84}$$

$$b'' = b' + (\theta_+' - \theta_-')$$

$$\lambda_{\pm}' = \left(\frac{1}{4} + (q \pm x)^2\right)^{1/2}$$

$$\theta_{\pm}' = \tan^{-1} 2(q \pm x)$$

θ_+' and θ_-' have the same range of values as θ_+ and θ_- (Eq. III.66)

Using the above notation and Eq. III.67, we have

$$L_{c_{2S}} = \frac{\sqrt{\mu}}{\pi c} \frac{\sqrt{2}}{2\alpha x} \int_1^\infty I_{2S}\, d\varepsilon \qquad \text{III.85a}$$

with $$I_{2S} = \frac{(\coth \pi/q + 1)\left[e^{-a'} \sin b' + e^{-a''}\left(\frac{1}{2}\sin b'' + x \cos b''\right)\right]}{\varepsilon - \lambda' + 2\alpha x} \qquad \text{III.85b}$$

λ' is defined in III.78.

$L_{c_{2S}}$ was evaluated in the same manner as $L_{c_{1S}}$, i.e. as the sum of two terms

$$L_{c_{2S}} = L^{(1)}_{c_{2S}} + L^{(2)}_{c_{2S}} \qquad \text{III.86a}$$

with $$L^{(1)}_{c_{2S}} = \frac{\sqrt{\mu}}{\pi c} \cdot \frac{\sqrt{2}}{2\alpha x} \int_1^{\varepsilon_0} I_{2S}\, d\varepsilon \qquad \text{III.86b}$$

$$L^{(2)}_{c_{2S}} = \frac{\sqrt{\mu}}{\pi c} \cdot \frac{\sqrt{2}}{2\alpha x} \int_{\varepsilon_0}^\infty \tilde{I}_{2S}\, d\varepsilon \qquad \text{III.86c}$$

$L^{(1)}_{c_{2S}}$ is the part of $L_{c_{2S}}$ evaluated numerically, and $L^{(2)}_{c_{2S}}$ the part evaluated analytically, $\tilde{I}_{2S}$ being an approximation for I_{2S} at high energies. ε_0 is chosen such that the corresponding q_0 (Eq. III.62) satisfies the relation:

$$\left| \frac{\frac{1}{2} \pm i\lambda}{q_0} \right| < 1 \qquad \text{III.87}$$

The approximate integrand $\tilde{I}_{2S}$ is derived by developing the expression III.85b in powers of 1/q. The first two terms of the expansion are

$$\tilde{I}_{2S} \simeq \frac{\alpha}{\pi q^5} \left(\frac{4\lambda^2}{3} + \frac{5}{2} \right) \left(\frac{1}{2\alpha q} + \frac{\lambda' - 2\alpha\lambda}{2\alpha q} \right) \qquad \text{III.88}$$

It follows from 86c and from the relation $d\varepsilon \simeq 2\alpha\, dq$ that

$$L^{(2)}_{C_{2S}} = \frac{\sqrt{\mu}}{\hbar c} \frac{\sqrt{2}\left(\frac{4\lambda^2}{3} + \frac{5}{2} \right)}{5\pi\, 2\alpha q_0^5} \left(1 + \frac{5}{6} \frac{\lambda' - 2\alpha\lambda}{2\alpha q_0} \right) \qquad \text{III.89}$$

We have finally, for L_{2S}

$$L_{2S} = L_{D_{2S}} + L_{C_{2S}} \qquad \text{III.90}$$

with $L_{D_{2S}}$ given by Eqs. III.45 and III.47 and $L_{C_{2S}}$ given by Eqs. III.86a, 86b and 89.

3° Results and Conclusions

We have applied the formulae and methods of this Section to the case of A^{37} ($Z = 18$). Among the few elements for which reliable experimental data exist this is the one with the smallest value of **Z** so that the non-relativistic approximation is not unjustified. In addition to that, we have evaluated one point of the ls - spectrum for the case of Cs^{131} ($Z = 55$) using our formulae, with a view to comparing the result with Hess's result for the same case.

a) The Case of A^{37}

In the case of A^{37} ($Z = 18$), we have computed the ratio $\omega_K d\mathcal{N}/\omega_c$ for four different points of the photon spectrum:

For $\hbar ck = 135$ Kev corresponding to $x = 2$
$\hbar ck = 269$ " " " $x = 4$
$\hbar ck = 404$ " " " $x = 6$
$\hbar ck = 673$ " " " $x = 10$

The limit of the spectrum is at $\hbar ck = 816$ Kev.

The results for this case are summarized in Tables I, II and III and in Fig. 5.

In Table I, we list the various contributions to the integral L_{1S} (Eq. II.30, ($n = 1$)), for the four values of the photon energy listed above. $L^{(1)}_{D_{1S}}$, $L^{(2)}_{D_{1S}}$, $L^{(3)}_{D_{1S}}$, $L^{(4)}_{D_{1S}}$ and $L^{\sim}_{D_{1S}}$ are given by the formulae III. 28, 29, 30, 31 and

40 respectively. To get an idea about the reliability of Eq. III.40, $L^{(4)}_{D_{1S}}$ has also been calculated from the approximate expression III.39. The values obtained (in italics) when compared with the exact values for $L^{(4)}_{D_{1S}}$, show a deviation of less than 0.5 percent. The error in evaluating $\tilde{L}_{D_{1S}}$ is of the same order of magnitude. The values for $L^{(1)}_{C_{1S}}$ are obtained by numerical integration of Eq. III.70a for four different values of x. Since the integrand is too complicated to be studied analytically, we give in Fig. 1, 2, 3 and 4 the curves representing the integrand as a function of the integration variable q for the four values of x. The curves just helped us to choose the appropriate lengths of intervals when carrying out the numerical integration. The upper limit of integration q_0 is different in each case. $L^{(2)}_{C_{1S}}$ is evaluated analytically from Eq. III.75b. The main error in the expression for L_{1S} comes from the numerical integration of $L^{(1)}_{C_{1S}}$; the error made in evaluating $\tilde{L}_{D_{1S}}$ and $L^{(2)}_{C_{1S}}$ are small compared to it. The total error on L_{1S}, however, is probably less than one unit in the third significant figure.

In Table II we list the contributions to the integral L_{2S}, (Eq. II.32 (n = 2)) for the same four values of the photon energy. $L^{(1)}_{D_{2S}}$, $L^{(2)}_{D_{2S}}$, $L^{(3)}_{D_{2S}}$, $L^{(4)}_{D_{2S}}$, $\tilde{L}_{D_{2S}}$ are evaluated from Eq. III.45, 46. $L^{(4)}_{D_{2S}}$, calculated from the approximate Eq. III.45e is also included. $L^{(1)}_{C_{2S}}$ is given by Eq. III.86b which was also integrated numerically. However, the curves for the integrand I_{2S} (Eq. III.85b) have not been included. $L^{(2)}_{C_{2S}}$ is given by Eq. III.89. The error in the values obtained for L_{2S} are of the same order of magnitude as in the case of L_{1S}.

In Table III, we give the values for the probability ratio $w_R dR/w_c$ as evaluated from Eq. II.30 and from the values of Table I and Table II for L_{1s} and L_{2s}. The quantity ρ_A which appears in Table III is defined as

$$\rho_A = \frac{\left[\left(\frac{w_R dR}{w_c}\right)_{1s} + \left(\frac{w_R dR}{w_c}\right)_{2s}\right]_{\text{This thesis}}}{\left[\left(\frac{w_R dR}{w_c}\right)_{1s} + \left(\frac{w_R dR}{w_c}\right)_{2s}\right]_{\text{Glauber and Martin (54)}}}$$

ρ_A is therefore a measure of the influence of the retardation factor on the $1s + 2s$ contributions to the probability ratio $w_R dR/w_c$.

In Fig. 5, we have plotted the two quantities $\frac{\pi}{\alpha}\left(\frac{w_R dR}{w_c}\right)_{1s}$ and $\frac{\pi}{\alpha}\left(\frac{w_R dR}{w_c}\right)_{1s+2s}$ both in our case and in the case of Glauber and Martin (54), as a function of the energy of the emitted photon. The curve $\frac{\pi}{\alpha}\left(\frac{w_R dR}{w_c}\right)_{1s}$ in the case of Glauber and Martin is identical with that which would be obtained from Morrison and Schiff's formula.

We can say very little, at the present time, about the comparison of our theoretical results for $w_R dR/w_c$ in case of A^{37} with the experimental results of Lindqvist and Wu (55). The procedure used by these authors to compare experiments and theory consists, first, in applying all kinds of experimental corrections to the theoretical gamma spectrum, and, next, in normalizing the measured spectrum to the spectrum so obtained (so that only relative intensities are being compared). The corrections would thus have to be applied to our theoretical spectrum, which we cannot do solely on the basis of the data published by Lindqvist and Wu (55). It is not impossible that the difference in the slope of the curves A(1s + 2s) and B(1s + 2s) in Fig. 5 may be reduced considerably after the

corrections have been applied.

b) The Case of Cs^{131}

In the case of Cs^{131} ($Z = 55$) we have calculated $w_R dR/w_C$ only for one value of the photon energy, namely for $\hbar ck = 205$ Kev ($x = 1$), and we restricted ourselves to the 1s - electron contribution.

An application of the formulae of this Section and a numerical integration carried out in the way indicated in Subsection a) give, for Cs^{131}:

$$L_{D_{1S}} = 1.438 \frac{\sqrt{\mu}}{\hbar c} \quad (x = 1)$$

$$L_{C_{1S}} = 0.343 \frac{\sqrt{\mu}}{\hbar c} \quad (x = 1)$$

Therefore, $$L_{1S} = 1.78 \frac{\sqrt{\mu}}{\hbar c}$$

The ratio

$$\rho_{Cs} = \frac{\left[\left(\frac{w_R dR}{w_C}\right)_{1S}\right] \text{This thesis}}{\left[\left(\frac{w_R dR}{w_C}\right)_{1S}\right] \text{Morrison - Schiff (40)}}$$

is found to be equal to 0.79.

If only the integration over the intermediate continuous states is taken into account, $L_{D_{1S}} = 0$, and the ratio ρ_{Cs} becomes only 0.03. This small value for ρ_{Cs} accounts for the larger part of the discrepancy between the results of Hess (who neglected the sum over the discrete states) and the results of Morrison and Schiff.

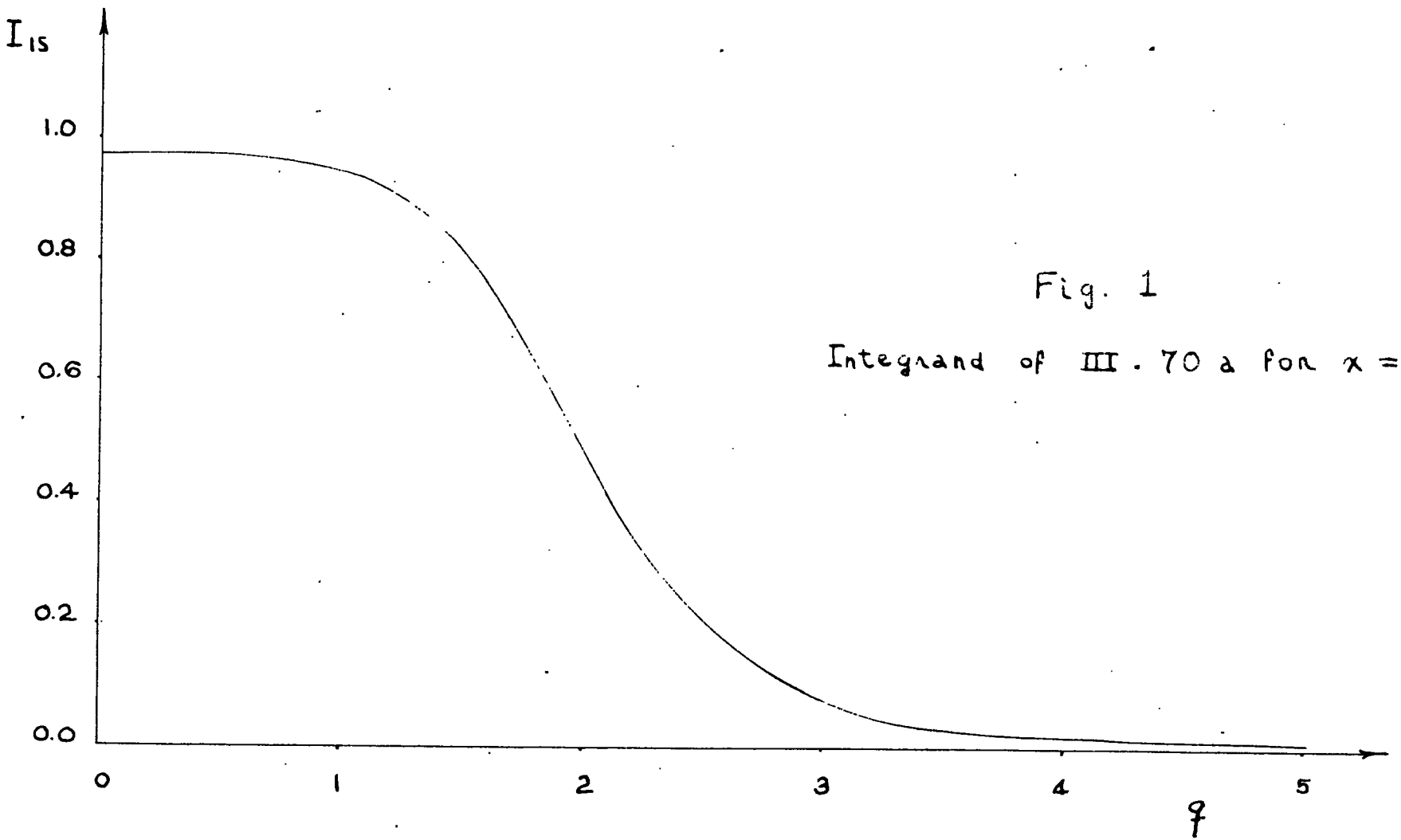

Fig. 1

Integrand of III . 70 a for $x = 2$

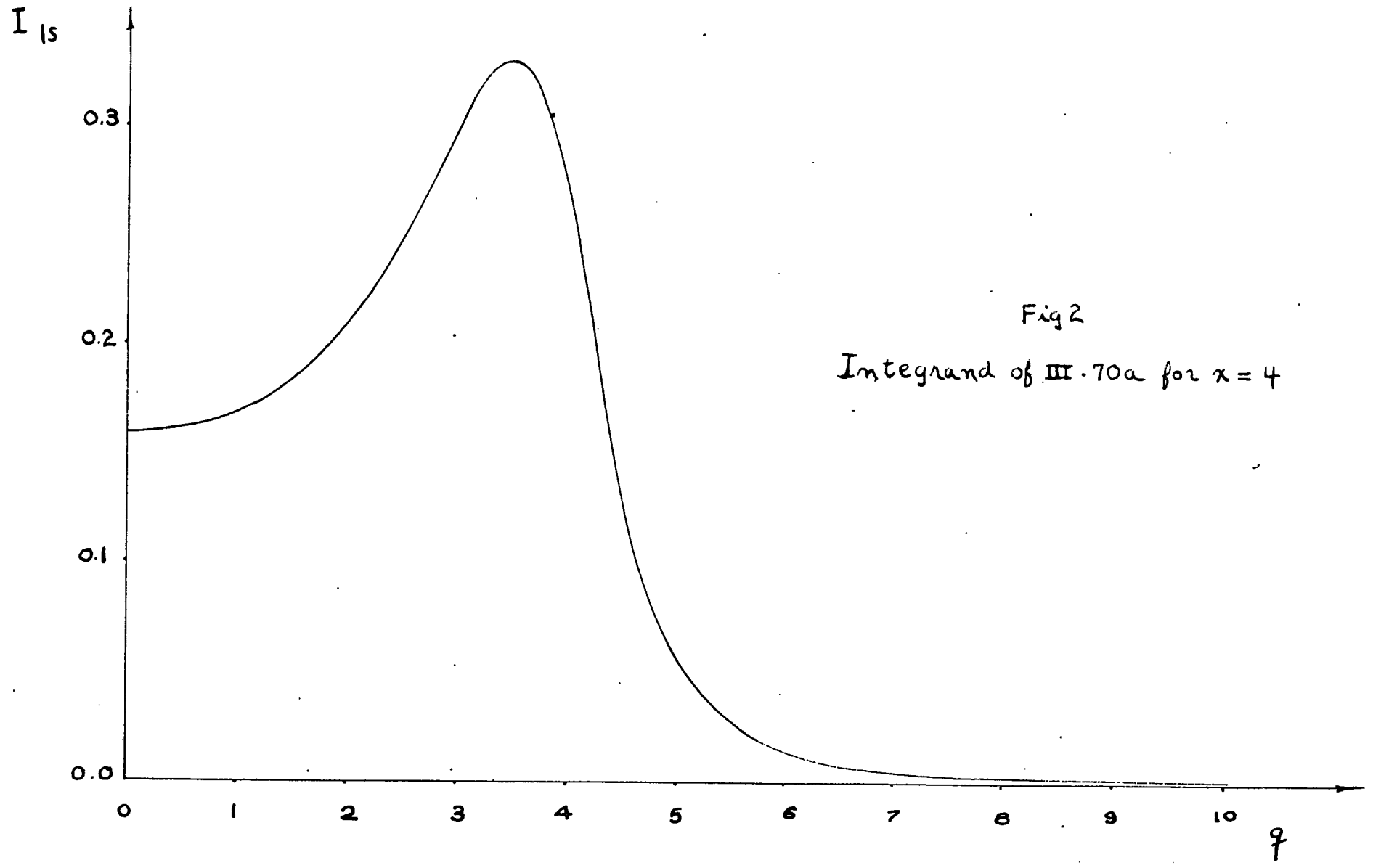

Fig 2

Integrand of III·70a for $x = 4$

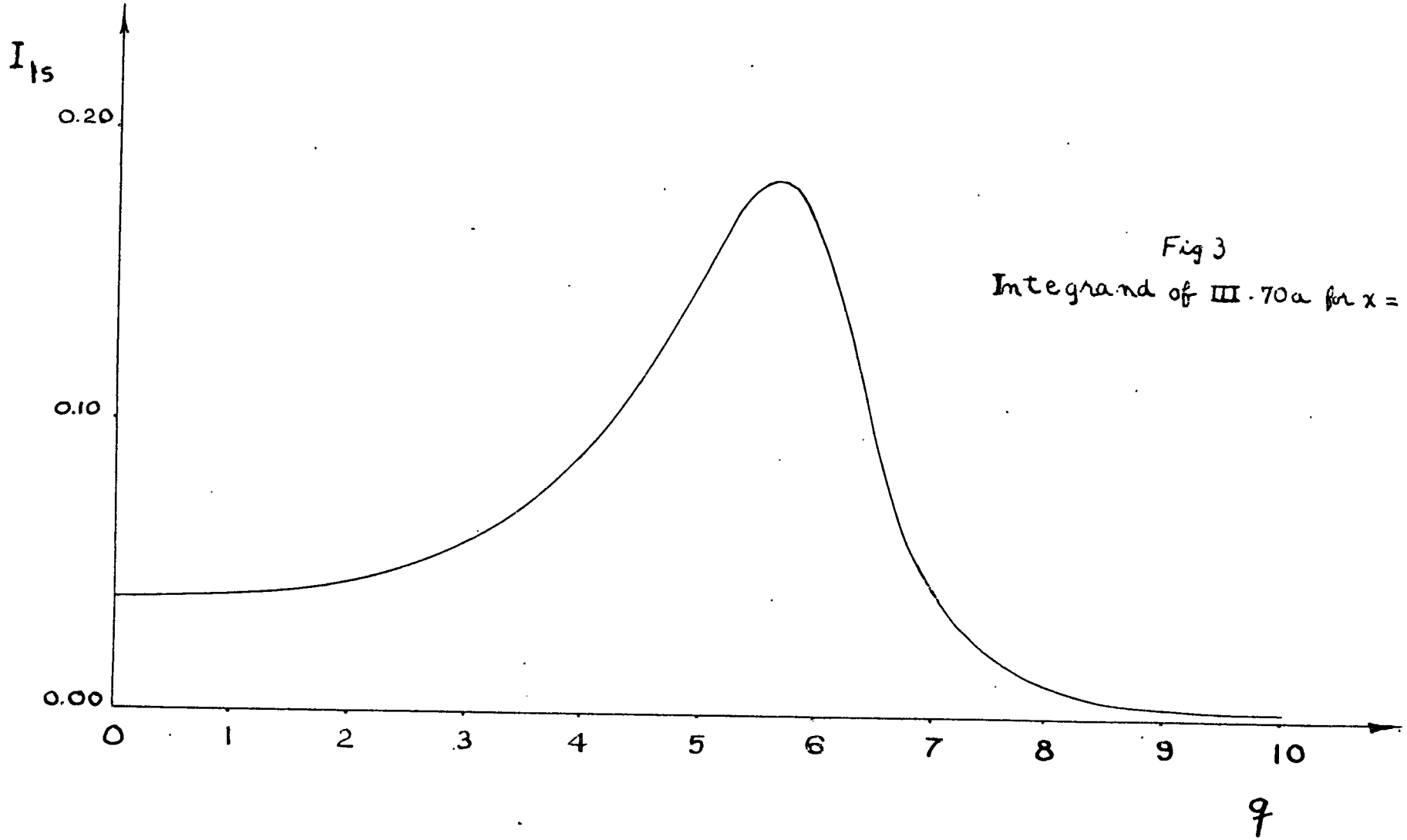

Fig 3
Integrand of III.70a for x = 6

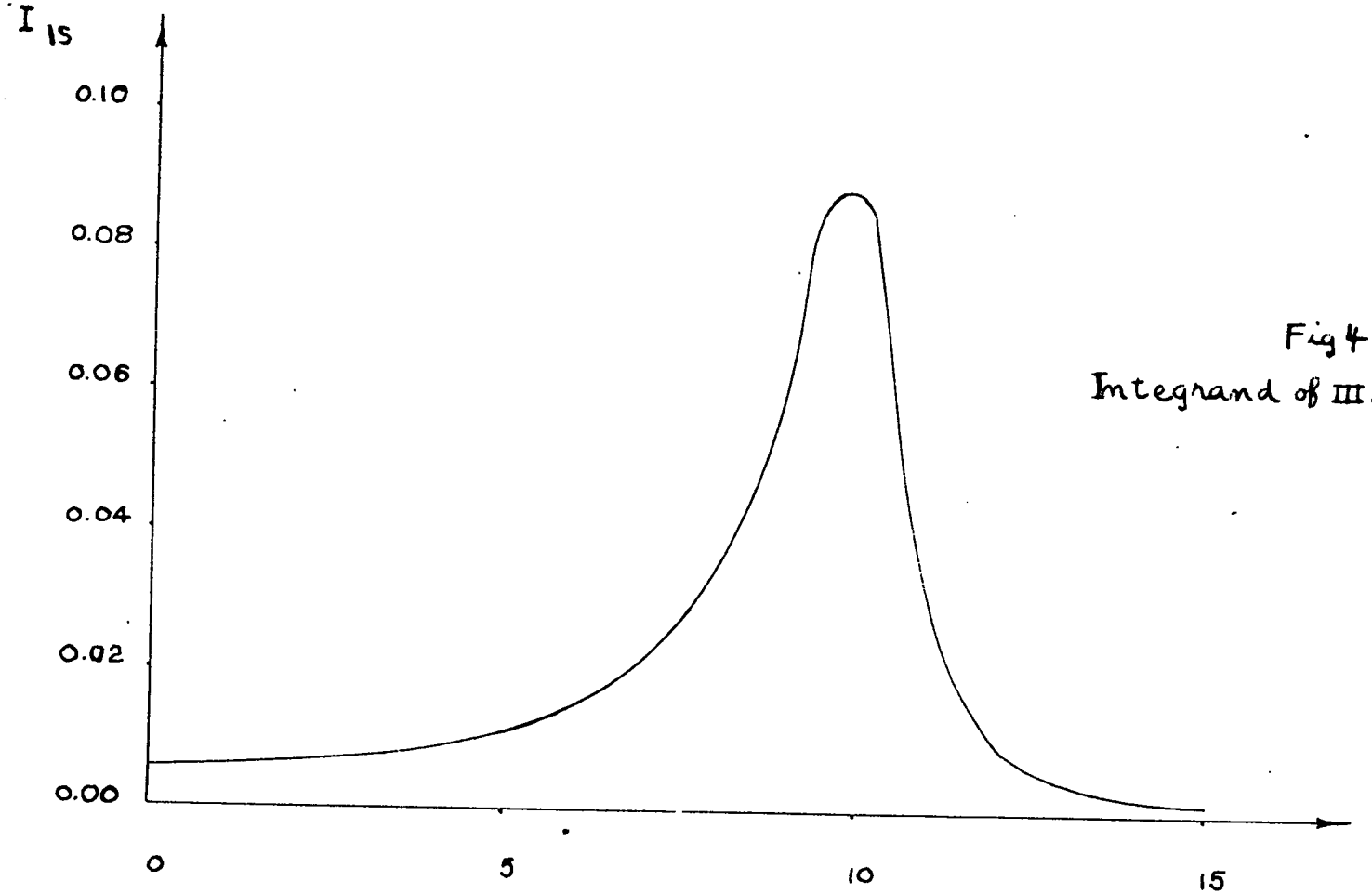

Fig 4
Integrand of III.70a for $x = 10$

Table I

1s	$\hbar ck = 135$ (x = 2)	$\hbar ck = 269$ (x = 4)	$\hbar ck = 404$ (x = 6)	$\hbar ck = 673$ (x = 10)
$L_D^{(1)}$	0.25000	0.02000	0.003333	0.0002959
$L_D^{(2)}$	0.03198	0.00266	0.000425	0.0000372
$L_D^{(3)}$	0.01225	0.00103	0.000168	0.0000147
$L_D^{(4)}$	0.00401	0.00033	0.000053	0.0000047
$L_D^{(4)\sim}$	0.004007	0.000328	0.0000539	0.00000469
$L_D^{\sim}$	0.00513	0.00042	0.000069	0.00000601
L_D	0.3034	0.0244	0.0040	0.00036
$L_C^{(1)}$	0.5962	0.3677	0.2093	0.09953
$L_C^{(2)}$	0.0063	0.0005	0.0012	0.00029
L_C	0.6025	0.3682	0.2105	0.09982
L	0.906	0.393	0.215	0.100

Table I showing the various contributions to the integral L_{1S} (in units of $\left(\frac{2\alpha m}{\hbar^3 c}\right)^{1/2}$) for four values of the photon energy $\hbar ck$ (in Kev)

$$L_D = L_D^{(1)} + L_D^{(2)} + L_D^{(3)} + L_D^{(4)} + L_D^{\sim}$$

$$L_C = L_C^{(1)} + L_C^{(2)}$$

$$L = L_C + L_D$$

Table II

$2S$	$\hbar ck = 135$ ($x = 2$)	$\hbar ck = 269$ ($x = 4$)	$\hbar ck = 404$ ($x = 6$)	$\hbar ck = 673$ ($x = 10$)
$L_D^{(1)}$	0.08385	0.007306	0.001206	0.0001079
$L_D^{(2)}$	0.00594	0.000984	0.000156	0.0000134
$L_D^{(3)}$	0.00451	0.000308	0.000047	0.0000040
$L_D^{(4)}$	0.00147	0.000124	0.000020	0.0000017
$L_D^{(4)\sim}$	0.001464	0.0001249	0.0000197	0.00000168
$L_D^{\sim}$	0.00187	0.000160	0.000025	0.0000022
L_D	0.0977	0.0089	0.00146	0.00013
$L_C^{(1)}$	0.2084	0.1312	0.07327	0.03062
$L_C^{(2)}$	0.0019	0.0007	0.00039	0.00015
L_C	0.2103	0.1319	0.07366	0.03077
L	0.308	0.141	0.0752	0.0309

Table II showing the various contributions to the integral L_{2S} (in units of $\left(\frac{Z\alpha m}{\hbar^3 c}\right)^{1/2}$) for four values of the photon energy $\hbar ck$ (in Kev)

$$L_D = L_D^{(1)} + L_D^{(2)} + L_D^{(3)} + L_D^{(4)} + L_D^{\sim}$$

$$L_C = L_C^{(1)} + L_C^{(2)}$$

$$L = L_D + L_C$$

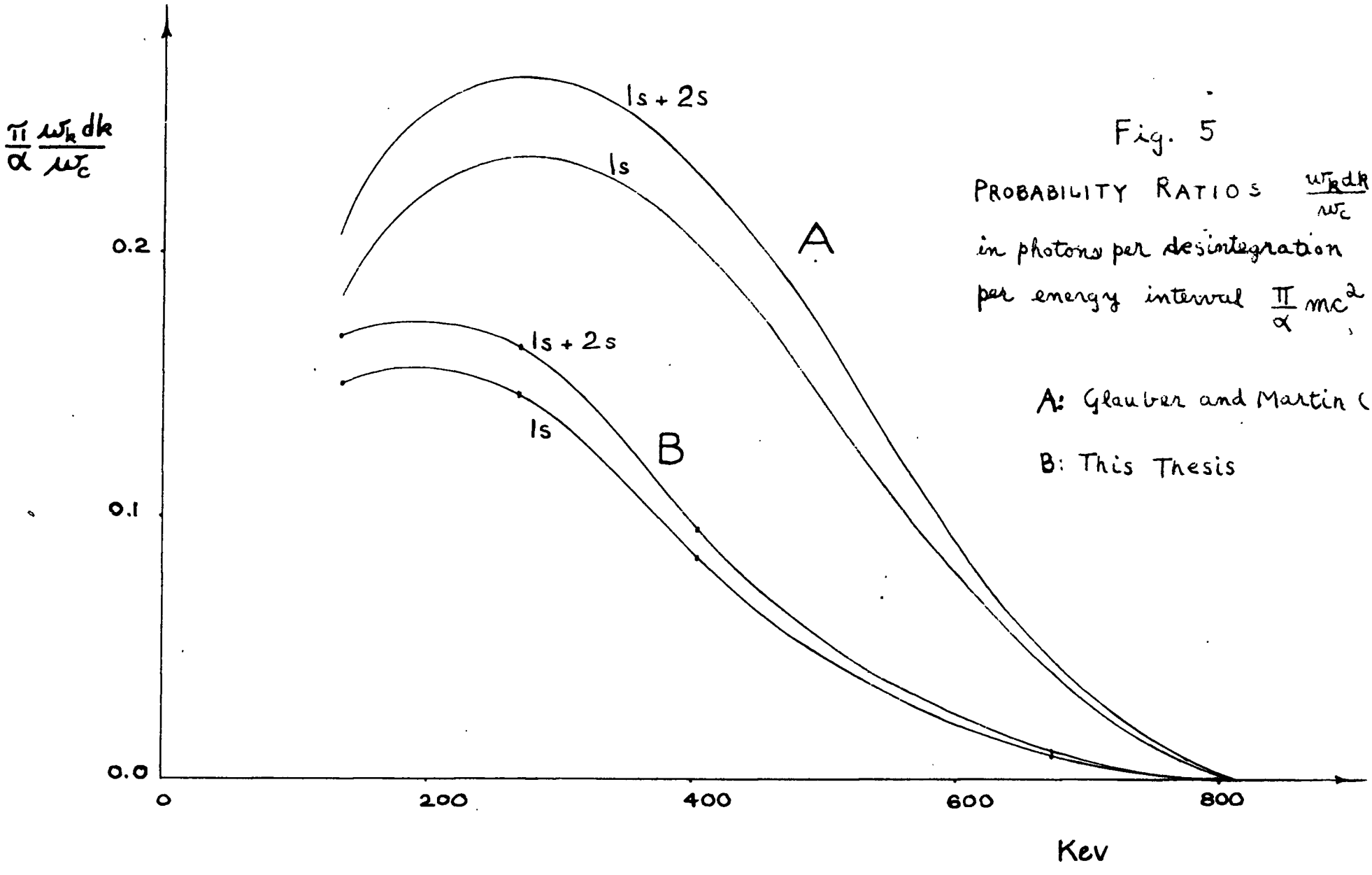

Fig. 5

PROBABILITY RATIOS $\frac{w_k dk}{w_c}$ in photons per desintegration per energy interval $\frac{\pi}{\alpha} mc^2$

A: Glauber and Martin (54)

B: This Thesis

Table III

	$\hbar ck = 135$ (x = 2)	$\hbar ck = 269$ (x = 4)	$\hbar ck = 404$ (x = 6)	$\hbar ck = 673$ (x = 10)
$\left(\frac{w_R dR}{w_C}\right)_{1s}$	0.687	0.665	0.384	0.0470
$\left(\frac{w_R dR}{w_C}\right)_{2s}$	0.080	0.087	0.047	0.0047
ρ_A	0.814	0.617	0.415	0.243

Table III showing the contributions to $w_R dR/w_C$ from the 1s and 2s electrons (in photons per desintegration per unit Kev energy interval $\times 10^6$) for four values of the photon energy $\hbar ck$ (in Kev). The table also shows the ratio ρ_A of the sum of these contributions to the corresponding result of Glauber and Martin (54).

Appendix A

We want to sketch the proof of the statement that

$$\frac{\beta}{\hbar c R} \sum_{\lambda} C_{\lambda}(SA') \varphi^{+}(R) A^{\wedge} \int d\vec{r} \sum_{E} \psi_{E}(R) \psi_{E}^{+}(\vec{r}) \beta \vec{\alpha} \cdot \vec{e}_{R} Q \psi_{ms} \qquad \text{A.1}$$

is negligible for small values of R.

Making use of the closure property,

$$\sum_{E} \psi_{E}(\vec{r}') \psi_{E}^{+}(\vec{r}) = \delta(\vec{r}-\vec{r}') I$$

(where I is the unit matrix), expanding $e^{-i\vec{R}\cdot\vec{r}}$ into products of spherical harmonics and the Bessel functions, and finally integrating over angles, one obtains for A.1 an expression proportional to

$$\int_{0}^{\infty} \delta(r-R) \frac{\sin kr}{kr} \varphi_{ms}(r) r^{2} dr \qquad \text{A.2}$$

(we have here assumed, for simplicity, the non-relativistic form for the wave function of the K-electron). Hence A.2 and, consequently, A.1 becomes proportional to

$$R^{2} \frac{\sin kR}{kR} \varphi_{ms}(R) \qquad \text{A.3}$$

which is of the order R^{2} for $R \to 0$

Appendix B

We sketch the proof of the identity:

$$\beta(i\vec{\sigma}\cdot\vec{u}-\vec{\alpha}\cdot\vec{e})\frac{1+\beta}{2}(-i\vec{\sigma}\cdot\vec{u}-\vec{\alpha}\cdot\vec{e})\beta = 1-\vec{\alpha}\cdot\frac{\vec{R}}{R} \qquad \text{B.1}$$

where $\vec{u} = \vec{e}\times\frac{\vec{R}}{R}$ and $\vec{e}\cdot\vec{R} = 0$

Making use of the relations $\beta\vec{\sigma} = \vec{\sigma}\beta$, $\beta\vec{\alpha} = -\vec{\alpha}\beta$, $\beta^2=1$, the expression on the left-hand side of B.1 can be written as

$$\frac{1}{2}(i\vec{\sigma}\cdot\vec{u}+\vec{e}\cdot\vec{\alpha})(-i\vec{\sigma}\cdot\vec{u}+\vec{e}\cdot\vec{\alpha}) + \qquad \text{B.2}$$

$$+\frac{1}{2}\beta(i\vec{\sigma}\cdot\vec{u}-\vec{e}\cdot\vec{\alpha})(-i\vec{\sigma}\cdot\vec{u}+\vec{e}\cdot\vec{\alpha})$$

or

$$\frac{1}{2}\left\{(\vec{\sigma}\cdot\vec{u})^2+(\vec{\alpha}\cdot\vec{e})^2+i\left[(\vec{\sigma}\cdot\vec{u})(\vec{\alpha}\cdot\vec{e})-(\vec{\alpha}\cdot\vec{e})(\vec{\sigma}\cdot\vec{u})\right]\right\} \qquad \text{B.3}$$

$$+\frac{1}{2}\beta\left\{(\vec{\sigma}\cdot\vec{u})^2-(\vec{\alpha}\cdot\vec{e})^2+i\left[(\vec{\sigma}\cdot\vec{u})(\vec{\alpha}\cdot\vec{e})+(\vec{\alpha}\cdot\vec{e})(\vec{\sigma}\cdot\vec{u})\right]\right\}$$

Now,

$$(\vec{\sigma}\cdot\vec{u})^2 = \vec{u}^2 = 1$$
$$(\vec{\alpha}\cdot\vec{e})^2 = \vec{e}^2 = 1$$

$$i\left[(\vec{\sigma}\cdot\vec{u})(\vec{\alpha}\cdot\vec{e})\pm(\vec{\alpha}\cdot\vec{e})(\vec{\sigma}\cdot\vec{u})\right] = \begin{cases} 0 \\ -2(\vec{\alpha}\cdot\frac{\vec{R}}{R})+2(\vec{\alpha}\cdot\vec{e})(\vec{e}\cdot\frac{\vec{R}}{R}) = -2(\vec{\alpha}\cdot\frac{\vec{R}}{R}) \end{cases}$$

So that the second line of B.3 vanishes, and the first line gives just the expression on the right-hand side of B.1.

Appendix C

We want to make it plausible that the factor

$$e^{-\frac{ipR}{\hbar}} \Phi\left(1+i\gamma;\, 2;\, \frac{2ipR}{\hbar}\right)$$

in Eq. III.48 may be set equal to unity over the whole range of integration, without too much error.

The general form of Eq. III.54 is (see Eq. III.68)

$$L_{C_{1S}} = \frac{\sqrt{\mu}}{\hbar c}\,\frac{4}{z\alpha\chi}\,\mu^2 \int_{mc^2}^{\infty} \frac{dE\,(\coth \pi/\varphi + 1)\,\mathcal{K}_{1S}\, f}{E - E_{1S} + \hbar c R} \qquad \text{C.1}$$

where

$$f = e^{-i\varphi\mu R}\,\Phi\left(1+i\gamma;\, 2;\, 2i\varphi\mu R\right)$$

is the factor in question, and $\mathcal{K}_{1S}$ is given by III.64.

Since $\mu R \simeq 10^{-3}$, one has, in fact, $f \simeq 1$ in the integration region where the remaining factor of the integrand is large, i.e. for $0 < \varphi < 15$, as can be seen from the graphs in Fig. 1 to 4.

For $\varphi > 15$, the integrand in C.1 can be replaced, without appreciable error, by a simpler expression (see Eq. III.75a) so that

$$\tilde{L}_{C_{1S}} \simeq \frac{\sqrt{\mu}}{\hbar c}\,\frac{1}{z\alpha\chi} \int_{15}^{\infty} \tilde{I}_{1S}\, f\, d\varepsilon$$

Consider now very large values of q. The behavious of f for large q's can be obtained from the asymptotic expansion of the

confluent hypergeometric function (Jahnke and Emde, p.275); we find

$$f \simeq \frac{e^{iq\mu R}}{(i/q)!}(2i\mu R q)^{-1+i/q} + c.c.$$

and $f \to 0$ for $q \to \infty$, because $(i/q)! \to 1$ (Jahnke and Emde, p. 10). But for large q's, the integrand, excluding f, is practically zero, so that putting $f \simeq 1$ (instead of $f \ll 1$) is harmless.

For the intermediate values of q, f remains finite while the remainder of the integrand is still very small, so that putting f = 1 is of no great consequence.

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